Deutsche Physikalische Gesellschaft DPG

Virtual DPG Spring Meeting 2021

of the Divisions

Biological Physics, Chemical and Polymer Physics, Dynamics and Statistical Physics, Physics of Socio-economic Systems

22 – 24 March 2021

bpcppdysoe21.dpg-tagungen.de/

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Content

Dear Conference Guests,

I would personally like to welcome you to the virtual DPG-Frühjahrstagung (DPG Spring Meeting) of the DPG Divisions Biological Physics, Chemical and Polymer Physics, Dynamics and Statistical Physics and Physics of Socio-Economic Systems (BP-CPP-DY-SOE).

I am very pleased that despite of the ongoing pandemic, we are able to hold this conference with an outstanding programme to promote the communication and exchange that is so important for science, and is invaluable especially for the next generation of physicists for the further scientific development and career planning. Here young researchers can present their theses to a larger scientific audience for the first time and enabling them to network with potential employers.

Our conference this year also shows the great potential for the innovation that currently lies undiscovered within the DPG. Thanks to the extraordinary commitment of our members, new and digital formats for events were developed and implemented in a very short time. These are not only temporary alternatives, but they can also help to promote DPG events in the future – and thus the visibility of physics in politics and the public.

For the success of this DPG Spring Meeting, I would like to express my sincere thanks to all those involved; the participating divisions for organising the scientific programme, and also the Wilhelm and Else Heraeus-Foundation for again generously supporting all DPG Spring Meetings. Furthermore, my special thanks goes to the staff of the DPG Head Office.

Dr. Lutz Schröter
President of the
Deutsche Physikalische Gesellschaft e.V.

Organisation

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Thematic Sessions and Mini-Symposia
Division Biological Physics (BP)

Active Biological Matter
Organisation:
Oliver Bäumchen, Universität Bayreuth
Stefan Klumpp, Universität Göttingen

Single molecule biophysics, Protein structure and dynamics
Organisation:
Ville Kaila, Stockholm University
Markus Zweckstetter, Max-Planck-Institut für Biophysikalische Chemie Göttingen

Cell Adhesion and Migration, Multicellular Systems
Organisation:
Jens Elgeti, Forschungszentrum Jülich
Florian Rehfeld, Universität Göttingen

Cell mechanics, Cytoskeletal filaments, Membranes and vesicles
Organisation:
Kerstin Göpfrich, Max-Planck-Institut für medizinische Forschung Heidelberg
Benedikt Sabass, Ludwig-Maximilians-Universität München
Ana-Suncana Smith, Friedrich-Alexander-Universität Erlangen-Nürnberg

Systems biology, Evolution, Statistical and Computational Biophysics
Organisation:
Hannes Mutschler, Max-Planck-Institut für Biochemie München
Pawel Romanczuk, Humboldt-Universität zu Berlin
Gunnar Schröder, Forschungszentrum Jülich

Bioimaging and Biospectroscopy
Organisation:
Ulrike Alexiev, Freie Universität Berlin
Katrin Heinze, Universität Würzburg

Focus Session: Cells in Microfluidics
Organisation:
Dmitry Fedosov, Forschungszentrum Jülich
Oliver Otto, Universität Greifswald

Focus Session: Stem Cells
Organisation:
Fabian Rost, Max-Planck-Institut für Physik Komplexer Systeme Dresden
Steffen Rulands, Max-Planck-Institut für Physik Komplexer Systeme Dresden

Focus Session: Lipid-lipid phase separation in cells
Organisation:
Christoph Weber, Max-Planck-Institut für Physik Komplexer Systeme Dresden
David Zwicker, Max-Planck-Institut für Dynamik und Selbstorganisation Göttingen

Thematic Sessions and Mini-Symposia
Division Chemical and Polymer Physics (CPP)

Charged Soft Matter
Organisation:
Joachim Dzubiella, Albert-Ludwigs-Universität

Complex fluids
Organisation:
Christine Papadakis, Technische Universität München

Molecular Electronics
Organisation:
Derck Schlettwein, Justus-Liebig-Universität Gießen

Perovskites
Organisation:
Eva M. Herzig, Universität Bayreuth

Theory & Simulation
Organisation:
Jens-Uwe Sommer, Leibniz-Institut für Polymerforschung Dresden

Wetting
Organisation:
Stefan Karpitschka, Max-Planck-Institut für Dynamik und Selbstorganisation

Thematic Sessions and Mini-Symposia
Division Dynamics and Statistical Physics (DY)

Statistical Physics, Nonequilibrium Phenomena and Stochastic Thermodynamics
Organisation:
Barbara Drossel, Technische Universität Darmstadt
Sabine Klapp, Technische Universität Berlin
Thomas Speck, Johannes Gutenberg-Universität Mainz

Fluid Physics of Turbulence, Convection and Life
Organisation:
Stephan Weiss, Max-Planck-Institut für Dynamik und Selbstorganisation
Michael Wilczek, Max-Planck-Institut für Dynamik und Selbstorganisation

Active Matter and Microswimmers
Organisation:
Carsten Beta, Universität Potsdam
Andreas Menzel, Otto-von-Guericke Universität Magdeburg
Holger Stark, Technische Universität Berlin

Complex Fluids, Soft Matter and Microfluidics
Organisation:
Uwe Thiele, Westfälische Wilhelms-Universität Münster

Nonlinear Dynamics and Pattern Formation
Organisation:
Azam Gholami, Max-Planck-Institut für Dynamik und Selbstorganisation

Brownian Motion and Anomalous Transport
Organisation:
Ralf Metzler, Universität Potsdam

Granular Physics
Organisation:
Matthias Sperl, Deutsches Zentrum für Luft- und Raumfahrt (DLR)

Glasses and Glass Transition
Organisation:
Andreas Heuer, Westfälische Wilhelms-Universität Münster

Thematic Sessions and Mini-Symposia
Division Physics of Socio-Economic Systems (SOE)

COVID-19 pandemics through the lens of physics
Organisation:
Fakhteh Ghanbarnejad
Philipp Hövel, Technische Universität Berlin

Data Analytics for Complex Dynamical Systems

Data Science in Biological and Interdisciplinary Physics

Partial Synchronization in Networks

Opinion Formation

Financial Markets and Risk Management

Economic Models and Evolutionary Game Theory

Transport, Urban and Regional Systems

Social Dynamics

Networks: from Structure to Dynamics

Programme
The scientific programme consists of **584** contributions:

34	Invited talks
319	Talks
231	Posters

Information for Participants

The virtuell conference will be held in the period 22–24 March, 2021

Conference Information

Conference Location
Web-based Conference - Login information will be provided a few days before the event starts.

Conference Time Zone
All times are in Central European Time (CET)

Conference Website
https://bpcppdysoe21.dpg-tagungen.de/

Conference Office
The virtual conference office is open during all breaks for questions about the conference. You will find it on the conference platform under the *„Welcome"* tab immediately after signed up.

Conference Platform functionalities

Supported Browsers
Google Chrome is currently the most stable and reliable browser for using the conference platform.

Firefox and Safari are browsers that should work but often less performant. The support staff is highly trained in resolving Google Chrome issues. If you are using a different browser than Google Chrome, we cannot provide in-depth troubleshooting support for you.

Joining the Event
To join an event space, you must first sign up and attend the event. All you have to do is visiting the event landing page and follow these steps.

⇨ Step 1
Click on *„Attend event"*. You will then be prompted to sign up.

⇨ Step 2
Once you signed up, go back to the event space and click *„Enter event space"* to join the event.

Navigating during the Event
To navigate on the conference platform you simply have to select the floor (1.) and then click on either *„JOIN"* (2.) or *„OPEN"*.

„JOIN" means you are joining a video call or joining a stage. Once you hover on a button a small tooltip gives some more details.

„OPEN" will open a popup with embedded websites, PDFs, or similar.

Test Browser Video Chat before the Event
If you want to test our default browser video chat before the event starts, you can visit the following page here: http://test.meetanyway.com . Here you simply have to click the green button *„Join meeting"*.

You can also invite your colleagues to that link and test together. Please note that you might meet other people, who test at the same time as you do.

Deutsche Physikalische Gesellschaft DPG

Jetzt bewerben!

DPG-Mentoring-Programm und Leading for Tomorrow

An der Schwelle zum Berufseinstieg bietet die DPG zwei besondere Programme an, gerade wenn der Berufseinstieg eventuell in Industrie und Wirtschaft erfolgen soll.

Bewerbungszeitraum 1. bis 31. März

Weitere Infos unter: www.mentoring_L4T.dpg-physik.de

Meet the Speaker
In the header you will find the „meet-the-speaker"-rooms of the four divisions (BP, CPP, DY, SOE). In these rooms, the respective speakers are listed sorted by lecture number. There you have the opportunity to discuss with the speakers and ask questions.

Notice Board
All changes regarding the schedule of the conference will be updated currently. The information is identical to the programme updates of the scientific programme and available at the scientific programme in other formats as well (ordered by publication date, filterable by conference part and as an rss-feed). Please use the form at *https://bpcppdysoe21.dpg-tagungen.de/programm/notice-board-form* to submit amendments, cancellations, etc.

Wilhelm and Else Heraeus Communication Programme
Within this programme, the active participation by young DPG members – from Germany and abroad – at the virtual DPG-Frühjahrstagungen (DPG Spring Meetings) is financially supported.
For the virtual DPG Spring Meetings, the conference fee (and exclusively the "early bird rate") is subsidised at 100 % (*submission of an application was open until 28 February 2021. Subsequent applications are unfortunately not possible*). After the conference, your participation in the conference will be checked on the basis of the login data and the funding will be finally confirmed or rejected if no participation took place.

Payment will be made – after prior notification by e-mail – by the end of April 2021 at the latest by bank transfer to the account you specified in your application.

The Deutsche Physikalische Gesellschaft thanks the Wilhelm and Else Heraeus Foundation for the generous financial support of young academic talents. We hope that young physicists will continue to seize the offered opportunity for active scientific communication at scientific conferences. A total of about 35,000 young academics were supported by this programme so far.

Social Events

Annual General Meetings of the Divisions:

Division	Date	Room
Biological Physics Division (BP)	Tuesday, 23 March 2021, 18:30	BPa
Physics of Socio-economics Physics (SOE)	Tuesday, 23 March 2021, 19:00	SOEa

The DPG on Instagram
Since the anniversary year 2020 the DPG is presenting an inspiring personality or an everyday physical phenomenon on Instagram (@dpgphysik) every day. Who inspires you? What fascinates you? Submit online suggestions for the 175 Inspirers and the 175 Impulses.
You can find the entries at http://175inspirierende.dpg-physik.de and http://175impulse.dpg-physik.de. Contact: 175inspirierende@dpg-physik.de or impulse@dpg-mail.de.

Acknowledgement
The Deutsche Physikalische Gesellschaft (DPG) wants to thank the Wilhelm and Else Heraeus-Foundation, Hanau, and all staff who make the success of the conference possible.

Synopsis of the Daily Programme

Monday, March 22, 2021

BP

Invited Talks

09:40	BPa	BP 1.3	Cyclic Strain Steers Animal Cells •Rudolf Merkel
09:00	BPb	BP 2.1	The tortoise and hare: how moving slower allows groups of bacteria to spread across surfaces Oliver Meacock, Amin Doostmohammadi, Kevin Foster, Julia Yeomans, •William Durham
14:40	BPa	BP 7.3	Towards the mechanical characterization of neuronal network formation Paulina Wysmolek, Florian Huhnke, Katja Salbaum, Joachim Spatz, •Friedhelm Serwane
14:00	BPc	BP 9.1	From individual to collective intermittent motion: from bacteria to sheep •Fernando Peruani

Sessions

09:00	BPa	BP 1	Cell Mechanics I
09:00	BPb	BP 2	Active Biological Matter I
09:00	BPc	BP 3	Focus Physics of Stem Cells
11:00	BPa	BP 4	Cell Mechanics II
11:00	BPb	BP 5	Active Biological Matter II
11:00	BPc	BP 6	Systems Biology I
14:00	BPa	BP 7	Cell Mechanics III
14:00	BPb	BP 8	Bioimaging and Biospectroscopy
14:00	BPc	BP 9	Systems Biology II
14:00	DYp	BP 10	Posters DY – Fluid Physics, Active Matter, Complex Fluids, Soft Matter and Glasses
16:30	BPp	BP 11	Poster A: Single Molecule, Multicellular, Bioimaging, Focus Sessions, etc.

CPP

Invited Talks

11:00	CPPa	CPP 2.6	Singlet fission in blends of organic semiconductors •Katharina Broch, Clemens Zeiser, Luca Moretti, Chad Cruz, Giulio Cerullo, Roel Tempelaar, Christopher Bardeen
14:00	CPPa	CPP 2.11	Small, but highly effective: Functional molecules in polymer devices •Ulrike Kraft
11:00	CPPb	CPP 3.5	Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates •Ralf Seemann, Roghayeh Shiri, Stefan Bommer, Dirk Peschka, Sebastian Jachalski, Lenoie Schmeller, Barbara Wagner
14:00	CPPb	CPP 3.10	Sinking droplet durotaxis and engulfment •Anne Juel

Sessions

08:50	CPPa	CPP 1	Welcome
09:00	CPPa	CPP 2	Molecular Electronics – organized by Derck Schlettwein (Justus Liebig University Giessen, Giessen)
09:00	CPPb	CPP 3	Wetting – organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen)
09:00	BPb	CPP 4	Active Biological Matter I
11:00	BPb	CPP 5	Active Biological Matter II
16:30	CPPp	CPP 6	Poster Session I – Molecular Electronics and Wetting

Monday, March 22, 2021

DY

Invited Talks

09:00	DYc	DY 4.1	X-ray tomography investigation of cyclically sheared granular materials •Yujie Wang
10:00	DYa	DY 7.1	Can convective heat transport be more efficient than the so-called ‚ultimate' regime? •Basile Gallet
16:00	DYb	DY 15.1	Glassy physics: from liquids to living cells •Liesbeth Janssen

Sessions

09:00	CPPb	DY 1	Wetting – organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen)
09:00	DYa	DY 2	Fluid Physics 1 – organized by Stephan Weiss and Michael Wilczek (Göttingen)
09:00	DYb	DY 3	Statistical Physics 1 – organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)
09:00	DYc	DY 4	Invited Talk: Yujie Wang (Shanghai)
09:00	BPb	DY 5	Active Biological Matter I
09:30	DYc	DY 6	Granular Physics 1 – organized by Matthias Sperl (Köln)
10:00	DYa	DY 7	Invited Talk: Basile Gallet (Saclay)
11:00	DYa	DY 8	Fluid Physics 2 – organized by Stephan Weiss and Michael Wilczek (Göttingen)
11:00	DYb	DY 9	Statistical Physics 2 – organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) und Thomas Speck (Mainz)
11:00	DYc	DY 10	Granular Physics 2 – organized by Matthias Sperl (Köln)
11:00	BPb	DY 11	Active Biological Matter II
14:00	DYp	DY 12	Posters DY – Fluid Physics, Active Matter, Complex Fluids, Soft Matter and Glasses
15:00	DYc	DY 13	Granular Physics 3 – organized by Matthias Sperl (Köln)
16:00	DYa	DY 14	Microfluidics and Droplets – organized by Uwe Thiele (Münster)
16:00	DYb	DY 15	Invited Talk: Liesbeth Janssen (Eindhoven)
16:30	DYb	DY 16	Statistical Physics 3 – organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)

SOE

Invited Talks

09:00	SOEa	SOE 1.1	Mathematical modelling of COVID-19: dynamics and containment •Yuliya Kyrychko
11:00	SOEa	SOE 1.5	data-driven modeling of COVID-19 pandemic •Yamir Moreno

Sessions

09:00	SOEa	SOE 1	COVID-19 pandemics through the lens of physics (org.: Fakhteh Ghanbarnejad and Philipp Hövel)
14:00	SOEa	SOE 2	Networks and Social Dynamics
17:30	SOEp	SOE 3	Poster

Deutsche Physikalische Gesellschaft DPG

2021

Physik im Kopf?

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10.09. - 12.09.2021

Physikzentrum Bad Honnef

Teilnahme kostenlos

Anmeldung:
19.04. - 30.05.
schuelertagung.dpg-physik.de

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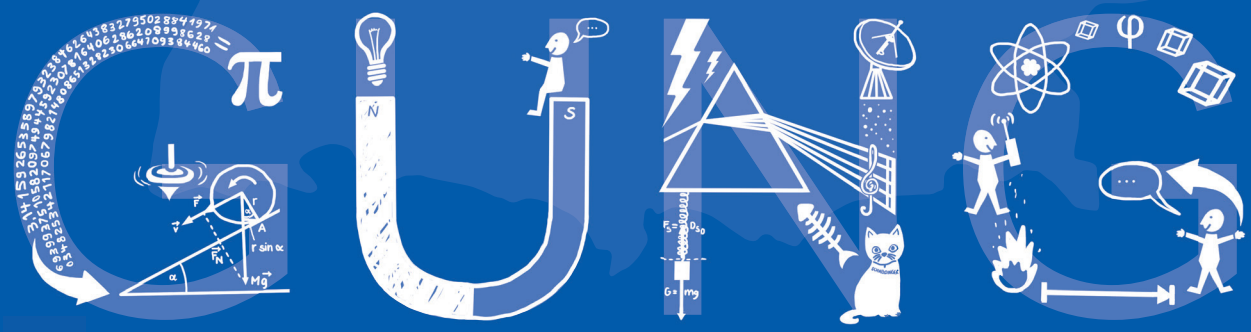

DPG Schüler Tagung

Illustration und Gestaltung: Annemarie Woeste

schuelertagung.dpg-physik.de

Tuesday, March 23, 2021

BP

Invited Talks

09:00	BPa	BP 12.1	Molecular simulation meets cryo electron tomography •Gerhard Hummer
09:40	BPb	BP 13.3	Active behaviors of cellular monolayers. •Benoit Ladoux
14:00	BPa	BP 21.1	Predicting Protein and RNA Structures: from statistical physics to machine learning •Alexander Schug
15:00	BPc	BP 23.4	Synthetic cells: De novo assembly with microfluidics and DNA nanotechnology •Kerstin Göpfrich

Sessions

09:00	BPa	BP 12	Single Molecule Biophysics I
09:00	BPb	BP 13	Multicellular Systems I
09:00	BPc	BP 14	Focus Phase Separation in Biological Systems I
09:30	DYa	BP 15	Active Matter 1 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
11:00	BPa	BP 16	Single Molecule Biophysics II
11:00	BPb	BP 17	Multicellular Systems II
11:00	BPc	BP 18	Cell Mechanics IV
11:00	DYa	BP 19	Active Matter 2 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
12:00	BPc	BP 20	Focus Biological Cells in Microfluidics I
14:00	BPa	BP 21	Systems Biology III
14:00	BPb	BP 22	Focus Phase Separation in Biological Systems II
14:00	BPc	BP 23	Focus Biological Cells in Microfluidics II
16:00	BPp	BP 24	Poster B: Active Biological Matter, Cell Mechanics, Systems Biology, Computational Biophysics, etc.
17:45	BPb	BP 25	Nationale Forschungsdateninfrastruktur (NDFI)
18:30	BPa	BP 26	Annual General Meeting of the Biological Physics Division

CPP

Invited Talks

11:00	CPPa	CPP 7.5	Ultrafast spectroscopy of charge and structural dynamics in hybrid perovskites •Felix Deschler
14:00	CPPa	CPP 7.9	Structural dynamics of halide perovskites via in-situ electron microscopy •Chen Li
09:00	CPPb	CPP 8.1	Polymer Micelles with Crystalline Cores: confinement effects, molecular exchange kinetics and mechanical response Nico Koenig, Lutz Willner, •Reidar Lund
11:00	CPPb	CPP 8.4	Dynamic behaviour of anisotropic magnetic particles in suspensions •Sofia Kantorovich

Sessions

09:00	CPPa	CPP 7	Perovskites – organized by Eva M. Herzig (University of Bayreuth, Bayreuth)
09:00	CPPb	CPP 8	Complex Fluids – organized by Christine M. Papadakis (Technical University of Munich, Garching)
09:00	BPc	CPP 9	Focus Phase Separation in Biological Systems I
09:30	DYa	CPP 10	Active Matter 1 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
11:00	DYa	CPP 11	Active Matter 2 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
14:00	BPb	CPP 12	Focus Phase Separation in Biological Systems II
14:30	DYc	CPP 13	Complex Fluids and Soft Matter 3
16:30	CPPp	CPP 14	Poster Session II – Complex Fluids and Perovskites
17:45	BPb	CPP 15	Nationale Forschungsdateninfrastruktur (NDFI)

Tuesday, March 23, 2021

DY

Invited Talks

09:00	DYa	DY 18.1	Reinforcement learning of microswimmer chemotaxis using genetic algorithms •Andreas Zöttl, Benedikt Hartl, Maximilian Hübl, Gerhard Kahl
10:00	DYc	DY 22.1	Stability and dynamics of convection in dry salt lakes •Lucas Goehring, Jana Lasser, Marcel Ernst, Matthew Threadgold, Cédric Beaume, Steven Tobias
14:00	DYa	DY 27.1	Human exhaled particles from nanometres to millimetres •Gholamhossein Bagheri
14:00	DYc	DY 29.1	Fingers, fractals, and flow in liquid metals •Karen Daniels
15:40	DYb	DY 31.1	Fixation and ancestry of competing species growing on a rugged front •Mehran Kardar

Sessions

09:00	CPPb	DY 17	Complex Fluids – organized by Christine M. Papadakis (Technical University of Munich, Garching)
09:00	DYa	DY 18	Invited Talk: Andreas Zöttl (Vienna)
09:00	DYb	DY 19	Statistical Physics 4 – organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)
09:00	DYc	DY 20	Nonlinear Dynamics 1 – organized by Azam Gholami (Göttingen)
09:30	DYa	DY 21	Active Matter 1 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
10:00	DYc	DY 22	Invited Talk: Lucas Goehring (Nottingham)
11:00	DYa	DY 23	Active Matter 2 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
11:00	DYb	DY 24	Dynamics and Statistical Physics – Open Session
11:00	DYc	DY 25	Nonlinear Dynamics 2 – organized by Azam Gholami (Göttingen)
11:00	SOEa	DY 26	Data Analytics for Complex Dynamical Systems (joint SOE/DY Focus Session)
14:00	DYa	DY 27	Fluid Physics 3 – organized by Stephan Weiss and Michael Wilczek (Göttingen)
14:00	DYb	DY 28	Statistical Physics 5 – organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)
14:00	DYc	DY 29	Invited Talk: Karen Daniels (Raleigh)
14:30	DYc	DY 30	Complex Fluids and Soft Matter 1 – organized by Uwe Thiele (Münster)
15:40	DYb	DY 31	Invited Talk: Mehran Kardar (Boston)
16:30	DYp	DY 32	Posters DY – Statistical Physics, Brownian Motion and Nonlinear Dynamics
17:45	BPb	DY 33	Nationale Forschungsdateninfrastruktur (NDFI)

SOE

Sessions

11:00	SOEa	SOE 4	Data Analytics for Complex Dynamical Systems (joint SOE/DY Focus Session)
14:00	SOEa	SOE 5	Financial and Economic Systems and Evolutionary Game Theory
17:45	BPb	SOE 6	Nationale Forschungsdateninfrastruktur (NDFI)
19:00	SOEa	SOE 7	Annual General Meeting of the Physics of Socio-economic Systems Division

Wednesday, March 24, 2021

BP

Sessions

09:00	DYb	BP 27	Active Matter 3 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
11:00	DYb	BP 28	Active Matter 4 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
14:30	DYb	BP 29	Active Matter 5 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)

CPP

Invited Talks

09:00	CPPa	CPP 16.1	Charging Dynamics and Structure of Ionic Liquids in Nanoporous Supercapacitors •Christian Holm, Konrad Breitsprecher, Svyatoslav Kondrat
11:00	CPPa	CPP 16.4	Interaction of polyelectrolytes with proteins •Matthias Ballauff
09:00	CPPb	CPP 17.1	Data-driven methods in polymer physics: exploring the sequence space of copolymers •Marco Werner
11:40	CPPb	CPP 17.6	Structure formation in drying films and droplets •Arash Nikoubashman, Michael Howard, Michael Kappl, Hans-Jürgen Butt

Sessions

09:00	CPPa	CPP 16	Charged Soft Matter – organized by Joachim Dzubiella (Albert Ludwigs University Freiburg, Freiburg)
09:00	CPPb	CPP 17	Theorie and Simulation – organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden)
09:00	DYa	CPP 18	Complex Fluids and Soft Matter 1
09:30	DYc	CPP 19	Glasses and Glass Transition 1
11:00	DYa	CPP 20	Complex Fluids and Soft Matter 2
11:00	DYc	CPP 21	Glasses and Glass Transition 2
16:30	CPPp	CPP 22	Poster Session III – Charged Soft Matter and Theory and Simulation

DY

Invited Talks

10:00	DYa	DY 35.4	When surface viscosities rule: Bubble relaxation and thin film wrinkling •Kirsten Harth
09:00	DYc	DY 37.1	Physical properties of ultrastable computer-generated glasses •Ludovic Berthier
14:00	DYb	DY 44.1	Life in a tight spot: How bacteria swim in complex spaces •Sujit Datta
14:00	DYc	DY 45.1	Small diffusive systems warm up faster than they cool down Alessio Lapolla, •Aljaz Godec

Sessions

09:00	CPPb	DY 34	Theorie and Simulation – organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden)
09:00	DYa	DY 35	Complex Fluids and Soft Matter 2 – organized by Uwe Thiele (Münster)
09:00	DYb	DY 36	Active Matter 3 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)
09:00	DYc	DY 37	Invited Talk: Ludovic Berthier (Montpellier)
09:00	SOEa	DY 38	Partial Synchronization in Networks (Focus Session joint with DY and BP)
09:30	DYc	DY 39	Glasses and Glass Transition 1 – organized by Andreas Heuer (Münster)
11:00	DYa	DY 40	Complex Fluids and Soft Matter 3 – organized by Uwe Thiele (Münster)
11:00	DYb	DY 41	Active Matter 4 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)

Wednesday, March 24, 2021

BP

11:00	DYc	DY 42	Glasses and Glass Transition 2 – organized by Andreas Heuer (Münster)
14:00	DYa	DY 43	Pattern Formation – organized by Azam Gholami (Göttingen)
14:00	DYb	DY 44	Invited Talk Sujit S. Datta (Princeton)
14:00	DYc	DY 45	Brownian Motion and Anomalous Transport – organized by Ralf Metzler (Potsdam)
14:30	DYb	DY 46	Active Matter 5 – organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin)

SOE

Sessions

09:00	SOEa	SOE 8	Partial Synchronization in Networks (Focus Session joint with DY and BP)
11:00	SOEa	SOE 9	Opinion Formation
13:00	SOEa	SOE 10	Transport, Regional and Urban Dynamics

Biological Physics Division
Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions

Invited Talks

BP 1.3	Mon	9:40–10:10	BPa	**Cyclic Strain Steers Animal Cells** — •Rudolf Merkel
BP 2.1	Mon	9:00– 9:30	BPb	**The tortoise and hare: how moving slower allows groups of bacteria to spread across surfaces** — Oliver Meacock, Amin Doostmohammadi, Kevin Foster, Julia Yeomans, •William Durham
BP 7.3	Mon	14:40–15:10	BPa	**Towards the mechanical characterization of neuronal network formation** — Paulina Wysmolek, Florian Huhnke, Katja Salbaum, Joachim Spatz, •Friedhelm Serwane
BP 9.1	Mon	14:00–14:30	BPc	**From individual to collective intermittent motion: from bacteria to sheep** — •Fernando Peruani
BP 12.1	Tue	9:00– 9:30	BPa	**Molecular simulation meets cryo electron tomography** — •Gerhard Hummer
BP 13.3	Tue	9:40–10:10	BPb	**Active behaviors of cellular monolayers.** — •Benoit Ladoux
BP 21.1	Tue	14:00–14:30	BPa	**Predicting Protein and RNA Structures: from statistical physics to machine learning** — •Alexander Schug
BP 23.4	Tue	15:00–15:30	BPc	**Synthetic cells: De novo assembly with microfluidics and DNA nanotechnology** — •Kerstin Göpfrich

Sessions

BP 1.1–1.4	Mon	9:00–11:00	BPa	**Cell Mechanics I**
BP 2.1–2.4	Mon	9:00–11:00	BPb	**Active Biological Matter I (joint session BP/DY/CPP)**
BP 3.1–3.4	Mon	9:00–11:00	BPc	**Focus Physics of Stem Cells**
BP 4.1–4.6	Mon	11:00–13:30	BPa	**Cell Mechanics II**
BP 5.1–5.6	Mon	11:00–13:30	BPb	**Active Biological Matter II (joint session BP/CPP/DY)**
BP 6.1–6.6	Mon	11:00–13:30	BPc	**Systems Biology I**
BP 7.1–7.5	Mon	14:00–16:30	BPa	**Cell Mechanics III**
BP 8.1–8.6	Mon	14:00–16:30	BPb	**Bioimaging and Biospectroscopy**
BP 9.1–9.5	Mon	14:00–16:30	BPc	**Systems Biology II**
BP 10.1–10.22	Mon	14:00–16:30	DYp	**Posters DY - Fluid Physics, Active Matter, Complex Fluids, Soft Matter and Glasses (joint session DY/BP)**
BP 11.1–11.41	Mon	16:30–19:00	BPp	**Poster A: Single Molecule, Multicellular, Bioimaging, Focus Sessions, etc.**
BP 12.1–12.4	Tue	9:00–11:00	BPa	**Single Molecule Biophysics I**
BP 13.1–13.4	Tue	9:00–11:00	BPb	**Multicellular Systems I**
BP 14.1–14.4	Tue	9:00–11:00	BPc	**Focus Phase Separation in Biological Systems I (joint session BP/CPP)**
BP 15.1–15.3	Tue	9:30–10:30	DYa	**Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)**
BP 16.1–16.6	Tue	11:00–13:30	BPa	**Single Molecule Biophysics II**
BP 17.1–17.6	Tue	11:00–13:30	BPb	**Multicellular Systems II**
BP 18.1–18.3	Tue	11:00–12:00	BPc	**Cell Mechanics IV**
BP 19.1–19.6	Tue	11:00–13:00	DYa	**Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)**
BP 20.1–20.3	Tue	12:00–13:30	BPc	**Focus Biological Cells in Microfluidics I**
BP 21.1–21.4	Tue	14:00–16:00	BPa	**Systems Biology III**
BP 22.1–22.4	Tue	14:00–16:00	BPb	**Focus Phase Separation in Biological Systems II (joint session BP/CPP)**
BP 23.1–23.4	Tue	14:00–16:00	BPc	**Focus Biological Cells in Microfluidics II**

BP 24.1–24.50	Tue	16:00–18:30	BPp	**Poster B: Active Biological Matter, Cell Mechanics, Systems Biology, Computational Biophysics, etc.**
BP 25	Tue	17:45–18:30	BPb	**Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)**
BP 26	Tue	18:30–19:00	BPa	**Annual General Meeting**
BP 27.1–27.5	Wed	9:00–10:40	DYb	**Active Matter 3 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)**
BP 28.1–28.6	Wed	11:00–13:00	DYb	**Active Matter 4 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)**
BP 29.1–29.4	Wed	14:30–15:50	DYb	**Active Matter 5 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)**

Annual General Meeting of the Biological Physics Division

Tue 18:30–19:00 BPa

Virtual DPG Meeting "Biological Physics", March 22-23, 2021

Monday 22.03.2021

Time	Cell Mechanics	Active Matter	Focus Stem Cells
09:00 - 09:10	Alexander Rohrbach	William Durham (Invited)	Allyson Quin Ryan
09:10 - 09:20			
09:20 - 09:30	Swetha Raghuraman		Aneta Koseska
09:30 - 09:40		Alexandros Fragkopoulos	
09:40 - 09:50	Rudolf Merkel (Invited)		Fabrizio Olmeda
09:50 - 10:00		Jayabrata Dhar	
10:00 - 10:10			David J. Jörg
10:10 - 10:20	Marta Urbanska	Robert Großmann	
10:20 - 10:30			
10:30 - 10:40	Meet the Speaker / Coffee Break		
10:40 - 10:50			
10:50 - 11:00			
	Cell Mechanics	Active Matter	Systems Biology
11:00 - 11:10	Anil Kumar Dasanna	Ludwig Hoffmann	Annalena Salditt
11:10 - 11:20			
11:20 - 11:30	Alexander Ziepke	Alexander Mietke	Mona Förster
11:30 - 11:40			
11:40 - 11:50	Ivan Hornak	Fenna Stegemerten	Philip Bitthin
11:50 - 12:00			
12:00 - 12:10	Falko Ziebert	Felix Rühle	Tobias Kühn
12:10 - 12:20			
12:20 - 12:30	Niladri Sarkar	Theresa Jakuszeit	Johanna Dickmann
12:30 - 12:40			
12:40 - 12:50	Mehdi Abbasi	Judit Clopes	Julian Rode
12:50 - 13:00			
13:00 -14:00	Meet the Speaker / Lunch Break		

Time	Cell Mechanics	Bioimaging	Systems Biology
14:00 - 14:10	Paul Heo	Sebastian Kruss	Fernado Peruani (Invited)
14:10 - 14:20			
14:20 - 14:30	Justus Bednár	Till Korten	
14:30 - 14:40			Adolfo Alsina
14:40 - 14:50	Friedhelm Serwane (Invited)	Jakob Tomas Bullerjahn	
14:50 - 15:00			Marko Popovic
15:00 - 15:10		Katharina Preißinger	
15:10 - 15:20	Katrin John		Giacomo Bartolucci
15:20 - 15:30		Konstantin Speckner	
15:30 - 15:40	Cordula Reuther		Philipp Fleig
15:40 - 15:50		Robert Magerle	
15:50 - 16:00	Meet the Speaker / Coffee Break		
16:00 - 16:10			
16:10 - 16:20			
16:20 - 16:30			
16:30 - 19:00	Poster Session A		

Virtual DPG Meeting "Biological Physics", March 22-23, 2021

Tuesday 23.03.2021

Time	Proteins	Multicellular	Focus LLPS
09:00 - 09:10	Gerhard Hummer (Invited)	Steffen Grosser	Davide Michieletto
09:10 - 09:20			
09:20 - 09:30		Maxime Hubert	Patrick M. McCall
09:30 - 09:40	Michael Thorwart		
09:40 - 09:50		Benoit Ladoux (Invited)	Lars Hubatsch
09:50 - 10:00	Luman Haris		
10:00 - 10:10			Thomas Böddeker
10:10 - 10:20	Jochen S. Hub	Gabriele Lubatti	
10:20 - 10:30			
10:30 - 10:40	Meet the Speaker / Coffee Break		
10:40 - 10:50			
10:50 - 11:00			
	Proteins	Multicellular	Cell Mechanics / Focus Microfluidics
11:00 - 11:10	Benjamin Lickert	Mirna Kramar	Anna Schepers
11:10 - 11:20			
11:20 - 11:30	Jan Lipfert	Christina Oettmeier	Felix Schwietert
11:30 - 11:40			
11:40 - 11:50	Henrike Müller-Werkmeister	Pierre A. Haas	Luncina Kainka
11:50 - 12:00			
12:00 - 12:10	Benedikt Rennekamp	Doriane Vesperini	Sebastian Johannes Müller
12:10 - 12:20			
12:20 - 12:30	Martin Stöhr	Simon Syga	Tom Robinson
12:30 - 12:40			
12:40 - 12:50	Clark Zahn	David Brückner	Felix Reichel
12:50 - 13:00			
13:00 -14:00	Meet the Speaker / Lunch Break		

Time	Systems Biology	Focus LLPS	Focus Microfluidics
14:00 - 14:10	Alexander Schug (Invited)	Florian Oltsch	Yesaswini Komaragiri
14:10 - 14:20			
14:20 - 14:30		Patrick Schwarz	Alexander Kihm
14:30 - 14:40	Bernadette Mohr		
14:40 - 14:50			Kirsty Y. Wan
14:50 - 15:00	Aboutaleb Amiri	Sandeep Choubey	
15:00 - 15:10			Kerstin Göpfrich (Invited)
15:10 - 15:20	Julia M. Riede	Wojciech Lipinski	
15:20 - 15:30			
15:30 - 15:40	Meet the Speaker / Coffee Break		
15:40 - 15:50			
15:50 - 16:00			
16:00 - 18:30	Poster Session B		

Sessions

– Invited Talks, Contributed Talks, and Posters –

BP 1: Cell Mechanics I

Time: Monday 9:00–11:00 Location: BPa

BP 1.1 Mon 9:00 BPa

Pulling, failing and adaptation of macrophage filopodia — •Alexander Rohrbach and Rebecca Michiels — Bio- und Nano-Photonik, Universität Freiburg

Macrophages are cells of the immune system, which use filopodia to connect to pathogens and withdraw them towards the cell body for phagocytosis. The withdrawal of living targets requires to overcome counteracting forces, which the cell generates after a mechanical stimulus is transmitted to the filopodium. Adaptation to mechanical cues is an essential biological function of cells, but it is unclear whether optimization strategies are essential for filopodia pulling. We use optically trapped beads as artificial targets and interferometric particle tracking to investigate factors contributing to filopodia performance. We find that bead retractions are interrupted by sudden failure events caused by mechanical rupture of the actin-membrane connection. Filopodia resume pulling only milliseconds after ruptures by reconnecting to the actin backbone. Remarkably, we see a gradual increase of filopodia force after failures, which points towards a previously unknown adaptation mechanism. Fluorescence microscopy reveals that particles are transported in a stop-and-go behavior with the actin retrograde flow via a force-dependent linker at the filopodium tip. Additionally, we see that the strength of the attachment between bead and filopodium increases under load, a characteristic of catch bond adhesion proteins. Our findings show how mechanical adaptation enable macrophage cells to optimize their performance under load.

BP 1.2 Mon 9:20 BPa

The dynamics of burst-like collective migration in 3D cancer spheroids — •Swetha Raghuraman[1], Raphael Wittkowski[2], and Timo Betz[1] — [1]Institute of Cell Biology, ZMBE, Münster, Germany — [2]Center for Soft Nanoscience

Collective migration of cells is a striking behavior observed during morphogenesis, wound healing and cancer cell invasion. Spherical aggregates of cells are known to migrate in 3D matrices like collagen, matrigel or fibronectin *in-vitro*. Although biochemical signaling is a main research focus, the biophysical properties of the spheroid leading to an invasion is less explored. We observe a striking phenotypical difference when HeLa cervical cancer spheroids were embedded in different concentrations of collagen I matrices. HeLa spheroids in lower collagen concentration (LCC) 0.5 mg/ml, displayed an explosion invasion-like behavior within 6 hours, while those in higher collagen concentration (HCC) 2.5 mg/ml were consistently growing over 48 hours, without any invasion like behavior. The migration dynamics of cells in HCC were more fluid-like with lower velocity as compared to the burst-like phenotype in LCC, which showed higher velocity and super diffusive characteristics. We hypothesize that in LCC, spheroids generate an increased pressure due to a volume increase when they fail to engage rigid ECM contacts because of the soft environment. The volume increase then pushed the cells into the soft regions of the ECM, which tends to be inhomogeneous at the LCC. We believe that such mechanical interplay can pave the way to understand migration behavior of cancer cells with respect to their biophysical properties.

Invited Talk BP 1.3 Mon 9:40 BPa

Cyclic Strain Steers Animal Cells — •Rudolf Merkel — Forschungszentrum Jülich, IBI-2 Mechanobiology, 52428 Jülich, Germany

Throughout the organism, all tissue cells experience mechanical strain, e.g. due to the pulsating blood flow. Cells recognize, process, and act upon this signal. To study this mechanoresponse we applied well-defined mechanical strain cyclically to cultivated cells [1]. Cellular mechanoresponses were quantified via reorientation of cytoskeletal fibers. In cultivated endothelial cells we compared responses of actin, microtubules, and vimentin using a correlation-based algorithm and observed distinctly different ordering dynamics and amplitudes [2].

Even though the rigid skull protects the brain, it experiences intense mechanical deformations. Therefore we studied mechanoresponses of primary neurons from cortices of rat embryos. We observed a pronounced reorientation of neuronal dendrites upon cyclic strain and found a surprising mechanical resilience of these cells that survived even several days of uniaxial, cyclic stretching at an amplitude of 28% and a frequency of 300 mHz [3]. Moreover, results on neuronal activity and on the mechanobiology of further cell types of the brain will be shown.

[1] U. Faust et al., PLOS ONE 6, e28963 (2011).
[2] R. Springer et al., PLOS ONE 14, e0210570 (2019)
[3] J.-A. Abraham et al., Langmuir 35, 7423 (2019)

BP 1.4 Mon 10:10 BPa

Elucidating cell mechanics regulators from mechano-transcriptomic data using discriminative network analysis — •Marta Urbanska[1,2], Yan Ge[1], Maria Winzi[1], Shada Abuhattum[1,2], Maik Herbig[1,2], Martin Kräter[1,2], Nicole Töpfner[1], Anna Taubenberger[1], Carlo V. Cannistraci[1], and Jochen Guck[1,2] — [1]BIOTEC, TU Dresden, Dresden, Germany — [2]Max Planck Institute for the Science of Light, Erlangen, Germany

Mechanical properties of cells determine their capability to perform many physiological functions, such as migration, differentiation or circulation through vasculature. Identifying molecular factors that govern the mechanical phenotype is therefore a subject of great interest. Here we present an approach that enables establishing links between mechanical phenotype changes and the genes responsible for driving them. In particular, we employ a discriminative network analysis method termed PC-corr to associate cell mechanical states, measured by real- time deformability cytometry, with large-scale transcriptomic datasets across different biological systems. We obtain a conserved module of five target genes and validate their capacity to discriminate between soft and stiff cell states in silico, obtaining AUC-ROC values of 72-94%. We then show experimentally that the top scoring gene, CAV1, changes the mechanical phenotype of cells when silenced or overexpressed. The data-driven approach presented here has the power of de novo identification of genes involved in cell mechanics, thereby extending the toolbox for tuning the mechanical properties of cells on demand to enable biological function or prevent pathologies.

30 min. Meet the Speaker & coffee break

BP 2: Active Biological Matter I (joint session BP/DY/CPP)

Time: Monday 9:00–11:00 Location: BPb

Invited Talk BP 2.1 Mon 9:00 BPb

The tortoise and hare: how moving slower allows groups of bacteria to spread across surfaces — Oliver Meacock[1,2], Amin Doostmohammadi[3], Kevin Foster[1], Julia Yeomans[1], and •William Durham[1,2] — [1]University of Oxford, United Kingdom — [2]University of Sheffield, United Kingdom — [3]University of Copenhagen, Denmark

Bacteria use tiny grappling hook like appendages called pili to pull themselves across solid surfaces. While pili-based motility has been widely studied in solitary Pseudomonas aeruginosa cells, this species also uses pili to collectively migrate across surfaces when they are densely packed together in a colony. Interestingly, we find genotypes that individually move slower can collectively migrate faster as a group. Using theory developed to study liquid crystals, we demonstrate that this effect is mediated by the physics of topological defects, points where cells with different orientations meet one another. Our analyses reveal that when defects with a topological charge of +1/2 collide with one another, the fast-moving mutant cells rotate vertically and become trapped. By moving more slowly, wild-type cells avoid this trapping mechanism, allowing them to collectively migrate faster. Our work suggests that the physics of liquid crystals has played a pivotal role in the evolution of collective bacterial motility by exerting a strong selection for cells that exercise restraint in their movement.

Full paper in Nature Physics available free of charge at: https://rdcu.be/cbcgc

BP 2.2 Mon 9:30 BPb

Light-regulated cell aggregation in confinement — •Alexandros Fragkopoulos[1], Jeremy Vachier[1], Johannes Frey[1], Flora-Maud Le Menn[1], Marco Mazza[1,2], Michael Wilczek[1], David Zwicker[1], and Oliver Bäumchen[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany — [2]Department of

Mathematical Sciences, Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom — [3]Experimental Physics V, University of Bayreuth, D-95447 Bayreuth, Germany

Photoactive microbes live in complex environments with spatially and temporally fluctuating light conditions. They survive in such habitats by switching their metabolic activity from photosynthesis to aerobic respiration in unfavorable light conditions. We demonstrate that this adaptation in a suspension of soil-dwelling *Chlamydomonas reinhardtii* cells under confinement leads to a spontaneous separation into regions of high and low cell densities. We show that the inhibition of the photosynthetic machinery is necessary but insufficient to generate the observed aggregation. Microfluidic experiments, simulations, and mean-field theory approaches demonstrate that the emergence of microbial aggregations is governed by the oxygen concentration field inside the microhabitat. In fact, in regions where the energy production is completely arrested by both, the photosynthetic and respiratory systems, the cell speed decreases resulting in an aggregation, which thus takes the form of the underline oxygen field.

BP 2.3 Mon 9:50 BPb

Emergent activity of motile phytoplankton in nutrient landscapes — •Jayabrata Dhar, Francesco Danza, Arkajyoti Ghoshal, and Anupam Sengupta — Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, 162 A, Avenue de la Faencerie, L-1511, Luxembourg City, Luxembourg

Despite their minuscule size, microbes mediate a range of processes in ecology, medicine, and industrial settings that span orders of nutrient concentrations. Yet, to date, we lack a biophysical framework that could link nutrient availability to phytoplankton behavior and predict the impact of dynamic nutrient conditions on motility. Using a combination of micro-scale imaging, microbiology and fluid dynamic models, we quantify how nutrient availability regulates motility, at both individual and population scales [1]. We extract the time-scales over which phytoplankton actively regulate swimming and morphological characteristics, thus shedding light on the finely tuned biophysical mechanisms that equip cells to tackle spatial and temporal heterogeneity of nutrient landscapes. Our results propose local nutrient levels as a handle to control the activity of motile phytoplankton species, promising an exciting model of tunable motile active matter.

[1] Danza, Dhar, Ghoshal and Sengupta (in prep.)

BP 2.4 Mon 10:10 BPb

Chemotaxis strategies of bacteria with multiple run-modes — Zahra Alirezaeizanjani[1,2], •Robert Grossmann[1], Veronika Pfeifer[1], Marius Hintsche[1], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Bacterial chemotaxis – a fundamental example of directional navigation in the living world – is key to many biological processes, including the spreading of bacterial infections. Many bacterial species were recently reported to exhibit several distinct swimming modes – the flagella may, for example, push the cell body or wrap around it. How do the different run modes shape the chemotaxis strategy of a multi-mode swimmer? Here, we investigate chemotactic motion of the soil bacterium *Pseudomonas putida* as a model organism. By simultaneously tracking the position of the cell body and the configuration of its flagella, we demonstrate that individual run modes show different chemotactic responses in nutrition gradients and thus constitute distinct behavioral states. Based on an active particle model, we demonstrate that switching between multiple run states that differ in their speed and responsiveness provide the basis for robust and efficient chemotaxis in complex natural habitats.

30 min. Meet the Speaker

BP 3: Focus Physics of Stem Cells

Time: Monday 9:00–11:00 Location: BPc

BP 3.1 Mon 9:00 BPc

How Tissue Microenvironment Impacts Pluripotent Cell Differentiation — •Allyson Quinn Ryan[1,2], Diana Alves-Afonso[1], Jacqueline M. Tabler[1], and Carl D. Modes[1,2] — [1]Max Planck Institute for Molecular Cell Biology and Genetics — [2]Center for Systems Biology Dresden

The importance of stem cell population maintenance throughout both development and adulthood has been evident for several decades. Classically, how these populations are regulated is investigated through genetic and cell biological studies. However, work in recent years has shown forces exerted by and through tissue microenvironments to be of equal importance as molecular and transcriptional profiles to cell potency and identity. Here we show that collagen organization and tissue stiffness of the midline suture, a stem cell like niche in the cranial mesenchyme, is distinct from that of adjacent tissues. Surprisingly, Lamin A/C nuclear envelope expression is higher in suture than bone, despite the soft nature of the tissue. When collagen crosslinking is perturbed, Lamin A/C localization patterns, nuclear morphology and neighbor relationships within the suture are significantly altered. These results point towards a framework of non-cellular tissue entities and collective organization influencing the maintenance of potency in developmental tissues.

BP 3.2 Mon 9:20 BPc

Robustness and timing of cellular differentiation through population based symmetry-breaking — Angel Stanoev[1], Dhruv Raina[1], Christian Schröter[1], and •Aneta Koseska[2] — [1]Department of Systemic Cell Biology, Max Planck Institute of Molecular Physiology, Dortmund — [2]Cellular computations and learning, caesar, Bonn

During mammalian development, cell types expressing mutually exclusive genetic markers are iteratively differentiated from a multilineage primed state. The current dynamical framework of differentiation, single-cell multistability, however requires that initial conditions in the multilineage primed state are appropriately controlled to result in robust proportions of differentiated fates.

We propose a fundamentally different dynamical treatment in which cellular identities emerge and are maintained on population level, as a novel unique solution of the coupled system. We show that the subcritical organization of such a coupled system close to the bifurcation point enables symmetry-breaking to be triggered by cell number increase in a timed, self-organized manner. Robust cell type proportions are thereby an inherent feature of the resulting inhomogeneous solution. In accordance with this theory, we demonstrate experimentally that a population-based mechanism governs cell differentiation in an embryonic stem cell model for an early lineage decision of mammalian embryogenesis. Our results therefore suggest that robustness and accuracy can emerge from the cooperative behavior of growing cell populations during development.

BP 3.3 Mon 9:40 BPc

Inference of emergent spatio-temporal processes from single-cell sequencing reveals feedback between de novo DNA methylation and chromatin condensates — •Fabrizio Olmeda[1], Tim Lohoff[2], Stephen Clark[2], Laura Benson[2], Felix Krueger[2], Wolf Reik[2,3], and Steffen Rulands[1,4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]The Babraham Institute, Cambridge, UK — [3]University of Cambridge, Cambridge, UK — [4]Center for Systems Biology Dresden, Dresden, Germany

Recent breakthroughs in single-cell genomics allow probing molecular states of cells with unprecedented detail along the sequence of the DNA. Biological function relies, however, on emergent processes in the three-dimensional space of the nucleus, such as droplet formation through phase separation. Here, we use single-cell multi-omics sequencing to develop a theoretical framework to rigorously map epigenome profiling along the DNA sequence onto a description of the emergent spatial dynamics in the nucleus. We show how DNA methylation patterns of the embryonic genome are established through the interplay between spatially correlated DNA methylation and topological changes to the DNA. This feedback leads to the predicted formation of condensates of methylated DNA. Our work provides a general framework of how mechanistic insights into emergent processes underlying cell fate decisions can be gained by the combination of single-cell multi-omics and methods from theoretical physics.

BP 3.4 Mon 10:00 BPc

Competition for stem cell fate determinants as a mechanism for tissue homeostasis — •David J. Jörg[1,2], Yu Kitadate[3,4], Shosei Yoshida[3,4], and Benjamin D. Simons[1,2,5] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [2]Gurdon Institute, University of Cambridge, Cambridge CB2 1QN, UK — [3]Division of Germ Cell Biology, National Institute for Basic Biology, National Institutes of Natural Sciences, Okazaki, Japan — [4]Department of Basic Biology, School of Life Science, Graduate University for Advanced Studies (Sokendai), Okazaki, Japan — [5]Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK

Stem cells maintain tissues by generating differentiated cell types while simultaneously self-renewing their own population. The mechanisms that allow stem cell populations to control their density, maintain robust homeostasis and recover from injury remain elusive. Motivated by recent experimental advances, here we develop a robust mechanism of stem cell self-renewal based on competition for diffusible fate determinants. We show that the mechanism is characterized by signature dynamic and statistical properties, from stem cell density fluctuations and transient large-scale oscillation dynamics during recovery, to scaling clonal dynamics and front-like boundary propagation. We suggest that com-

petition for fate determinants provides a generic mechanism by which stem cells can self-organize to achieve density homeostasis in an open niche environment.

30 min. Meet the Speaker

BP 4: Cell Mechanics II

Time: Monday 11:00–13:30 Location: BPa

BP 4.1 Mon 11:00 BPa

Stochastic bond dynamics induce optimal alignment of malaria parasite — •Anil Kumar Dasanna, Sebastian Hillringhaus, Gerhard Gompper, and Dmitry Fedosov — Theoretical Physics of Living Matter, IBI-5 and IAS-2, Forschungszentrum Jülich, Germany

Merozoites, malaria parasites during the blood-stage of infection, invade healthy red blood cells (RBCs) to escape from the immune system and multiply inside the host. The invasion occurs only when the parasite apex is aligned with RBC membrane, making the parasite alignment a crucial step for the invasion. Recent experiments have also demonstrated that there is a considerable membrane deformation during the alignment process. In this work, using mesoscopic simulations we assess the exact roles of RBC deformations and parasite adhesion during the alignment. Using coarse-grained models of a deformable RBC and a rigid parasite, we show that both RBC deformation and parasite adhesion bond dynamics are important for an optimal alignment. By calibrating the parasite's motion properties against experiments, we show that simulated alignment times match quantitatively the experimental alignment times. We find that the stochastic nature of adhesion bond kinetics is the key for inducing optimal alignment times. We also show that alignment times increase drastically for rigid RBC which signifies that parasite invasion is less probable into already infected RBC and that membrane deformations during the parasite alignment. Finally, we will demonstrate the importance of parasite shape in the alignment process.

BP 4.2 Mon 11:20 BPa

Mechano-chemical interactions in a one-dimensional description of intracellular reaction-diffusion systems — •Alexander Ziepke and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

The understanding of self-organization processes in biological systems represents a key challenge in the field of theoretical biology. There are various studies on reaction-diffusion (RD) models in a single spatial dimension (1D) that give insights on the fundamental behavior of pattern formation in biological systems [1]. However, effects of a spatial confinement, e.g. the cell geometry, are not captured by most of the 1D models. With our new approach we bridge this gap between biological systems in a spatio-temporally varying confinement and simple 1D-RD equations. On the basis of an asymptotic perturbation analysis, we reduce the dimensionality of the confined system [2]. The resulting description incorporates the effects of mechano-chemical coupling and, therefore, extends significantly the applicability of 1D models beyond free dynamics on straight lines. Studying the derived equation for mass-conserving RD systems with interacting membrane-bound and cytosolic species, we find conditions for geometry induced pattern formation. Moreover, mechano-chemical interactions can lead to a feedback between RD kinetics and a deformation of the cell membrane, giving rise to a variety of interesting phenomena.

[1] J. Halatek and E. Frey, Nat. Phys., 14, 507 (2018)
[2] A. Ziepke, S. Martens, and H. Engel, J. Chem. Phys., 145, 094108 (2016)

BP 4.3 Mon 11:40 BPa

Stochastic model of T Cell repolarization during target elimination — •Ivan Hornak and Heiko Rieger — Saarland University, Dep. Theoretical Physics, Center for Biophysics

Cytotoxic T lymphocytes (T) and natural killer cells are the main cytotoxic killer cells of the human body to eliminate pathogen-infected or tumorigenic cells (target cells). Once a T or NK cell has identified a target cell, they form a tight contact zone, the immunological synapse (IS). One then observes a rotation of the microtubule (MT) cytoskeleton and a movement of the microtubule organizing center (MTOC) to the center of the IS. Since the mechanism of this relocation remains elusive, we devise a theoretical model for the molecular motor driven motion of the MT cytoskeleton. We analyze the cortical sliding and the capture-shrinkage mechanisms currently discussed in the literature and compare quantitative predictions about the spatio-temporal evolution of the MTOC position and spindle morphology with experiments. The model predicts the experimentally observed biphasic nature of the repositioning process. We confirm that the capture-shrinkage mechanism is dominant over the cortical sliding mechanism when MTOC and IS are initially diametrically opposed and inferior to the cortical sliding in other configurations. We find that the two mechanisms act synergistically reducing the resources necessary for repositioning. When two IS are present, the MTOC undergoes irregular transitions between the two IS and we determine the dependency of the dwell times and transition frequency on the dynein density for both mechanisms.

BP 4.4 Mon 12:00 BPa

Virus motility - Ifluenza's spike protein dynamics as a self-organized motor — •Falko Ziebert[1] and Igor Kulic[2,3] — [1]Institute for Theoretical Physics, Heidelberg University, D-69120 Heidelberg, Germany — [2]Institut Charles Sadron UPR22-CNRS, F-67034 Strasbourg, France — [3]Institute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany

Directed self-sustained motion is a hallmark of life employed by both eukaryotic cells and bacteria. While viruses are commonly believed to be just passive agents, influenza has recently been shown to actively move across glycan-coated surfaces, mimicking those of to be infected host cells. Starting from known properties of influenza's spike proteins, we develop a physical model. It predicts a collectively emerging dynamics of spike proteins and surface bound ligands that combined with the virus' geometry give rise to self-organized rolling propulsion. We show that in contrast to most Brownian ratchets, the rotary spike drive is not fluctuation driven but operates optimally as a macroscopic engine in the deterministic regime. The mechanism also applies to man-made analogues like DNA-monowheels and should give guidelines for their optimization.

BP 4.5 Mon 12:20 BPa

Thermodynamics of caveolae formation and mechanosensing — •Niladri Sarkar[1,2] and Pierre Sens[2] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, Netherlands. — [2]Laboratoire Physico Chimie Curie, Institut Curie, CNRS, 75005 Paris, France.

Caveolae are invaginations in cell membranes formed by proteins in the caveolin and cavin family self-aggregating in the membrane to form buds. These buds also have some proteins from the EHD family aggregating at their necks. We have developed a two component equilibrium model for the thermodynamics of these bud formation process using energy considerations, where the caveolin proteins are considered as one component and the neck proteins are taken to be another. We have found that depending on the surface tension of the membrane, the line tension associated with the different proteins and the concentration of the different proteins, invaginations of different shapes and sizes can be obtained, and there can be a transition from a fully budded state to a non-budded state via a partial budded state. Also neck proteins are found to provide extra mechano-protection against disassembly due to surface tension.

BP 4.6 Mon 12:40 BPa

Erythrocyte-erythrocyte aggregation dynamics under shear flow — •Mehdi Abbasi[1], Alexander Farutin[1], Hamid Ez-Zahraouy[2], Abdelilah Benyoussef[3], and Chaouqi Misbah[1] — [1]Univ Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France — [2]LaMCScI, Faculty of Sciences, Mohammed V University of Rabat, Rabat 1014, Morocco — [3]Hassan II Academy of Science and Technology, Rabat 10220, Morocco

In a previous work [Blood cells, molecules, and diseases 25, 339 (1999)], it has been shown that the Red blood cells (RBCs) aggregation process starts by the formation of RBC doublets. In this work we study, by means of numerical simulations, the dynamics of RBCs doublets under shear flow and the impact on rheology. We present a rich phase diagram of RBCs doublets configurations showing features never evoked before. In particular, we show that RBCs doublet may be robust even for very high shear stress compromizing oxygen delivery to organs and tissues. A link to pathological conditions (several common blood diseases) is highlighted.

30 min. Meet the Speaker

BP 5: Active Biological Matter II (joint session BP/CPP/DY)

Time: Monday 11:00–13:30 Location: BPb

BP 5.1 Mon 11:00 BPb

Chiral stresses in nematic cell monolayers — •Ludwig A. Hoffmann[1], Koen Schakenraad[1,2], Roeland M. H. Merks[2,3], and Luca Giomi[1] — [1]Instituut-Lorentz, Leiden University, The Netherlands — [2]Mathematical Institute, Leiden University, The Netherlands — [3]Institute of Biology, Leiden University, The Netherlands

Recent experiments on monolayers of spindle-like cells have provided a convincing demonstration that certain types of collective phenomena in epithelia are well described by active nematic hydrodynamics. While recovering some of the predictions of this framework, however, these experiments have also revealed unexpected features that could be ascribed to the existence of chirality over length scales larger than the typical size of a cell.

We elaborate on the microscopic origin of chiral stresses in nematic cell monolayers and investigate how chirality affects the motion of topological defects, as well as the collective motion in stripe-shaped domains. We find that chirality introduces a characteristic asymmetry in the collective cellular flow, from which the ratio between chiral and non-chiral active stresses can be measured. Furthermore, we find that chirality changes the nature of the spontaneous flow transition under confinement and that, for specific anchoring conditions, the latter has the structure of an imperfect pitchfork bifurcation.

BP 5.2 Mon 11:20 BPb

Developmentally driven self-assembly of living chiral crystals — •Alexander Mietke[1], Tzer Han Tan[2], Hugh Higinbotham[2], Yuchao Chen[2], Peter Foster[2], Shreyas Gokhale[2], Jörn Dunkel[1], and Nikta Fakhri[2] — [1]Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA

The emergent dynamics exhibited by self-organizing collections of living organisms often shows signatures of symmetries that are broken at the single-organism level. At the same time, early organism development itself is accompanied by a sequence of symmetry breaking events that eventually establish the body plan. Combining these key aspects of collective phenomena and embryonic development, we describe here the spontaneous formation of hydrodynamically stabilized active crystals made of hundreds of starfish embryos during early development. As development progresses and embryos change morphology, crystals become increasingly disordered and eventually stop forming. We show that these structures exhibit distinct macroscopic chiral features as a direct consequence of the embryo's chiral swimming properties. We introduce a hydrodynamic near-field model that quantitatively describes the formation and rotation of crystals, as well as the emergence of long-lived chiral deformation waves, all of which can be understood as consequences of broken symmetries on the single-embryo level.

BP 5.3 Mon 11:40 BPb

Thin-Film Model of Resting and Moving Active Droplets — •Fenna Stegemerten[1], Sarah Trinscheck[1,2], Karin John[2], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Münster, Germany — [2]Université Grenoble-Alpes, CNRS Laboratoire Interdisciplinaire de Physique, Grenoble, France — [3]Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Münster, Germany

We propose a long-wave model for free-surface drops of polar active liquid on a solid substrate. The coupled evolution equations for the film height and the local polarization profile are written in the form of a gradient dynamics supplemented with active stresses and fluxes. A wetting energy for a partially wetting liquid is incorporated allowing for motion of the liquid-solid-gas contact line. This gives a consistent basis for the description of drops of dense bacterial suspensions or compact aggregates of living cells on solid substrates. As example, we analyze the dynamics of active drops and demonstrate how active forces compete with passive surface forces to shape droplets and drive contact line motion. We perform parameter continuation in the activity parameters discussing both, resting and moving droplets. Additional direct time simulations investigate transitions from non-uniformly to uniformly polarized as well as resting to moving states.

BP 5.4 Mon 12:00 BPb

Sedimentation and Convection of Bottom-Heavy Squirmers — •Felix Rühle, Jan-Timm Kuhr, and Holger Stark — TU Berlin, Institut für Theoretische Physik, Berlin, Germany

Active particles form appealing patterns, in particular, when hydrodynamic interactions are present [1-3]. A fascinating example known from biology is bioconvection of microswimmers under gravity [4]. In order to study such systems, we simulate bottom-heavy squirmers (neutral squirmers, pushers, and pullers) under different gravitational forces and torques [3]. The relevant parameters are the ratio of swimming to bulk sedimentation velocity α and the normalized torque.

In the state diagram of these parameters, for neutral squirmers at low α we observe sedimentation states, where bottom-heaviness leads to the formation of clusters of different sizes. For high α, finite torques lead to inverted sedimentation. In between, we identify plumes of collectively sinking squirmers that feed convective rolls of circling squirmers at the bottom of the simulation cell. At $\alpha \gtrapprox 1$ and large torques squirmers form a spawning cluster above the wall, from which squirmers occasionally escape. For strong pushers and pullers, we find that the dipolar flow fields weaken the formation of plumes and convective rolls.

[1] M. Hennes, *et al.*, PRL **112**, 238104 (2014)
[2] H. Jeckel, *et al.*, PNAS **116**, 1489 (2019).
[3] F. Rühle, and H. Stark, Eur. Phys. J. E **43**, 26 (2020).
[4] T.J. Pedley, and J.O. Kessler, Annu. Rev. Fluid Mech. **24**, 313 (1992).

BP 5.5 Mon 12:20 BPb

Microscopic scattering of pusher particles in complex environments — •Theresa Jakuszeit[1], Samuel Bell[2], and Ottavio A. Croze[1] — [1]Cavendish Laboratory, JJ Thomson Avenue, CB3 0HE, Cambridge, United Kingdom — [2]Laboratoire Physico Chimie Curie, Institut Curie,PSL Research University, CNRS UMR168, 75005 Paris, France

Active propulsion as performed by bacteria and Janus particles, in combination with hydrodynamic interaction at boundaries, can lead to the breaking of time reversibility. One typical example of this is the accumulation of bacteria on a flat wall. However, in microfluidic devices with cylindrical pillars of sufficiently small radius, self-propelled particles can slide along the surface of a pillar without becoming trapped over long times. This non-equilibrium scattering process can result in large diffusivities even at high obstacle density, unlike particles that undergo classical specular reflection, as in the Lorentz gas. We experimentally study the non-equilibrium scattering as well as the long-term diffusive transport of pusher-like particles by tracking wild-type and smooth-swimming mutants of the model bacterium Escherichia coli in microfluidic obstacle lattices. We relate the determined parameters of the scattering process to previously proposed models and discuss their relevance. Finally, we discuss the potential interpretation of the role of tumbles in the scattering process.

BP 5.6 Mon 12:40 BPb

Swimming behavior of squirmer dumbbells and polymers — •Judit Clopés Llahí, Gerhard Gompper, and Roland G. Winkler — Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany

Nature provides a plethora of microswimmers, which can be rather elongated, filament- or polymer-like. Examples are bacteria swarmer cells or marine phytoplankton dinoflagellates assembling in a linear fashion. In order to address the relevance of hydrodynamic interactions for the collective behavior of such organisms, we study the swimming properties of linear polymer-like assemblies by mesoscale hydrodynamic simulations, where an active unit (monomer) is described by a spherical squirmer – which can be a pusher, a neutral swimmer, or a puller. We find that the monomer hydrodynamic flow field leads to correlations in the relative orientation of adjacent monomers, and consequently the swimming efficiency differs from that of active Brownian linear assemblies. In particular, puller dumbbells and chains show a pronounced increase in the rotational diffusion coefficient compared to pushers, while for neutral squirmers, the rotational diffusion coefficient is similar to that of active Brownian particles. Hence, the large-scale conformational and dynamical properties depend on the specific propulsion mechanism. Refs.: J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. 78, (2015). R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, (2017). J. Clopés, G. Gompper, R. G. Winkler, Soft Matter 16, 10676 (2020).

30 min. Meet the Speaker

BP 6: Systems Biology I

Time: Monday 11:00–13:30 Location: BPc

BP 6.1 Mon 11:00 BPc

Ligation Chain Reactions in Non-Equilibrium Convection Compartments with Microscale pH Cycles — •Annalena Salditt, Dieter Braun, Patrick Kudella, and Leonie Karr — Ludwig-Maximilians-Universität

Early replication mechanisms for the origin of life rely on periodic strand separation to start new rounds of replication necessary to stabilize and accumulate information of long nucleic acids. Especially for catalytically active RNAs, high temperatures required for strand separation promote their hydrolysis, leading to a loss of information. Therefore, a geophysical non-equilibrium environment on early Earth would have required means to separate hybridized strands after replication and to localize long, potentially functional molecules against diffusion while protecting them from hydrolysis. We perform ligation extension experiments in moderate temperature gradients across micrometer thick, water-filled chambers with a water-CO2 interface to induce a miniaturized water cycle while maintaining thermophoretic trapping conditions. In addition to more realistic early atmospheric conditions of the Earth, the CO2-water interface causes periodic pH changes, that induce the hybridization of double strands. We expect this to be a promising autonomous setting for ligation chain reactions starting from a random or semi-random oligomer pool.

BP 6.2 Mon 11:20 BPc

The effects of cross-species gene transfer on genome dynamics — •Mona Förster[1], Isabel Rathmann[1], Jeffrey Power[2], Melih Yüksel[1], and Berenike Maier[1] — [1]Universität zu Köln, Deutschland — [2]Universität Tübingen, Deutschland

Phylogenetic studies have provided strong evidence that gene transfer happens frequently and acts across species. However, the rate at which gene transfer occurs and its short-term effect on genome dynamics are poorly understood. To address the effect of intra- and inter-species gene transfer on genome dynamics we developed an evolution experiment and analysis method to detect horizontal gene transfer. To investigate mechanistic contributions to gene transfer probability, we ensured minimal selection by not allowing for population dynamics. We were able to detect a remarkably high gene transfer rate of 0.4 $\%h^{-1}$ across subspecies of *Bacillus subtilis*. This rate was four times lower when gene transfer was probed between *B. subtilis* and *Bacillus vallismortis* and 125 times lower between *B. subtilis* and *Bacillus atrophaeus*. Interestingly, the average sequence divergence of integrated segments is comparable between all three donors with a mean of about 7 %. We observed that the fraction of replaced genome increases linearly throughout 40 h of DNA uptake, which suggests that transfer of genes, is not yet saturated and could be probed further in evolutionary runs. Following up on this, it will be interesting to use the fitness distribution of the minimal selection replicates to design an evolution experiment with strong selection.

BP 6.3 Mon 11:40 BPc

Genetically engineered control of phenotypic structure in microbial colonies — •Philip Bittihn[1,4], Andriy Didovyk[1,5], Lev S. Tsimring[1], and Jeff Hasty[1,2,3] — [1]BioCircuits Institute — [2]Department of Bioengineering — [3]Molecular Biology Section, Division of Biological Sciences, University of California, San Diego, La Jolla, CA, USA — [4]Department of Living Matter Physics, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [5]Vertex Pharmaceuticals, San Diego, California, USA

Many essential biological behaviors originate from an entanglement of biological (cellular) and physical processes. This is a challenge not only for traditional biology and physics methodology, but also for synthetic biology, where such interactions severely limit the ability to engineer desired behavior with artificial gene regulatory networks. We show how to achieve control of phenotypic structure in bacterial microcolonies by simultaneously exploiting internal gene expression and metabolism, as well as physical coordination through nutrient diffusion and growth, which leads to self-generated nutrient gradients and a heterogeneous population consisting of both dividing and dormant cells. In microfluidic experiments and a mathematical model, we show that gene circuits which sense and control growth can create a spatio-temporal feedback loop via nutrient transport and generate sustained growth oscillations, while a phenotype-specific lysis circuit can selectively eliminate dormant cells. Our results demonstrate how to understand and control multicellular substrates as complex active physical systems.

Reference: *Nature Microbiology* **5**, 697–705 (2020)

BP 6.4 Mon 12:00 BPc

Dynamics, Statistics and Coding in Random Rate and Binary Networks — •Tobias Kühn[1,2,3], Christian Keup[2,3], David Dahmen[2], and Moritz Helias[2,3] — [1]MSC de l'Université de Paris, ENS, CNRS, Paris, France — [2]INM-6, Forschungszentrum Jülich, Germany — [3]Department of Physics, RWTH Aachen, Germany

Cortical neurons communicate with spikes, discrete events in time. Functional network models often employ rate units that are continuously coupled by analog signals. Is there a benefit of discrete signaling? By a unified mean-field theory for large random networks of rate and binary units, we show that both models can be matched to have identical statistics up to second order. Their stimulus processing properties, however, are different: contrary to rate networks, the chaos transition in binary networks strongly depends on network size, and we discover a chaotic submanifold in binary networks that does not exist in rate models. Its dimensionality increases with time after stimulus onset and reaches a fixed point that depends on the synaptic coupling strength. Low-dimensional stimuli are transiently expanded into higher-dimensional representations that live within the manifold. We find that classification performance first increases and then degrades due to variability in the manifold. During this transient, resilience to noise by far exceeds that of rate models with matched statistics, which are always regular. In their respective chaotic regime, however, rate networks show similar a mechanism of transient signal amplification, same for spiking networks [Keup et al. arXiv:2002.11006]. Ack.: Helmholtz assn. (VH-NG-1028); RWTH (ERS seed fund neuroIC002).

BP 6.5 Mon 12:20 BPc

Long-range and rapid signalling gradient formation by cell-to-cell relay — •Johanna Dickmann[1], Jochen Rink[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Development, regeneration and tissue renewal are spectacular tissue patterning events. Tissue patterning, the adaptation of the correct cell fate at the correct position, requires information. This information can be provided by spatially graded distributions of signalling molecules, called signalling gradients. While the formation of signalling gradients is thought to result from diffusion and degradation in the context of embryonic development, it remains controversial how such signalling gradients can be generated on long length scales e.g. during regeneration. We introduce a relay mechanism for gradient formation in which the signal is propagated from cell to cell via a positive feedback loop. That is, each cell produces signalling molecules in response to receiving a signal. We show that polarised secretion of signalling molecules produced in response to the received signal results in an effective drift of signalling molecule concentration through the system, markedly accelerating the formation of signalling gradients. This way, the relay mechanism explains gradient formation on millimetre length scales within hours to days for physiological parameter choices.

BP 6.6 Mon 12:40 BPc

Model for inference of cell dynamics from C14 data — •Julian Rode[1], Fabian Rost[2], Paula Heinke[1], Enikö Lazar[3], Lutz Brusch[1], and Olaf Bergmann[1] — [1]Technische Universität Dresden, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Karolinska Institutet, Stockholm, Sweden

Carbon dating is an established method to determine the age of ancient artefacts. Traditionally, radioactive decay changes the C14 ratio of the sample which can be used to determine the age. Recently, a second route has become available as the drastic change of atmospheric C14 due to atomic bomb tests in the 60's allows to invert this classic C14 dating method. Now, the C14 decay is negligible, but the atmospheric C14 changes quickly, allowing an accurate age measurement even of human samples. This method allows to estimate the cell turnover in vivo using the C14 carbon ratio of the DNA from many cells. But a simple matching of C14 values is not sufficient because the measured C14 values are the average of cells with different ages. We introduce a C14-structured population model to predict the average C14 content and accounting for cell division, cell inflow from a fast cycling stem cell population and cell death. Additionally, a priori knowledge such as tissue growth has to be considered resulting in constrains for the model solution. We use variations of this model to analyse C14 data from human liver and muscle tissue.

30 min. Meet the Speaker

BP 7: Cell Mechanics III

Time: Monday 14:00–16:30 Location: BPa

BP 7.1 Mon 14:00 BPa

Highly Reproducible Physiological Asymmetric Membrane with Freely Diffusing Embedded Proteins in a 3D Printed Microfluidic Setup — Paul Heo[1], Sathish Ramakrishnan[1,2], Jeff Coleman[2], James E. Rothman[2], •Jean Baptiste Fleury[3], and Frederic Pincet[1] — [1]Laboratoire de Physiqe Statistique ENS, Paris, France — [2]Department of Cell Biology Yale School of Medicine, New Haven, USA — [3]Department of Experimental Physics and Center for Biophysics, Saarland University Saarbruecken, Germany

Experimental setups to produce and to monitor model membranes have been successfully used for decades and brought invaluable insights into many areas of biology. However, they all have limitations that prevent the full in vitro mimicking and monitoring of most biological processes. Here, a suspended physiological bilayer-forming chip is designed from 3D-printing techniques. This chip can be simultaneously integrated to a confocal microscope and a path-clamp amplifier. The bilayer, formed by the zipping of two lipid leaflets, is free-standing, horizontal, stable, fluid, solvent-free, and flat with the 14 types of physiologically relevant lipids, and the bilayer formation process is highly reproducible. Furthermore, different proteins family can be added to the bilayer in controlled orientation and keep their native mobility and activity. These features allow in vitro recapitulation of membrane process close to physiological conditions, as shown in the following references: Small, 2019, 10.1002/smll.201900725 Advanced Materials, 2020, 10.1002/adma.202070389 PNAS, 2021 (in press)

BP 7.2 Mon 14:20 BPa

Tracking Electrostatically Driven Membrane Transfer between Lipid Vesicles and a Supported Lipid Bilayer on a QCM — •Justus Bednár[1,2], Anastasia Svetlova[1,2], Vanessa Maybeck[1], and Andreas Offenhäusser[1] — [1]Forschungszentrum Jülich, Institute of Biological Information Processing: Bioelectronics (IBI-3) — [2]Fakultät für Mathematik, Informatik und Naturwissenschaften RWTH Aachen

Lipid bilayer systems are used widely in medicine and biotechnology. Supported lipid bilayers (SLBs) for example, can be employed as a biomimetic platform for cell cultures or can be studied as a model system of the cell membrane itself. If SLB and lipid vesicles have opposite surface charges, their electrostatic interaction can be used to modify the lipid composition of the SLB. Studying the underlying process, the quartz crystal microbalance (QCM) stands out for its ability to precisely monitor the acoustic response of a macroscopic SLB and coupled objects with a sub-second time resolution. Unfortunately, standard models that relate the QCM signal response to physical properties of the sample do not apply in this case.

Here, a viscoelastic model for an ensemble of lipid vesicles, coupled to an SLB, is presented. Experimental results demonstrate the capability of this model to estimate relative concentrations of extracellular vesicles (EVs) in bulk solution. Furthermore, throughout numerous experiments of electrostatically driven membrane transfer between lipid vesicles and an SLB, a non-trivial time-dependence of vesicle-adsorption is observed.

Invited Talk BP 7.3 Mon 14:40 BPa

Towards the mechanical characterization of neuronal network formation — Paulina Wysmolek[2], Florian Huhnke[2], Katja Salbaum[1], Joachim Spatz[2], and •Friedhelm Serwane[1,2] — [1]LMU, Department of Physics, Munich — [2]Max Planck Institute for Medical Research, Heidelberg

In recent years, researchers have engineered multicellular 3D systems, organoids, which share the same cell types and tissue organization as their in vivo counterparts. Those in vitro models provide an opportunity to glimpse at how biology self-assembles neuronal networks and how nanoscale building blocks, such as cell-cell adhesion molecules, contribute to the formation of tissue shape, structure and function. In this talk I will present the current and future research of our newly established ERC-group. We will explore, how tissue mechanical properties affect the formation and function of retina organoids. For this, we build on our expertise in mechanics measurements (1,2) and retina organoid technology. Quantifying the mechanics of neuronal systems opens the door to neurodegenerative disease modeling as it will be performed by our group. In addition, it allows developing a biophysical understanding how neuronal networks are initially formed.

(1) Serwane et al., In vivo quantification of spatially-varying mechanical properties in developing tissues. Nature Methods, 2017

(2) Mongera et al., A fluid-to-solid jamming transition underlies vertebrate body axis elongation. Nature, 2018

BP 7.4 Mon 15:10 BPa

Lattice defects induce microtubule self-renewal — Laura Schaedel[1], Sarah Triclin[1], Denis Chrétien[2], Ariane Abrieu[3], Charlotte Aumeier[1], Jérémie Gaillard[1], Laurent Blanchoin[1,4], Manuel Théry[1,4], and •Karin John[5] — [1]Univ. Grenoble-Alpes, CEA, CNRS, INRA, Biosciences & Biotechnology Institute of Grenoble, Laboratoire de Physiologie Cellulaire & Végétale, CytoMorpho Lab, 38054 Grenoble, France — [2]Univ. Rennes, CNRS, IGDR (Institute of Genetics and Development of Rennes) - UMR 6290, F-35000 Rennes, France — [3]CRBM, CNRS, University of Montpellier, Montpellier, France — [4]Univ. Paris Diderot, INSERM, CEA, Hôpital Saint Louis, Institut Universitaire d'Hematologie, UMRS1160, CytoMorpho Lab, 75010 Paris, France — [5]Univ. Grenoble-Alpes, CNRS, Laboratoire Interdisciplinaire de Physique, 38000 Grenoble, France

Microtubules are dynamic polymers, which grow and shrink at their extremities. Within the microtubule shaft, tubulin dimers adopt a highly ordered lattice structure, which is generally not considered to be dynamic. Here we report a new aspect of microtubule dynamics, whereby thermal forces are sufficient to remodel the lattice, despite its apparent stability. Our combined experimental data and numerical simulations on lattice dynamics and structure demonstrate that dimers can spontaneously leave and be incorporated into the lattice at structural defects. We propose a model mechanism, where the lattice dynamics is initiated via a passive breathing mechanism at dislocations, which are frequent in rapidly growing microtubules.

BP 7.5 Mon 15:30 BPa

Multiplication of gliding microtubules for biocomputational applications — •Cordula Reuther[1], Paula Santos Otte[1], Rahul Grover[1], Till Korten[1], Günther Woehlke[3], and Stefan Diez[1,2] — [1]B CUBE, TU Dresden, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, 01062 Dresden, Germany — [3]Department of Physics, TU München, Garching, Germany

Recently, an approach to solve combinatorial problems was demonstrated by kinesin-1 driven microtubules exploring, as autonomous agents, physical networks of nanometer-sized channels [Nicolau et al., PNAS, 113(10), 2016]. The possibility to multiply the agents exponentially while traversing such networks is crucial for the scalability of these systems. We developed a method for the multiplication of microtubules gliding on surface-immobilized kinesin-1 and kinesin-14 molecules, respectively. Specifically, our method comprises two simultaneously proceeding processes: (1) elongation of microtubules by self-assembly of tubulin dimers and (2) cutting of microtubules by the severing enzyme spastin. The main challenge in doing so is to optimize both processes such that the average length of the filaments stays roughly constant over time while the number of filaments increases exponentially. Additionally, nucleation of new filaments ought to be avoided in order to prevent errors in the calculations performed by the microtubules. Thus, we first studied each of the two processes separately under various conditions before combining the optimized protocols to actually multiply microtubules. Finally, we aim to multiply microtubules in a physical network with channel structures.

40 min. Meet the Speaker

BP 8: Bioimaging and Biospectroscopy

Time: Monday 14:00–16:30 Location: BPb

BP 8.1 Mon 14:00 BPb

Near Infrared Fluorescence Imaging with Carbon nanotubes and Nanosheets — •Sebastian Kruss — Ruhr-Universität Bochum, Germany

We are interested in 1D and 2D materials that provide novel photophysical properties such as near Infrared (NIR) fluorescence. The NIR range (800-1700 nm) of the spectrum is beneficial for many optical applications because it falls into the tissue transparency window. One example of such a material is semiconducting single-walled carbon nanotubes (SWCNTs). SWCNTs fluoresce in the NIR and their optoelectronic properties are very sensitive to changes in the chemical environment and they are therefore versatile building blocks for fluorescent labels and sensors. In my talk I will show fundamental insights into SWCNT photophysics/surface chemistry and how selectivity of SWCNT-based fluorescent sensors can be enhanced. These sensors can be used for multiscale imaging to resolve single molecules such as kinesin motors in vivo, efflux of neurotransmitters (dopamine, serotonin) from cells, identification of pathogens or stress

in whole plants. Furthermore, I introduce a novel class of ultrabright 2D NIR fluorescent silicate nanosheets and demonstrate in vivo particle tracking as well as standoff detection in living plants.

BP 8.2 Mon 14:20 BPb

Motion-based segmentation for particle tracking: A fully-convolutional neuronal network that analyses movement — •Till Korten[1], Walter de Back[2], Christoph Robert Meinecke[3], Danny Reuter[3,4], and Stefan Diez[1] — [1]B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, Dresden, Germany — [2]Institute for Medical Informatics and Biometry (IMB), Carl Gustav Carus Faculty of Medicine, Technische Universität Dresden, Dresden, Germany — [3]Center for Microtechnologies, TU-Chemnitz, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany

For single-particle tracking it is often necessary to separate particles of interest from background particles based on their movement pattern. Here we introduce a deep neuronal network that employed convolutional long-short-term-memory layers in order to be able to perform image segmentation based on the motion pattern of particles. Training was performed with ≈ 500 manually annotated 128x128 pixel frames. The segmentation result was used as input for a conventional single particle tracking algorithm. With this workflow 100% of all tracks belonged to microtubules that were propelled by kinesin-1 motor proteins along guiding channels and no tracks belonged to microtubules diffusing in the background. Furthermore, microtubules moving in a different orientation than the guiding channels during training, did not show up during inference. In conclusion, the deep-learning-based tracking resulted in almost twice as many (2800 vs. 1500) usable tracks that were 35 % longer compared to filtering after tracking.

BP 8.3 Mon 14:40 BPb

Molecule counts in complex oligomers with single-molecule localization microscopy — Tim Niklas Baldering[1], •Jakob Tómas Bullerjahn[2], Gerhard Hummer[2], Mike Heilemann[1], and Sebastian Malkusch[1] — [1]Institute of Physical and Theoretical Chemistry, Goethe-University Frankfurt, Frankfurt am Main, Germany — [2]Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Frankfurt am Main, Germany

Single-molecule localization microscopy resolves nano-scale protein clusters in cells, and in addition can extract protein copy numbers from within these clusters. A powerful approach for such molecular counting is the analysis of fluorophore blinking using stochastic model functions. Here, we develop a theoretical model for quantitative analysis of photoactivated localization microscopy (PALM) data that accounts for the detection efficiency. By this, we are able to extract populations of different oligomers reliably and in complex mixtures. We demonstrate this approach analyzing simulated PALM data of a photoactivatable fluorescent protein. We generate simulations of blinking data of oligomers and of mixtures of oligomers, and show robust oligomer identification. In addition, we demonstrate this approach for experimental PALM data.
https://doi.org/10.1088/1361-6463/ab3b65

BP 8.4 Mon 15:00 BPb

Dissection of Plasmodium falciparum developmental stages with multiple imaging methods — •Katharina Preissinger[1,2], Beáta Vértessy[1,2], István Készmárki[3,4], and Miklós Kellermayer[5] — [1]Department of Applied Biotechnology and Food Sciences, BME, Budapest, Hungary — [2]Institute of Enzymology, Research Center for Natural Sciences, Budapest, Hungary — [3]Department of Physics, BME, Budapest, Hungary — [4]Department of Experimental Physics V, University of Augsburg, Germany — [5]Department of Biophysics and Radiation Biology, Semmelweis University, Budapest, Hungary

Efficient malaria treatment is a global challenge, requiring in-depth insight into the maturation of malaria parasites during the intraerythrocytic cycle. Exploring structural and functional variations of the parasites and their impact on red blood cells (RBCs) is a cornerstone of antimalarial drug development. In order to trace such changes in fine steps of parasite development, we performed an imaging study of RBCs infected by Plasmodium falciparum, using atomic force microscopy (AFM) and total internal reflection fluorescence microscopy (TIRF), further supplemented with bright field microscopy for the direct assignment of the stages. This multifaceted imaging approach allows to reveal correlations of the parasite maturation with morphological and fluorescence properties of the stages. We established identification patterns characteristic to the different parasite stages based on the height profile of infected RBCs which show close correlation with typical fluorescence (TIRF) maps of RBCs.

BP 8.5 Mon 15:20 BPb

Self-organization of endoplasmic reticulum exit sites — •Konstantin Speckner, Lorenz Stadler, and Matthias Weiss — Experimentalphysik 1, Universität Bayreuth

The endoplasmic reticulum (ER) is a highly dynamic organelle that pervades the entire cell and hosts a variety of vital processes. For example, the exchange of proteins with the secretory pathway occurs at specialized and long-lived membrane domains, called ER exit sites (ERES). In mammalian cells, ERES form protein assemblies that emerge as a lattice-like arrangement of dispersed droplets on the ER membrane. Although ERES were seen to diffuse on short timescales, they appear stationary on longer periods. Notably, their dynamics is different from the cytoskeleton-dependent, shivering motion of ER tubules. To gain insights into the self-organization of ERES patterns, we have studied biochemical perturbations on the morphology of the ER and analyzed the spatial arrangement of ERES by quantitative fluorescence imaging. As a result, we found a significantly changed patterns of ERES components when reducing the amount of curvature-inducing membrane proteins. In contrast, disrupting the ER network into fragments or affecting the cytoskeletons integrity had only mild effects on the ERES patterns. Our findings can be well explained by modelling ER junctions as diffusion barriers for the exchange of ERES protein constituents. Altogether, we provide evidence that the native ERES patterns are the result of a quenched fluctuation-driven two-dimensional demixing process.

BP 8.6 Mon 15:40 BPb

A multisensory interface for exploring nanomechanical tissue properties with human senses — •Robert Magerle, Paul Zech, Martin Dehnert, Alexandra Bendixen, and Andreas Otto — Fakultät für Naturwissenschaften, TU Chemnitz

Tissues display a complex spatial structure and their mechanical properties remain largely unexplored on the nanometer scale. Here we present a multisensory interface that makes nanomechanical tissue properties accessible to human perception and cognition. With a haptic device, we translate the 3D force fields measured with an atomic force microscope (AFM) on the nanometer scale into forces perceivable to humans. This allows human users to explore haptically the specimen's surface shape as well as its local nanomechanical properties while simultaneously employing multiple senses. First tissues studied include native (unfixed), hydrated tendon of sheep, chickens, and mice. AFM imaging in air with controlled humidity preserves the tissue's water content and allows for high-resolution imaging. The force-vs.-distance (FD) data measured with the AFM display a rate-independent hysteresis with return-point memory. A generic hysteresis model that uses FD data collected during one approach-retract cycle predicts the force (output) for an arbitrary indentation trajectory (input). We implemented this hysteresis model with a haptic device which allows human users to perceive a physically plausible tip–sample interaction. They can discriminate the specimen's local hardness, its elastic response, as well as the energy dissipation due to the rate-independent hysteretic process.

30 min. Meet the Speaker

BP 9: Systems Biology II

Time: Monday 14:00–16:30 Location: BPc

Invited Talk BP 9.1 Mon 14:00 BPc

From individual to collective intermittent motion: from bacteria to sheep — •Fernando Peruani — CY Cergy Paris University, Cergy, France

Intermittent behavior is observed in biological systems at all scales, from bacterial systems to sheep herds. First, I will discuss how Escherichia coli explores surfaces by alternating stop and moving phases. Specifically, I will show that a stochastic three behavioral state model is consistent with the empirical data. The model reveals that the stop frequency of bacteria is tuned at the optimal value that maximizes the diffusion coefficient. These results provide a new perspective on how evolution may have reshaped the bacterial motility apparatus. Intermittent motion is also observed in Merino sheep, where again a stochastic three behavioral state model provides a quantitative understanding of the empirical data. However, in sheep, individual transition rates depend on the behavioral state of other individuals and collective behaviors emerge. Specifically, I will show that small sheep herds display highly synchronized intermittent collective motion, with the herd behaving as a self-excitable system. Based on the analysis of these two biological systems (bacteria and sheep), we will discuss the need of three behavioral states to describe intermittent motion in biological systems, providing a unified picture of such behavior across scales.

Refs.: Perez Ipina et al. Nature Physics 15, 610-615 (2019); Gascuel et al. Animal behavior (2021); Gomez Nava et al. (2021)

BP 9.2 Mon 14:30 BPc

Specialisation and plasticity in a primitive social insect — •Adolfo Alsina[1], Solenn Patalano[2], Martin Bachman[3], Irene Gonzalez-Navarrete[4], Stephanie Dreier[5], Shankar Balasubramanian[3], Seirian Sumner[5], Carlos Gregorio-Rodriguez[6], Wolf Reik[2], and Steffen Rulands[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]The Babraham Institute, Cambridge, UK — [3]University of Cambridge, Cambridge , UK — [4]Centre for Genomic Regulation (CRG), Barcelona , Spain — [5]Institute of Zoology, London , UK — [6]Universidad Complutense de Madrid (UCM), Madrid, Spain

Biological systems not only have the remarkable capacity to build and maintain complex spatio-temporal structures in noisy environments, they can also rapidly break up and rebuild such structures. How can such systems can simultaneously achieve both robust specialisation and plasticity is poorly understood. Here we use primitive societies of Polistes wasps as a model system where we experimentally perturb the social structure by removing the queen and follow the relaxation dynamics back to the social steady state over time. We combine a unique experimental strategy correlating measurements across vastly different spatial scales with a theoretical approach. We show that Polistes integrates antagonistic processes on multiple scales to distinguish between extrinsic and intrinsic perturbations and thereby achieve both robust specialisation and rapid plasticity. Such dynamics provide a general principle of how both specialization and plasticity can be achieved in biological systems.

BP 9.3 Mon 14:50 BPc

Plasticity in vertex model of epithelial tissues — •Marko Popović[1,2], Valentin Druelle[1,3], Natalie Dye[4,5], Frank Julicher[2,5], and Matthieu Wyart[1] — [1]Institue of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]Max Planck Institute for Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [3]Biozentrum, University of Basel, Klingelberstrasse 70, 4056 Basel, Switzerland — [4]Max Planck Institute for Molecular Cell Biology and Genetics, Pfotenhauerstrasse 108, 10307 Dresden, Germany — [5]Cluster of Excellence Physics of Life, TU Dresden, 01307 Dresden, Germany

Developing tissues are often described as viscoelastic liquids. However, tissues can also be plastic and respond elastically to stresses below the critical value, while flowing plastically at higher stresses. Plasticity is exhibited by a wide class of amorphous solids such as colloidal gels, emulsions, and foams where it corresponds to a yielding transition. Are features of yielding transition, such as dependence on system preparation and non-linear rheology, relevant in developing tissues? Motivated by similarities of disordered tissues and amorphous solids we study the plasticity of the vertex model of epithelial tissues, where the mechanical properties of cells are prescribed and tissue mechanics is obtained from their collective behavior. We describe the mechanics of T1 transitions, which are the elementary plastic events in epithelial tissues. We find that interactions between T1 transitions are analogous to those of particle rearrangements in amorphous solids and our simulations suggest that the vertex model belongs to the same class of universality.

BP 9.4 Mon 15:10 BPc

Selection via phase separation — •Giacomo Bartolucci[1,2], Adriana Serrao[3], Philipp Schwintek[3], Alexandra Kühnlein[3], Yash Rana[4], Dieter Braun[3], Christof Mast[3], and Christoph A. Weber[1,2] — [1]Max Planck for the Physics of Complex Systems, Dresden — [2]Center for Systems Biology Dresden — [3]Ludwig Maximilian University, München — [4]Harvard University, Cambridge, USA

Living cells and pre-biotic systems are complex aqueous mixtures composed of thousands of different heteropolymers. In such multi-component mixtures, enrichment and selection of a small set of components are important to achieve biological function. However, when the number of components increases, each of them becomes more diluted impeding a significant enrichment of selected components. Here, we propose a selection mechanism relevant for prebiotic mixtures based on cycles of phase separation combined with material exchange of the dense phase with a reservoir. We find a selective enrichment of components up to two orders of magnitude coinciding with a growth of the dense phase up to the system volume. Such enrichment of selective components is robust also in mixtures composed of a large number of components. For a prebiotic soup, our findings indicate that cycles of phase separation and material exchange with a reservoir, e.g. the accumulation DNA gel in rock pores periodically filled with DNA rich aqueous solution, could provide a mechanism for the selection and enrichment of specific heteropolymers sequences in a multi-component mixture at the origin of life.

BP 9.5 Mon 15:30 BPc

Towards an alphabet of random matrix models for large biological networks — •Philipp Fleig[1] and Ilya Nemenman[2] — [1]University of Pennsylvania, Philadelphia, USA — [2]Emory University, Atlanta, USA

Biological interaction networks such as populations of neurons or amino acid sequences in proteins are critical to the functioning of any biological system. The trend of modern high-throughput experiments is to record data from a rapidly increasing number of simultaneously measured network units. Such data recorded from a biological network has characteristics of a large random matrix with hidden structures encoded in it. We present first steps towards the design of an alphabet of random matrix models to describe data of biological networks. Here, we focus on how to detect different random matrix structures in data from simple observable quantities such as pairwise correlations and the eigenvalue spectrum of the correlation matrix. Using random matrix theory we show analytically how properties of the data, such as a hidden dimensionality, are encoded in these observables. Finally, we use a neural network classifier with the observables as input to detect different types of random matrix structures in our alphabet and their hidden dimensionality in noisy data of finite size. Our approach can likely be used to model large and complex data of diverse types of biological networks.

40 min. Meet the Speaker

BP 10: Posters DY - Fluid Physics, Active Matter, Complex Fluids, Soft Matter and Glasses (joint session DY/BP)

Time: Monday 14:00–16:30 Location: DYp

See DY 12 for details of this session.

BP 11: Poster A: Single Molecule, Multicellular, Bioimaging, Focus Sessions, etc.

Time: Monday 16:30–19:00 Location: BPp

BP 11.1 Mon 16:30 BPp

How fast do PMCA pumps transport Ca^{2+}? — •Barbara Schmidt[1], Cristina E. Constantin[2], Bernd Fakler[2], and Heiko Rieger[1] — [1]Center for Biophysics and Dep. Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Institute of Physiology, University of Freiburg, 79104 Freiburg, Germany

Plasma membrane protein complexes of two PMCA subunits and two Neuroplastin or Basigin proteins are responsible for Ca^{2+} ion transport out of cells. Here we make use of BK-type Ca^{2+}-activated K^+ channels to determine the Ca^{2+} transport activity of PMCA. Due to their large conductance and their particular gating kinetics the BK channels may be used as fast and reliable sensors for intracellular Ca^{2+}-concentration ($[Ca^{2+}]_i$) beneath the plasma membrane. Experimentally we monitor the PMCA-mediated Ca^{2+} clearance (or transport) by the decay of BK-currents following their activation by a short (0.8 ms) period of Ca^{2+}-influx through Cav2.2 channels. To relate the experimentally observed temporal evolution of the K^+ current to the underlying temporal evolution of the Ca^{2+} concentration we implement a theoretical model for the Ca^{2+}-dependence of the BK-current and of the PMCA pump strength. The maximum PMCA pump strength is used to fit the predicted time course of the K^+ current to the experimental data, which turns out to be at least 2 orders of magnitude larger than what has been assumed so far. Implication of this finding for Ca^{2+} signaling in general are discussed.

BP 11.2 Mon 16:30 BPp

Molecular Friction and Adhesion on Porous Membranes — •Kordula Schellnhuber[1,2], Hanna Hübner[2], Johanna Blass[1], Markus Gallei[2], and Roland Bennewitz[1] — [1]INM-Institut für Neue Materialien, Campus D.2.2 Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Lehrstuhl für Polymerchemie, Naturwissenschaftlich-Technische Fakultät, Universität des Saarlandes, 66123 Saarbrücken, Germany

Understanding and controlling the dynamics of polymer-surface interactions are key to a functional design of nanoscale objects and to reveal mechanisms underlying biological processes. We study friction and adhesion of single polymers at the solid-liquid interface by means of atomic force microscopy (AFM) with focus on entanglement dynamics. As a model system, a single M13mp18 DNA-molecule with a length of 2.5 μm is attached to an AFM probe. Friction measurements are performed by moving the cantilever in parallel to the surface at a height of a few hundred nanometers. Deflection of the cantilever reveals adhesive interactions between the DNA polymer and the membrane. Entanglement of the DNA in the membrane pores is probed by adhesion measurements after varying waiting time at a constant height of few hundred nanometers above the surface.

BP 11.3 Mon 16:30 BPp

The mechanics of single cross-links which mediate cell attachment at a hydrogel surface — Arzu Colak, Bin Li, Johanna Blass, Aranzazu del Campo, and •Roland Bennewitz — INM - Leibniz Institute for New Materials, Saarbrücken, Germany

Cells attach to the surface of a poly(ethylene glycol diacrylate) (PEGDA) hydrogel if linkers are functionalized with the RGD cell adhesive motif. Attachment and spreading of cells on the hydrogel depend on its mechanical properties, for examples when Young*s modulus E of the hydrogel is varied. We were interested in the effective stiffness of those linkers which mediate cell attachment and measured it by means of single-molecule force spectroscopy [1]. For these experiments, the linkers were functionalized with biotin and the tip of an atomic force microscope with streptavidin. A factor of ten in the elastic modulus E of the hydrogel corresponded to a factor of five in the effective spring constant k of single crosslinks, indicating a transition in scaling with the mesh size ζ from the macroscopic $E \propto \zeta^{-3}$ to the molecular $k \propto \zeta^{-2}$. The effective stiffness of single linkers was also measured for a second polymer network based on four-arm star-PEG molecules which interpenetrated the PEGDA hydrogel. The quantification of stiffness and deformation at the molecular length scale contributes to the discussion of mechanisms in force-regulated phenomena in cell biology. [1] A. Colak, B. Li, J. Blass, K. Koynov, A. del Campo, R. Bennewitz, The mechanics of single cross-links which mediate cell attachment at a hydrogel surface, Nanoscale, 11 (2019) 11596-11604.

BP 11.4 Mon 16:30 BPp

Deep reinforcement learning of molecular mechanisms — •Roberto Covino[1], Hendrik Jung[2], Arjun Wadhawan[3], Peter G. Bolhuis[3], and Gerhard Hummer[2,4] — [1]Frankfurt Insitute for Advanced Studies, Frankfurt am Main, Germany — [2]Max Planck Institute of Biophysics, Frankfurt am Main, Germany — [3]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands — [4]Institute of Biophysics, Goethe-University Frankfurt, Frankfurt, Germany

We present a deep reinforcement learning artificial intelligence (AI) that learns the molecular mechanism from computer simulations. The AI simulates molecular reorganizations and progressively learns how to predict their outcome. We integrate path theory, transition path sampling (TPS), and deep learning. TPS is a Markov Chain Monte Carlo method to sample the rare trajectories connecting metastable states. Using reinforcement learning, we iteratively train a deep neural network on the outcomes of TPS simulation attempts. In this way, we increase the rare-event sampling efficiency while gradually revealing the underlying mechanism. At convergence, the AI learns the rare events' committor function, encoded in the trained neural network. By using symbolic regression, we distill simplified quantitative models that reveal mechanistic insight in a human-understandable form. Our innovative AI enables the sampling of rare events by autonomously driving many parallel simulations with minimal human intervention and aids their mechanistic interpretation.

BP 11.5 Mon 16:30 BPp

Acidic amino acids do not affect the robustness of protein hydration layers to changes in KCl concentration — •Hosein Geraili[1] and Ana Vila Verde[2] — [1]MPI of Colloids and Interfaces, Dept Theory and Bio-Systems, Potsdam, Germany — [2]U. Duisburg-Essen, Physics, Duisburg, Germany

The proteins of halophilic microorganisms have a higher content in negatively charged amino acids compared to microorganisms living in normal environments. One proposed hypothesis explaining this large content in acidic residues is that they are necessary to maintain the proteins at normal hydration levels in an environment with high salt concentration, i.e., in low water activity. To investigate protein hydration in high salt concentration using Molecular Dynamics, we optimized the interaction potential between potassium ions and the carboxylate side-chain of acidic amino acids; the optimized potential is compatible with the widely-used suite of AMBER force fields and the TIP3P water model. We compared hydration levels of 5 halophilic proteins and 5 non-halophilic ones. Our simulations show that all proteins have almost identical levels of hydration in high and low KCl concentrations: the large fraction of acidic amino acids in halophilic proteins is not necessary to ensure that they remain hydrated. We quantified the translational dynamics of the solvation shell of the halophilic and non-halophilic proteins, and observe almost no difference between them. The claim that acidic residues cooperatively interacting with the solvated network of ions would markedly decrease the dynamics of the protein solvation shell is not supported by our calculations.

BP 11.6 Mon 16:30 BPp

Optical tweezers and multimodality imaging: a platform for dynamic single-molecule analysis — •Bärbel Lorenz, Ann Mukhortava, and Philipp Rauch — LUMICKS B.V. Amsterdam, Pilotenstraat 51, 1059CH Amsterdam, The Netherlands

The possibility to investigate molecular interactions, structure, and dynamics using single-molecule fluorescence- and force spectroscopybased methods has led to many new insights over the past decades. Here, we present our efforts in establishing the easy and reliable experimental workflow for further enabling discoveries in the field of biology and biophysics using both the combination of optical tweezers with single-molecule fluorescence microscopy (C-Trap). As a proof of concept, we will discuss an overview of the experimental designs and the workflow for combining FRET with an ultra-stable optical trap for studying binding and colocalization dynamics of histones and a helper protein on DNA and observing protein/DNA hairpin folding dynamics. These experiments show that the technological advances in hybrid single-molecule methods can be turned into an easy-to-use and stable instrument that opens up new venues in many research areas.

BP 11.7 Mon 16:30 BPp

Molecular mechanisms of single alpha helix deformation under tension — Ana Bergues-Pupo[1], Reinhard Lipowsky[2], and •Ana Vila Verde[3] — [1]Max Delbrück Center for Molecular Medicine, Berlin, Germany — [2]MPI of Colloids and Interfaces, Dept Theory and Bio-Systems, Potsdam, Germany — [3]U. Duisburg-Essen, Physics, Duisburg, Germany

Alpha helices (SAHs) that are stable in isolated form have been found in motor proteins, where they connect spatially separated domains. We investigate the force-estension curve and molecular deformation mechanisms of SAHs pulled from the termini, at pull speeds approaching the quasi-static limit, using molecular dynamics simulations with atomistic resolution of the protein and an implicit model for the solvent. SAHs unravel starting from the termini, in a residue-by-residue manner. Contrary to prior simulations of metastable helices, hydrogen bond breaking is not the main event determining the barrier to unfolding of SAHs at all pull speeds we tested. We fit the force-extension curves to the cooperative Sticky Chain model, and extract the distance, x_E = 0.13 nm, to the transition state, the natural frequency of bond vibration, ν_0 = 0.82 ns^{-1}, and the height, V_0=2.9 kcal/mol, of the free energy barrier associated with the deformation of single residues. The results confirm that the Sticky Chain model could be used to analyze experimental force-extension curves of SAHs and other biopolymers.

BP 11.8 Mon 16:30 BPp

Structural Dynamics Correlation of Peptides derived from Nucleoporins: Time-resolved X-ray Scattering and Computational Modelling — •Naireeta Biswas[1,2], Markus Osterhoff[2], Jakob Soltau[2], Sheung Chun Ng[3], Dirk Görlich[3], and Simone Techert[1,2] — [1]FS-SCS, Deutsches Elektronen-Synchrotron (DESY), Notkestraβe 85, 22607 Hamburg, Germany — [2]University of Göttingen, Institute for X-ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Department of Cellular Logistics, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

FG nucleoporins are intrinsically disordered proteins located in the nuclear pore complexes (NPCs) consist of FG repeating motifs. It has been proposed that repeating motifs play an important role in the formation of hydrogel due to their cohesive interactions and hydrophobic nature. These protein hydrogels show unique features of non-covalent interactions such as hydrogen bonding, Vander Waals interaction or π-π stacking, driving the protein self-assembly, leading to an anisotropic structural growth, thus forming hydrogels with unusual materials properties. Our computational simulations, suggest different conformations and interactions between these FG repeating motifs and that these conformational variety may be the driving forces for the co-existing domains. To understand this molecular rationale of the protein kinetics during their gelation process, we have studied the first steps of self-assembling and structural organization of the protein hydrogels during the formation .

BP 11.9 Mon 16:30 BPp

Heat flows adjust local ion concentrations in favor of prebiotic chemistry — •T. Matreux[1], K. LeVay[2], A. Schmid[1], P. Aikkila[1], L. Belohlavek[3], Z. Caliskanoglu[3], E. Salibi[2], A. Kühnlein[1], C. Springsklee[3], B. Scheu[3], D.B. Dingwell[3], D. Braun[1], H. Mutschler[2], and C.B. Mast[1] — [1]Systems Biophysics, LMU, Amalienstr. 54, 80799 Munich, Germany — [2]MPI für Biochemie, Am Klopferspitz 18, 82152 Martinsried, Germany — [3]Earth and Environmental Sciences, LMU, Theresienstr. 41, 80333 Munich, Germany

Prebiotic reactions often require certain initial concentrations of ions. For example, the activity of RNA enzymes requires a lot of divalent magnesium salt,

whereas too much monovalent sodium salt leads to a reduction in enzyme function. However, it is known from leaching experiments that prebiotically relevant geomaterial such as basalt releases mainly a lot of sodium and only little magnesium. A natural solution to this problem is heat fluxes through thin rock fractures, through which magnesium is actively enriched and sodium is depleted by thermogravitational convection and thermophoresis. This process establishes suitable conditions for ribozyme function from a basaltic leach. It can take place in a spatially distributed system of rock cracks and is therefore particularly stable to natural fluctuations and disturbances.

BP 11.10 Mon 16:30 BPp

Structured keratin films as artificial nail plate model — •Kim Thomann, Andreas Späth, and Rainer H. Fink — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

Human fingernails can be studied ex vivo only in form of clippings which offer limited insight as they do not necessarily reflect the behavior of the whole nail. Keratin films (KFs) can potentially serve as human fingernail substitute which is especially relevant for the medical and beauty sector. In order to model the nail's adhesive characteristics, structured and unstructured films from keratin extracted from human hair and nails were produced.

The fingernail being the reference, the KFs were characterized with a number of methods, including SEM, AFM, contact angle (CA) measurements, XPS, ATR-FTIR and Raman spectroscopy. In terms of composition, KFs show a good resemblance, regardless of keratin origin. The nail's microstructured topography is well matched by the structured KFs. CA measurements revealed that the surface free energy is in the same range for both KF types. However, the unstructured KFs exhibit a much stronger polar component compared to the nail while the structured KFs fit the nail's component composition well. Thus, the structured KFs represent a good approach to achieve a satisfying model in terms of wetting while combining both composition and topography aspects. The research is funded by the BMBF within project 05K19WE2.

BP 11.11 Mon 16:30 BPp

Activity of hydrogel-encapsulated cells monitored by atomic force microscopy — •Mengxiao Li[1,2], Kordula Schellnhuber[1,2], Shardul Bhusari[1,2], Johanna Blass[1], Shrikrishnan Sankaran[1], and Roland Bennewitz[1,2] — [1]INM - Leibniz for New Materials, Campus D22, 66123 Saarbrücken — [2]Saarland University, Naturwissenschaftlich Technische Fakultät, 66123 Saarbrücken

Living materials are an emerging concept in biomaterial research. Living organisms become part of the material and equip it with tailored functions. For example, genetically engineered bacteria are encapsulated in hydrogels to release drugs when triggered by an external stimulus [1]. The aim of this study is to develop a new technique for highly sensitive measurements of mechanical perturbances arising from growth and motion of bacteria trapped in a thin hydrogel film by means of Atomic Force Microscopy (AFM). To probe the activity of E. coli bacteria enclosed in a pluronic diacrylate hydrogel, we contact its surface with a colloidal probe cantilever. Normal and lateral displacements of the contact caused by motion or division of bacteria are recorded for a contact time of 300s at various positions of the hydrogel surface. Over 24 hours, we observe an increase of the mechanical signals with time that we attribute to bacterial colony growth inside the hydrogel film. Characteristic time scales of the processes are determined by means of continuous wavelet transform.

[1] S. Sankaran et al., Small 15 (2019) 1804717.

BP 11.12 Mon 16:30 BPp

Cohesin and condensin extrude DNA loops in a cell cycle-dependent manner — •Stefan Golfier[1,2], Thomas Quail[1,2], and Jan Brugues[1,2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]MPI-PKS, Nöthnitzer Straße 38, Dresden, Germany

How cells spatially organise long DNA polymers inside the confinements of the cell nucleus without creating knots and tangles has been a central question in cell biology. Recent observations have unveiled the physical architecture of the genome as a hierarchy of higher-order structures that deeply impact biological function. Despite their role for gene regulation, DNA repair and genome propagation, the underlying mechanisms shaping the 3D genome remained elusive. The active formation of vast DNA loops by the molecular motors cohesin and condensins has been proposed as a general mechanism to spatially organize the genome across the cell cycle. However, the requirements for genome organisation change dramatically during the cell cycle. To date it remained unclear, if DNA loops shape the drastically different chromatin architectures in inter- and metaphase. Using Xenopus laevis egg extracts, we reconstitute and directly observe DNA loop formation for the first time in a native environment and dependence of the cell cycle. We show that DNA loops are actively formed in both meta- and interphase, but with distinct biophysical properties and responsible factors. Our findings provide fundamental evidence that DNA loops are the physical building blocks of genome architecture, that are molecularly regulated during the cell cycle.

BP 11.13 Mon 16:30 BPp

UV-Induced Selectivity of Short DNA Oligonucleotides in Early Evolution — •Corinna L. Kufner[1], Dominik B. Bucher[2], Wolfgang Zinth[3], Christof B. Mast[3], Gabriella G. Lozano[1], Sukrit Ranjan[4], Zoe R. Todd[5], and Dimitar D. Sasselov[1] — [1]Harvard University, USA — [2]TU München — [3]LMU München — [4]Northwestern University, USA — [5]University of Washington, USA

At early stages of the evolution of life, between 3.5 and 4.2 billion years ago, the ultraviolet (UV) irradiation on the surface of the Earth was much higher than today. In the prebiotic era, particularly in the absence of complex enzymes, UV light both served as an important energy source for photochemical reactions and imposed a strong selection pressure on the building blocks of life. Here, we study the photophysics of short DNA oligonucleotides by irradiation experiments and ultrafast UV pump (266 nm) IR probe (5-7 um) spectroscopy. We find a strong sequence selectivity in the photostability of short oligonucleotides. Charge transfer states can promote sequence selective self-repair of adjacent photolesions via an entirely intrinsic mechanism which resembles the enzymatic repair by photolyases. Particularly charge transfer states which involve Guanine, the strongest electron donor among the canonical nucleobases, play a key role in the photostability of short oligonucleotides. It may be assumed that photophysical mechanisms have strongly influenced the selection of base sequences at early stages of evolution.

BP 11.14 Mon 16:30 BPp

Nanomechanics of DNA self-assemblies and light driven molecular motors — Michael Penth[1,2], Yijun Yijun[1], Arzu Çolak[1], Kordula Schellnhuber[1,2], Mitchell K.L. Han[1], Aránzazu del Campo[1,3], Roland Bennewitz[1,2], and •Johanna Blass[1] — [1]INM - Leibniz for New Materials, Campus D22, 66123 Saarbrücken — [2]Saarland University, Physics Department, 66123 Saarbrücken — [3]Saarland University, Chemistry Department, 66123 Saarbrücken

Single-molecule force spectroscopy has become an essential tool to unravel the structural and nanomechanical properties of biomolecules. In this study, we present Flow Force Microscopy (FlowFM) as a massively parallel approach to study the nanomechanics of hundreds of molecules in parallel. The high-throughput experiments performed in a simple microfluidic channel enable statistically meaningful studies with nanometer scale precision in a time frame of several minutes. A surprisingly high flexibility was observed for a self-assembled DNA construct typically used in DNA origami. The persistence length was determined to be 12.6 nm, a factor of four smaller than for native DNA. The enhanced flexibility is attributed to the discontinuous backbone of DNA self-assemblies. We also quantified the forces actuated by a unique molecular machine that can apply forces at cell-matrix and cell-cell junctions using light as an energy source. Micrometer-sized beads tethered to the surface via entangled rotary motors were retracted against drag forces from 1 pN to 5 pN within the first minute of UV-irradiation.

BP 11.15 Mon 16:30 BPp

In-situ GiSAXS investigations of sprayed drugs on Peptide Hydrogel based matrix — •Naireeta Biswas[1,2], Elisabeth Erbes[1,2], Krishnayan Basuroy[1], Jose Velaquez Garcia[1], Sreevidya Thekku Veedu[1], Matthias Schwartzkopf[1], Calvin Brett[1,4], Stephan Roth[1,3], and Simone Techert[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestraβe 85, 22607 Hamburg, Germany — [2]University of Göttingen, Institute for X-ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, 100 44 Stockholm, Sweden. — [4]Department of Mechanics, KT Royal Institute of Technology, 100 44 Stockholm, Sweden

A controlled and personalized treatment is key to successful medication. We have designed a novel hybrid material- a matrix made of a mixture of hydrophilic carboxymethylated nanocellulose (CMC) hydrogel and disordered hydrophobic peptide hydrogel (P). Our investigations into this material are the first steps towards a novel drug delivery/carrier strategy that allows a controlled dosage of anti-COVID drugs embedded in the system. This gives us the opportunity to vary the local uptake in a hydrophobic or hydrophilic compartment in the matrix. The structural intercalation and the time-resolved process were investigated with in-situ grazing-incidence small-angle X-ray scattering (GISAXS) experiments while spraying the drug on the matrix. In this work, we have focused on the structural analysis of the peptide hydrogel system with the drugs. The structural analysis of the CMC fibers will be presented in the poster of Elisabeth Erbes.

BP 11.16 Mon 16:30 BPp

Cytoplasmic streaming enables inter-nuclear signaling in the giant syncytium *Physarum polycephalum* — •Nico Schramma[1], Siyu Chen[1,2], and Karen Alim[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Technical University of Munich, Physics Department, Munich, Germany

The slime mold *Physarum polycephalum* is known for its optimized active transport network, which is utilized to spread signals and nutrients over its up to meter-sized cell-body. Intriguingly, this syncytium contains up to billions of nu-

clei, which are said to divide in a mitotic wave. However, direct experimental evidence of this finding is still missing and the possibility of inter-nuclear signaling remains elusive. Here, by observing fluorescent labeled nuclei with high-speed microscopy, we uncover that individual nuclei not only can be transported in the tubes of the network, but can also get immobilized in the porous, gel-like endoplasm wrapping the tubes. Then, using particle image velocimetry, we resolve the slow flow within the endoplasmic tube-walls. Furthermore, we use a simplified advection-diffusion-reaction model to show that inter-nuclear exchange of large molecules such as mRNA can only happen within physiological time scales between stuck nuclei in the endoplasm, rather than between transported nuclei. Our study provides evidence that immobilised nuclei may play a crucial role in the coordination of mitotic waves or gene-expression patterns in *Physarum* and may pave the way to use *Physarum* as a model syncytium to understand the interplay of fluid-driven transport and signaling of nuclei.

BP 11.17 Mon 16:30 BPp

Resolving Energy Storage in Extra-Embryonic Membranes — •Zoë Lange[1,2], Franziska Krämer[1,3,4], Frederic Strobl[3,4], Ernst Stelzer[3,4], and Franziska Matthäus[1,4] — [1]Frankfurt Institute for Advanced Studies (FIAS) — [2]IfB, FB Physik, Uni Frankfurt/Main — [3]Buchmann Institute for Molecular Life Sciences (BMLS) — [4]IZN, FB Biowissenschaften, Uni Frankfurt/Main

Efficient energy use and storage is crucial in living organisms. In the context of evolution, energy management is continuously optimized to ensure an individual's ability to successfully compete. This is especially true for oviparous species, as all required energy has to be provided at the moment of oviposition in order to give rise to a fully functional organism. Based on our preliminary imaging data in the emerging insect model *Tribolium castaneum*, we formulate the hypothesis that extra-embryonic serosa cells utilize shape change during gastrulation to allocate and store energy that is later on required for their extensive movement during dorsal closure. To investigate this possible functional connection, we want to gain further insights into the multi-scale effects of force propagation from cellular to tissue level. Spatial and temporal dynamics of forces are calculated using non-invasive Force Inference (FI). FI utilizes a biomechanical model, a mathematical inverse method and a Bayesian framework to estimate cell and tissue stress from segmented image data and for the whole system simultaneously. Here we highlight our workflow from obtaining 3D time-lapse light sheet-based fluorescent microscopy images of live *Tribolium* embryos to multi-scale estimation of tensions and pressures acting in the serosa membrane.

BP 11.18 Mon 16:30 BPp

Cell Fate Clusters in Inner Cell Mass Organoids Arise from Cell Fate Heredity — •Tim Liebisch[1,2], Armin Drusko[1,2], Biena Mathew[1,3], Ernst Stelzer[1,3], Sabine Fischer[4], and Franziska Matthäus[1,2] — [1]GU Frankfurt — [2]FIAS — [3]BLMS — [4]JMU Würzburg

Recently, inner cell mass (ICM) organoids have been published as an in vitro model system towards preimplantational development. ICM organoids mimic the second cell fate decision taking place in in vivo mouse embryos. It was shown that cells of the same fate tend to cluster stronger than expected for the currently hypothesised random cell fate distribution. Three major processes contribute to the cell fate arrangements at the 24 h old and 48 h old ICM organoids or mid and late blastocyst, respectively: chemical signalling; cell sorting process; cell proliferation.

An agent-based model was developed, accounting for cellular interactions, cell growth and division. The model was applied to compare current assumptions of how the ICM neighbourhood is formed. The model supports the hypothesis that initial cell fate acquisition is a stochastically driven process. Subsequently, the observed neighbourhood structures can emerge due to cell fate heredity.

Simulations show that the initial cell differentiation process takes place only during a small time window, during ICM organoid composition. Our results leave little room for cellular signalling believed to be important in cell fate decision. Hence, we are discussing an alternative role of chemical signalling in this process.

BP 11.19 Mon 16:30 BPp

Migration of Cytotoxic T Lymphocytes in Collagen Matrices — •Zeinab Sadjadi[1], Heiko Rieger[1], Markus Hoth[2], Bin Qu[2], and Renping Zhao[2] — [1]Department of Theoretical Physics and Center for Biophysics, Saarland University — [2]Department of Biophysics, Center for Integrative Physiology and Molecular Medicine, School of Medicine, Saarland University

Cytotoxic T lymphocytes (CTLs) need to migrate to search for their target cells in complex biological microenvironments, a key component of which is extracellular matrix (ECM). The mechanisms underlying CTL*s navigation are not well understood so far. Here we use a collagen assay as a model for the ECM and analyze the migration trajectories of primary human CTLs in collagen matrices with different concentrations. We observe different migration patterns for individual T cells. Three different motility types can be distinguished: slow, fast and mixed motilities. Slow CTLs remain nearly stationary within the collagen matrix and show slightly anti-persistent motility, while the fast ones move quickly and persistent. We hypothesize that the slow mode describes CTLs creating channels through the collagen matrix by deforming and tearing apart collagen fibers, and that the fast motility mode describes CTLs moving within these channels. The dynamics of the mixed type consists of periods of slow and fast motions. The dynamics can be well described by a two-state persistent random walk model. We extract the parameters of the model by analyzing experimental data.

BP 11.20 Mon 16:30 BPp

Is Cell segregation just like oil and water: A phase field approach — •Florian Franke, Steffen Lange, Hans-Joachim Böhme, Sebastian Aland, and Anja Voss-Böhme — Hochschule für Technik und Wirtschaft Dresden (HTW), Dresden, Germany

Understanding the segregation of cells is crucial to answer questions about tissue formation in embryos or tumor progression. According to Steinberg's differential adhesion hypothesis the separation of cells can be compared to the separation of two liquids, e.g. water and oil. Specifically, it was proposed, that similarly to the demixing of fluids, differences in the strengths of the adhesive forces in homo- and heterotypic cell contact lead to all sorting. This hypothesis has been tested on the basis of cell-based models which simulate motile cells with differential adhesive interaction on the basis of probability cellular automaton models. On the other hand, the segregation of fluids like water and Oil can be well described by phase-field models as the Cahn-Hilliard-Navier-Stokes-equation.

Here we investigate the relation between the two approaches and to what extent parameters can be transformed between the two models. Further, by comparing simulations of either model to in-vitro experiments from the literature, we conclude that cells segregation is best described by the cellular automaton. Only a specific time regime of the segregation resembles the demixing of two liquids. However, experimentally observed cell segregation displays both regimes of logarithmic and power-law segregation with varying exponent. This rich behavior is reproduced by the cellular automaton model.

BP 11.21 Mon 16:30 BPp

Theoretical approaches to mechanics of biofilms — •Hui-Shun Kuan[1], Wolfram Pönisch[2], Leander Self[3], Frank Jülicher[4], Michael Schmiedeberg[3], and Vasily Zaburdaev[1] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]MRC Laboratory for Molecular Cell Biology, University College London, United Kingdom — [3]Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg — [4]Max Planck Institute for the Physics of Complex Systems

Mechanics of biofilms is intrinsically affected by biological processes at different scales: from the activity of molecular motors to motility, and to cell death and division. As a result, the rheological properties of these bacterial colonies are markedly different from those exhibited by systems at thermal equilibrium. In this work, motivated by biofilms of *Neisseria gonorrhoeae* bacteria, we use a continuum theory and agent-based numerical simulations to study dense bacterial colonies shaped by attractive intercellular interactions. We can describe the formation of a colony as a phase separation process while the colony itself behaves as a viscoelastic material. By studying the behaviour of the colonies under oscillatory shear, we can link their mechanical properties to the dynamics of the intercellular forces. Due to the turnover of these active forces, the colonies show a liquid-like behaviour at large times and strong shear-thinning effect under the large amplitude of the oscillatory shear. Our study provides an important insight on how the active intercellular forces define the material properties of living aggregates which can now also be tested experimentally.

BP 11.22 Mon 16:30 BPp

Nanoprobing of osteoblasts adhered to molecular landscapes of dendrimer and protein — Christian Völkner[1], Issam Assi[1], Willi Karberg[1], •Regina Lange[1], Martina Grüning[2], Barbara Nebe[2], Ingo Barke[1], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, Physics of Surfaces & Interfaces, 18059 Rostock — [2]Rostock University Medical Center, Dept. of Cell Biology, 18057 Rostock

Molecular surface gradients can constitute electric field landscapes and serve to control local cell adhesion and migration. This may allow the discovery of routes to improve osseointegration of implants. Flat molecule aggregate landscapes of amine-terminated dendrimers (PAMAM, generation 1) or proteins (BSA) were prepared on glass by micro contact printing [1] to provide lateral electric field gradients through their less negative zeta potentials compared to the glass substrate.

The local as well as the mesoscopic responses of adhered osteoblasts (MG-63) were studied by means of Scanning Ion Conductance Microscopy (SICM) [2] and Fluorescence Microscopy, in situ.

A distinct spindle shape oriented parallel to the stripe pattern as well as a preferential adhesion of the cells on the glass site have been observed when the width of the stripes and the spacing is 6 or 20 μm. To explain this effect, we suggest a retraction mechanism according to cathodic taxis, a subtype of galvanotaxis [3].

[1] Whitesides et al., Chem. Rev. 105, 1171 (2005)
[2] Korchev et al., Biophys. J. 73, 653 (1997)
[3] Djamgoz et al., J.of Cell Science 117, 1631 (2004)

BP 11.23 Mon 16:30 BPp

Kinetics of light-switchable surface association of *C. reinhardtii* populations — •Rodrigo Catalan[1], Alexandros Fragkopoulos[1], Nicolas von Trott[1], Simon Kelterborn[2], Peter Hegemann[2], and Oliver Bäumchen[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany — [2]Humboldt University of Berlin, Institute of Biology, 10115 Berlin, Germany. — [3]University of Bayreuth, Experimental Physics V, 95440 Bayreuth, Germany

Bacterial and microalgal colonization on surfaces produce favorable and adverse effects in technological and medical settings. Therefore, the fundamental aspects of biofilm formation on solid substrates are actively studied. While bacteria have been the main focus of research to understand microbial surface colonization, analogous studies using archetypes in microalgae are thus far elusive. We exploit light-switchable flagellar adhesion of *C. reinhardtii* [Kreis et al., Nature Physics, 2018] to study the kinetics of adsorption and desorption of cell suspensions on glass using bright field microscopy and image analysis. We observe that both processes exhibit a lag response relative to the time at which blue- or red-light conditions are set and we model this feature using time-delayed Langmuir kinetics. We find that adsorption occurs significantly faster than desorption, with the delay to be an order of magnitude larger. Adsorption experiments of phototactically blind *C. reinhardtii* mutants show that phototaxis does not affect the kinetics of either process. Hence, our method can be used as an assay for characterizing surface colonization.

BP 11.24 Mon 16:30 BPp

Unravelling the biomolecular origin of light-switchable adhesion of *Chlamydomonas* to surfaces — •Antoine Girot[1], Rodrigo Catalán[1], Alexandros Fragkopoulos[1], Marzieh Karimi[1], Simon Kelterborn[2], Peter Hegemann[2], Michael Hippler[3], and Oliver Bäumchen[1,4] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Institute of Biology, Humboldt University of Berlin, 10099 Berlin, Germany — [3]Institute of Plant Biotechnology and Biology, University of Münster, 48143 Münster, Germany — [4]Experimental Physics V, University of Bayreuth, 95440 Bayreuth, Germany

In this work, we focus on the adhesion of the biflagellated microalga *Chlamydomonas reinhardtii*. We discovered that this alga exhibits light-switchable adhesion, i.e. the flagella of the cells stick to surfaces under blue but not under red light. In order to unravel the biomolecular origin of this specific light-regulated behaviour, two different experimental approaches are carried out. First, we record the kinetics of the adsorption and desorption of a cell suspension to a surface in response to a light switch. Second, we employ *in vivo* micropipette force spectroscopy to measure the adhesion force of single cells. By applying these methods for different wild-type strains, we aim at identifying characteristic gene sequences associated to cells adhesion. To unravel the blue-light sensitive photoreceptor responsible for adhesion, these experiments are performed with specific photoreceptor-deleted mutants. Finally, we investigate how the glycosylation of the flagellar membrane proteins affects the adhesion of *Chlamydomonas*.

BP 11.25 Mon 16:30 BPp

Determination of the effective adhesion parameter for the sorting behavior of a cell system with several cell types using statistical learning methods — •Philipp Rossbach, Steffen Lange, Hans-Joachim Böhme, and Anja Voss-Böhme — Hochschule für Technik und Wirtschaft Dresden

The process of cell sorting plays an essential role in development and maintenance of tissues. To understand this process, mathematical modeling can assist cell biological research by providing means to analyze the consequences of different hypotheses on the underlying mechanisms. In the Differential Adhesion Hypothesis (DAH) by Steinberg (1962) it is assumed that cell sorting is determined by quantitative differences in cell type specific intercellular adhesion strengths. An implementation of the DAH is the Differential Migration Model (DMM) by Voss-Böhme and Deutsch (2010). From this DMM an effective adhesion parameter (EAP) for systems with two cell types can be derived analytically which predicts the asymptotic sorting pattern. However, the existence and form of such an parameter for more than two cell types is unclear.

Here, we investigate numerically the existence of an EAP for systems with more than two cell types. We rely on in-silico time-series data that is produced by a cellular automaton which emulates the DMM and classify the segregation behavior using statistical learning methods such as SVM and Logit Model. We use these tools to demonstrate the existence of an EAP for three cell types which matches our analytical prediction for systems with arbitrary many cell types.

BP 11.26 Mon 16:30 BPp

Optogenetic control of intracellular flows and cell migration: a minimal active gel model — •Oliver M. Drozdowski[1,2], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]BioQuant, Heidelberg University, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany

The actin cytoskeleton of cells is in continuous motion due to both polymerization of new filaments and their contraction by myosin II molecular motors. Through adhesion to the substrate, such intracellular flow can be converted into cell migration. Recently, optogenetics has emerged as a new powerful experimental method to control both actin polymerization and myosin II contraction. While optogenetic control of polymerization can initiate cell migration by effecting protrusions, it is less clear if and how optogenetic control of contraction can effect cell migration. Here we analyze the latter situation using a minimal variant of active gel theory into which we include optogenetic activation as a spatiotemporally constrained perturbation. The model can describe the symmetrical flow of the actomyosin system observed in optogenetic experiments but not the long-lasting polarization required for cell migration. Motile solutions become possible if cytoskeletal polymerization is added to the boundary conditions. Optogenetic activation of contraction can then initiate locomotion in a symmetrically spreading cell and strengthen motility in an asymmetrically polymerizing one. If designed appropriately, it can also arrest motility even for protrusive boundaries.

BP 11.27 Mon 16:30 BPp

Reversible elastic phase field approach and application to cell monolayers — •Robert Chojowski, Ulrich S. Schwarz, and Falko Ziebert — Institute for Theoretical Physics and BioQuant, Heidelberg University, Germany

Force generation and motion of individual cells and cell collectives are fundamental constituents for many biological processes, including development, wound healing and cancer metastasis. Wound healing assays are quantitative experiments in which a 2D cell monolayer moves into empty space, often forming finger-like protrusions. Such experiments have revealed that migrating cell monolayers are both dynamic and elastic at the same time. However, such a combination of properties is very challenging to model with conventional approaches. Here we present a new phase field approach enabling us to predict the dynamics of thin elastic sheets under the action of active stresses and localized forces while ensuring reversibility as required by elasticity[1]. The continuum equations of our model can be solved by a combination of spectral and matrix methods and the numerical solutions can be compared to analytical ones. We demonstrate the potential of our modelling approach by studying several biologically relevant situations and geometries for single cells and cell monolayers, including elastic bars, contractile discs and the formation of elastic protrusions in an expanding monolayer scenario.

[1] R. Chojowski, U.S. Schwarz, F. Ziebert, Reversible elastic phase field approach and application to cell monolayers, Eur. Phys. J. E 43, 63 (2020)

BP 11.28 Mon 16:30 BPp

Morphodynamics in the Foraging of *Physarum polycephalum* — •Lisa Schick and Karen Alim — Technische Universit"at M"unchen

Foraging behaviour of animals is generally described as optimized for maximal energy uptake per time spend foraging within optimal foraging theory. Food sources often occur as food patches, so that foraging becomes a balance between time spent for exploration and time spent for patch exploitation leading to the question at which point a patch should be abandoned. Foraging behaviour in a patchy habitat can also be observed in unicellular but spatially extended organisms like *Physarum polycephalum*. However, it is unclear which foraging strategy the large and adaptive network-like morphology allows for. The plasmodial network of *P. polycephalum* adapts its morphology in the process of foraging by mass transport. Recent observations show that on encounter of a food patch, depending on body size, the whole body is relocated for exploitation. We here study the morphological changes as a function of network size and nutritional state by introducing a model for the exploration and exploitation phases in *P. polycephalum*. We estimate the energy uptake from our foraging observations in order to obtain rules for the foraging behaviour.

BP 11.29 Mon 16:30 BPp

A general theoretical framework to describe the influence of electric field on Mesechymal stem cell differentiation — •Jonathan Dawson[1], Ursula van Rienen[1,2,4], Poh Soo Lee[3], and Revathi Appali[1,4] — [1]Institute of General Electrical Engineering, University of Rostock, Germany — [2]Life, Light and Matter, Interdisciplinary Faculty, University of Rostock, Germany — [3]Max Bergmann Center for Biomaterials, Institute for Materials Science, Technical University of Dresden, Dresden, Germany — [4]Ageing of Individuals and Society, Interdisciplinary Faculty, University of Rostock, Germany

Bone regeneration is a highly complex and tightly regulated process which involves concerted and controlled action of human mesenchymal stem cell (hMSC) proliferation and differentiation into osteoblasts. Multiple physiological and environment factors influence the osteogenic differentiation and proliferation of hMSCs. Here we present a quantitative study investigating the influence of external electric field on stem cell dynamics, specifically proliferation and differentiation. In experiments, hMSCs were exposed to a low-frequency electrical field applied via a transformer-like-coupling (TLC). Osteogenic differentiation was quantified by measuring expression levels of cell alkaline phosphate (ALP) activity over time. Our mean-field theory describes the dynamics of a population of ALP stained hMSCs and takes into account cell division, cell differentiation, and intracellular ALP activity. Our results show that the stem cell differentiation rate is electric field dependent, and the proliferation rate is cell-density dependent.

BP 11.30 Mon 16:30 BPp

Asymmetries & gradients during early C. elegans embryogenesis — •Rebecca Benelli, Philipp Struntz, Dirk Hoffmann, and Matthias Weiss — Universität Bayreuth

To enable differentiation of cells and to facilitate cell organization the establishment of gradients is crucial in early embryogenesis. We have used the model organism C. elegans and a custom built light-sheet microscope to study the formation of protein and organelle gradients in three dimensions over time. Due to the low phototoxicity and reduced bleaching induced by this selective illumination long term observations without developmental perturbations are made possible. The focus of the current study is on evolution until the first cell division, which, next to the different sized daugther cells, is characterized by a lot of accompanying asymmetries. We study the protein concentration of two vital proteins in early development with respect to their axial as well as radial distribution. Also, two organelles with opposing gradients are investigated. Since diffusion plays a vital role in the establishment of gradients a new multiplexed diffusion measurement technique (SPIM-FCS) is used to quantify changes in diffusive behavior of proteins in space and time.

BP 11.31 Mon 16:30 BPp

Characterisation of local membrane height fluctuations on live cells — •Max Ulbrich[1], Christian Völkner[1], Regina Lange[1], Sophie Kussauer[2], Robert David[2], Martina Grüning[3], Barbara Nebe[3], Ingo Barke[1], and Sylvia Speller[1] — [1]Institute of Physics, Physics of Surfaces & Interfaces, University of Rostock, 18059 Rostock — [2]University Medical Center, Cardial Regeneration, University of Rostock, 18057 Rostock — [3]Rostock University Medical Center, 18057 Rostock

Assessment of cellular membrane fluctuations may aid monitoring of physiologic and pharmacologic effects [1]. Scanning Ion Conductance Microscopy (SICM) is a nanoprobing method to acquire morphology and dynamics on live cells. We operate the nanopipette-probe on fixed lateral locations and record SICM time traces in order to assess membrane fluctuations and cell activities [2]. Membrane fluctuations of live osteoblasts and cardiomyocytes are analysed in the time and frequency domain. Living osteoblasts and paused pacemaker cells, in average, exhibit scaling exponents of -2.8 and -2.5, respectively, however with large variations from cell to cell and site to site. We discuss this behavior in view of reference measurements on fixed cells and in the context of optically obtained results [3].

[1] B Rappaz, et al, Blood Cells Mol. Dis. 42 (2009) 228
[2] S-O Kim, et al, Nano Convergence (2017) 4:5
[3] B Sinha, et al, Biophys. J. (2017) 113

BP 11.32 Mon 16:30 BPp

A single-molecule view of the cytosolic membrane of Trypanosoma brucei — •Paula Büttner, Marie Schwebs, and Susanne Fenz — Julius-Maximilians-Universität Würzburg, Würzburg, Germany

African trypanosomes are the causative agents of sleeping sickness. In the bloodstream of their host, they express a dense coat of GPI-anchored variant surface glycoproteins (VSGs). Fluidity of this coat is fundamental for the evasion of the hosts immune system and thus for the survival of the parasite. However, VSG dynamics is also limited by the lipid matrix. We have recently introduced super-resolution imaging of intrinsically fast-moving flagellates based on cytocompatible hydrogel embedding and found that the inner membrane leaflet appears to be structured [Glogger et al. JPD 17 & Exp. Parsitol. 17]. We hypothesize that the WCB (whole cell body) protein, that connects the cytoskeleton with the plasma membrane, causes this structure. We present two-color single-molecule measurements of a lipid probe and WCB to address this hypothesis.

BP 11.33 Mon 16:30 BPp

Multi-color fluorescence fluctuation spectroscopy in living cells via spectral detection — •Valentin Dunsing, Annett Petrich, and Salvatore Chiantia — Universität Potsdam, Potsdam, Deutschland

Signaling pathways in biological systems rely on specific interactions between multiple biomolecules. Fluorescence fluctuation spectroscopy is a powerful toolbox to quantify such interactions directly in living cells. Cross-correlation analysis of spectrally separated fluctuations provides information about intermolecular interactions, but is conventionally limited to two fluorophore species. Here, we present scanning fluorescence spectral correlation spectroscopy (SFSCS), a versatile approach that can be implemented on standard confocal microscopes, allowing the investigation of interactions between multiple protein species at the plasma membrane of cells. We demonstrate that SFSCS enables cross-talk-free cross-correlation, diffusion and oligomerization analysis of up to four protein species labeled with strongly overlapping fluorophores. As an example, we investigate the interactions of influenza A virus (IAV) matrix protein 2 with two cellular host factors simultaneously. We furthermore extend raster spectral image correlation spectroscopy (RSICS) to four species analysis and apply it to determine the stoichiometry of ternary IAV polymerase complexes in the cell nucleus. Based on triple correlation analysis of RSICS data, i.e. detection of coincident fluctuations of fluorescence signals emitted by three fluorophore species, we provide direct evidence for the assembly of ternary protein complexes.

BP 11.34 Mon 16:30 BPp

Conditions for thermodynamic stability and critical points in multicomponent mixtures with structured interactions — •Isabella Graf and Benjamin Machta — Yale University, New Haven, CT, USA

Multicomponent mixtures are ubiquitous in biology, ranging from cellular membranes to liquid-like droplets. There is experimental evidence that their phase behavior plays a functional role for signaling and control of biochemical reactions and is under regulation itself. For instance, it has been demonstrated recently that membranes composed of a large variety of lipids are tuned close to a miscibility critical point. Theoretical work has shed light on the phase behavior of idealized systems with many components and random, mutually independent interactions, but there is little understanding of how these results generalize to systems with more structured interactions. To address this open question, we consider a family of multicomponent models with an interaction matrix of variable rank. The matrix is constructed so that each component is characterized by several scalar "features", each of which conveys an Ising-like interaction between neighboring components and could be interpreted as lipid tail length, headgroup or saturation in the case of membrane lipids. We derive analytical, mean-field conditions for the occurrence of thermodynamic stability and (higher-order) critical points and find that these conditions depend on the cumulants of the principal components of the feature distribution. These results might provide important insights into critical membrane behavior and phase behavior of multicomponent mixtures more generally.

BP 11.35 Mon 16:30 BPp

Modeling RNA Polymerase II clusters by lattice kinetic Monte Carlo simulations — •Tim Klingberg[1,2], Lennart Hilbert[3], and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max-Planck-Zentrum für Physik und Medizin — [3]Karlsruher Institut für Technologie

Eukaryotic genes are mainly transcribed by RNA polymerase II (Pol II). Before active transcription starts, Pol II is recruited to the promoter region of a specific gene and then released from a paused state into transcript elongation. Clusters of paused Pol II of various sizes and morphologies can be observed in zebrafish embryos (Pancholi et al.). Here, we aim to understand the physical mechanisms that are essential for the cluster formation and determine their emerging properties. To this end, we apply two-dimensional lattice kinetic Monte Carlo simulations with single Pol II particles interacting with DNA polymers, whose dynamics are determined by the Verdier-Stockmayer algorithm. The model suggests that formation of Pol II clusters can be rationalized as phase separating phenomenon where polymerases form a liquid phase that wets the chromatin at the promoter region. Cluster properties such as size and morphology can be linked to the size of the promoter region and the respective gene. Despite the simplicity of the model, it is sufficient to qualitatively describe the experimentally observed cluster properties in normal conditions and under drug treatments interfering with the transcription process.

BP 11.36 Mon 16:30 BPp

Euchromatin reorganisation during transcription resembles active microemulsion — •Rakesh Chatterjee[1,2], Hui-Shun Kuan[1,2], and Vasily Zaburdaev[1,2] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Max Planck Zentrum für Physik und Medizin, 91058 Erlangen, Germany

During transcription RNA polymerase II (Pol II) attaches and moves along the DNA strand to produce messenger-RNA (mRNA). The selective induction of transcription from DNA into RNA shapes and is being shaped by the chromatin organisation. To investigate this complex interplay, we aim to establish a phenomenological model, which qualitatively mimics the experimental results regarding transcription process in primary cell cultures obtained from zebrafish embryos. Our phenomenological lattice model is based on the framework of microphase separation or microemulsion. DNA, mRNA and Pol II serve as the three basic components similar to the oil-water-surfactant system, which exhibits two and three phase coexistence. Freely diffusing Pol II undergoes chemical transitions reflecting different stages of the transcription process. Similar behaviour can be realised by assuming transient dynamics of the surfactants which switches between active and inactive states. We use lattice model simulations and the correlation function approach to characterises different phases of this three component system. The resulting structures can be understood via the continuum theory that we derive by coarse-graining the lattice model.

BP 11.37 Mon 16:30 BPp

Deformability-based cell sorting by a microfluidic ratchet effect — •Sebastian W. Krauss, Pierre-Yves Gires, Winfried Schmidt, Walter Zimmermann, and Matthias Weiss — University Bayreuth, Bayreuth, Germany

Various physiological states impact on the rigidity of cells, e.g. aging, infection, or cancer. Cellular rigidity can be quantified with a high throughput by monitoring cell deformations during passage through a narrow constriction in a microfluidic device [1]. In contrast to this mere feed-forward approach, we use an asymmetric periodic flow protocol to exploit flow-induced deformations for

sorting cells according to their stiffness. In particular, we apply an asymmetrically oscillating flow in a microfluidic channel that leads to a zero net drift of solid polystyrene particles, whereas deformable objects, here taken as red blood cells, experience a nonzero deformation-dependent displacement in each cycle. Preliminary results suggest this approach to be a versatile tool for screening the physiological state of cells.

[1] Otto, O., et al. (2015) Nature Methods 12.3, 199

BP 11.38 Mon 16:30 BPp

Mechanical phenotyping beyond geometrical constraints using virtual fluidic channels — •Muzaffar Panhwar[1], Fabian Czerwinski[1], Venkata A.S. Dabbirru[1], Yesaswini Komaragiri[1], Peter Nestler[1], Bob Fregin[1], Ricardo H. Pires[1], Doreen Biedenweg[2], and Oliver Otto[1] — [1]AG Biomechanic, ZIK-HIKE, Universität Greifswald, Greifswald, Deutschland — [2]Universitätsmedizin Greifswald, Greifswald, Deutschland

Microfluidic techniques have proven to be of key importance for achieving high-throughput cell mechanical measurements. However, their design modifications require sophisticated cleanroom equipment. Here, we introduce virtual fluidic channels as a flexible and robust alternative to Poly-dimethylsiloxane chips. Virtual channels are liquid-bound fluid flows that can be tailored in three dimensions within seconds for rheological studies on a wide size range of biological samples. While cell deformation inside standard hard-wall constrictions is mainly driven by shear stress, virtual channel possess an additional normal stress component originating from the liquid-liquid interface. We demonstrate that this interface acts as a high-frequency liquid cantilever for probing cell rheology on a millisecond timescale. In proof-of principle experiments, cells are treated with cytochalasin D to inhibit actin polymerization. A significant reduction in the Young's modulus is found compared to untreated cells. In addition, we utilize virtual channels to measure the mechanical properties of single cells and spheroids as a tissue model system. Our results indicate that the Young's modulus of single cells exceeds the one of tissue by one order of magnitude.

BP 11.39 Mon 16:30 BPp

Monitor, categorize and manipulate label-free water-in-oil droplets in microfluidic systems — •Tobias Neckernuss[1,3], Chrostoph Frey[2], Jonas Pfeil[1,3], Daniel Geiger[1,3], Ilia Platzman[2], Joachim Spatz[2], and Othmar Marti[1] — [1]Institute for Experimental Physics, Ulm University — [2]Max-Planck-Institute for Medical Research, Heidelberg — [3]Sensific GmbH, Germany

A key point of droplet based microfluidics is the availability of powerful but easy-to-implement methods for high throughput real-time analysis and automated manipulation of the droplets. We developed a novel optical device, consisting of a fast camera with integrated data processing for smart and fast algorithms enabling label-free real-time monitoring and active manipulation of passing droplets. The device continuously analyzes up to 3000 particles per second in real-time with respect to bright-field image parameters like size, brightness, granularity, circumference, speed and many more. According to these parameters and combinations thereof, the passing droplets can be sorted. We measure different droplet production parameters and demonstrate label-free detection of cells encapsulated in droplets. Furthermore, we performed label-free sorting of cell laden droplets from empty droplets. The peripheral sorting electronics are controlled by our device. Decision making is based on predefined parameter ranges that are compared to the measurement results of the droplets right before the sorting gate. Similarly, in another experiment we demonstrate efficient sorting of droplets depending on size.

BP 11.40 Mon 16:30 BPp

Transition of adherent to suspension state: relevance to cell mechanical properties — •Venkata Dabbiru[1], Emmanual Manu[1], Huy Tung Dau[1], Nora Bödecker[1], Doreen Biedenweg[2], Ricardo Pires[1], and Oliver Otto[1] — [1]University of Greifswald, Germany — [2]University Medicine Greifswald, Germany

Adherent cells often detach from their native surface as a result of important physiological changes such as those, for example, found in cancer. While many studies have examined the mechanical properties of cells in their native adherent or suspended state, few studies have addressed the consequences associated with the transition between them. We have approached this question by using atomic force microscopy for adherent and semi-adherent cells as well as real-time deformability cytometry to study the mechanical properties of cells in suspension. As a model system, HEK293T cells have been cultured in the presence and absence of surface-tethering molecules, respectively, to mimic the transition state. Our results show that cell detachment is associated with increased stiffening of cells. Interestingly, surface-tethered transiently suspended cells and fully suspended cells differ in their mechanical properties. Analysing the F-actin distribution by confocal microscopy indicates a passive cell-surface interaction, which is not driven by adhesion molecules.

BP 11.41 Mon 16:30 BPp

Brillouin microscopy studies on phase separated FUS protein droplets — •Timon Beck[1,2], Mark Leaver[2], Raimund Schlüssler[2], and Jochen Guck[1,2] — [1]Max-Planck-Institut für die Physik des Lichts, Erlangen — [2]Biotec TUD, Dresden

The reversible phase separation of protein-RNA condensates plays an important role in intracellular organization and is involved, for example, in metabolic control and DNA repair. These phase-separated compartments can undergo an irreversible solidification, which has been associated with neurodegenerative diseases. This phenomenon has been mostly studied qualitatively and indirectly, and a direct quantitative determination of the bulk material properties during the solidification is still missing. Here, we use Brillouin microscopy to investigate phase-separated FUS protein droplets in vitro. Brillouin microscopy is a non-invasive technique which measures optomechanical properties with optical resolution using (spontaneous) Brillouin scattering. This non-elastic scattering process occurs when light is scattered by (thermally excited) soundwaves. Quantification of the Brillouin frequency shift gives direct access to the longitudinal modulus, refractive index and mass density, while the linewidth is linked to the viscosity. We followed the solidification of FUS protein droplets over time in a controlled environment monitoring the changes in Brillouin shift and linewidth. Our measurements aim to reveal the relevant time-scales and the impact of different buffer conditions on the solidification process. This establishes Brillouin microscopy as a promising quantitative tool for unraveling the mechanisms of this type of phase transition.

BP 12: Single Molecule Biophysics I

Time: Tuesday 9:00–11:00 Location: BPa

Invited Talk BP 12.1 Tue 9:00 BPa

Molecular simulation meets cryo electron tomography — •Gerhard Hummer — Max Planck Institute of Biophysics, Frankfurt am Main, Germany

Cryo electron tomography and molecular dynamics simulations perfectly complement each other. Electron tomograms provide us with a remarkably detailed, three-dimensional view of the molecular architecture of cells and viruses in situ, that is in the natural context; however, this view is essentially static and atomic resolution remains largely out of reach, in particular for dynamic biomolecular machineries. By contrast, molecular dynamics simulations naturally give us an atomistic view that includes dynamics, albeit in an idealized context. The synergistic potential of tomography and simulation can now be realized thanks to an increase in the resolution achievable by cryo electron tomography, a rapid growth in raw computational power, significant improvements in the quality of the potential energy functions entering classical molecular dynamics simulations, and the availability of simulation codes that can handle the complex molecular systems encountered in situ. To illustrate the power of combining molecular simulations with cryo electron tomography, I will present results from studies of the spike protein of the SARS-CoV-2 virus (Turoňová, Sikora, Schürmann et al., Science 2020) and from desmosome cell-cell junctions (Sikora, Ermel, Seybold et al., PNAS 2020).

BP 12.2 Tue 9:30 BPa

Electronic Quantum Coherence in Photosynthetic Protein Complexes — Hong-Guan Duan Duan[1], Ajay Jha[1], Vandana Tiwari[1], Richard J. Cogdell[2], Khuram Ashraf[2], Valentyn I. Prokhorenko[1], •Michael Thorwart[3], and R. J. Dwayne Miller[4] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [2]Institute of Molecular, Cell & Systems Biology, University of Glasgow, UK — [3]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [4]University of Toronto, Canada

The search for quantum effects in biological systems led previous experiments to report long-lived electronic quantum coherence in the primary step of the energy transfer in photosynthetic protein complexes. However, the origin of the coherence became a topic of intense debate. We have revisited this in a joint experimental and theoretical effort studying the quantum dynamics in the Fenna-Matthews-Olson (FMO) complex by two-dimensional electronic spectroscopy at different temperatures. We found that the electronic coherence time is significantly shorter under ambient conditions than previously reported. To capture solid evidence of quantum coherence, lower temperatures are required. We have clearly observed electronic coherence with a time scale of 500 fs at low temperature (20 K). However, the coherence lifetime is rapidly reduced with increasing temperature. At room temperature, electronic coherence is too short (60 fs) to play any functional role in the energy transfer which occurs on a time scale of

picoseconds. The long-lived oscillations previously reported in 2D spectra are due to Raman vibrational modes on the electronic ground state.

BP 12.3 Tue 9:50 BPa

Conformational Changes of IDP under Influence of Guanidinium Chloride: Integrative Approach using X-ray/Neutron Scattering and Single Molecule Spectrosopy — •Luman Haris[1,2], Iwo König[4], Martin Dulle[1], Aurel Radulescu[3], Ingo Hoffmann[5], Olaf Holderer[3], Tobias Erich Schrader[3], Ben Schuler[4], and Andreas Maximilian Stadler[1,2] — [1]FZ Jülich, JCNS-1 & IBI-8, Jülich — [2]IPC, RWTH Aachen, Aachen — [3]FZ Jülich, Outstation MLZ, Garching — [4]Biochemisches Institut, Universität Zürich, Zürich — [5]Institut Laue-Langevin, Grenoble

IDPs are identified by the presence of unfolded region due to relatively abundant polar residues content within its amino acid sequence. Together with other residues, IDPs exhibit not only high flexibility but also sensitivity to physicochemical fluctuation such as pH, temperature, and ions concentration. For this reason, IDPs are involved in cellular processes such as DNA repair scheme and chromatin modification. In this project, we pursue a quantitative description of structure and dynamics of IDPs with different net charges: namely Prothymosin Alpha and Myelin Basic Protein. Here, we employed neutron spin-echo spectroscopy (NSE) and small angle X-ray scattering (SAXS) to gain insight on the emergence of internal friction within the peptide and its conformational change as a function of Guanidinium Chloride (GndCl) concentration respectively. The experimental results obtained from SAXS shows contraction and expansion as measured by FRET. Similarly, from NSE data, we are able to extract the internal friction which is in good agreement with FCS result.

BP 12.4 Tue 10:10 BPa

Do the loops in the N-SH2 binding cleft truly serve as allosteric switch in SHP2 activation? A tale of disorder, crystal contacts, and activation free energies — Massimiliano Anselmi and •Jochen S Hub — Unvierstität des Saarlandes, Saarbrücken, Germany

SHP2 is a multi-domain protein, playing an important role in upregulating cellular processes such as cell survival, proliferation, and programmed cell death. SHP2 mutations cause developmental disorders and were found in many cancer types. In healthy cells, SHP2 mainly takes an autoinhibited, inactive form, and SHP2 is activated upon binding of a phosphopeptide to the N-SH2 domain. For the past two decades, the widening of the binding cleft upon peptide binding has been considered as the key event driving SHP2 activation.

We re-analyzed the manifold amount of crystallographic data of SHP2, and we carried out extensive MD simulations and free energy calculations of SHP2 in solution and in a crystal environment. We found that the "allosteric switch" model is in fact compromised by crystal contacts and flexible, poorly resolved loops, and that the degree of openness of the binding cleft does not even influence the free energy of SHP2 opening. Instead, we detected an alternative allosteric mechanism, namely the unzipping of a central beta sheet of N-SH2, which drives SHP2 activation. Apart from the implications on SHP2 activation and inhibition, the study highlights that MD simulations in crystal and solution environments are a powerful tool to avoid misinterpretation of crystal structures.

30 min. Meet the Speaker

BP 13: Multicellular Systems I

Time: Tuesday 9:00–11:00 Location: BPb

BP 13.1 Tue 9:00 BPb

Elongated Cells Fluidize Malignant Tissues — •Steffen Grosser, Jürgen Lippoldt, Linda Oswald, Frédéric Renner, and Josef A. Käs — Peter Debye Institute for Soft Matter Physics, Universität Leipzig

Tissue morphology changes during tumour progression. In 2D cell cultures, different tissue states, such as fluid, jammed and nematic, are linked to cell shapes. While it is not clear if these results hold true in three dimensions, they suggest to investigate cell shapes and tissue states of matter in 3D. To explain cell motility in tumors, we compare 3D cell spheroids composed of cells from a cancerous and a non-cancerous cell line. Through spheroid fusion experiments and live cell tracking, we show that the epithelial sample behaves solid-like and the malignant sample is fluidized by active cells moving through the tissue. Full 3D-segmentations of the samples show that the fluid-like tissue has elongated cell shapes. This links cell shapes to cell motility and bulk mechanical behaviour. We reveal two active states of matter in 3D tissues: an amorphous glass-like state with characteristics of 3D cell jamming, and a disordered fluid state.

BP 13.2 Tue 9:20 BPb

Relation between tissue homeostasis and mechnosensitivity in model epithelium — •Maxime Hubert[1], Sara Kaliman[1], Carina Wollnik[2], Simone Gehrer[1], Damir Vurnek[1], Diana Dudziak[3], Florian Rehfeldt[2], and Ana-Suncana Smith[1,4] — [1]PULS Group, Friedrich Alexander University Erlangen-Nurnberg, Erlangen, Germany — [2]Cell & Matrix Mechanics Group, Georg-August-University Gottingen, Gottingen, Germany — [3]Group for the Biology of Dendritic Cells, University Clinic Erlangen-Nurnberg, Erlangen, Germany — [4]Group for Computational Life Sciences, Ruder Boskovic Institute, Zagreb, Croatia

Despite recent efforts to understand homeostasis in epithelial tissues, there are many unknowns surrounding this cooperative steady state. In the context of cell morphology, single cell studies set mechanosensitivity as an important regulatory process. However, mechanoresponse in tissues remains heavily debated. Here we show that changes in matrix stiffness induce a non-equilibrium transition from tubular to squamous tissues. Despite adopting different cell shapes and densities, all homeostatic states display equivalent topologies. This suggests that the latter property is actively targeted in homeostasis. On the contrary, we observe a dramatic change in the self-assembled organization of the colonies on the macroscopic scale. Such behavior is recovered in simulations by introducing stiffness-dependent activity. Our results unequivocally relate the mechanosensitive properties of individual cells to the evolving macroscopic structures, an effect that could be important for understanding the emergent pathology of living tissues.

Invited Talk BP 13.3 Tue 9:40 BPb

Active behaviors of cellular monolayers. — •Benoit Ladoux — Institut Jacques Monod, CNRS & Université de Paris, Paris, France

The actomyosin machinery endows cells with contractility at a single cell level. Within a tissue, cells are not only interacting with their substrate but also with their neighbors. The way forces from adhesion complexes are transmitted leads to various collective behaviors and plays a role in the active nature of cellular monolayers. In the first part, I will show how these active behaviours and stresses govern fundamental biological processes such as cell extrusion. By modelling the epithelium as an active nematic liquid crystal and measuring mechanical parameters such as strain rates and stresses measurements within cellular monolayers, we show that apoptotic cell extrusion is provoked by singularities in cell alignments in the form of comet-shaped topological defects. Cellular monolayers display various active behaviors as exemplified by the contractile nature of fibroblasts and the extensile nature of epithelial cells or neural crest cells. In the second part, I will discuss how these two contradictory modes of force generation can coexist. Through a combination of experiments and in silico modeling, we uncover the mechanism behind this switch in behaviour of cell monolayers from extensile to contractile as the weakening of intercellular contacts. We find that this switch in active behaviour also promotes the buildup of tension at the cell-substrate interface through an increase in actin stress fibers and higher traction forces. Such differences in extensility and contractility act to sort cells, thus determining a general mechanism for mechanobiological pattern formation.

BP 13.4 Tue 10:10 BPb

cell competition in mouse embryo — •Gabriele Lubatti[1], Antonio Scialdone[1], Tristan Tristan[2], Ana Lima[2], and Shankar Srinivas[3] — [1]Institute of Epigenetics and Stem Cells, Helmholtz Zentrum Munich, Munich, Germany — [2]National Heart and Lung Institute, Imperial College London, Hammersmith Hospital Campus, London, UK — [3]Department of Physiology Anatomy & Genetics, University of Oxford, Oxford, UK

Cell competition is a biological process whereby cells eliminate their less fitted neighbours [1] [2]. It has myriad positive roles in the organism: it selects against mutant cells in developing tissues, prevents the propagation of oncogenic cells and eliminates damaged cells during ageing. While it was first characterized in drosophila [3], it is currently unclear what are the transcriptional features of cells eliminated through competition and what are the roles of cell competition during mammalian development. We analysed single-cell transcriptomic data from mouse embryos around the time gastrulation starts (stage E6.5) where apoptosis was inhibited. We show that in these embryos a new population of epiblast cells emerges, expressing markers of cell competition previously characterized [4]. Our analysis also identifies additional features of eliminated cells, including disrupted mitochondrial activity that we validate in vivo. Moreover, by using physical modelling, we show that cell competition might play a role in the regulation of embryo size, which could be particularly important around gastrulation [5].

30 min. Meet the Speaker

BP 14: Focus Phase Separation in Biological Systems I (joint session BP/CPP)

Time: Tuesday 9:00–11:00 Location: BPc

BP 14.1 Tue 9:00 BPc

Intranuclear Phase Separation of a Chromatin Scaffolding Protein — •Davide Michieletto[1], Mattia Marenda[1], David Zwicker[2], and Jan Kirschbaum[2] — [1]University of Edinburgh — [2]Max Planck Institute for Dynamics and Self-Organization

The formation and regulation of phase separated condensates is now widely seen in vitro and cytoplasm, but far more challenging to observe and test in the cell nucleus. In this talk I will present recent work on an abundant nuclear RNA-binding protein called Scaffold Attachment Factor A, or SAF-A, that regulates chromatin decompaction at transcriptionally active loci through its interaction with RNA. Here I show that the intrinsically disordered RNA binding domain of SAFA * known as an RGG domain – undergoes phase separation upon transcriptional inhibition and that the size of the condensates can be controlled by tuning the amount arginine/lysine residues in the RGG domain. By expressing a longer, and closer to native, SAFA domain we observe that the phase separation is suppressed. To explain our findings, we propose an equilibrium model in which a slowly diffusing RNA substrate can sequester RGG fragments; upon transcriptional inhibition the freed up fragments can undergo phase separation via weak self-interactions.

BP 14.2 Tue 9:20 BPc

Quantitative phase microscopy enables precise and efficient determination of biomolecular condensate composition — •Patrick M McCall[1,2], K Kim[3,4], AW Fritsch[1], JM Iglesias-Artola[1], LM Jawerth[1,2], J Wang[1], M Ruer[1], A Poznyakovskiy[1], J Peychl[1], J Guck[3,4], S Alberti[3], AA Hyman[1], and J Brugués[1,2] — [1]MPI-CBG, Dresden — [2]MPI-PKS, Dresden — [3]TU Dresden — [4]MPI Science of Light

Many cellular processes rely on condensed macromolecular phases termed biomolecular condensates. Despite progress in measurements and theoretical descriptions of several condensate properties, an understanding of their most basic feature, composition, remains elusive. Here we combined quantitative phase microscopy and sessile droplet physics to measure the shape and composition of individual model condensates. This technique requires 1000-fold less material than traditional approaches, achieves a precision of better than 2 %, and does not rely on fluorescent tags, which we show can significantly alter phase behavior. The protein concentrations measured in three model condensates span a broad range, from 80 to 500 mg/ml, pointing to a natural diversity in condensate composition specified by protein sequence. We report salt- and temperature-dependent binodals as well as time-resolved measurements revealing that PGL3 condensates undergo a contraction-like process during aging. This leads to doubling of the internal protein concentration coupled to condensate shrinkage. We anticipate that this new approach will enable understanding the physical properties of biomolecular condensates and their function.

BP 14.3 Tue 9:40 BPc

Quantitative Theory for the Diffusive Dynamics of Liquid Condensates — •Lars Hubatsch[1,2], Louise M Jawerth[1,2], Celina Love[2], Jonathan Bauermann[1], Stefano Bo[1], T-Y Dora Tang[2], Anthony A Hyman[2], and Christoph A Weber[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

To unravel the biological functions of membraneless liquid condensates it is crucial to develop a quantitative understanding of the physics underlying their dynamics. Key properties of such condensates are diffusion and exchange of material with their environment. Experimentally, such diffusive dynamics are typically probed through the direct observation of the individual or collective motion of fluorescently labelled molecules. However, to date we lack a physics-based quantitative framework for the dynamics of labeled condensate components. Here, we derive the corresponding theory, building on the physics of phase separation, and quantitatively validate this framework via experiments. We show that using our theory we can precisely determine diffusion coefficients inside liquid condensates via a spatio-temporal analysis of fluorescence recovery after photobleaching (FRAP) experiments. We showcase the accuracy and precision of our approach by considering space and time resolved data of protein condensates and two different coacervate systems. Strikingly, our theory can be used to determine the diffusion coefficient in the dilute phase and the partition coefficient, purely based on fluorescence measurements in the droplet.

BP 14.4 Tue 10:00 BPc

Interactions of droplets with polymer networks at the mesh and continuum scale — •Thomas J Boeddeker[1], Estefania Vidal[2], Kathryn A Rosowski[1], David Zwicker[2], and Eric R Dufresne[1] — [1]ETH Zurich, Zurich, Switzerland — [2]MPI DS, Göttingen, Germany

Phase-separation of biomolecules in cells takes place in a complex environment crossed by multiple filaments of the cytoskeleton or chromatin. Interactions between the emerging protein droplets and filaments take place over different length scales and may lead to motion and deformation of both network and droplet. In this shared talk, Thomas presents experimental work on the interactions of stress granules, a phase-separated protein-RNA droplet in the cytosol, with the heterogeneous microtubule network at the mesh scale. Inspired by observations in the cell, we then turn to synthetic gels where elastic effects produce ripening in stiffer materials leading to a dissolution front. Estefania presents a theoretical framework for the observed ripening in gradients of network stiffness at the continuum scale. Our combined results present an initial approach to understand the complex interactions throughout phase separation in an elastic network.

30 min. Meet the Speaker

BP 15: Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)

Time: Tuesday 9:30–10:30 Location: DYa

See DY 21 for details of this session.

BP 16: Single Molecule Biophysics II

Time: Tuesday 11:00–13:30 Location: BPa

BP 16.1 Tue 11:00 BPa

Comparison of continuous and discrete Markov models of biomolecular dynamics — •Benjamin Lickert and Gerhard Stock — Universität Freiburg

Motions of biomolecular systems, recorded by molecular dynamics simulations, are often modeled as Markov processes. A very popular approach is given by Markov state models where the conformational space is divided into different states [1]. To be Markovian, the intrastate dynamics need to be significantly faster than the interstate dynamics. On the other hand, the observed dynamics can be modeled as a continuous diffusive process, called Langevin dynamics, on some low-dimensional free energy landscapes $F(\vec{x})$. In this case, Markovianity is given if the system, i.e., $\vec{x}(t)$, evolves substantially slower than the neglected degrees of freedom, i.e., the bath surrounding the system. Recently, a data-driven approach was formulated to estimate such a Langevin model from a given trajectory $\vec{x}(t)$. Here, we compare the features of both modeling frameworks. While Markov state models are very appealing due to their clearly structured generation and interpretation, Langevin dynamics have the advantage that they allow for the estimation of continuously defined observables, like free energy and autocorrelations. Using molecular dynamics simulations of systems with varying complexity we have a look at these points in practice [2].

[1]: J.H.Prinz et al., J.Chem.Phys. 134, 174105 (2011)
[2]: B.Lickert and G.Stock, J.Chem.Phys. 153, 244112 (2020)

BP 16.2 Tue 11:20 BPa

Magnetic Tweezers Protein Force Spectroscopy: Applications to Von Willebrand Factor and SARS-CoV-2 Cell Adhesion — •Jan Lipfert[1], Magnus Bauer[1], Steffen Sedlak[1], Achim Löf[1], Tobias Obser[2], Maria Brehm[2], Martin Benoit[1], Adina Hausch[1], and Sophia Gruber[1] — [1]Department of Physics, LMU Munich — [2]Department of Pediatric Hematology and Oncology, University Medical Center Hamburg Eppendorf

The physiological function of proteins is often critically affected by forces acting on them. We have developed a versatile and modular approach for force measurements on proteins in magnetic tweezers [Löf et al. PNAS 2019; Gruber et al. Nanoscale 2020] that enables ultra-stable (>days) and parallel measurements (>50) in a wide force range, in particular at low forces (<1 pN).

We apply our new assay to two systems critical in human pathologies: the blood protein von Willebrand Factor (VWF) and the Spike-mediated adhesion of SARS-CoV-2, the causative agent of the current pandemic. First, we probe regulatory transitions at low forces within VWF. Our results reveal fast (~250 ms) transitions in the dimeric VWF stem around 1 pN, which likely constitute the first steps in its mechano-activation. Second, we use a tethered ligand assay to quantitate how the SARS-CoV-2 spike protein binds to its cellular receptor ACE2. We find that SARS-CoV-2 has a higher force stability and lower off-rate than the previous SARS-CoV-1, which caused the 2002 pandemic, which might contribute to different infection patterns observed for the two viruses.

BP 16.3 Tue 11:40 BPa

Watching an enzyme at work: Time-Resolved Serial Crystallography reveals water mediated allosteric regulation — •Henrike Müller-Werkmeister — Uni Potsdam, Institut für Chemie, Physikalische Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam

We have studied the homodimeric enzyme fluoroacetate dehalogenase by time-resolved serial synchrotron crystallography (TR-SSX). Using a fixed target based sample delivery [1] with an efficient interlacing pattern allowed us to realize "hit-and-return" (HARE) TR-SSX to cover the full timescale from 30 milliseconds to 30 seconds [2]. With a photocaged substrate for reaction initiation, four catalytic turnovers could be resolved [3]. The total of 18 independent structures not only provide unprecedented insight into the reaction mechanism, showing the substrate binding, the Michaelis-Menten-complex and the covalent intermediate, but also reveal the allosteric mechanism leading to half-the-sites reactivity. In fact, a molecular water wire can be observed that together with molecular breathing is clocked to the enzymatic reaction.

[1] I. Martiel, H. M. Müller-Werkmeister, A. E. Cohen, Acta Cryst. D, 2019, D75, 160*177 [2] E. C. Schulz*, P. Mehrabi*, H. M. Müller-Werkmeister*, F. Tellkamp, A. Jha, W. Stuart, E. Persch, R. De Gasparo, F. Diederich, E. F. Pai, R. J. D. Miller, Nature Methods, 2018, 15 (11), 901-904 [3] P. Mehrabi*, E. C. Schulz*, R. Dsouza, H. M. Müller-Werkmeister, F. Tellkamp, R. J. D. Miller, E. F. Pai, Science, 2019, 365 (6458), 1167-1170

BP 16.4 Tue 12:00 BPa

Hybrid Kinetic Monte Carlo / Molecular Dynamics Simulations of Bond Scissions in Proteins — •Benedikt Rennekamp[1,2] and Frauke Gräter[1,2] — [1]Heidelberg Institute for Theoretical Studies, Schloss-Wolfsbrunnenweg 35, 69118 Heidelberg, Germany — [2]Interdisciplinary Center for Scientific Computing, Heidelberg University, INF 205, 69120 Heidelberg, Germany

Proteins are exposed to various mechanical loads that can lead to covalent bond scissions even before macroscopic failure occurs. In regular Molecular Dynamics (MD) simulations covalent bonds are, however, predefined and reactions cannot occur. Furthermore, such events rarely take place on MD time scales.

We have developed a hybrid Kinetic Monte Carlo / Molecular Dynamics (KIMMDY) scheme that overcomes the separation of time scales of these processes and drastically increases the accessible time scales for reactive MD simulations. Here, bond rupture rates are calculated in the spirit of a transition state model based on the interatomic distances in the MD simulation and then serve as an input for a Kinetic Monte Carlo step.

With this new technique we investigated bond ruptures in a multi-million atom system of tensed collagen, a structural protein found in skin, bones and tendons. Our simulations show a clear concentration of homolytic bond scissions near chemical crosslinks in collagen. We suggest that these created mechanoradicals are a yet unknown connection converting mechanical into oxidative stress. This application also demonstrates the scalability of our hybrid computational approach.

BP 16.5 Tue 12:20 BPa

van der Waals Forces in Biomolecular Systems: from Solvation to Long-range Interaction Mechanisms — •Martin Stöhr and Alexandre Tkatchenko — Department of Physics and Materials Science, University of Luxembourg

A decisive characteristic of the biomolecular machinery is the access to a rich set of coordinated processes within a small energy window. Most of these processes involve collective conformational changes and occur in an aqueous environment. Conformational changes of (bio)molecules as well as their interaction with water are thereby largely governed by non-covalent van der Waals (vdW) dispersion interactions. By virtue of their intrinsically collective nature, vdW forces also represent a key influence on collective nuclear behavior. Our understanding of vdW interactions in large-scale (bio)molecular systems, however, is still rather limited. Here, we employ the Many-Body Dispersion framework to investigate the vdW interaction in biomolecular systems and its spatial and spectral aspects. In particular, we show the role of beyond-pairwise vdW forces for protein stability and highlight the delocalized character of the protein-water vdW interaction. We further examine intrinsic electronic behaviors and reveal a coexistence of strong delocalization with spatially-separated, yet correlated, local domains. This, ultimately, forms the basis for a potential, efficient long-range interaction mechanism for coordinated processes in biomolecular systems such as enzymatic action, regulation and allostery.

BP 16.6 Tue 12:40 BPa

Q band mixing in chlorophyll a - spectral decomposition of Qx and Qy absorption bands — •Clark Zahn[1], Till Stensitzki[1], Angelica Zacarias[2], and Karsten Heyne[1] — [1]Institutfür Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D06120 Halle, Germany and ETSF

Chlorophyll a (Chl a) is one of the most abundant pigments on earth. Despite extensive research, the composition of its absorption spectrum is yet not well understood. Here, we apply polarization resolved femtosecond Vis pump - IR probe spectroscopy, providing a detailed insight into Q band mixing of Chl a. The excitation was tuned to various wavelengths covering the Q band absorption. We show, that the dichroic ratio of the keto-C=O stretching vibration at 1698 cm-1 strongly depends on the excitation wavelength. Hence, the angle between the excited electronic transition dipole moment (tdm) and the vibrational keto-C=O tdm changes significantly across the Q band. By tracing this angle Θ for different excitation wavelengths, we are able to determine the Qx contribution along the Q band region. We find that Qx contributes 42-71% to the absorption of the lower energetic peak at 618 nm and to 59-100% to the absorption of the high energy flank at around 580 nm. Complementary measurements on the C=C stretching vibration at 1608 cm-1 provide corroborating evidence for our findings. Our results provide a direct spectral disentanglement of the Q band, without any previous assumptions. Thus, making them a reliable benchmark for quantum chemical calculations.

30 min. Meet the Speaker

BP 17: Multicellular Systems II

Time: Tuesday 11:00–13:30 Location: BPb

BP 17.1 Tue 11:00 BPb

Encoding memory in biological network hierarchy — •Mirna Kramar[1] and Karen Alim[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany

Remembering sources of food and threat is essential for survival. Even very simple organisms are able to encode sensory information that aids them in tackling complex environments. The slime mould *Physarum polycephalum* is a giant unicellular eukaryote whose body consists of a network of tubes which undergoes constant reorganization. The mechanism behind the network reorganization upon food encounter has not been explained previously. Here, we identify the imprint the food stimulus leaves on network morphology as memory and show that the network relies on tube growth and flows to encode stimulus information. We hypothesise an encoding mechanism introducing a local release of a chemical agent that affects the mechanical properties of the tubes and spreading through the network by protoplasmic flows. Using a theoretical model, we test our hypothesis and find the model yields a correct prediction of flow-dependent stimulus response. Finally, we investigate the role of network hierarchy in memory encoding and show that the network directly relies on existing tube diameter hierarchy to encode the stimulus. Our findings [1] demonstrate *P.polycephalum*'s ability to encode and read stored memory and likely open doors to the use of the organism in bioinspired design.

[1] Kramar and Alim, PNAS, in press (2021)

BP 17.2 Tue 11:20 BPb

A lumped-parameter model illustrates information processing and migration in the slime mold *Physarum polycephalum* — •Christina Oettmeier and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen

The slime mold *P. polycephalum* exhibits rich spatiotemporal oscillatory behavior. The organism's size spans orders of magnitude, from large meter-sized stationary transport networks down to micrometer-sized amoebae. All morphotypes show actomyosin-based contraction-relaxation cycles resulting in proto-

plasmic streaming. Furthermore, the giant amoeba shows a very high behavioral plasticity, leading to speculations about the origins of cellular minimal cognition. The underlying functions are not neuron-based, but are emergent phenomena, resulting from mechanochemical processes on the tubular network. In this context, we investigate how the slime mold processes information. At different parts of a migrating amoeba, oscillation frequencies vary. Oscillations in the back cause endoplasm flows through the internal vein system and expand the frontal membrane. We use the electronic-hydraulic analogy, implemented in a lumped-parameter model, to investigate this special case of information processing. A single vein segment can be described as a flexible tube, possessing a fluidic resistance (R) and fluidic capacitance (C) due to wall elasticity. The electronic equivalent is a passive RC low pass filter. Thus, the oscillation frequencies at the back are higher than those at the front due to filtering. The model can also explain the onset of locomotion.

BP 17.3 Tue 11:40 BPb

Morphoelasticity of Large Bending Deformations of Cell Sheets during Development — •Pierre A. Haas[1,2,3] and Raymond E. Goldstein[4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Center for Systems Biology, Dresden, Germany — [4]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom

Deformations of cell sheets during morphogenesis are driven by developmental processes such as cell division and cell shape changes. In elastic shell theories of development, these processes appear as variations of the intrinsic geometry of a thin shell. However, morphogenesis often involves large bending deformations that are outside the formal range of validity of classical shell theories.

In this talk, I will therefore discuss a shell theory valid in this new geometric limit of large bending deformations [1]. I will emphasise the geometric material anisotropy that arises in this theory and the elastic role of cell constriction. Finally, taking the invagination of the spherical embryos of the alga *Volvox* as a model, I will compare this shell theory to a classical theory not formally valid for large bending deformations and reveal how the geometry of large bending deformations stabilises invagination [1].

[1] P. A. Haas and R. E. Goldstein, Phys. Rev. E **103** (2021, in press)

BP 17.4 Tue 12:00 BPb

Migration of immune cells in an obstacle park — •Doriane Vesperini[1], Zeinab Sadjadi[2], Heiko Rieger[2], and Franziska Lautenschläger[1] — [1]Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Several crucial processes in biological systems can be described as a search problem such as: finding food resources or pathogens. The presence of obstacles like non-targeted cells or extracellular matrix in biological environments induces a perturbation of the initial cell trajectory. For example, the presence of bystander cells has been shown to increase the velocity and the persistence of natural killer cells [1]. Besides obstacles density, their spatial disposition may also influence the search efficiency. It has been demonstrated that the density and geometry of pillar lattices affect migration strategies of cells [2].

We investigate how search efficiency is influenced by spatial arrangement of obstacles. A microfluidic device is designed to track HL60 cells differentiated into neutrophils in confined 2D environments. Our device consists of pillar forests distributed in triangular or square arrangements. We calculate the escape time and diffusion properties of the searcher in different densities and height of pillars and investigate which key parameters influence the search efficiency.

[1] Zhou X., et al. Scientific Reports (2017)
[2] Gorelashvili M., et al. New Journal of Physics (2014)

BP 17.5 Tue 12:20 BPb

Cell-cell adhesion and 3D matrix confinement explain plasticity of breast cancer invasion — •Simon Syga[1], Peter Friedl[2,3,4], and Andreas Deutsch[1] — [1]Center for Information Services and High Performance Computing, Technische Universität Dresden, Germany — [2]Department of Cell Biology, Radboud Institute for Molecular Life Sciences, Radboud University Medical Center, Nijmegen, the Netherlands — [3]David H. Koch Center for Applied Genitourinary Cancers, The University of Texas MD Anderson Cancer Center, Houston, TX, USA — [4]Cancer Genomics Centre, Utrecht, the Netherlands

Plasticity of cancer invasion and metastasis depends on the ability of cancer cells to switch between collective invasion modes and single cell dissemination, under the control of cadherin-mediated cell-cell junctions. E-cadherin is considered a tumor suppressor, the downregulation of which causes single-cell scattering in 2D environments. In clinical samples, however, E-cadherin expressing and deficient tumors both invade collectively and metastasize equally, implicating additional mechanisms controlling cell-cell cooperation and dissemination. Using a cellular automaton model we identify physical confinement by the extracellular matrix (ECM) as the dominant physical mechanism that supports collective invasion irrespective of the composition and stability of cell-cell junctions. In particular, we predict that downregulation of E-cadherin results in a transition from coordinated to uncoordinated collective movement along extracellular boundaries, whereas single-cell escape depends on locally free tissue space.

BP 17.6 Tue 12:40 BPb

Learning the dynamics of cell-cell interactions in confined cell migration — •David Brückner[1], Nicolas Arlt[2], Alexandra Fink[1], Pierre Ronceray[3], Joachim Rädler[2], and Chase Broedersz[1,4] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, München — [2]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-Universität, München — [3]Center for the Physics of Biological Function, Princeton University, Princeton, NJ 08544, USA — [4]Department of Physics and Astronomy, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands

Contact-mediated cell-cell interactions play a key role in shaping the stochastic trajectories of migrating cells. But how can we describe the stochastic dynamics of colliding cells in a unifying theoretical framework? To address this question, we monitor stochastic cell trajectories in a micropatterned cell collider in which pairs of cells perform repeated cellular collisions. Capitalizing on this large experimental data set of coupled cell trajectories, we infer an interacting stochastic equation of motion that accurately predicts the observed interaction behaviors. Our approach reveals that interacting non-cancerous MCF10A cells can be described by repulsion and friction interactions. In contrast, cancerous MDA-MB-231 cells exhibit novel and surprising attraction and anti-friction interactions, promoting the predominant relative sliding behavior observed for these cells. Based on the inferred interactions, we show how our framework may generalize to provide a unifying theoretical description of diverse cellular interaction behaviors.

30 min. Meet the Speaker

BP 18: Cell Mechanics IV

Time: Tuesday 11:00–12:00 Location: BPc

BP 18.1 Tue 11:00 BPc

Direct measurements of interactions between intermediate filaments — •Anna V. Schepers[1], Charlotta Lorenz[1], Peter Nietmann[2], Andreas Janshoff[2], Stefan Klumpp[3], and Sarah Köster[1] — [1]Insitute for X-Ray Physics, Georg August University Göttingen — [2]Institute of Physical Chemistry, Georg August University Göttingen — [3]Institute for Dynamics of Complex Systems, Georg August University Göttingen

The cytoskeleton consists of F-actin, microtublues and intermediate filaments (IFs), which form a complex composite network. F-actin and microtubule networks have been studied extensively and a large variety of cross-linkers are known. By contrast, the interactions in reconstituted IF networks are less well understood. It has, however, been shown that multivalent ions cause bundling and network stiffening. While rheological experiments give insight into the slow stiffening and mechanics of vimentin IF networks, it is challenging to distinguish the contributions of filament stiffening and of increased attraction. Combining optical trapping and fluorescence microscopy enables us to bring two single vimentin IFs in contact and directly study the interactions between the filaments. By amplifying electrostatic attraction or diminishing the hydrophobic interactions we are able to study the nature of the interactions between IFs. These results, in combination with studies of the mechanical properties of single IFs, allow us to model the interactions with Monte-Carlo simulations, thereby gaining a deeper understanding of cytoskeletal structures.

BP 18.2 Tue 11:20 BPc

Stiffening of the Ndc80 complex, the main mirotubule-kinetochore linker — •Felix Schwietert and Jan Kierfeld — TU Dortmund University, 44221 Dortmund, Germany

In the mitotic spindle microtubules attach to chromosomes via kinetochores, whose molecular structure and mechanical properties are not completely understood. Over the past years, it became evident that the Ndc80 complex plays a major role for attaching microtubules to the kinetochore and transmitting forces from depolymerizing microtubules to the chromosome. The Ndc80 complex is a rod-like coiled-coil with globular end domains that bind to the kinetochore and the microtubule, respectively. Due to its force transmitting function, its elastic properties are of great interest for modeling and understanding chromosome dynamics in the mitotic spindle. Here, we theoretically explain the recent ex-

perimental result that the effective stiffness of a Ndc80 complex increases under tension [1]. Our model is based on the specific architecture of the Ndc80 complex, which has a characteristic flexible kink at approximately one third of its length.

[1] V. A. Volkov, P. J. Huis in 't Veld, M. Dogterom, and A. Musacchio, eLife 7:e36764 (2018)

BP 18.3 Tue 11:40 BPc

Development of microtentacles in suspended cells upon weakening of the actin cortex — •Lucina Kainka, Reza Shaebani, Ludger Santen, and Franziska Lautenschläger — Saarland University, Center for Biophysics, 66123 Saarbrücken

Circulating Tumor Cells (CTCs) pose a significant threat due to their role in metastasis: It has been proposed that CTCs are able to escape the blood stream and reattach to the tissue by the formation of so-called microtentacles (McTNs). McTNs are microtubule based membrane protrusions with a diameter of less than 1 μm and a length of tens of μm.

In CTCs the balance of the outward growing microtubule and the contractive forces of the actin cortex is disrupted enabling microtubules to form these kind of protrusions. Using cytoskeletal drugs which are targeting the actin cortex integrity we induce McTNs even in non-cancerous RPE1 cells. We investigate the presence of microtubules and actin as well as vimentin under those conditions. Furthermore, we established a statistic over the number and lengths of McTNs depending on different drug concentrations applied.

Scanning electron microscopy images of the cytoskeleton beneath the plasma membrane of McTNs give further insight into their cytoskeletal composition.

BP 19: Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)

Time: Tuesday 11:00–13:00 Location: DYa

See DY 23 for details of this session.

BP 20: Focus Biological Cells in Microfluidics I

Time: Tuesday 12:00–13:30 Location: BPc

BP 20.1 Tue 12:00 BPc

Numerical Investigation of Cell Deformation during Bioprinting — •Sebastian Johannes Müller and Stephan Gekle — Universität Bayreuth, Bayreuth, Deutschland

In 3D bioprinting, cells suspended in hydrogel are deposited through a fine nozzle, creating three dimensional biological tissues. Due to the high viscosity of the hydrogel, the cells experience hydrodynamic stresses that deform or damage the cells and can ultimately affect the viability and functionality of the cells in the printed construct.

Using numerical methods, we quantify these deformations in dependency of the flow parameters and cell elasticity. We consider shear thinning fluid rheology and validate our Lattice Boltzmann flow calculations with microfluidic flow experiments of typical hydrogel materials. Our hyperelastic cell, modeled as purely elastic continuum with neo-Hookean force calculations, is validated with experimental data for cells obtained via AFM indentation measurements.

By coupling our cell model with the fluid simulations, we investigate the cell deformation in typical flow scenarios, like capillary and shear flow. As essential part of the printing process, we further simulate the cell flowing through the transition from the printer nozzle into the free hydrogel strand, where additional radial flow components stretch the cell at short time scale.

BP 20.2 Tue 12:20 BPc

Microfluidic platforms to study forces on model cells — •Tom Robinson — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Biological cells in their natural environment experience a variety of external forces such as fluidic shear stresses, osmotic pressures, and mechanical loads. The response of cell membranes to such forces is of great interest and model systems such as giant unilamellar vesicles (GUVs) offer the chance to investigate individual components without interference from cellular complexity (Robinson, Adv Biosyst., 2019). However, being able to handle and apply forces to these delicate objects in a controllable manner is non-trivial. Therefore, we present several microfluidic platforms to create, capture, analyse, and apply forces to GUVs. First, we present platforms for surfactant-free GUV production (Yandrapalli, et al. bioRxiv, 2020) as well as their high-capacity capture and isolation (Yandrapalli & Robinson, Lab Chip, 2019; Yandrapalli, et al. Micromachines, 2020). Lipid rafts are thought to play an important role in the spatial organization of membrane proteins. Therefore, GUVs with membrane domains are used as models to explore their behaviour in response to external forces. We use valve-based systems to apply precise fluidic shear stresses vesicles (Sturzenegger, et al. Soft Matter, 2016) and a device with an integrated micro-stamp to mechanically compress GUVs to study the effects that deformation has on lipid rafts (Robinson & Dittrich, ChemBioChem 2019). Microfluidic valves are also used to apply precise osmotic changes to measure membrane permeability to water (Bhatia et al. Soft Matter, 2020).

BP 20.3 Tue 12:40 BPc

High Throughput Microfluidic Characterization of Erythrocyte Shapes and Mechanical Variability — •Felix Reichel[1,2], Johannes Mauer[3], Ahsan Nawaz[1], Gerhard Gompper[3], Jochen Guck[1], and Dmitry Fedosov[3] — [1]Max Planck Institute for the Science of Light and Max-Planck-Zentrum für Physik und Medizin, Erlangen — [2]Biotechnology Center, Center for Molecular and Cellular Bioengineering, Technische Universität Dresden, Dresden — [3]Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich

The circulation of red blood cells (RBCs) in microchannels is important in microvascular blood flow and biomedical applications such as blood analysis in microfluidics. Current understanding of the complexity of RBC shapes and dynamical changes in microchannels is mainly formed by a number of simulation studies, but there are few systematic experimental investigations. Here, we present a first systematical mapping of experimental RBC shapes and dynamics for a wide range of flow rates and channel sizes. Results are compared with simulations and show good agreement. A key difference to simulations is that in experiments there is no single well-defined RBC state for fixed flow conditions, but rather a distribution of states. This result can be attributed to the inherent variability in RBC mechanical properties, which is confirmed by a model that takes the variation in RBC shear elasticity into account. These results make a significant step toward a quantitative connection between RBC behavior in microfluidic devices and their mechanical properties.

30 min. Meet the Speaker

BP 21: Systems Biology III

Time: Tuesday 14:00–16:00 Location: BPa

Invited Talk BP 21.1 Tue 14:00 BPa

Predicting Protein and RNA Structures: from statistical physics to machine learning — •Alexander Schug — John von Neumann Institute for Computing, Jülich Supercomputer Centre, Forschungszentrum Jülich — Faculty of Biology, University of Duisburg-Essen

On the molecular level, life is orchestrated through an interplay of many biomolecules. To gain any detailed understanding of biomolecular function, one needs to know their structure. Yet the structural characterization of many important biomolecules and their complexes - typically preceding any detailed mechanistic exploration of their function- remains experimentally challenging. Tools rooted in statistical physics such as Direct Coupling Analysis (DCA) but also increasingly Machine Learning driven approaches take advantage of the explosive growth of sequence databases and infer residue co-evolution to guide structure prediction methods via spatial constraints. For proteins, systematic large-scale studies of >1000 protein families are already possible. Additional information, such as low-resolution experimental information (e.g. SAXS or FRET) can be

used as further constraints in simulations. For RNA there are significantly less data available, which hinders in particular ML based approaches. Still, DCA combined with ML can improve prediction quality.

BP 21.2 Tue 14:30 BPa

Rational optimization of drug-membrane selectivity by computational screening — •Bernadette Mohr and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Success rates of drug discovery are non-satisfactory considering the high cost in time and resources. This leads to an increased demand for development of improved screening methods. In our work, we explore the capabilities of using a coarse-grained (CG) model to efficiently find candidate structures with desired properties. The Martini CG force field is a physics-based model that incorporates both the essential chemical features with a robust treatment of statistical mechanics. Martini simplifies the molecular representation through a small set of bead types that encode a variety of functional groups present in organic chemistry. This offers two advantages: (i) many molecules map to the same CG representation and (ii) screening boils down to systematically varying among the set of CG bead types available. The combination of these two aspects makes Martini a remarkably efficient candidate for high-throughput screening. We apply this approach to the selective binding of drugs between Cardiolipin and phosphoglycerols in mitochondrial membranes. A systematic screening starting from an already-reported compound will be presented. We identify clear design rules for improved selectivity, and rationalize them on a physical basis. As an outlook, we explore prospects of further boosting screening at higher throughput by means of connecting the CG simulations within a deep-learning framework.

BP 21.3 Tue 14:50 BPa

Morphology of spherical epithelial monolayers — •Aboutaleb Amiri[1], Charlie Duclut[2,3], Carl Modes[2,3], and Frank Jülicher[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Max Plack Institute for Molecular Cell Biology and Genetics, 01037 Dresden, Germany — [3]Center for Systems Biology Dresden, 01307 Dresden, Germany

We develop a generalised vertex model off the mechanics of epithelial cell monolayers to study morphogenesis in three dimensions. In this approach, a cell is represented by a polyhedron which is characterised by the location of its vertices in 3D space. We take into account apical, basal, and lateral cell surface tension, as well as pressure differences between outside and inside the cells. We consider an epithelium with spherical topology enclosing a lumen and investigate mechanisms that can generate different morphologies. In particular, we are interested in the roles of mechanical feedback on cell behaviours for the morphogenesis of closed epithelial monolayers.

BP 21.4 Tue 15:10 BPa

Load distribution among the main structures of a passively flexed lumbar spine — •Julia M. Riede[1], Falk Mörl[2], Michael Günther[1], Maria Hammer[1], and Syn Schmitt[1] — [1]Computational Biophysics&Biorobotics, IMSB/Simtech, University of Stuttgart, Germany — [2]Biomechanics&Ergonomics, FSA mbH Erfurt, Germany

Mechanical loads may induce degeneration of spinal structures. It is still unknown how the load during spine motion is distributed among the spine's main structures: muscles, vertebrae and facet joints, ligaments, and intervertebral discs. Currently, there are no measurements that capture the load on all spinal structures at once. Therefore, computer simulations are the method of choice to overcome the lack of knowledge about the biophysical properties and processes determining spinal in vivo dynamics.

For predicting the load distribution of spinal structures, we combined experimental and simulation methods. In experiments, we determined the overall stiffness for forward-flexing rotations between the lumbar vertebrae L5 and L4 of subjects lying in sideways position and being bent by a machine, without active muscle resistance. Forward dynamics simulations of this experiment using our detailed musculo-skeletal multibody model of the human allowed for a structural resolution of the loads in the L4|5 region. The results indicated that stiffness values of particularly ligaments and passive muscle tissue put in from literature resources were too high. With now corrected values, our model has gained validity for future investigations on human movement dynamics and modelling applications like e.g. exoskeletons.

30 min. Meet the Speaker

BP 22: Focus Phase Separation in Biological Systems II (joint session BP/CPP)

Time: Tuesday 14:00–16:00 Location: BPb

BP 22.1 Tue 14:00 BPb

Phase separation provides a mechanism to reduce noise in cells — •Florian Oltsch[1,2], Adam Klosin[1], Tyler Harmon[1,3], Alf Honigmann[1,4], Frank Jülicher[2,3,4], Anthony Hyman[1,2,4], and Christoph Zechner[1,2,4] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — [2]Center for Systems Biology Dresden, 01307 Dresden, Germany — [3]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Cluster of Excellence Physics of Life, TU Dresden, 01062 Dresden, Germany

Noise in gene expression can cause significant variability in protein concentration. How cells buffer variation in protein concentration is an important question in biology. In this talk, I will show that liquid-liquid phase separation provides an effective mechanism to reduce variability in protein concentration. First, I will introduce our theoretical framework that discusses phase separation in the presence of active protein production and turnover. This stochastic non-equilibrium model allows us to study how fluctuations in protein concentration are affected by phase separation. I will then present under which physical conditions noise buffering by phase separation can be effective. Subsequently, I will show experimental data to test our theoretical predictions.

BP 22.2 Tue 14:20 BPb

Parasitic Behavior in Competing Dissipative Reaction Cycles — •Patrick Schwarz[1], Sudarshana Laha[3,4], Jacqueline Janssen[3,4], Tabea Huss[1], Christoph A. Weber[3,4], and Job Boekhoven[1,2] — [1]Department of Chemistry, Technische Universitat München, Lichtenbergstrasse 4, 85748 Garching, Germany — [2]Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2a, 85748 Garching, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [4]Center for Systems Biology Dresden, CSBD, Dresden, Germany

Fuel-driven reaction cycles serve as model systems of the intricate reaction network of life. Rich and dynamic behavior is observed when such reaction cycles regulate phase separation or assembly. However, it remains unclear how the interplay between multiple reaction cycles affects their fate. To tackle this question, we created a library of precursor molecules that compete for a common fuel to transiently activate products. Generally, the competition for fuel means that a competitor decreases the success of the cycle. However, in cases where the transient competitor product can phase separate, this relation can be inverted. The presence of assemblies formed by such a competitor can increase the survival time of one product, analogous to how the presence of a host can increase the survival time of a parasite. Our study of such a parasitic behavior in multiple fuel-driven reaction cycles represents a lifelike trait, paving the way for bottom-up design of synthetic life.

BP 22.3 Tue 14:50 BPb

Surface condensation of a pioneer transcription factor on DNA — •Jose A. Morin[1,2], Sina Wittmann[1], Sandeep Choubey[1,3], Adam Klosin[1], Stefan Golfier[1,3], Anthony A. Hyman[1,5], Frank Julicher[3,4,5], and Stephan W. Grill[1,2,5] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany. — [2]Biotechnologisches Zentrum, Technische Universitat Dresden,Dresden, Germany. — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [4]Center for Systems Biology Dresden, Dresden, Germany. — [5]Cluster of Excellence Physics of Life, Technische Universitat Dresden, Dresden, Germany.

Transcription factors cluster into sub-micrometer sized condensates while initiating transcription of their target genes. How cells achieve liquid-like clusters of constrained size at specific locations on DNA is not known. Here we investigate the role of DNA in the nucleation of condensates, using the pioneer transcription factor KLF-4. We show that KLF-4 forms liquid-like condensates on the DNA surface at physiological concentrations, below the one required for Klf4 phase separation. Through a dialogue between theory and experiments, we demonstrate that condensation occurs via a switch-like transition from a thin adsorbed layer to a thick condensed layer on DNA that is well described as a prewetting transition on a heterogeneous substrate. This phenomenon is thus a form of surface condensation mediated by and limited to the DNA surface.

BP 22.4 Tue 15:10 BPb

Slowing down protein aggregation in liquid compartments — •Wojciech P. Lipiński[1], Brent Visser[1], Mireille Claessens[2], Mohammad A. A. Fakhree[2], Saskia Lindhoud[3], and Evan Spruijt[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — [2]Nanobiophysics, Faculty of Science and Technology, University of Twente, Enschede, the Netherlands — [3]Molecular Nanofabrication, Faculty of Science and Technology, University of Twente, Enschede, the Netherlands

With increasing life expectancy in modern societies, amyloid-related diseases

are becoming alarmingly common. Extensive work has been done to investigate the kinetics of amyloid formation and the structure of aggregates. Recently it has been suggested that protein aggregation can be influenced by the presence of membraneless organelles. Aggregation-prone proteins may be sequestered by liquid compartments, leading to significant changes in concentration and altered aggregation kinetics.

Here, we present a combined computational and experimental study of the fate of aggregation-prone proteins that are sequestered by liquid droplets. We investigated computationally the influence of varying parameters describing aggregation and transport processes and showed that aggregation process can be either accelerated or inhibited by the presence of liquid compartments. Motivated by these findings we have undertaken efforts to develop experimental systems exhibiting diversified influence of the phase-separated environment on the protein aggregation process.

30 min. Meet the Speaker

BP 23: Focus Biological Cells in Microfluidics II

Time: Tuesday 14:00–16:00 Location: BPc

BP 23.1 Tue 14:00 BPc

ROS induces intracellular acidosis associated with increased cell stiffening — •Yesaswini Komaragiri[1,3], Huy T Dau[1], Doreen Biedenweg[2], Ricardo H Pires[1,3], and Oliver Otto[1,3] — [1]Biomechanics, ZIK-HIKE, Universität Greifswald, Greifswald, Germany — [2]Universitätsmedizin Greifswald, Greifswald, Germany — [3]Deutsches Zentrum für Herz-Kreislauf-Forschung e.V., Standort Greifswald, Universitätsmedizin Greifswald, Greifswald, Germany

Reactive oxygen species (ROS) are associated with important alterations in cell physiology. The impact that superoxides and other ROS have on the cytoskeleton has been extensively documented; however, the mechanism by which they may affect cell mechanics remain to be understood. By varying concentrations of hydrogen peroxide, we exposed the human myeloid precursor cell line (HL60) to different levels of ROS. Using real-time fluorescence and deformability cytometry, we coupled the mechanical characterization of cells with a simultaneous fluorometric assessment of intracellular superoxide levels. Our work reveals a direct correlation between the elastic modulus of cells and levels of superoxide. We did not detect global changes in the F-actin and microtubule network but demonstrate that cell stiffening at elevated ROS levels is driven by intracellular acidosis.

BP 23.2 Tue 14:20 BPc

Lingering dynamics of microvascular blood flow — •Alexander Kihm[1], Stephan Quint[1], Matthias Laschke[2], Michael Menger[2], Lars Kaestner[1], Thomas John[1], and Christian Wagner[1] — [1]Department of Experimental Physics, Saarland University, Saarbruecken, Germany — [2]Institute for Clinical and Experimental Surgery, Saarland University, Homburg, Germany

The microvascular networks in the body of vertebrates consist of the smallest vessels, such as arterioles, venules, and capillaries. The flow of red blood cells (RBCs) through these networks ensures the gas exchange in, as well as the transport of nutrients towards the tissues. Any alterations in this blood flow may have severe implications on the health state. Since the vessels in these networks obey dimensions similar to the diameter of RBCs, dynamic effects on the cellular scale play a key role. The steady progression in numerical modeling of RBCs even in complex networks has led to novel findings in the field of hemodynamics, especially concerning the impact and the dynamics of lingering events. However, these results are yet unmatched by a detailed analysis of the lingering in experiments in vivo. To quantify this lingering effect in in vivo experiments, we analyze branching vessels in the microvasculature of Syrian hamsters via intravital microscopy and the use of an implanted dorsal skinfold chamber. We present a detailed analysis of these lingering effects of cells at the apex of bifurcating vessels, affecting the temporal distribution of cell-free areas in the branches and even causing a partial blockage in severe cases.

BP 23.3 Tue 14:40 BPc

Phenotyping photokinetic and excitable behaviours of single microswimmers in confinement — Samuel Bentley, Vasileios Anagnostidis, Hannah Laeverenz-Schlogelhofer, Fabrice Gielen, and •Kirsty Y. Wan — Living Systems Institute, Exeter, United Kingdom, EX4 4QD

All living organisms are environmentally intelligent. This is the fundamental distinction between life, and other forms of matter. Even unicellular organisms are capable of complex behaviours. Here, we study the detailed motor actions of flagellated algal microswimmers, using motility as a dynamic read-out of whole-organism behaviour. Previous studies have focussed on locomotor transients over short timescales ranging from seconds to minutes. Here we present a novel microfluidic platform which can allow us to monitor single cells over unprecedented timescales. Two representative species of microswimmers were trapped and confined inside circular arenas: a biflagellate which exhibits a form of run-and-tumble, and an octoflagellate which exhibits a distinctive, tripartite behavioural repertoire termed run-stop-shock. Stochastic transitions in swimming gait are projected onto a low-dimensional behavioural state space. Single-cell motility signatures were analysed to reveal species-specific photokinetic and excitable behaviours. Finally, we conduct on-demand pharmacological perturbations within these microenvironments, to shed new light on the physiological basis of excitable flagellar dynamics.

Invited Talk BP 23.4 Tue 15:00 BPc

Synthetic cells: De novo assembly with microfluidics and DNA nanotechnology — •Kerstin Göpfrich — Max Planck Institute for Medical Research, Jahnstr. 29, 69120 Heidelberg, Germany

The future of manufacturing entails the construction of biological systems and synthetic cells from the bottom up. Instead of relying exclusively on biological building blocks, the integration of new tools and new materials may be a shortcut towards the assembly of active and eventually fully functional synthetic cells [Göpfrich *et al., Trends Biotechnol.*, 2018]. This is especially apparent when considering recent advances in DNA nanotechnology and microfluidics. Exemplifying this approach, we use microfluidics for the assembly of synthetic cellular compartments that we equip with natural or synthetic cytoskeletons. Light serves as a non-invasive stimulus to trigger their symmetry-breaking contraction [Jahnke *et al., Adv. Biosys.*, 2020; *Adv. Funct. Mater.*, 2019]. We further demonstrate the division of giant unilamellar lipid vesicles (GUVs) as synthetic cell models based on phase separation and osmosis rather than the biological building blocks of a cell's division machinery. We derive a parameter-free analytical model which makes quantitative predictions that we verify experimentally [Dreher *et al., Angew. Chem.*, 2020]. Remarkably, we show that caged compounds provide full spatio-temporal control to increase the osmolarity locally in an illuminated area, such that a target-GUV undergoes division whereas the surrounding GUVs remain unaffected. All in all, we believe that precision technologies, like microfluidics, can help to accelerate synthetic biology research.

30 min. Meet the Speaker

BP 24: Poster B: Active Biological Matter, Cell Mechanics, Systems Biology, Computational Biophysics, etc.

Time: Tuesday 16:00–18:30 Location: BPp

BP 24.1 Tue 16:00 BPp

Chirality-induced rheotaxis of bacteria in bulk shear flows — •Guangyin Jing[1,2], Andreas Zöttl[2,3], Eric Clement[2], and Anke Lindner[2] — [1]Northwest University, Xian, China — [2]ESPCI Paris, France — [3]TU Wien, Austria

The interaction of swimming bacteria with shear flows controls their ability to explore complex environments [1], crucial to many societal and environmental challenges and relevant for microfluidic applications such as cell sorting. We combine experimental, numerical, and theoretical analysis, and present a comprehensive study of the transport of motile bacteria in shear flows [2]. Experimentally, we obtain with high accuracy and, for a large range of flow rates, the spatially resolved velocity and orientation distributions of run-and-tumble E. coli bacteria. They are in excellent agreement with the simulations of a kinematic model accounting for stochastic and microhydrodynamic properties and,

in particular, the flagella chirality. Theoretical analysis reveals the scaling laws behind the average rheotactic velocity at moderate shear rates using a chirality parameter and explains the reorientation dynamics leading to saturation at large shear rates from the marginal stability of a fixed point. Our findings constitute a full understanding of the physical mechanisms and relevant parameters of bacteria bulk rheotaxis.

[1] A. J. T. M. Mathijssen, N. Figueroa-Morales, G. Junot, E. Clément, A. Lindner, and A. Zöttl, Nat. Comm. 10, 3434 (2019).

[2] G. Jing, A. Zöttl, E. Clement, and A. Lindner, Sci. Adv. 6, eabb2012 (2020).

BP 24.2 Tue 16:00 BPp

Resistive force theory and wave dynamics in swimming flagellar apparatus isolated from C. reinhardtii — Samira Goli Pozveh[1], Albert Bae[2], and •Azam Gholami[1] — [1]MPI for Dynamics and Self-organization, Göttingen, Germany — [2]Department of Biomedical Engineering, University of Rochester, USA

Cilia-driven motility and fluid transport is ubiquitous in nature and essential for many biological processes. The biflagellated micro-swimmer Chlamydomonas reinhardtii is a model organism to study dynamics of flagellar synchronization. Hydrodynamic interactions, intracellular mechanical coupling or cell body rocking are believed to play crucial role in synchronization of flagellar beating in green algae. Here, we use freely swimming intact flagellar apparatus isolated from wall-less strain of Chlamydomonas to investigate wave dynamics. Our analysis in phase coordinates show that, when the frequency difference between the flagella is high (10-41% of the mean), neither mechanical coupling via basal body nor hydrodynamics interactions are strong enough to synchronize two flagella, indicating that beating frequency is perhaps controlled internally by the cell. We also examined the validity of resistive force theory for a flagellar apparatus swimming freely in the vicinity of a substrate and found a quantitative agreement between experimental data and simulations with drag anisotropy of ratio 2. Finally, using a simplified wave form, we show that by controlling phase or frequency differences between two flagella, steering can occur.

BP 24.3 Tue 16:00 BPp

Magnetic stirbars as a tunable stirrer for cell-like systems — •Mithun Thampi, Pierre-Yves Gires, and Matthias Weiss — University of Bayreuth, Bayreuth, Germany

Transport inside living systems or biofluid droplets is governed by diffusion and energy-dependent active transport. Speeding up these processes remains challenging: here we report on an easy way to gently stir biofluid droplets. We produce micrometer long magnetic stirbars (MSBs) by aligning Fe_3O_4 nanoparticles and stabilizing them by a biocompatible silica coating. The successful production of these MSBs is confirmed by scanning electron microscopy[1]. The rotating magnetic field is achieved by using two pairs of Helmholtz-like coils with a custom build controller, which can tune both the frequency and the strength of the magnetic field. Using single-particle tracking of tracer beads, we demonstrate via a broad palette of measures that local stirring of the fluid at different frequencies leads to an enhanced but apparently normal and homogeneous diffusion process. The signature of stirring is visible in the power-spectral density and in the autocorrelation function of the trajectories[2]. We finally look at their stirring effects on the out of equilibrium self-organization of *Xenopus laevis* egg extract[1].

References:

1. P.-Y. Gires, M. Thampi, M. Weiss. "Miniaturized magnetic stirbars for controlled agitation of aqueous microdroplet". Sci. Rep., 10, 10911, (2020).

2. P.-Y. Gires, M. Thampi, M. Weiss. "Quantifying active diffusion in an agitated fluid". Phys. Chem. Chem. Phys., 22, 21678, (2020).

BP 24.4 Tue 16:00 BPp

RNA polymerase II forms clusters in line with liquid-phase wetting of chromatin — Agnieszka Pancholi[1], Tim Klingberg[2], Weichun Zhang[1], Roshan Prizak[1], Irina Mamontova[1], Amra Noa[1], Gerd Ulrich Nienhaus[1], Vasily Zaburdaev[2], and •Lennart Hilbert[1] — [1]Karlsruhe Institute of Technology — [2]Friedrich-Alexander-University Erlangen-Nuremberg

Two major control points for transcription in eukaryotic cells are recruitment of RNA polymerase II (Pol II) into a paused state and subsequent pause release to begin transcript elongation. Pol II associates with macromolecular clusters during recruitment, but it remains unclear how Pol II recruitment and pause release might affect these clusters. Here, we show that clusters exhibit morphologies that are in line with wetting of chromatin by a liquid phase enriched in recruited Pol II. Applying super-resolution microscopy to zebrafish embryos, we find recruited Pol II associated with large clusters, and elongating Pol II with dispersed clusters. A lattice kinetic Monte Carlo model representing recruited Pol II as a liquid phase and chromatin as a condensation surface reproduced the observed cluster morphologies, see Klingberg et al. Considering previous *in vitro* observations of condensate formation by wetting of DNA, our work indicates that similar liquid-phase wetting of chromatin might occur *in vivo*.

BP 24.5 Tue 16:00 BPp

Hydrodynamic interactions between microswimmers and particles in viscosity gradients — •Sebastian Ziegler[1], Maxime Hubert[1], Thomas Scheel[2], Jens Harting[2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Friedrich-Alexander-University Erlangen-Nürnberg, Germany — [2]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany — [3]Division of Physical Chemistry, Ruder Bošković Institute Zagreb, Croatia

A common theoretical approach to model systems of microswimmers is to prescribe the swimming stroke of each individual. If the system consists of more than one device, the problem of hydrodynamic interactions becomes a purely geometric one. This limitation is overcome by prescribing the forcing instead of the stroke, as shown by our novel perturbative approach, applicable to arbitrary geometries. We elaborate the effects of nearby swimmers on the stroke, swimming speed and direction. We find that for two swimmers, a significant fraction of the parameter space results in both swimmers experiencing a boost from one another.

We furthermore study the interaction of spherical particles in fluids with viscosity gradients. Using an analytical approach we show that a particle in a linear viscosity gradient induces a locally distance-independent flow field. Moreover, we characterize the effect of asymmetric particle placement in the finite-size gradient. Finally, we study the interactions between two particles that are at different temperatures than the surrounding fluid, and calculate the first order correction to the mobility matrix in the regime of low Peclet numbers.

BP 24.6 Tue 16:00 BPp

Motion of Magnetic Microswimmers in Complex Environments — •Konrad Marx[1], Vitali Telezki[1], Omar Muñoz[1], Agnese Codutti[2], Damien Faivre[2,3], and Stefan Klumpp[1,2] — [1]Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [3]Aix Marseille Université, CNRS, CEA, BIAM, Saint Paul lez Durance, France

We study magnetic microswimmers that tend to align their active motion with the direction of a magnetic field. A biological example are magnetotactic bacteria, which use this effect to navigate towards favorable oxygen conditions. Their natural environment is sediment at the bottom of lakes. Motivated by this, we study a computational model for how magnetic microswimmers attempt to cross a channel of circular obstacles. Our model accounts for diffusion, interaction with the obstacles and the walls, and for a magnetic field acting along the channel. We generate obstacle configurations from experimental data on size distribution of sand grains. We find that obstacles can play a decisive role for the trajectories of the microswimmers and their chance to cross the channel. Specifically, we identify regions that necessitate backwards swimming ("traps") as a dominant factor and investigate which geometrical parameters of the obstacle configurations determine the arrival rates of the swimmers at the end of the channel.

BP 24.7 Tue 16:00 BPp

Capillary Action In Active Brownian Particles — •Shauri Chakraborty, Adam Wysocki, and Heiko Rieger — Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbruecken 66123, Germany

We study the rise of active Brownian particles against gravity in a thin capillary tube. Capillarity, a well-understood phenomena in classical liquids, is known to originate due to attractive interactions between the liquid molecules and the capillary walls and the inter-molecular attractive forces among the liquid molecules. By contrast, we observe capillary rise in a minimal model of active Brownian particles with purely repulsive interactions. In such a system, an effective force of attraction emerges because of a damping due to the inter-particle collisions and the particle-wall interactions. We also validate in our numerical simulations, whether our findings agree with the results obtained for a similar system, previously studied in an active lattice gas (ALG) setting which can be described by exact hydrodynamic equations on macroscopic scales.

BP 24.8 Tue 16:00 BPp

Light-powered reactivation of flagella and contraction of microtubules network: towards building an artificial cell — Raheel Ahmad, Vahid Nasirimarekhani, Albert Bae, Samira Goli, Yu-Jung Su, Eberhard Bodenschatz, Isabella Guido, and •Azam Gholami — MPI for Dynamics and Self-organization, Göttingen, Germany

The bottom-up assembly of such systems in the context of synthetic biology is still a challenging task. In this paper, we demonstrate biocompatibility and efficiency of an artificial light-driven energy module and a motility functional unit by integration of light-switchable photosynthetic vesicles with demembranated flagella, thereby supplying ATP for dynein molecular motors upon illumination. Flagellar propulsion is coupled to its beating frequency and light- driven dynamic synthesis of ATP allows us to control beating frequency of flagella as a function of illumination. Additionally, we verified the functionality of light-powered synthetic vesicles in in vitro motility assays by encapsulation of microtubules assembled with force-generating kinesin-1 motors and energy module to investigate dynamics of a contractile filamentous network in cell-like compartments by optical stimulation. Integration of this photosynthetic system with

different biological building blocks such as cytoskeletal filaments and molecular motors may contribute to the bottom-up synthesis of artificial cells that are able to undergo motor-driven morphological deformations and exhibit directional motion in a light-controllable fashion. *In collaboration with C. Kleineberg, K. Sundmacher, and T. Vidakovich-Koch from MPI-Magdeburg.

BP 24.9 Tue 16:00 BPp

Mechanochemical dynamics of spherical active surfaces subject to load-dependent cross-linkers — •Mirco Bonati[1,2], Lucas Wittwer[3], Elisabeth Fischer-Friedrich[1,2], and Sebastian Aland[4] — [1]Fischer-Friedrich Lab, Biotechnologisches Zentrum, Technische Universitat Dresden, Dresden, Germany. — [2]DFG Excellence Cluster Physics of Life — [3]HTW Dresden, Friedrich-List-Platz 1, 01069 Dresden, Germany — [4]TU Bergakademie Freiberg, Akademiestrasse 6, 09599 Freiberg, Germany

Mechanochemical dynamics of active surfaces, as the thin cellular actin cortex, play a crucial role in several biological processes such as cell shape regulation and morphogenesis. Relying on a hydrodynamic theory of curved active surfaces and elastic thin shell theory, we aim to study both theoretical and numerical aspects of the self-organized pattern formation of the cell cortex. Our goal is to develop a mathematical model that takes into accounts biologically relevant facts, such as load-dependence of molecular unbinding and cortical strain stiffening. In particular, we want to study the influence of catch and slip bond cross-linkers on active gel pattern formation as it has been shown that the mechanical stiffness of the actin cytoskeleton can vary greatly with small changes in cross-linkers concentration. This force-sensing may give rise to new aspects of pattern formation.

BP 24.10 Tue 16:00 BPp

Simulations of Structure Formation by Dipolar Active Particles — •Vitali Telezki and Stefan Klumpp — Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Dipolar swimmers describe a class of artificial and biological active particles with an internal magnetic moment. Because of the interplay between different physical interactions such as steric, hydrodynamic and magnetic interactions, complex collective behaviour is expected to emerge in dense systems of dipolar swimmers.

We use Brownian dynamics simulations to investigate the collective behaviour of these dipolar swimmers. We focus on the structure formation of dipolar swimmers in small confined systems and analyze what structures can emerge and how they depend on the self-propulsion speed and the magnetic strength of the swimmers. We are particularly interested in the effect of the geometry and the interactions with the confinement on the emerging structures. In addition, we study how external magnetic fields influence the collective behaviour of large systems of dipolar swimmers.

BP 24.11 Tue 16:00 BPp

Minimum Dissipation Theorem for Microswimmers — •Babak Nasouri[1], Andrej Vilfan[1,2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, Germany — [2]J. Stefan Institute, Ljubljana, Slovenia — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom

We derive a theorem for the lower bound on the energy dissipation rate by a rigid surface-driven active microswimmer of arbitrary shape in a fluid at a low Reynolds number. We show that, for any swimmer, the minimum dissipation at a given velocity can be expressed in terms of the resistance tensors of two passive bodies of the same shape with a no-slip and perfect-slip boundary. To achieve the absolute minimum dissipation, the optimal swimmer needs a surface velocity profile that corresponds to the flow around the perfect-slip body, and a propulsive force density that corresponds to the no-slip body. Using this theorem, we propose an alternative definition of the energetic efficiency of microswimmers that, unlike the commonly used Lighthill efficiency, can never exceed unity. We validate the theory by calculating the efficiency limits of spheroidal swimmers.

BP 24.12 Tue 16:00 BPp

Vimentin Intermediate Filaments Stabilize Dynamic Microtubules by Direct Interactions — •Charlotta Lorenz[1,4], Laura Schaedel[1,4], Anna V. Schepers[1,3], Stefan Klumpp[2,3], and Sarah Köster[1,3] — [1]Institute for X-Ray Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Max Planck School "Matter to Life" — [4]Equal contribution.

Many cellular functions such as cell shape, mechanics and intracellular transport rely on the organization and interaction of actin filaments, microtubules (MTs) and intermediate filaments (IFs), which are the main constituents of the eukaryotic cytoskeleton. Here, we study the interaction between vimentin IFs and MTs in a minimal in vitro system and show that MTs are stabilized against depolymerization by the presence of vimentin IFs. To explore the nature of this interaction and in particular probe for electrostatic and hydrophobic contributions, we directly measure attractive forces occurring between individual MTs and vimentin IFs using optical tweezers in different buffer conditions. Theoretical modeling enables us to determine the corresponding energy landscape. Feeding back the physical parameters describing the interactions into a Monte Carlo simulation that mimicks dynamic MTs confirms that the additional interaction with IFs stabilizes them. We suggest that within cells, the interactions we observe might be a mechanism for cells to fine-tune cytoskeletal crosstalk and MT stability.

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BP 24.13 Tue 16:00 BPp

Post-Translational Modifications Soften Vimentin Filaments — •Julia Kraxner, Charlotta Lorenz, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

The mechanical properties of biological cells greatly influence their function, such as the ability to move, contract and divide and they need to flexibly adapt, for example during wound healing or cancer metastasis. These mechanical properties are determined by the so-called cytoskeleton, a complex network consisting of three filamentous protein systems, microtubules, actin filaments and intermediate filaments (IFs). A rather slow way to adapt cell mechanics to varying requirements on the cell is differential expression of the cytoskeleton proteins which affects the network architecture and the interaction between the filaments. Here, we focus on the intermediate filament vimentin and introduce post-translational modifications (PTMs), i.e. changes applied to specific amino acids in the protein after expression in the cell. By such PTMs, e.g. the charge pattern along the protein may be altered. Interestingly, PTMs occur comparatively fast and thus provide a mechanism for mechanical modulation on short time scales. We study the impact of one such PTM, phosphorylation, which is the addition of a phosphate group to an amino acid, on filament mechanics by stretching single filaments using optical traps. Whereas full phosphorylation leads to disassembly of IFs, partial phosphorylation results in softening of the filaments. By employing mutants that mimic phosphorylation as well as Monte Carlo simulations, we explain our observation through the additional charges introduced during phosphorylation.

BP 24.14 Tue 16:00 BPp

Growing with vacancies: Eden growth models suggest that flat clathrin lattices assemble with spatial heterogeneity — •Felix Frey[1,2], Delia Bucher[3], Kem A. Sochacki[4], Justin W. Taraska[4], Steeve Boulant[3], and Ulrich S. Schwarz[1] — [1]ITP and BioQuant, Heidelberg University, DE — [2]Department of Bionanoscience, TU Delft, NL — [3]CIID, University Hospital Heidelberg and DKFZ, DE — [4]NHLBI, NIH, Bethesda, US

Biological cells constantly transport material across their plasma membrane and clathrin-mediated endocytosis is one of the main uptake mechanisms. Recently, it has been shown that clathrin lattices first assemble flat before the clathrin-coated membrane starts to invaginate [1]. However, how this flat-to-curved transition proceeds in detail is still unclear, since energetic and topological barriers exist and it is difficult to observe the assembly process in time and space. Here we hypothesize that clathrin lattices grow with lattice vacancies that would facilitate the flat-to-curved transition. We identify the Eden growth model as the most suitable framework for clathrin lattice growth. We then derive four distinct variants of the model that represent the different binding modes of clathrin triskelia based on their geometry. Our computer simulations show that the different model variants lead to distinct lattice shapes and densities. Comparison with experimental electron microscopy and correlative light microscopy data suggests that clathrin lattices grow with a moderate level of lattice vacancies [2]. [1] D. Bucher*, F. Frey*, et al., Nat. Communs. 9, 1109 (2018). [2] F. Frey et al., New J. of Phys. 22, 073043 (2020).

BP 24.15 Tue 16:00 BPp

Dynamic RT-DC: red blood cell viscoelasticity as a label-free biomarker — •Bob Fregin[1,3], Fabian Czerwinski[1], Konstanze Aurich[2], Doreen Biedenweg[2], Stefan Gross[3], Gerald Kerth[4], and Oliver Otto[1,3] — [1]ZIK HIKE, Universität Greifswald, Greifswald, Germany — [2]Universitätsklinikum Greifswald, Greifswald, Germany — [3]DZHK, Universität Greifswald, Greifswald, Germany — [4]Angewandte Zoologie und Naturschutz, Universität Greifswald, Greifswald, Germany

Real-Time Deformability Cytometry (RT-DC) is a label-free technique for single-cell mechanical analysis with high throughput of up to 1,000 cells/s. Initially, RT-DC was limited to steady-state deformation captured at the end of a microfluidic channel yielding Young's modulus.

Dynamic RT-DC (dRT-DC) introduces the possibility to capture full viscoelastic properties at up to 100 cells/s. Single-cell shape-changes along the entire length of the microfluidic channel are tracked in real-time and are subsequently analyzed by a Fourier decomposition discriminating cell responses to interfering stress distributions. We demonstrate that dRT-DC allows for cell mechanical assays at the millisecond time scale fully independent of cell shape. We use this approach for a fundamental comparison of peripheral blood cells based on their Young's modulus as well as viscosity.

In proof-of-principle experiments, we use dRT-DC to approach the question of temperature control in hibernating animals. Initial experiments on bats and humans suggest a role of red blood cell viscoelasticity to maintain blood flow at low temperatures.

BP 24.16 Tue 16:00 BPp

3D direct and inverse traction force microscopy — •Johannes Wolfram Blumberg and Ulrich Sebastian Schwarz — Institute for Theoretical Physics and BioQuant, Heidelberg University

In traction force microscopy (TFM), the mechanical forces of cells adhering to an elastic substrate are estimated from the substrate displacements as measured by the movement of embedded fiducial marker beads. Usually, this estimate is obtained by minimizing the mean squared distance between experimentally observed and predicted displacements (inverse TFM). In direct TFM, in contrast, the stress tensor and the surface tractions are calculated directly and locally from the deformation field using the underlying material law. This procedure makes it easier to estimate not only tangential, but also normal forces, and to deal with non-planar substrates, but it is also more sensitive to noise. In general, it is not clear how well direct TFM performs compared with inverse TFM. We have compared the direct method for TFM to the standard inverse method, which is Fourier transformed traction cytometry (FTTC). In particular, we developed a method to estimating the local inaccuracy based on the divergence-freeness of the stress tensor. We discuss the relative strengths and weakness of the two methods and find that each of them can be preferable for certain settings.

BP 24.17 Tue 16:00 BPp

Time-resolved MIET measurements of blood platelet spreading and adhesion — •Anna Zelená and Sarah Köster — Institute for X-Ray Physics, Georg-August-University Göttingen, Germany

Human blood platelets are non-nucleated fragments of larger cells (*megakaryocytes*) and highly important for blood clotting. The hemostatic function of platelets is directly linked to their mechanics and cytoskeletal morphology. However, the exact mechanism of spreading and contraction remains elusive. In our study, we employ metal-induced energy transfer (MIET) imaging in time-resolved and static modes to investigate, in vitro, single blood platelets with nanometer resolution. Using static MIET, we are able to quantitatively determine three-dimensional height profiles of the basal platelet membrane above a rigid metal substrate. We observe areas, where the basal platelet membrane approaches the rigid metal substrate more closely than the rest of the membrane. This may be related to previously observed "hot spots" of high traction forces. Time-resolved MIET experiments allow us to follow the temporal evolution of the membrane-to-surface distance during adhesion and spreading. Our experiments reveal distinct behaviors between the outermost rim and the central part of the platelets. Overall, the combination of static and time-resolved MIET provides insights into the platelet adhesion system and improves our understanding of blood clot formation. Additionally, our approach demonstrates the potential of MIET as a three-dimensional reconstruction method for thin membrane formations.

BP 24.18 Tue 16:00 BPp

EMT-induced cell-mechanical changes enhance mitotic rounding strength — •Kamran Hosseini[1,2], Anna Taubenberger[2], Carsten Werner[3], and Elisabeth Fischer-Friedrich[1,2] — [1]Cluster of Excellence Physics of Life, TU Dresden, Germany — [2]Biotechnology Center, TU Dresden, Germany — [3]Leibniz Institute of Polymer Research Dresden, Max Bergmann Center, Dresden, Germany

To undergo mitosis successfully, most animal cells need to acquire a round shape to provide space for the mitotic spindle. This mitotic rounding relies on mechanical deformation of surrounding tissue and is driven by forces emanating from actomyosin contractility. Cancer cells are able to maintain successful mitosis in mechanically challenging environments such as the increasingly crowded environment of a growing tumor, thus, suggesting an enhanced ability of mitotic rounding in cancer. Here, it is shown that the epithelial-mesenchymal transition (EMT), a hallmark of cancer progression and metastasis, gives rise to cell-mechanical changes in breast epithelial cells. These changes are opposite in interphase and mitosis and correspond to an enhanced mitotic rounding strength. Furthermore, it is shown that cell-mechanical changes correlate with a strong EMT-induced change in the activity of Rho GTPases RhoA and Rac1. Accordingly, it is found that Rac1 inhibition rescues the EMT-induced cortex-mechanical phenotype. The findings hint at a new role of EMT in successful mitotic rounding and division in mechanically confined environments such as a growing tumor.

BP 24.19 Tue 16:00 BPp

Measurement of the mechanosensitive binding of actin crosslinkers in the cytoskeleton of live cells — •Valentin Ruffine, Kamran Hosseini, and Elisabeth Fischer-Friedrich — DFG Cluster of Excellence Physics of Life, BIOTEC, Technische Universität Dresden, Germany

In mammalian cells, actin filaments (F-actin) are bundled and crosslinked by multiple actin-binding proteins. The cytoskeletal structures they form are essential for cell motility, division, mechanosensitivity, intracellular transport and the mechanical protection of the cell. They have a highly nonlinear rheological behavior, which is tuned through their microscopic structure and their composition: the length of the microfilaments, the concentration of filaments and crosslinkers, and the nature of the crosslinkers.

Actin-binding proteins mostly form transient bonds with the filaments. This enable both a protective solid-like response on short timescales and large reorganization of the biopolymer network on longer ones. The average lifetime of these bonds typically depends on the mechanical load applied to them, thus on the mechanical stress in the actin network. Interestingly, this lifetime increases with increasing load for some actin crosslinkers. This behavior is termed "catch-bond" and is far less intuitive than the opposite, "slip-bond" behavior. Here, we report experimental results showing a catch-bond behavior for three major human actin crosslinkers: α-actinin 4, filamin A and filamin B. These were obtained in mitotic HeLa cells, using AFM-based cortical tension measurements coupled with FRAP and confocal imaging.

BP 24.20 Tue 16:00 BPp

Simulating Cells Going Through Constrictions - A Cellular Potts Model Approach — •Miriam Schnitzerlein[1,3], Felix Reichel[2,3], Martin Kräter[2,3], Hui-Shun Kuan[1,3], Jochen Guck[2,3], and Vasily Zaburdaev[1,3] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Biological Optomechanics, Max-Planck Institute for the Science of Light, Erlangen, Germany — [3]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

In the human body, many cells types regularly have to struggle through confinements. For example in the blood system where not only blood cells but also cancer cells may encounter capillaries with cross-sections below the cell size. One in vitro experiments to mimic and study such processes is using microfluidic techniques, where living cells suspended in an aqueous solution could be forced through a channel with recurring constrictions. By analyzing cell deformation and passage times we can learn about their mechanical properties. Ultimately linking the characteristics of the passage to cell mechanics requires a simple and tractable model. Here we suggest using a well known Cellular Potts Model (CPM), which represents cells as a set of adjacent spins on a lattice with cell dynamics arising from an energy minimization principle. The major challenge is to link phenomenological parameters of the model to experimental space and time scales and also to mechanical properties of living cells. Our first results demonstrate qualitative agreement with experimental observations and thus indicate the CPM as a promising tool to quantify cell passage through constrictions.

BP 24.21 Tue 16:00 BPp

Optimal hematocrit for ATP release by red blood cell in microcirculation — •Zhe Gou and Chaouqi Misbah — Laboratoire Interdisciplinaire de Physique, Grenoble, France

ATP release by red blood cells (RBCs) acts as an important signaling molecule for various physiological functions, such as vasodilation. When flowing in microcirculation, RBCs experience a cascade of branching vessels, from arterioles to capillaries, and finally to venules, which affects not just flow behavior of blood but also ATP release. In a previous study, we have proposed a model of ATP release by RBCs through two pathways of cell membrane: pannexin 1 channel (Px1), sensitive to shear stress, and cystic fibrosis transmembrane conductance regulator (CFTR) which responds to cell deformation. As a continuation, present work further investigates the effect of flow strength, hematocrit, and vascular diameter by numerical simulations. We found a nontrivial spatial RBC organization and ATP patterns due to application of shear stress on the RBC suspension. Conditions for optimal ATP release per cell are identified, which depend on vessel size and hematocrit Ht. Increasing further Ht beyond optimum enhances the total ATP release but should degrade oxygen transport capacity, a compromise between an efficient ATP release and minimal blood dissipation. Moreover, ATP is boosted in capillaries suggesting a vasomotor activity coordination throughout the resistance network. Further studies of vascular network may help to explore the whole signaling cascade of ATP.

BP 24.22 Tue 16:00 BPp

Influence of NaCl on Neuronal Membranes — •Sebastian Jaksch[1], Alexandros Koutsioubas[1], Piotr Zolnierczuk[1], Olaf Holderer[1], Henrich Frielinghaus[1], Stephan Förster[1], and Peter Müller-Buschbaum[2] — [1]Jülich Centre for Neutron Science (JCNS), Garching (Germany), Jülich (Germany) and Oak Ridge TN (USA) — [2]Lehrstuhl für funktionelle Materialien, Physik-Department, Technische Universität München (Germany)

We previously investigated the structure and the dynamic behavior of L-α-phosphatidylcholine (SoyPC) phospholipid membranes, [1,2] by means of GISANS and GINSES and established a multi-lamellar structure as well as a surface mode, attributed to transient waves in the membranes. Extending those measurements to include various NaCl concentrations within the membrane we could identify two main features:[3] (1) The thickening of the membrane layers as reported by SAXS measurements is due to an enriched ion layer close to the head group of the phospholipid membranes, and not, as for hydrophobic molecules an actual swelling of the membrane. (2) The in-plane dynamics of the membranes is enhanced by the addition of NaCl, while retaining the previously reported surface mode. Those features can play an important role in the under-

standing of membrane functions, such as the formation of ion channels, and thus their biological function on a fundamental level. [1] S. Jaksch, et al, Phys. Rev. E 91(2), 2015, 022716. [2] S. Jaksch, et al, Scientific Reports 7(1), 2017, 4417. [3] S. Jaksch, et al, Influence of NaCl on the structure and dynamics of phospholipid layers, submitted.

BP 24.23 Tue 16:00 BPp

Viscoelastic properties of Pancreatic cancer cells on Soft supports — •Shruti G Kulkarni[1,2], Malgorzata Lekka[2], and Manfred Radmacher[1] — [1]University of Bremen, Bremen, Germany — [2]Institute of Nuclear Physics, Krakow, Poland

Pancreatic ductal adenocarcinoma (PDAC) is one of the leading causes of cancer-related mortality, with less than 5% of patients having a 5-year survival rate. The dense extra-cellular matrix (ECM) prevents drug-delivery and its remarkably high stiffness may play a role in cancer initiation and progression. Invasive potential of pancreatic cancer cells has also been related to cellular stiffness. We tested the effect of substrate stiffness on stiffness of pancreatic cancer cells using atomic force microscopy. Force curves were measured on primary tumor cell lines (PANC1 and PL45) grown on collagen-coated polyacrylamide gels (PAG) of stiffness 2.8 kPa and 16.6 kPa and plastic petri dishes. PANC1 shape changes in gradient from well-spread to round as stiffness of the substrate decreases. Mechanical parameters like Young's (~1.4 kPa), storage and loss moduli remain the same, indicating that they display a loss of mechanosensitivity when cultured on PAG. PL45 is rounded on PAG but well-spread on plastic. Cells on the 2.8 kPa gel are 3.5 kPa stiff, while those on 16.6 kPa gel are only 2.2 kPa stiff. PL45 cells may have an increased potential to invade through soft ECMs, because their stiffness increases as the substrate's stiffness decreases. Further experimentation to study the connection between metastatic and invasive cell lines, and other biomimetic substrates, as well as the role of specific ECM proteins has been planned.

BP 24.24 Tue 16:00 BPp

Calcium Dynamics Model in Endothelial Cells — •Ananta Kumar Nayak[1], Zhe Gou[1], Sovan Lal Das[2], and Chaouqi Misbah[1] — [1]Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble 38000, France. — [2]Department of Mechanical Engineering, Indian Institute of Technology Palakkad, Palakkad 678557, India.

Calcium is a ubiquitous molecule and a second messenger that regulates many cellular functions ranging from the exocytosis to the proliferation of cell. Endothelial cells (ECs) form a inner lining of blood vessels and play an important role in transduction of extracellular environment information to the cytoplasm. A robust calcium dynamics model is required to understand these cellular functions occurring at (patho) physiological conditions in the ECs. In this work, we have developed a single cell minimal calcium dynamics model by including cytosol and endoplasmic reticulum (ER) calcium, Inp3 (Inositol Trisphosphate) kinetics, and the receptor dynamics. We find that the receptor desensitization due to phosphorylation and recycling of receptor play a vital role in maintaining the calcium homeostasis in the presence of a constant stimulus due to adenosine triphosphate (ATP). Apart from this, our model is able to capture other experimental facts like refilling of calcium in ER, which is dependent on the extracellular calcium concentration. Overall the model is able to account for the natural physiological recovery towards homeostasis of active components in the calcium generation cascade. Furthermore, in a future work, we plan to extend this model to include blood flow through the blood vessel to gain insights in the development of vascular diseases.

BP 24.25 Tue 16:00 BPp

Computational Modeling of Nuclear Blebs — •Silvia Bonfanti[1], Maria Chiara Lionetti[2], Maria Rita Fumagalli[3], Francesc Font-Clos[1], Stefano Zapperi[1,4], and Caterina A.M. La Porta[2,3] — [1]Center for Complexity and Biosystems Department of Physics, University of Milan, Milano, Italy — [2]Center for Complexity and Biosystems Department of Environmental Science and Policy, University of Milan, Milano, Italy — [3]CNR-Consiglio Nazionale delle Ricerche, Biophysics institute, Genova, Italy — [4]CNR-Consiglio Nazionale delle Ricerche, Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia, Milano, Italy

The morphology of the nucleus of eukaryotic cells is determined by the complex interactions among the nuclear lamina forming the nuclear scaffold, the internal chromatin filaments and the coupling with the external cytoskeleton. It is known that nuclear morphological alterations such as blebs are often associated with pathological conditions such as Hutchinson-Gilford progeria syndrome. Here, we investigate the role of mechanical factors in nuclear morphological alterations constructing a model of the cell nucleus, consisting of a flexible coarse-grained shell representing nuclear envelope and lamina endowed with stretching and bending rigidity, coupled to a set of coarse-grained polymers representing chromatin and also to a set of oscillating points modeling contractions of the cytoskeleton. We compare the simulations results with experimental results on a cellular model of progeria and shed light on the important role played by chromatin and nuclear tethering in determining nuclear morphology and fluctuations.

BP 24.26 Tue 16:00 BPp

Contractile activity inhibition of Dupuytren fibroblasts: AFM mechanical approach — •Sandra Pérez-Domínguez and Manfred Radmacher — Institute of Biophysics, University of Bremen, Bremen, Germany

Dupuytren's disease is a fibromatosis of the connective tissue of the palm that causes progressive and permanent contracture of the digits. The mechanical properties of healthy, scar and Dupuytren fibroblasts, all from the same patient, were investigated employing the AFM after inhibiting the myosin light chain kinase. For this purpose, ML-7 was used to block the actin-myosin activity, therefore, reducing inhibiting the cell contraction. The stiffness of Dupuytren fibroblasts was around 3 kPa before adding ML-7 and in almost all cases a decrease to 400 Pa was observed after ML-7 addition. 60% of Dupuytren cells did not recover; nevertheless, 30% of them showed a recovery over time. Scar fibroblasts have a Young's modulus of 2.5 kPa before adding ML-7 and showed a decrease to 300 Pa after adding ML-7 similar to what we observed with the Dupuytren fibroblasts. Most scar fibroblasts reacted to the inhibitor; however, some 20% did not show any response. Healthy fibroblasts showed - in preliminary experiments using a different AFM cantilever tip - a smaller response when ML-7 has been added, and some of the cells did not respond to the inhibitor considerably. This is actually conceivable since healthy fibroblasts shall have less cortical tensity, i.e. less myosin activity, and consequently applying a myosin inhibitor will result in less change.

BP 24.27 Tue 16:00 BPp

A matter of size: Understanding size-dependent organelle transport in cells — •Simon Wieland[1,2], David Gitschier[1], Marius M. Kaiser[1], Christina Steininger[1], Wolfgang Gross[1], Adam G. Hendricks[3], and Holger Kress[1] — [1]Biological Physics Group, University of Bayreuth, Bayreuth — [2]Animal Ecology I, University of Bayreuth, Bayreuth — [3]Department of Bioengineering, McGill University, Montreal

Intracellular transport of organelles is essential for numerous cellular processes, including phagocytosis. Earlier findings indicate that the persistence of organelle transport during phagocytosis strongly depends on cargo size. To understand this behavior on a molecular level, we systematically quantified the size-dependence of phagosomal transport forces using magnetic tweezers. We found that transport forces increase with organelle size. With a simple geometrical model taking the distribution of microtubules around the organelles into account, we explain the scaling behavior of the transport forces. Our findings indicate that intracellular organelles displace microtubules from their original positions, leading to an increased microtubule density at the organelles surface, and thus an increased number of binding possibilities for molecular motors. Additionally, we performed immunofluorescence experiments on isolated phagosomes, allowing us to identify and estimate the relative number of molecular motors on the organelles. Quantifying the size-dependence of phagosomal transport can lead to a deeper understanding of intracellular organelle transport and the dynamics of interactions between molecular motors and the cytoskeleton.

BP 24.28 Tue 16:00 BPp

Extracellular matrix mechanical prestress during morphogenesis of Drosophila wing discs — •Yanín Guerra[2], Elisabeth Fischer-Friederich[2], and Christian Dahmann[1] — [1]Institute of Genetics, Technische Universität Dresden, 01062 Dresden, Germany. — [2]Biotechnology Center of the TU Dresden (Biotec), Tatzberg 47/49, 01062 Dresden, Germany

The folding of tissues is the manner in which two dimensional sheets transform into three dimensional structures. There are many mechanisms involved in fold formation such as apical constriction, cell proliferation, collective migration and cell-ECM adhesion. For a long time it has been thought that the most important process is apical constriction, notwithstanding, how this mechanisms organise to construct healthy three dimensional structures remains as an open question.

A recent study on the mechanical processes involved during hinge fold formation of the Drosophila wing imaginal disc found that there is a decrease of basal tension in the central fold (H/H fold), but no apical constriction [1]. Moreover, they report that this fold exhibits a depletion of the extracellular matrix (ECM) suggesting that the dynamics of such structure drive fold formation. So, how does the interaction between the ECM and the actomyosin networks contributes to basal tension in the morphogenesis of the H/H fold in Drosophila wing disc?

The main goal of this research is to elucidate the role of ECM in the formation of H/H fold in Drosophila wing. To achieve this goal I will culture the wing imaginal discs ex vivo in order tomeasure its mechanical properties using atomic force microscopy.

BP 24.29 Tue 16:00 BPp

Profilin Regulating the Polymerisation Velocity of Actin — •Lina Heydenreich and Jan Kierfeld — TU Dortmund

F-Actin, as a part of the cytoskeleton, drives crucial biological processes like cell motility, where the control of the polymerisation speed is essential. Experiments in [1] show a maximal polymerisation speed of F-actin at high concentrations of profilin and actin.

We present a kinetic model of F-actin growth in the presence of profilin and obtain an exact result for the mean growth velocity which is in agreement with

stochastic simulations, and explains the experimental data. The maximal growth speed is limited by the release rate of profilin from filamentous actin. In the limit where nearly all actin monomers are bound to profilin, the polymerisation speed follows the Michaelis-Menten kinetics.

We analyse the influence of an external force on the polymerisation speed. The stall force for energetically balanced rates is identical to the stall force for F-Actin without profilin.

[1] Johanna Funk et al. "Profilin and formin constitute a pacemaker system for robust actin filament growth". eLife 8 (2019), e50963

BP 24.30 Tue 16:00 BPp

Tailored ensembles of neural networks optimize sensitivity to stimulus statistics — •Johannes Zierenberg[1,2], Jens Wilting[1], Viola Priesemann[1,2], and Anna Levina[3,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany — [2]Bernstein Center for Computational Neuroscience, Am Fassberg 17, 37077 Göttingen, Germany — [3]University of Tübingen, Max Planck Ring 8, 72076 Tübingen, Germany — [4]Max Planck Institute for Biological Cybernetics, Max Planck Ring 8, 72076 Tübingen, Germany

The capability of a living organism to process stimuli with nontrivial intensity distributions cannot be explained by the proficiency of a single neural network. Moreover, it is not sufficient to maximize the dynamic range of the neural response; it is also necessary to tune the response to the intervals of stimulus intensities that should be reliably discriminated. We derive a class of neural networks where these intervals can be tuned to the desired interval. This allows us to tailor ensembles of networks optimized for arbitrary stimulus intensity distributions. We discuss potential applications in machine learning.

BP 24.31 Tue 16:00 BPp

Timing cellular decisions using transient cues — •Felix Meigel[1], Lina Hellwig[2], Jörg Contzen[2], Philipp Mergenthaler[2], and Steffen Rulands[1,3] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]Neurology Department, Charité University Medicine Berlin — [3]Center for Systems Biology Dresden

The maintenance of intact tissues relies on precise cellular decision-making despite strongly fluctuating extrinsic cues. These decisions involve processes on vastly different scales, from molecules to organelles and cells in tissues. How can cells manipulate the propagation of fluctuations across these scales to perform biological function? Here, we show how the non-equilibrium interplay between microscopic and mesoscopic dynamics leads to a kinetic low-pass filter facilitating precise sensing of fluctuating cellular states. Specifically, we find that the interplay between molecular and organelle dynamics gives rise to a single, collective degree of freedom. We show that this degree of freedom exhibits rich dynamical behaviour showing different kinetics on different temporal scales and thereby leading to the suppression of fast fluctuations. We demonstrate our findings in the context of the metabolic regulation of cell death via the interplay of Bax protein dynamics with rapid mitochondrial fusion and fission and find an order of magnitude effect on the error rate of the cell death decision. Our work shows paradigmatically how biological function relies on the non-equilibrium integration of processes on different spatial scales to control and respond to fluctuations.

BP 24.32 Tue 16:00 BPp

Dynamic analysis of the SinR/SlrR/SinI genetic circuit for biofilm formation in Bacillus subtilis — •Simon Dannenberg, Jonas Penning, and Stefan Klumpp — Institut für Dynamik komplexer Systeme Georg-August-Universität Göttingen Friedrich-Hund-Platz 1 37077 Göttingen, Germany

Switching between different lifestyles in bacteria serves as a survival strategy under changing environmental conditions. It allows genetically identical cells to develop different phenotypic traits and creates diversity in a colony of cells. Such switches either occur stochastically due to fluctuations in gene expression or are the result of a deterministic process. In our work we investigate biofilm formation by mathematical analysis of the SinR/SlrR/SinI genetic circuit in Bacillus subtilis. Via a rate equation approach for the involved proteins, steady state solutions are found in which parameter regions for bistability exists. For those regions we conducted a stochastic analysis using a Gillespie algorithm, which shows that typical fluctuations are not sufficient to induce the transitions between these states. Instead, we propose a deterministic switching mechanism and analyzed its dynamic.

BP 24.33 Tue 16:00 BPp

Intermediate scattering function in multi-channel dynamics: from model systems to particle-tracking data in live cells — •Cai Dieball[1], Adal Sabri[2], Xinran Xu[3], Diego Krapf[3,4], Matthias Weiss[2], and Aljaz Godec[1] — [1]Mathematical bioPhysics Group, Max Planck Institute for Biophysical Chemistry, 37077 Göttingen, Germany — [2]Experimental Physics I, University of Bayreuth, 95440 Bayreuth, Germany — [3]Department of Electrical and Computer Engineering, Colorado State University, Fort Collins, Colorado 80523, USA — [4]School of Biomedical Engineering, Colorado State University, Fort Collins, Colorado 80523, USA

Several experimental techniques probe collective observables related to the intermediate scattering function, i.e. the expectation value of the Fourier-transformed displacement vectors of the system's particles. These techniques include neutron, X-ray and dynamic light scattering, neutron spin echo and Fourier imaging correlation spectroscopy, and differential dynamic microscopy. Intermediate scattering functions provide useful, complementary information even when applied to experiments that are able to track the motion of individual particles. In our work we analyze the intermediate scattering function in systems with "multi-channel" dynamics, i.e. dynamics stochastically switching between different modes of motion. We first inspect scattering fingerprints in simple model systems with two-channel dynamics. We then analyze trajectories from particle-tracking experiments in the cytoplasm of mammalian cells, and confirm that these display characteristics of anomalous, two-channel fractional Brownian motion.

BP 24.34 Tue 16:00 BPp

Nonlinear Allosteric Effect in Elastic Network Models of Proteins — •Maximilian Vossel and Aljaž Godec — Mathematical bioPhysics Group, Max Planck Institute for Biophysical Chemistry, 37077 Göttingen, Germany

Allostery is a ubiquitous phenomenon in proteins, where the binding of a ligand at one site induces perturbations at another, often spatially distant site. The large scale dynamics of biomolecules is often effectively described by coarse-grained elastic network models that encode the collective motion of proteins around their equilibrium structure. However, despite their conceptual simplicity the manner in which these network models respond to local structural perturbations, such as the binding of a ligand molecule, is highly non-trivial and in the context of allostery remains an unsolved problem. We develop a simple and efficient algorithm for determining the full, nonlinear response of such networks to arbitrary structural perturbations that mimic the binding of a ligand molecule in the limit of high stiffness (or low temperature). Applying the algorithm we find that the response often displays pronounced nonlinearities. This suggests that recent attempts to explain allostery in proteins based on linear response theory are not necessarily accurate and may not always be meaningful.

BP 24.35 Tue 16:00 BPp

Comparative analysis of metabolic and transcriptomic features of Nothobranchius furzeri — •Maria Rita Fumagalli[1,2,3], Francesc Font-Clos[1,4], Simone Milan[1], Stefano Zapperi[1,4,5], and Caterina A.M. La Porta[1,2,3] — [1]Center for Complexity and Biosystems, University of Milan — [2]Biophysics Institute, CNR, Genova — [3]Dep. of Environmental Science and Policy, University of Milan — [4]Dep. of Physics, University of Milan — [5]ICMATE, CNR, Milan

Nothobranchius furzeri is a killifish with an extremely rapid growth and short lifespan with respect to other vertebrates. Despite its short life, N. furzeri shows hallmarks typical of aging. We investigated the aging process of N. furzeri in comparison with other two well characterized animal models (Danio rerio and Mus Musculus) with a combination of computational analysis and modeling.

The analysis of gene expression changes during ageing suggests the presence of alterations in regulatory mechanisms happening early during N. furzeri lifetime. Coherently, N. furzeri shows a specific deregulation pattern of genes involved in chromatin remodeling as well as histone acetylation and deacetylation. Enzymes deregulation could affect metabolic reactions, but changes in terms of efficiency in the production/consumption of metabolites are not easy to address. To this end, we implemented a metabolic network model based on flux balance analysis applying it to the fundamental glycolysis pathway.

Overall, our analysis shows that N. furzeri ageing process is associated to very peculiar chromatin and metabolic dynamics.

BP 24.36 Tue 16:00 BPp

Dynamics of tethered polymers in a circular confinement — •Meng Wang[1,2], Tim Klingberg[1,2], Mauro Battipede[1,2], Vasily Zaburdaev[1,2], and Hui-Shun Kuan[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max-Planck-Zentrum für Physik und Medizin

During meiosis, the paternal and maternal chromosomes find each other to pair and exchange parts of their genetic material in the process of recombination, which is the major mechanism contributing to genetic diversity in sexually reproducing organisms. As the first steppingstone in understanding how physical mechanisms help chromosomes to align, we study the dynamics of chromosomes in the nucleus. In this poster, we consider meiotic DNA as a freely jointed chain confined in a circle with the ends of the chain being tethered and free to move along the circle. We use the kinetic Monte Carlo algorithms to simulate the stochastic motion of the polymer and compare the results to the Rouse model. Although the Rouse model successfully describes the simulation results, especially the transient subdiffusive regimes, the global motion of the polymer is very different due to the constraint of the circle. For small monomer numbers, the polymer can stretch to match the diameter of the circle, and the trajectory of its each end can wind around the circle. However, with fixed polymer length, for large monomer numbers, the chain tends to form a contracted coil, stochastically moving along the circle like a composite particle in the long-time limit.

BP 24.37 Tue 16:00 BPp

Dimensionality of neural circuit manifolds associated with a salt-and-pepper organization of cortical stimulus preferences — •Michael Sternbach[1,2,3] and Fred Wolf[1,2,3,4,5] — [1]Campus Institute for Dynamics of Biological Networks, Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization — [3]Bernstein Center for Computational Neuroscience Göttingen — [4]Institute for Dynamics of Complex Systems, Georg-August University Göttinge — [5]Max Planck Institute of Experimental Medicine

Biological neural circuits are expected to converge to one of many stable network configurations. For the form vision core circuit of primate/carnivore V1 prior work indicates that stable network configurations form toroid high-dimensional continua (Wolf 2005, Kaschube et al. 2010). Similar results for network configurations in rodents V1, called salt-and-pepper organizations (SaP), are currently not available. Here we utilize techniques from the study of spin liquid states (Chalker 2015) to construct mathematically tractable models with SaP optimal states. We demonstrate that these models can exhibit ground state manifolds with extensive dimensionality. This result is consistent with the general expectation that there are a very high number of equivalent SaP configurations. These studies expand the toolbox for analyzing the multiplicity of stable cortical circuit configurations. Our first results suggest that the evolutionary transition from a rodent ancestral circuit configurations of V1 to a primate/carnivore V1 architecture was accompanied by a reduction in cortical circuit state dimension.

BP 24.38 Tue 16:00 BPp

Trading bits in the readout from a genetic network — •Marianne Bauer[1], Mariela Petkova[2], Thomas Gregor[1,3], Eric Wieschaus[1], and William Bialek[1,4] — [1]Princeton University, Princeton, USA — [2]Harvard University, Boston, USA — [3]Institut Pasteur, Paris, France — [4]City University of New York, New York, USA

In genetic networks, information of relevance to the organism is represented by the concentrations of transcription factor molecules. In order to extract this information the cell must effectively "measure" these concentrations, but there are physical limits to the precision of these measurements. We explore this trading between bits of precision in measuring concentration and bits of relevant information that can be extracted, using the gap gene network in the early fly embryo as an example. We argue that cells in the embryo can extract all the available information about their position, but only if the concentration measurements approach the physical limits to information capacity. These limits necessitate the observed proliferation of enhancer elements with sensitivities to combinations of transcription factors, but fine tuning of the parameters of these multiple enhancers is not required.

BP 24.39 Tue 16:00 BPp

Coupling of growth, replication and division in E. coli — •Mareike Berger — AMOLF, Amsterdam, The Netherlands

Growth, DNA replication and division are key features of every living organism. The precise temporal control of these processes is essential for survival. We investigate how the model organism E. coli couples its replication to its division cycle under different growth conditions. According to the phenomenological general growth law, E. coli on average initiates replication at a constant volume per origin of replication and divides a constant time later. This simple mechanism allows E. coli to divide faster than it takes to replicate its DNA while maintaining cell size homeostasis. It is a longstanding open question how the general growth law is realized on a molecular level. We present a theoretical model that is based on experimentally observed molecular mechanisms and that can reproduce the phenomenological general growth law. This novel model allows us to make quantitative predictions on the regulation of replication in E. coli.

BP 24.40 Tue 16:00 BPp

DNA accumulates and concentrates in artificial hydrothermal chimneys mimicking prebiotic geophysical conditions — •Maximilian Weingart, Lea Gigou, Ömer Coskun, William Orsi, and Dieter Braun — LMU München, Munich, Germany

The so called concentration problem on early Earth represents one of the greatest challenges for molecular evolution forcing it to proceed from highly diluted prebiotically formed molecules in an extensive ocean. Origin of Life research is therefore inclined to think about potential locations that provide necessary geophysical conditions to overcome this hurdle.

Recently, Barge and Coworkers [1] showed the formation of oxyhydroxide minerals in alkaline hydrothremal vents suggesting that prebiotic chemical reactions could have happened in such a scenario. Additionally, diffusiophoresis driven by the ionic gradient across the mineral membrane could move dissolved DNA molecules towards the chimneys where the charged strands adsorb to the mineral surface. This could locally increase DNA concentration while prohibiting back diffusion into the ocean at the same time.

To test this hypothesis, herein we used an artificial hydrothermal vent mimic [1] by using crimp flasks and injecting hydrothermal fluid (pH 12) into the Fe(II) containing ocean simulant (pH 5.5) with dissolved DNA ladders. Preliminary results showed higher DNA concentration in the mineral sample after selective analysis of remaining ocean and chimney. [1] Barge et al. PNAS (2019) doi.org/10.1073/pnas.1812098116

BP 24.41 Tue 16:00 BPp

Phase separation in membranes due to matter exchange — •Nirvana Caballero[1], Karsten Kruse[2], and Thierry Giamarchi[1] — [1]Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva, Switzerland — [2]Department of Biochemistry, Department of Theoretical Physics and National Center of Competence in Research Chemical Biology, University of Geneva, CH-1211 Geneva, Switzerland

Heterogeneous lipid composition in cell membranes is key to biological function, acting as one of the main mechanisms to exchange information between cells or between a cell an its environment. The underlying mechanisms controlling pattern formation are still under debate. In this work, we consider a theoretical phase-field model to describe the composition of a two-dimensional membrane exchanging matter with a reservoir. The model includes matter absorption and desorption in the membrane with different rates. By only assuming matter conservation in the system membrane-reservoir, we show with extensive numerical simulations that, depending on these rates, a complex patterned composition distribution emerges in the membrane. The pattern emergence is due to spatio-temporal "memory" effects. Our results show that the causes of heterogeneous lipid composition may be justified in simple physical terms.

BP 24.42 Tue 16:00 BPp

DNA Replication:Accuracy and Speed of elongation — •Mamata Sahoo[1], Arsha Nousad[1], Priyaranjan Baral[2], and Stefan Klumpp[3] — [1]Department of Physics, University of Kerala, Kariavattom Campus-6955881, India — [2]Department of Physics, — [3]Institute for the Dynamics of Complex Systems, University of Gottingen, Gottingen, Germany

Being a dual purpose enzyme, the DNA polymerase is responsible for elongation of the newly formed DNA strand as well as cleaving the erroneous growth in case of a misincorporation. Though this is an efficient mechanism, sometimes DNAP with misincorporated nucleotide may escape to the next site as well as a correctly incorporated nucleotide causing a replication error may get cleaved unnecessarily from the exonuclease site. An error in 10^9 correct nucleotides incorporation has been observed experimentally. Here we propose a theory based kinetic model of DNA replication and find out the exact results for the velocity of elongation as well as the accuracy of replication. Surprisingly it is observed that the velocity of elongation with erroneous stepping passes through a crossover showing exact opposite behaviors at above and below the crossover point. Moreover, we ask the question that how the erroneous stepping with other parameters of the model have to be set in order to have a control over the speed of elongation mechanism. Finally we argue that the theoretical analysis of our results provide a simple picture of the design of a more accurate replication system and follows up with the speed-accuracy linear trade-off rule.

BP 24.43 Tue 16:00 BPp

Protein-ligand dynamics on multisecond timescales from sub-μs atomistic simulations — •Steffen Wolf, Benjamin Lickert, Simon Bray, and Gerhard Stock — Biomolecular Dynamics, Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3a, 79104 Freiburg

Coarse-graining of fully atomistic molecular dynamics simulations is a long-standing goal to allow the prediction of processes occurring on biologically relevant timescales. To achieve the necessary enhanced sampling, we first perform dissipation-corrected targeted molecular dynamics simulations which yield free energy and friction profiles of the molecular process of interest. In a second step, we use these fields to perform Langevin equation simulations which account for the desired molecular kinetics. By introducing the concept of temperature boosting of the Langevin equation, this combination of methods allows for the simulation of biomolecular processes occurring on multisecond timescales and beyond. Adopting the dissociation of solvated sodium chloride and several protein-ligand complexes as test problems, we are able to reproduce rates from atomistic MD simulation and experiments within a factor of 1.5–4 for rates up to the range of millseconds and 2–20 in the range of seconds.

BP 24.44 Tue 16:00 BPp

Structuring of the epithelial tissue — •Jakov Lovrić[1,3], Michael A. Klatt[2], Sara Kaliman[3], Gerd E. Schröder-Turk[4], and Ana-Sunčana Smith[1,3] — [1]Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia — [2]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA — [3]PULS Group, Institute for Theoretical Physics, Interdisciplinary Center for Nanostructured Films,Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [4]Murdoch University, College of Science, Health, Engineering and Education, Murdoch, Australia

Structural properties of space tessellations are important to understand various problems in many fields of science and industry. One of the existing questions is how to tessellate space with the maximized centrality of the cells, usually known as the Quantizer problem. Here we study stable solutions of the Quantizer problem by applying Lloyd's algorithm on various disordered random point pro-

cesses. We find that Lloyd's algorithm converges to a universal amorphous structure with long-range order. Furthermore, we investigate the role of cell centrality in the epithelium tissue. First, we find that the tissue can be represented by the tessellation based on the nuclear shape of constituting cells. In the following, we explore the interplay between finite-size effects and the Lloyd minimization and find that during the epithelial tissue development, centrality as a concept may play a role and is tightly controlled by the activity of the cell.

BP 24.45 Tue 16:00 BPp

Processive motors as active agents of microtubule lattice regulation — William Lecompte and •Karin John — University of Grenoble-Alpes, CNRS, Laboratoire Interdisciplinaire de Physique, 38000 Grenoble, France

Microtubules and molecular motors are ubiquitous in eukaryotic cells and are vital for many key cellular functions (cell division, organelle transport, motion). Recent experiments have shown that molecular motors modify the underlying microtubule lattice, yet a mechanistic model has remained elusive. Here we investigate theoretically how molecular motors could potentially participate in remodelling the shaft lattice. Our key idea is, that the walk of molecular motors locally destabilizes the lattice and may facilitate the exchange of tubulin dimers with the surrounding medium.

To test this assumption, we investigate a microtubule lattice model with lattice-motor interactions using kinetic Monte Carlo simulations. We propose a simple model with two key ingredients. The walk of molecular motors along the microtubule induces locally a conformational change with life time τ_r in the underlying lattice, which is less stable than the unperturbed lattice. Single lattice vacancies are stabilized via a steric hindrance for GTP dimers to integrate a GDP-lattice environment. As preliminary results we observed that a small flux of molecular motors which weakly destabilizes the lattice is sufficient to decrease the life-time of microtubules in the absence of free tubulin considerably.

BP 24.46 Tue 16:00 BPp

Analysis of cell contact inhibition during growth of epithelial tissue — •Sebastian Rühle, Anja Voss-Böhme, and Steffen Lange — University of applied sciences, Dresden, Germany

Dominating mechanisms in the development of healthy epithelial tissue are still subject to contemporary research, especially for tumour progression. While experiments suggest, that biomechanical cell-cell-interactions are crucial for the development of the tissue, it's usually oversimplified or neglected in theoretical approaches. For instance, the impact of cell migration, competition or contact inhibition on development of the cell colony is barely quantified. Puliafito et al. (2012) did experiments on MDCK-cells and proposed, that the behaviour of the colony during the growth phase can be solely explained by contact inhibition.

To test this hypothesis, we develop a cell-based model and compare the numerical results with the experimental data. using a cellular automaton we emulate single cell behaviour like cell migration, growth, proliferation, and cell-cell interactions like cell adhesion. The parameters are calibrated by experimental single cell tracking measurements. We show that without any mechanism of contact inhibition, this calibrated model reproduces emergent quantities like colony area, density, shape, cell size distribution, and collective cell motion from the experiment only to some extent. The discrepancies are most prominent for the long term cell density and cell size distribution and substantiate the role of contact inhibition in tissue growth.

BP 24.47 Tue 16:00 BPp

Analyzing the replication dynamics of malaria parasites — •Patrick Binder[1,2,3], Severina Klaus[4], Thomas Höfer[3], Nils Becker[3], Ulrich Schwarz[2,3], and Markus Ganter[4] — [1]Institute for Theoretical Physics, Heidelberg University, Germany — [2]BioQuant, Heidelberg University, Germany — [3]German Cancer Research Center (DKFZ), Heidelberg, Germany — [4]Center for Infectious Diseases, Heidelberg University Hospital, Heidelberg, Germany,

At around 200 million cases and half a million of fatalities each year, malaria remains a global health challenge. The predominant malaria-causing pathogen *Plasmodium falciparum* is a eukaryotic parasite with a complex life cycle that includes proliferation within red blood cells. After invasion, the parasite undergoes several rounds of nuclear division, eventually releasing around 24 daughter parasites into the blood. Intriguingly, the nuclei divide asynchronously although they reside in a shared cytoplasm. It is unknown how this process is controlled to yield a well-controlled and well-timed final outcome. We investigate the regulation of DNA replication and nuclear division by confronting simple stochastic branching models with high-resolution time-lapse confocal microscopy. We first found that successive rounds of replication speed up initially and slow down later on. Second, termination of replication is regulated by a counter mechanism and not a timer. Third, DNA replication is less synchronous than in stochastic lineages of mother-daughter correlated nuclei or even independent nuclei. Together, our analysis discovered the unusual mode of replication of a major human pathogen.

BP 24.48 Tue 16:00 BPp

Topology Control and Pruning in Intertwined Biological Flow Networks. — •Felix Kramer[1,2] and Carl Modes[1,2,3] — [1]Max Planck Institute for Molecular Cell Biology and Genetics (MPI-CBG), Dresden 01307, Germany — [2]Center for Systems Biology Dresden (CSBD), Dresden 01307, Germany — [3]Cluster of Excellence Physics of Life (PoL), Dresden 01062, Germany

Any larger organism is dependent on the proper distribution of supplies such as water, oxygen, nutrients etc, through extended and complex vessel systems. Naturally, the morphogenesis of these vessel networks during their earliest developmental stages has been extensively studied, in particular for slime-molds, leaf venation systems and vessel systems in vertebrates. Interestingly enough there is a universal hypothesis for the onset of maturation of any rudimentary network: Mechanic stresses, caused by the fluid flow, drive the development of the system toward a stationary state representing on optimum of dissipation, flow uniformity or metabolite distribution. Nevertheless, the influence of environmental factors on such long-term adaptation dynamics as well as the networks structure and function have not been fully understood. Therefore, interwoven channel systems such as found in the liver, kidney and pancreas, present a novel challenge and key opportunity regarding the field of coupled distribution networks. We here present an advanced version of the discrete Hu-Cai model, coupling two spatial networks in 3D. We show that spatial coupling of two flow-adapting networks can control the onset of topological complexity in concert with short-term flow fluctuations.

BP 24.49 Tue 16:00 BPp

Exploratory analysis and comparison of biomolecular structural ensembles with PENSA — •Martin Vögele[1] and Ron O. Dror[1,2,3,4] — [1]Department of Computer Science, Stanford University — [2]Department of Molecular and Cellular Physiology, Stanford University — [3]Department of Structural Biology, Stanford University — [4]Institute for Computational and Mathematical Engineering, Stanford University

Molecular simulations enable the study of proteins and other biomolecules and their dynamics on an atomistic scale. The large amount of data produced for ever more complex systems often makes it difficult to identify the structural features that are relevant for a particular phenomenon. Whilst most available analysis tools provide methods to analyze one simulation at a time, many common research pursuits necessitate analysis across several conditions - like mutations or different ligands - and finding significant differences between them.

We introduce PENSA, a collection of methods for exploratory analysis and comparison of structural ensembles such as those from molecular dynamics simulations. So far PENSA users can compare two conditions, e.g., via the relative entropy of their features or a Kolmogorov-Smirnov test, and visualize deviations on a reference structure. PENSA also implements exploratory analysis methods - like principal component analysis and clustering - that are applied across several ensembles. We demonstrate PENSA's usefulness on real-world examples by showing how it helps to determine molecular mechanisms efficiently.

BP 24.50 Tue 16:00 BPp

Morpheus: A user-friendly modeling and simulation framework for multicellular systems — Jörn Starruss, Diego Jahn, Robert Müller, Andreas Deutsch, and •Lutz Brusch — Center for Information Services and High Performance Computing (ZIH), Technische Universität Dresden, Germany

Computational modeling and simulation become increasingly important to analyze tissue morphogenesis. Existing software for multicellular models require scientists to encode their models in an imperative programming language. Morpheus (1,2), on the other hand, is an extensible open-source software framework that is entirely based on declarative modeling. It uses the domain-specific language MorpheusML to define multicellular models through a user-friendly GUI and has since proven applicable by a much broader community, including experimentalists. We here present how MorpheusML enables advanced scientific workflows (3) and cross-software exchange of multicellular models (4). MorpheusML can represent the spatial and mechanical aspects of interacting cells. A numerical simulation is then composed by automatic scheduling of predefined components in the simulator. Moreover, Morpheus supports simulations based on experimental data, e.g. segmented cell configurations, and offers a broad set of analysis tools to extract features right during simulation.

(1) Starruß et al. Bioinformatics 30, 1331, 2014. (2) Morpheus homepage: https://morpheus.gitlab.io (3) Parameter estimation workflow: https://fitmulticell.gitlab.io (4) Model standardization: https://multicellml.org

BP 25: Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)

Time: Tuesday 17:45–18:30 Location: BPb

Details will be published in a programme update.

BP 26: Annual General Meeting

Time: Tuesday 18:30–19:00 Location: BPa

Annual General Meeting

BP 27: Active Matter 3 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)

Time: Wednesday 9:00–10:40 Location: DYb

See DY 36 for details of this session.

BP 28: Active Matter 4 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)

Time: Wednesday 11:00–13:00 Location: DYb

See DY 41 for details of this session.

BP 29: Active Matter 5 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)

Time: Wednesday 14:30–15:50 Location: DYb

See DY 46 for details of this session.

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Overview of Invited Talks and Sessions

Invited Talks

CPP 2.6	Mon	11:00–11:40	CPPa	**Singlet fission in blends of organic semiconductors** — •Katharina Broch, Clemens Zeiser, Luca Moretti, Chad Cruz, Giulio Cerullo, Roel Tempelaar, Christopher Bardeen
CPP 2.11	Mon	14:00–14:40	CPPa	**Small, but highly effective: Functional molecules in polymer devices** — •Ulrike Kraft
CPP 3.5	Mon	11:00–11:40	CPPb	**Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates** — •Ralf Seemann, Roghayeh Shiri, Stefan Bommer, Dirk Peschka, Sebastian Jachalski, Lenoie Schmeller, Barbara Wagner
CPP 3.10	Mon	14:00–14:40	CPPb	**Sinking droplet durotaxis and engulfment** — •Anne Juel
CPP 7.5	Tue	11:00–11:40	CPPa	**Ultrafast spectroscopy of charge and structural dynamics in hybrid perovskites** — •Felix Deschler
CPP 7.9	Tue	14:00–14:40	CPPa	**Structural dynamics of halide perovskites via in-situ electron microscopy** — •Chen Li
CPP 8.1	Tue	9:00– 9:40	CPPb	**Polymer Micelles with Crystalline Cores: confinement effects, molecular exchange kinetics and mechanical response** — Nico Koenig, Lutz Willner, •Reidar Lund
CPP 8.4	Tue	11:00–11:40	CPPb	**Dynamic behaviour of anisotropic magnetic particles in suspensions** — •Sofia Kantorovich
CPP 16.1	Wed	9:00– 9:40	CPPa	**Charging Dynamics and Structure of Ionic Liquids in Nanoporous Supercapacitors** — •Christian Holm, Konrad Breitsprecher, Svyatoslav Kondrat
CPP 16.4	Wed	11:00–11:40	CPPa	**Interaction of polyelectrolytes with proteins** — •Matthias Ballauff
CPP 17.1	Wed	9:00– 9:40	CPPb	**Data-driven methods in polymer physics: exploring the sequence space of copolymers** — •Marco Werner
CPP 17.6	Wed	11:40–12:20	CPPb	**Structure formation in drying films and droplets** — •Arash Nikoubashman, Michael Howard, Michael Kappl, Hans-Jürgen Butt

Sessions

CPP 1	Mon	8:50– 9:00	CPPa	**Welcome**
CPP 2.1–2.15	Mon	9:00–16:30	CPPa	**Molecular Electronics - organized by Derck Schlettwein (Justus Liebig University Giessen, Giessen)**
CPP 3.1–3.14	Mon	9:00–16:30	CPPb	**Wetting - organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen) (joint session CPP/DY)**
CPP 4.1–4.4	Mon	9:00–11:00	BPb	**Active Biological Matter I (joint session BP/DY/CPP)**
CPP 5.1–5.6	Mon	11:00–13:30	BPb	**Active Biological Matter II (joint session BP/CPP/DY)**
CPP 6.1–6.17	Mon	16:30–18:30	CPPp	**Poster Session I - Molecular Electronics and Wetting**
CPP 7.1–7.12	Tue	9:00–16:30	CPPa	**Perovskites - organized by Eva M. Herzig (University of Bayreuth, Bayreuth)**
CPP 8.1–8.13	Tue	9:00–16:30	CPPb	**Complex Fluids - organized by Christine M. Papadakis (Technical University of Munich, Garching) (joint session CPP/DY)**
CPP 9.1–9.4	Tue	9:00–11:00	BPc	**Focus Phase Separation in Biological Systems I (joint session BP/CPP)**
CPP 10.1–10.3	Tue	9:30–10:30	DYa	**Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)**
CPP 11.1–11.6	Tue	11:00–13:00	DYa	**Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)**
CPP 12.1–12.4	Tue	14:00–16:00	BPb	**Focus Phase Separation in Biological Systems II (joint session BP/CPP)**

CPP 13.1–13.6	Tue	14:30–16:30	DYc	**Complex Fluids and Soft Matter 3 (joint session DY/CPP)**
CPP 14.1–14.26	Tue	16:30–18:30	CPPp	**Poster Session II - Complex Fluids and Perovskites**
CPP 15	Tue	17:45–18:30	BPb	**Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)**
CPP 16.1–16.12	Wed	9:00–15:20	CPPa	**Charged Soft Matter - organized by Joachim Dzubiella (Albert Ludwigs University Freiburg, Freiburg)**
CPP 17.1–17.10	Wed	9:00–14:40	CPPb	**Theorie and Simulation - organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden) (joint session CPP/DY)**
CPP 18.1–18.4	Wed	9:00–10:30	DYa	**Complex Fluids and Soft Matter 1 (joint session DY/CPP)**
CPP 19.1–19.3	Wed	9:30–10:30	DYc	**Glasses and Glass Transition 1 (joint session DY/CPP)**
CPP 20.1–20.6	Wed	11:00–13:00	DYa	**Complex Fluids and Soft Matter 2 (joint session DY/CPP)**
CPP 21.1–21.6	Wed	11:00–13:00	DYc	**Glasses and Glass Transition 2 (joint session DY/CPP)**
CPP 22.1–22.43	Wed	16:30–18:30	CPPp	**Poster Session III - Charged Soft Matter and Theory and Simulation**

Sessions

– Invited Talks, Contributed Talks, and Posters –

CPP 1: Welcome

Time: Monday 8:50–9:00 Location: CPPa

Welcome

CPP 2: Molecular Electronics - organized by Derck Schlettwein (Justus Liebig University Giessen, Giessen)

Time: Monday 9:00–16:30 Location: CPPa

CPP 2.1 Mon 9:00 CPPa

Organic light-emitting diodes for high-brightness operation: self-heating and switched-back regions — •Anton Kirch[1], Axel Fischer[1], Matthias Liero[2], Jürgen Fuhrmann[2], Annegret Glitzky[2], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Weierstrass Institute Berlin, Germany

Nonlinear effects typically involve switching phenomena that can lead to abrupt catastrophic device failure. For example, organic light-emitting diodes (OLEDs) suffer from strong electrothermal feedback that arises upon Joule self-heating. The interaction between temperature-dependent conductivity and power dissipation results in a positive feedback loop that finally destroys the device by thermal runaway. The situation becomes more severe for large-area OLEDs where the operation regime can locally differ. Former modeling studies, using a network of thermistors, led to the proposal that a so-called *switched-back* region arises. In this area, the current density, as well as the brightness, decreases although the total device current still increases when running an IV scan.

Here, we experimentally prove the existence of a switched-back region. We demonstrate that its appearance agrees with the simulation that solely uses electrothermal modeling. Our study aims to improve the long-term stability of high brightness OLED lighting tiles e.g. as applied in the automotive sector.

CPP 2.2 Mon 9:20 CPPa

Numerical Modeling of Transient Electroluminescence based on Thermally Activated Delayed Fluorescence — •Jeannine Grüne, Nikolai Bunzmann, Sebastian Weissenseel, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) show increased efficiencies due to effective upconversion from the non-emissive triplet states to the emissive singlet state via reverse intersystem crossing (RISC). A promising approach in this field are donor:acceptor configurations, whereby an intermolecular exciton is formed at the interface of two molecules, also called exciplex. A proven material combination is among others 4,4',4"-Tris[(3-methylphenyl)phenylamino]triphenylamine (m-MTDATA), as donor and Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB), as acceptor. The characterisitc behaviour especially in transient measurements differs from what is commonly observed in state of the art intramolecular emitters. In order to gain insight into the ongoing processes in exciplex based OLEDs, we performed numerical fits on transient electroluminescence (trEL) measurements at different temperatures. The kinetic model adapted for EL measurements on TADF systems includes second order terms to consider the existing annihilation processes such as triplet-triplet annihilation. Using this procedure, we can quantify the impact of efficiency-enhancing and efficiency-reducing processes as well as the time-dependent excited state populations.

CPP 2.3 Mon 9:40 CPPa

Two-dimensional electronic spectroscopy of phthalocyanine on rare gas clusters — •Ulrich Bangert, Lukas Bruder, Marcel Binz, Friedemann Landmesser, Elena Leissler, Daniel Uhl, and Frank Stienkemeier — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

With the recent advances of two-dimensional electronic spectroscopy (2DES) towards the gas phase, versatile samples like rare gas cluster beams become accessible [1]. Doping rare gas clusters with multiple molecules yields well defined many body systems. These systems are comparable to highly dilute thin film, however feature weak interaction with the substrate and are cooled down to ≤10 K. In previous experiments, such systems provided valuable details about singlet fission and super radiance in acene molecules [2,3]. We now apply for the first time 2DES to this approach and study free-base phthalocyanine in different environments: embedded in superfluid helium nanodroplets, deposited on the surface of neon clusters and as a thermal vapor. We find distinct differences in the photodynamics of the molecular assemblies.

[1] L. Bruder et al., J. Phys. B: At. Mol. Opt. Phys. 52 183501 (2019).
[2] S. Izadnia et al., J. Phys. Chem. Lett. 8, 2068 (2017).
[3] M. Müller et al., Phys. Rev. B 92 (12), 121408 (2015).

CPP 2.4 Mon 10:00 CPPa

Clarifying the orientation mechanism of homoleptic Iridium-carbene complexes — •Markus Schmid[1], Kristoffer Harms[2], Thomas Morgenstern[1], Alexander Hofmann[1], Hans-Hermann Johannes[2], Wolfgang Kowalsky[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institute for high frequency technology, TU Braunschweig, 38106 Braunschweig, Germany

Horizontal orientation of the emitting species is one of the most promising techniques to increase the efficiency of state of the art organic light emitting diodes. Especially metal-organic compounds have attracted great attention. While the alignment has been observed and explained for many heteroleptic Iridium complexes, there has been less progress for their homoleptic counterparts. Only few homoleptic compounds have been reported to show a beneficial morphology in guest-host systems. In this study, we investigated multiple derivatives and isomers of the sky-blue dye tris(N-dibenzofuranyl-N'-methylimidazole)iridium(III) ($Ir(dbfmi)_3$) doped in the hosts Bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) and 3,6-bis(diphenylphosphoryl)-9-phenylcarbazole (PO9). By a combination of optical techniques to probe the transition dipole orientation and electrical measurements to access the permanent dipole moment, we revealed that this homoleptic complex is significantly aligned in both matrices. From our insights into the film morphology we postulate that an anisotropic interaction is responsible for the orientation and even identified the region of the molecule that causes this behavior.

CPP 2.5 Mon 10:20 CPPa

Understanding Ultrafast Proton Transfer in Molecular Crystals — •Hyein Hwang[1,2], Vandana Tiwari[3], Simon /f. Bittmann[1], Hong-Guang Duan[4], Friedjof Tellkamp[1], Ajay Jha[5], and R. J. Dwayne Miller[6] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Chemistry, University of Hamburg, Germany — [3]European XFEL, Hamburg, Germany — [4]Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [5]RFI, Harwell Oxford, United Kingdom — [6]Department of Chemistry, University of Toronto, Ontario, Canada

Ultrafast proton transfer reaction is a topic of great interest particularly due to their association with the understanding of primary and elementary reaction pathways in functional electrochemical and biological systems. Although this reaction has been extensively investigated in solution for the role of interaction between the solute and the solvent-bath, but the dynamics in single molecular crystals remains elusive. Here, we study ultrafast intramolecular proton transfer reaction in hydroxyanthraquinones in crystalline form, where molecular system forms lattice. We use ultrafast transient absorption studies complemented with quantum chemistry calculations to reveal the role of spatial arrangement of the reactants within the lattice in reaction dynamics. Our work highlight the importance of intermolecular interactions guiding ultrafast dynamics in crystals.

20 min. meet the speakers - break

Invited Talk CPP 2.6 Mon 11:00 CPPa

Singlet fission in blends of organic semiconductors — •Katharina Broch[1], Clemens Zeiser[1], Luca Moretti[2], Chad Cruz[3], Giulio Cerullo[2], Roel Tempelaar[4], and Christopher Bardeen[3] — [1]Institute for Applied Physics, University of Tübingen, Germany — [2]Department of Physics, Polytechnic University of Milan, Italy — [3]Department of Chemistry, University of California at Riverside, USA — [4]Department of Chemistry, Northwestern University, USA

Singlet fission (SF), the photophysical process converting an singlet state into two triplets, is a promising approach to boost solar cell efficiencies [1], and is, due to a triplet-pair state intermediate, also interesting from the viewpoint of fundamental research. SF rates are controlled by the interplay of intermolecular interactions, energetics and electron-phonon coupling and a controlled modification of these parameters is key to a fundamental understanding of this complex process. Blends of organic semiconductors present an interesting alternative to established methods of chemical functionalization [2,3] and their potential for the study and control of SF pathways will be discussed using two examples of acene blends [3,4].

[1] M. B. Smith, J. Michl, Annu. Rev. Phys. Chem. 64 (2013); [2] D. Lubert-Perquel et al., Nat. Commun. 9 (2018); [3] K. Broch et al., Nat. Commun. 9 (2018); [4] C. Zeiser et al., Angew. Chem. Int. Ed. 59 (2020)

CPP 2.7 Mon 11:40 CPPa

Influence of alkyl chain variation on co-crystal formation and molecular charge transfer — •Nadine Russegger, Oleg Vladimirov, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

A very important and fundamental process for organic semiconductors is the charge transfer effect between electron donor and electron acceptor molecules in the ground state and in the excited state.

In this work, the charge transfer effect of weakly interacting organic semiconductor mixtures is comprehensively investigated depending on the influence of alkyl chain variation with different acceptor molecules. We choose dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different alkyl chain length in the imide position as acceptor molecules (PDIF-CN_2, PDI-C3, PDI-C5, and PDI-C8-CN_2).

For a full structural overview of the resulting molecularly mixed co-crystals, the bulk-heterojunction films were evaluated by surface X-ray scattering. The optical and electronic properties of the intermolecular interactions were characterized by optical absorption, photoluminescence as well as *in-situ* differential reflectance spectroscopy. For the various equimolar mixed systems of DNTT as well as DIP and different perylene-diimide derivatives charge transfer effects were estimated [1].

The results allow us to correlate the structural morphology and the charge transfer effects depending on the chain length and their configuration of the different mixed systems.

[1] V. Belova et al., *J. Am. Chem. Soc.*, **2017**, 139, 8474-8486.

CPP 2.8 Mon 12:00 CPPa

Anistropic Charge Transfer Formation at Crystalline Pentacene/Perfluoropentacene Interfaces — •Sebastian Hammer[1], Clemens Zeiser[2], Katharina Broch[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute for Applied Physics, University of Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

Strongly bound charge transfer (CT) states critically influence the performance of devices based on donor/acceptor (D/A) heterojunctions such as light emitting diodes or photovolatic cells. Whereas the excited states in the archetypical CT system Pentacene:Perfluoropentacene (P:PFP) have been vastly studied in thin films [1][2], the role of molecular orientation on CT formation and energetics has not been evaluated to the same extent, so far. Utilizing heteroepitaxial growth of PFP on P (001) single crystals surfaces we were able to prepare long-range ordered D/A heterojunctions in an edge-on molecular configuration as confirmed by XRD. Optical analyses by temperature dependent cw-fluorescence spectroscopy and *in-situ* differential reflectance spectroscopy on the PFP/P interfaces revealed no indication for CT formation in case of edge-on molecular orientation, in contrast to the face-to-face geometry. By means of bilayer as well as heterojunction diode structures we demonstrate that by controlling the molecular orientation at the PFP/P interface, thus, utilizing the anisotropic CT characteristics, the overall performance can be significantly improved.

[1] K. Broch et al., *Phys. Rev. B* **83**, 245307 (2011)
[2] T. Breuer, G. Witte, *J. Chem. Phys.* **21**, 138 (2013)

CPP 2.9 Mon 12:20 CPPa

Ab initio modelling of local interfaces in doped organic semiconductors — •Ana Maria Valencia, Guerrini Michele, and Caterina Cocchi — Humboldt-Universität zu Berlin

Despite the intensive efforts in the last decade, a clear and comprehensive understanding of the microscopic properties of doped organic semiconductors is still missing. Due to the complexity of these systems, which notoriously exhibit high level of disorder, also the results from quantum-mechanical ab initio methods are somehow constrained by the choice of the model structures. For a reliable prediction of electronic and optical properties, it is essential to rationalize the role of local interfaces between interacting donor and acceptor species. We address this problem from hybrid density-functional theory and many-body perturbation theory, investigating the structural, electronic, and optical properties of oligothiophenes doped by F4TCNQ. We consider different structures from isolated dimers and trimers, to periodic stacks and crystalline arrangements. Our results show that, depending on the amount and the nature of the local donor/acceptor interfaces, the choice of the simulated structure critically impacts the resulting electronic structure and degree of charge transfer. On the other hand, the optical spectra appear less sensitive to these characteristics, although a detailed inspection of the electron and hole densities discloses different excitation character depending on the relative donor/acceptor concentration [1] as well as on the donor length [2].

[1] Valencia, Guerrini, Cocchi, submitted (2019).
[2] Valencia & Cocchi, JPCC 123, 9617 (2019).

CPP 2.10 Mon 12:40 CPPa

Impact of electron-phonon-interaction on transport in organic molecular crystals: Naphthalene as a case study — •Konrad Merkel, Michel Panhans, Sebastian Hutsch, and Frank Ortmann — Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden

Understanding charge carrier transport in organic semiconductors is a key requirement for developing advanced electronic and opto-electronic devices such as OLEDs, OFETs and organic solar cells. However the general transport mechanism remains unclear. It is widely believed that electron-phonon-interaction plays an important role, due to the large fluctuations in the electronic coupling associated to the van-der-Waals-bonds between adjacent molecules. The interaction leads to a subtle interplay of scattering and phonon-assisted transport. Within the Kubo formalism, we derive a simulation technique, where we model the low-frequency phonon modes as local and non-local disorder in a tight-binding scheme and where all material parameters are calculated from density functional theory. We study the impact of such modes in naphthalene and compare our results to studies from literature.

60 min. meet the speakers - break

Invited Talk CPP 2.11 Mon 14:00 CPPa

Small, but highly effective: Functional molecules in polymer devices — •Ulrike Kraft — Max Planck Institute for Polymer Research, Mainz, Germany

The incorporation of small functional molecules such as dopants, plasticisers or molecular switches into polymer films can strongly affect their properties and even induce additional functionalities. Here, two examples will be discussed in which small functional molecules significantly influence the (electronic) properties of polymer devices:

Firstly, intrinsically stretchable interconnects and electrodes are printed from conductive inks consisting of PEDOT:PSS and ionic additives. In this approach, the ionic additives act as dopants and plasticisers and film properties can be tuned by orders of magnitude.

Secondly, the bias stress stability of polymer transistor is significantly improved by the addition of specific functional molecules. While on-state bias stress stability is widely studied, the off-state bias stress is mostly overlooked, even though equally important. We close this gap, focus on the off-state bias stress stability and show that threshold voltage shifts can be remarkably reduced.

CPP 2.12 Mon 14:40 CPPa

Single step production of a self-organized, low work function cathode interlayer from polymer blend solution — •Dominique Lungwitz[1], Keli Fabiana Seidel[2], Andreas Opitz[1], Thomas Krüger[3], Jan Behrends[3], Seth R. Marder[4], and Norbert Koch[1,5] — [1]Institut für Physik and IRIS Adlershof, Humboldt Universität zu Berlin, Germany — [2]Physics Department, Universidade Tecnológica Federal do Paraná, Brasil — [3]Berlin Joint EPR Lab and Institut für Experimentalphysik, Freie Universität Berlin, Germany — [4]School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics (COPE), Georgia Institute of Technology Atlanta, USA — [5]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Using cathode interlayers for reducing the work function of electrodes in organic electronic devices is a widely studied method. Here, we report a simple procedure to obtain a self-organized interlayer on ITO electrodes from a blend solution of P(NDI2OD-T2) and PEI. Reduced contact resistance and increased polymer conductivity are observed due to vertical phase separation. Fermi level pinning of P(NDI2OD-T2) at PEI covered ITO electrodes leads to the lowest possible electron injection barrier. Furthermore, an increased charge carrier density was measured. Finally, we relate the increase in polymer conductivity to a reduction of interfacial electron trapping and a morphology change. The results show clearly the importance of differentiation between work function reduction upon interfacial layers and conductivity increase upon changes of structural conformation.

CPP 2.13 Mon 15:00 CPPa

Morphological investigations on fullerene-free bulk heterojunction blends for photovoltaic applications — •Sebastian Grott[1], Lorenz Biessmann[1], Nitin Saxena[1], Wei Cao[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS funktionelle Materialien, 85748 Garching — [2]Elettra-Sincrotrone Trieste, 34149 Basovizza, Italy

In the last decades, the focus of research has been drawn towards the field of organic electronics due to their advantageous properties, such as versatility, flexibility, low-cost manufacturing processes, as well as their tuneable characteristics, such as solubility and absorption. These properties open up a wide range of applications, especially, in the field of photovoltaics. Hence, organic photovoltaics represent a promising alternative for the conventional inorganic photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional devices, values of over 10% have been reported and thus receive industrial attention for commercialization. We study the inner morphology of a low band gap, fullerene-free bulk heterojunction blend, namely PBDB-T and ITIC of different compositions with grazing-incidence small-angle X-ray scattering (GISAXS). The obtained structural information are correlated with current density voltage characteristics and the absorbance of the active layer in order to improve the efficiency.

CPP 2.14 Mon 15:20 CPPa

Fast Processing of Charge Transport Layers in Organic Solar Cells — •Harald Hoppe[1,2], Shahidul Alam[1,2], Aman Anand[1,2], Aurelien Sokeng Djourmessi[1,2], Jose Prince Madalaimuthu[1,2], Peter Fischer[4], and Ulrich S. Schubert[1,2,3] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University, Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University, Jena, Germany — [3]Jena Center for Soft Matter (JCSM), Friedrich Schiller University, Jena, Germany — [4]Faculty of Mechanical Engineering, Ilmenau University of Technology, Ilmenau, Germany

Charge transport layers (CTLs) are very important in organic solar cells to allow for an efficient and selective extraction of photogenerated charge carriers. Upon their optimization important photovoltaic parameters such as fill factors are being directly affected, for example since the series resistance and parallel resistance are often improved in combination with each other, when the contact becomes more selective. Unfortunately, CTLs often require an additional and rather intensive annealing process, which will add to the energy investment to such solar cells. In addition, such annealing processes may often either require too high temperatures to be compatible with flexible substrates or may be too time-consuming for fast web speeds. As one solution, we demonstrate the successful application of flash sintering for the annealing of CTLs.

CPP 2.15 Mon 15:40 CPPa

Polarized blue photoluminescence of mesoscopically ordered electrospun non-conjugated polyacrylonitrile nanofibers — Xiaojian Liao[1], •Frank-Julian Kahle[2], Bin Liu[3,4], Heinz Bässler[2], Xinghong Zhang[3], Seema Agarwal[1], Anna Köhler[2], and Andreas Greiner[1] — [1]Macromolecular Chemistry II, U Bayreuth, Germany — [2]Softmatter Optoelectronics, U Bayreuth, Germany — [3]MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Zhejiang University, P. R. China — [4]School of Energy and Power Engineering, North University of China, China

We demonstrate the fabrication of electrospun fibers from the non-conjugated polymer polyacrylonitrile (PAN) that can be aligned by a simple heat-stretching process. Upon excitation at 340 nm ribbons made from the nanofibres show polarized deep blue luminescence with an anisotropy of 0.37 and a quantum yield of about 0.31. Furthermore, they exhibit room temperature green phosphorescences with a lifetime of about 200 ms as well as a delayed deep blue fluorescence resulting from triplet-triplet annihilation (non-coherent photon upconversion). Wide and small angle X-ray scattering experiments show that the stretched electrospun nanofibers are highly aligned with nearly perfect uniaxial orientation within the fabricated ribbons. This results in mechanical robustness and flexibility, with a high specific tensile strength (534 ± 28) $MPa \cdot cm^3/g$ and toughness (79 ± 7) J/g. The combination of efficient polarized deep blue luminescence, room temperature phosphorescence, TTA, mechanical robustness and flexibility of these fibers opens up new avenues for applications.

30 min. meet the speakers - break

CPP 3: Wetting - organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen) (joint session CPP/DY)

Time: Monday 9:00–16:30 Location: CPPb

CPP 3.1 Mon 9:00 CPPb

Breakup Dynamics of Capillary Bridges on Hydrophobic Stripes — Maximilian Hartmann[1], •Mathis Fricke[2], Lukas Weimar[1], Dirk Gründing[2], Tomislav Maric[2], Dieter Bothe[2], and Steffen Hardt[1] — [1]Nano- and Microfluidics Group, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — [2]Mathematical Modeling and Analysis Group, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany

The breakup dynamics of a capillary bridge on a hydrophobic stripe between two hydrophilic stripes is studied both experimentally and numerically. The capillary bridge is formed from an evaporating water droplet wetting three neighboring stripes of a chemically patterned surface. The simulations are based on the Volume-of-Fluid (VOF) method implemented in Free Surface 3D (FS3D). By considering the breakup process in phase space, the breakup dynamics can be evaluated without the uncertainty in determining the precise breakup time. It is found that within an intermediate inviscid regime, the breakup dynamics follows a $t^{2/3}$-scaling, indicating that the breakup process is dominated by the balance of inertial and capillary forces. For smaller bridge widths, the breakup velocity reaches a plateau, which is due to viscous forces becoming more important. In the final stage of breakup, the capillary bridge forms a liquid thread that breaks up consistent with the Rayleigh-Plateau instability. The existence of satellite droplets in a regular pattern indicates that the primary breakup process is followed by self-similar secondary breakups.

CPP 3.2 Mon 9:20 CPPb

Simulating the hydrodynamics of droplets on photo-switchable substrates — •Josua Grawitter and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Interfaces between fluids and photo-switchable substrates provide a unique mechanism to precisely manipulate liquid droplets by creating and adapting a heterogeneous wettability landscape. Because droplets respond to changes in wettability, such interfaces provide a means to keep the droplets in non-equilibrium and thereby induce new states of dynamic wetting.

We present a boundary element method to determine the Stokes flow inside a droplet with its curved free surface and its flat interface at the substrate, where we apply the Navier boundary condition to permit motion of the contact line. In our approach we use the Cox-Voinov law [1] and introduce the velocity of the contact-line as a side condition. We also implement an iterative domain-splitting integration scheme capable of treating singular integrands, which are typical for the boundary element method. Using the implemented method, we study how droplets respond to specific spatiotemporal wettability patterns that either move or deform the droplet. Here, we present first studies of the spatio-temporal deformation dynamics induced by oscillating wettability along the contact line and of directed motion initiated by traveling wettability patterns. We specifically investigate how to design the patterns in order to maximize droplet speed.

[1] O. V. Voinov, Fluid Dyn. **11**, 714 (1976).

CPP 3.3 Mon 9:40 CPPb

Dynamics of liquid droplets on switchable prestructured substrates — •Moritz Stieneker[1] and Svetlana Gurevich[1,2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany — [2]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, D-48149 Münster, Germany

A mesoscopic continuum model is employed to model a thin, liquid film on a substrate with a spatio-temporal wettability. In particular, the effect of a switchable wettability pattern on the structure formation is analyzed for a one-dimensional case with the help of path-continuation techniques and direct numerical time simulations. It is found that if the periodic switching is introduced, the system reaction depends on the ratio between the time scale given by switching and the reaction time of the liquid. The behaviour of the contact angle during the slow and fast switching is investigated in details. Furthermore it is demonstrated that in the case of the slow switching the droplet solutions corresponding to the local minima of the free energy can be stabilized.

CPP 3.4 Mon 10:00 CPPb

Gradient dynamics model for drops spreading on polymer brushes — •Simon Hartmann and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Deutschland

When a liquid drop spreads on an adaptive substrate the latter changes its properties what may result in an intricate coupled dynamics of drop and substrate. We present a generic mesoscale hydrodynamic model for such processes that is written as a gradient dynamics on an underlying energy functional. We specify the model details for the example of a drop spreading on a dry polymer brush.

There, liquid absorption into the brush results in swelling of the brush causing changes in the brush topography and wettability. The liquid may also advance within the brush via diffusion (or wicking) resulting in coupled drop and brush dynamics. The specific model accounts for coupled spreading, absorption and wicking dynamics when the underlying energy functional incorporates capillarity, wettability and brush energy. We employ a simple version of such a model to numerically simulate a droplet spreading on a swelling brush and provide an in-depth analysis of the simulation results and some interesting quantities.

40 min. meet the speakers - break

Invited Talk CPP 3.5 Mon 11:00 CPPb

Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates — •Ralf Seemann[1], Roghayeh Shiri[1], Stefan Bommer[1], Dirk Peschka[2], Sebastian Jachalski[2], Lenoie Schmeller[2], and Barbara Wagner[2] — [1]Saarland University, Experimental Physics, D-66123 Saarbücken — [2]Weierstrass Institute, Mohrenstr. 39, D-10117 Berlin

The dewetting of liquid polystyrene (PS) from liquid polymethyl-methacrylate (PMMA) is studied. At dewetting temperatures, both polymers can be considered as Newtonian fluids with the same viscosity. Provided that the liquid PS layer is below 10 nm, breakup occurs by spinodal dewetting. Due to the low interfacial tension of the buried interface compared to the PS-air interface and the large mobility, a very short spinodal wavelength develops with a larger amplitude of the buried interface than that of the free PS-air interface. The spinodal patterns of PMMA-PS and PS-air interface are anti-correlated and the observed wavelength is within the range predicted from thin film models. For a later dewetting stage, when dewetting rims in the range of the PMMA film thickness have formed, characteristic profiles of both PMMA-PS and PS-air interface develop, which depend on the PMMA/PS thickness ratio. The dewetting rates are approximately linear but do not obey any well-defined scaling behavior. Based on the agreement of experimental results with theoretical predictions, we use the numerical simulations to predict local flow fields and energy dissipation that would otherwise be inaccessible to experiments.

CPP 3.6 Mon 11:40 CPPb

Wetting transitions on soft substrates — Marek Napiorkowski[1], •Lothar Schimmele[2], and Siegfried Dietrich[2,3] — [1]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [3]IV. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany

Within mean-field theory we study wetting of elastic substrates. Our analysis is based on a grand canonical free energy functional of the fluid number density and of the substrate displacement field. The substrate is described in terms of the linear theory of elasticity, parametrized by two Lamé coefficients. The fluid contribution is of the van der Waals type. Two potentials characterize the interparticle interactions in the system, the long-ranged attraction between the fluid particles and a potential characterizing the substrate-fluid interaction. By integrating out the elastic degrees of freedom we obtain an effective theory for the fluid number density alone. Its structure is similar to the one for wetting of an inert substrate. However, the long-ranged attraction between the fluid particles is replaced by an effective potential which also contains a term bilinear in the substrate-fluid interaction.

We discuss the corresponding wetting transitions in terms of an effective interface potential depending on the thickness of the wetting layer. We show that in the case of algebraically decaying interactions the elasticity of the substrate may suppress critical wetting transitions, and may even turn them first order.

CPP 3.7 Mon 12:00 CPPb

A Thermodynamic Consistent, Instantaneous Dividing Surface to Study Wetting Phenomena — •Amal Kanta Giri and Marcello Sega — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Straße 248, 90429 Nürnberg, Germany

A detailed knowledge of the microscopic structure and dynamics in the interfacial region of soft materials is a necessary step on the way to develop novel materials and is also key to a deeper understanding of the statistical mechanics of fluid interfaces out of equilibrium. The presence of thermal capillary waves, however, hinders efforts to investigate the local structure of interfaces by smearing out observable quantities computed in the global reference frame. To recover a detailed picture of the interface neighborhood, one needs to compute observables in the local, instantaneous reference frame located at the interface, although the determination of this frame is, in general, not unique.

Here, we report on the possibility of using computational geometry approaches to determine the set of instantaneous surface atoms in a way which is thermodynamically consistent with the Gibbs (equimolar) dividing surface. We apply these methods to the determination of the instantaneous, fluctuating contact line of droplets on solid substrates, with an outlook on the problem of dynamic wetting of soft, deformable substrates.

CPP 3.8 Mon 12:20 CPPb

Core-shell latex colloids as interfaces for tailoring wetting properties — Calvin J. Brett[1,2,3], Joakim Engström[3,4], Volker Körstgens[5], Peter Müller-Buschbaum[5,6], Eva Malmström[4], and •Stephan V. Roth[1,4] — [1]DESY, 22603 Hamburg, Germany — [2]KTH, Dept. Mechanics, SE-10044 Stockholm, Sweden — [3]WWSC, SE-10044 Stockholm, Sweden — [4]KTH, Dept. Fibre and Polymer Technology, SE-10044 Stockholm, Sweden — [5]TUM, Physik Department, 85748 Garching, Germany — [6]MLZ, TUM, 85748 Garching, Germany

Facile surface functionalisation of latex colloids makes them most promising materials for broad thin film applications. However, the effect of these colloids on chemical film and wetting properties is not easily evaluated. Core-shell particles can deform and coalesce on the nanoscale during thermal annealing yielding tailored physical properties. We investigated two different core-shell systems (soft and rigid) with identical shell but with chemically different core polymer and core size. These core-shell colloids are probed during thermal annealing on surfaces in order to investigate their behavior as a function of nanostructure size and rigidity. X-ray scattering allows us to follow the re-arrangement of the colloids and the structural evolution in situ during annealing. Evaluation by real-space imaging techniques reveals a disappearance of the structural integrity and a loss of colloids' boundaries. We present the possibility to tailor and fine-tune the wettability by tuning the core-shell colloid morphology in thin films, thus providing a facile template methodology for repellent surfaces.

CPP 3.9 Mon 12:40 CPPb

Drop Impact on Hot Plates: Contact, Lift-Off and the Formation of Holes — •Kirsten Harth[1,2], Sang.Hyeon Lee[3], Maaike Rump[2], Minwoo Kim[3], Detlef Lohse[2], Kamel Fezzaa[4], and Jung Ho Je[3] — [1]Institute of Physics, Otto von Guericke University Magdeburg — [2]Physics of Fluid and Max Planck Center, University of Twente, The Netherlands — [3]X-Ray Imaging Center, Pohang University of Science and Technology, Korea — [4]X-Ray Science Division, Argonne Ntnl. Laboratory, USA

Everyone who poured water into a hot pan has experienced the manifold boiling behaviours of drops impacting on a hot plate, a problem which is of high relevance in many technical applications. When the drop is gently deposited, and the surface temperature is sufficiently high, it hovers on a vapour layer (Leidenfrost effect). For impacting drops, this critical temperature for a contact-less rebound is substantially increased, and much harder to determine. In fact, determining contact times between drops and smooth substrates from side view imaging is impossible for most temperatures above the boiling point.

We combine High-Speed Total Internal Reflection and synchrotron X-Ray measurements to reliably determine contact times and the Leidenfrost temperature for drops impacting on smooth hot surfaces. Furthermore, we study the lift-off characteristics. A local minimum in lift-off times correlates with spontaneous lamella rupture and the morphology of the contact.

60 min. meet the speakers - break

Invited Talk CPP 3.10 Mon 14:00 CPPb

Sinking droplet durotaxis and engulfment — •Anne Juel — Department of Physics & Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Durotaxis refers to the spontaneous motion of objects along stiffness gradients of the supporting substrate. In droplet durotaxis migration occurs down rigidity gradients towards the softer regions of the substrate due to elasto-capillary interaction. We perform experiments in the limit of very soft PDMS substrates, where the cross-linked matrix of the gel can yield under the capillary stresses exerted by the sessile droplet. We find that the droplet moves towards the softest i.e. deepest parts of the gel layer while also sinking into the gel and that droplet durotaxis is much faster when engulfment is associated with the motion. For comparison, we focus on engulfment of aqueous droplets deposited onto a substrate layer of silicone oil. On substrates with a depth gradient, we observe qualitatively similar behaviour to the sinking durotaxis case. On deep layers, the droplet is ultimately engulfed in the oil layer. This involves rapid submersion of the droplet driven by capillary forces in the oil surface, followed by the much slower peeling of the droplet from the interface to which it is adhered. The later peeling stage is driven by a combination of geometric constraints at the apparent contact line and gravity pulling on the droplet. Gravitational effects are therefore essential to complete engulfment, even for micrometric droplets. Furthermore, the opposing effects of geometry and gravity result in the longest engulfment times for droplets of intermediate size.

CPP 3.11 Mon 14:40 CPPb

Droplets fighting contamination — •Abhinav Naga, William Wong, Anke Kaltbeitzel, Maria D'Acunzi, Hans-Jürgen Butt, and Doris Vollmer — Max Planck Institute for Polymer Research, Mainz, Germany

Lubricated surfaces are prone to accumulating contaminants due to their sticky yet slippery nature. The presence of contaminants, such as dust and dirt particles, alters their performance. An understanding of the effect of contaminated particles on the friction of surfaces is important not only from a fundamental per-

spective whereby further insight can be gained of the underlying mechanisms, but also from an applied perspective to predict the effectiveness of lubricated surfaces in the presence of contaminants.

In this study, we systematically contaminate lubricated silicone surfaces (Sylgard 184) and non-lubricated surfaces with spherical glass microparticles. We place a droplet on each surface and measure the force needed to push the droplet at different speeds towards an individual microparticle. We visualise this process with laser scanning confocal microscopy, focusing on the deformation inflicted by the microparticle on the droplet and its lubricant ridge. We combine these visualisations with our force measurements to suggest a mechanism for the removal of contaminated particles from surfaces using droplets, and we outline the differences between the outcomes on the lubricated and the non-lubricated surfaces. This work will help to understand droplet dynamics on imperfect or dirty lubricated surfaces.

CPP 3.12 Mon 15:00 CPPb

Lucas-Washburn equation applies for four phase contact point — •Peyman Rostami[1,2] and Günter Auernhammer[1,2] — [1]Max Planck Institute for Polymer Research, 55128, Mainz, Germany — [2]Leibniz Institute of Polymer Research, 01069, Dresden, Germany

A four-phase contact point, e.g., in merging of immiscible drops, is the point where the liquid-liquid interface advances along the contact line of one drop. The dynamics of drop merging involve various driving and dissipating forces in the dynamics of the four-phase contact point. The viscous friction, i.e. the flow field, within liquids is influenced by the different boundary conditions on the different interfaces (liquid-gas, liquid-liquid, liquid-solid). Additionally, Marangoni stresses between the two liquids and the spreading coefficients along the contact lines play a role. Effectively, these effects lead to a capillary force acting on the four-phase contact point. In total, the situation resembles the capillary flow in open V-shaped groove. The important difference is that, in the classical problem, the grooves are made out of two solid walls, but in the present case one of the *walls* is liquid, i.e., flowable and deformable. We investigate a range of liquids with different combination of physical properties (viscosity ratio, surface and interfacial tensions). The results show a good qualitative agreement for different liquids of the experimental results with the classical Washburn equation (h~square root of time), where h is the filled length of the *groove*.

CPP 3.13 Mon 15:20 CPPb

Imbibition-Induced Deformation Dynamics in Nanoporous Media — •Juan Sanchz[1], Zhuoqing Li[2], Michael Froeba[3], and Patrick Huber[4] — [1]Institute of Materials Physics, Hamburg University of Technology — [2]Institute of Materials Physics, Hamburg University of Technology — [3]Institute of Anorganic and Applied Chemistry, Hamburg University — [4]Institute of Materials Physics, Hamburg University of Technology

We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (carbon and silica) upon spontaneous, capillarity-driven invasion of water. We find two distinct dynamical regimes. One of them can be quantitatively traced to deformations originating in changes in the surface stress at the inner pore walls (dynamic Bangham's regime) upon water invasion, whereas the second one results from Laplace pressure effects. Our study demonstrates that it is possible to dynamically monitor imbibition dynamics by simple dilatometry measurements.

CPP 3.14 Mon 15:40 CPPb

Macroscopic Capillary Number for Characterization of Two-phase Flow in Porous Media — •Hu Guo and Rudolf Hilfer — Institute for Computational Physics, Universität Stuttgart, Stuttgart, Germany

The Capillary number (Ca) defined as the ratio of viscous force to capillary force is widely used to qualitatively characterize multiphase flow in porous media as in carbon dioxide geologic sequestration and chemical enhanced oil recovery (EOR). The main difficulty is to characterize forces porperly. There exists 22 definitions for Ca (Guo et al, IOR 2020). The most concise definition is $Ca = \frac{v\mu}{\sigma}$ with velocity v, viscosity μ and interfacial tension σ (Saffman and Taylor, 1958). It is supported by core flooding tests and most widely used. However, this definition is less sound than the one that involves the wettability parameter (Moore and Slobod, 1955). Meanwhile, the values of these Ca are regarded as too small to reflect the actual force balance (Dullien, 1979). It was shown theoretically, that this Ca is microscopic in nature and incorrectly used (Hilfer and Øren, 1996, Trans. Porous Media).

We study the new macroscopic capillary number $Ca = \frac{\mu\phi vL}{KP_b}$ with viscosity μ, porosity ϕ, velocity v, permeability K, length L and capillary breakthrough pressure P_b (Hilfer et al, 2015, Physical Review E). The new Ca explains some of the latest observations (Doorwar and Mohanty, 2017, SPE J; Qi et al, 2017, SPE J; Rabbani et al, 2018, PNAS; Zhao et al, 2019, PNAS) that contradict predictions obtained from the microscopic Ca. EOR field practice also verified that the macroscopic Ca is more profound.

30 min. meet the speakers - break

CPP 4: Active Biological Matter I (joint session BP/DY/CPP)

Time: Monday 9:00–11:00 Location: BPb

See BP 2 for details of this session.

CPP 5: Active Biological Matter II (joint session BP/CPP/DY)

Time: Monday 11:00–13:30 Location: BPb

See BP 5 for details of this session.

CPP 6: Poster Session I - Molecular Electronics and Wetting

Time: Monday 16:30–18:30 Location: CPPp

CPP 6.1 Mon 16:30 CPPp

Azobenzene molecular switches: Testing the charge transport in a self-assembled monolayer under light stimulus — •Vladyslav Savchenko and Olga Guskova — Leibniz Institute of Polymer Research Dresden (IPF Dresden), Hohe Str. 6, Dresden

The azobenzene-based molecules organized in chemisorbed self-assembled monolayers (SAMs) on the surfaces of electrodes work as photoswitches of the conductance, the electrode work function, and the magnetization/magnetic transitions. The aim of this computational study is to predict how the configurational rearrangements of the building blocks in a molecular switch consisting of azobenzene moiety and bithiophene spacer linked to a short alkanethiol affect the structural, electronic, and transport properties in SAMs.

The financial support of the Deutsche Forschungsgemeinschaft, project GU1510 5-1 "Optically reconfigurable nanoscale junctions for organic electronics" is highly appreciated.

CPP 6.2 Mon 16:30 CPPp

Ordered donor-acceptor complex formation and electron transfer in co-deposited films of structurally dissimilar molecules — •Andreas Opitz[1], C. Peter[1], B. Wegner[1,2], H.S.S.R. Matte[1], A. Röttger[1], T. Florian[1], X. Xu[1], P. Beyer[1], L. Grubert[1], S. Hecht[1], V. Belova[3], A. Hinderhofer[3], F. Schreiber[3], C. Kapser[4], J. Pflaum[4], Y. Zhang[5], S. Barlow[5], S.R. Marder[5], and N. Koch[1,2] — [1]Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]Universität Tübingen — [4]Universität Würzburg — [5]Georgia Institute of Technology Atlanta (USA)

Electrical and optoelectronic properties of organic semiconductor thin films can be tailored by co-deposition of molecular materials. At the moment it is difficult to predict a priori the resulting morphology (like phase separation or mixed crystals) for a selected material combination. Here, we study electron transfer between planar, rod-like electron donor molecules (DIP, PEN, DBTTF) and a non-planar electron acceptor molecule [Mo(tfd)$_3$] in co-evaporated films by analyzing morphological, vibrational and optical properties. [1]

The resulting morphology of the co-deposited films (phase separation or mixed crystals) can be rationalized within the laws of thermodynamics. Therefore, it is necessary to consider structural incompatibility of the molecules in terms of interaction energies between the molecules as well as the Coulomb attraction between molecular ions after the formation via ground-state electron transfer.

[1] A. Opitz et al., *J. Phys. Chem. C* **124** (2020) 11023-11031.

CPP 6.3 Mon 16:30 CPPp

Solid-state effects in the electronic and optical properties of donor-acceptor co-crystals — •Michele Guerrini[1,2], Ana M. Valencia[1,2], and Caterina Cocchi[1,2] — [1]Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany — [2]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin,Germany

In the framework of density functional theory and many-body perturbation theory, we investigate the role of solid-state effects (SSEs) in the electronic and optical properties of a donor-acceptor (DA) co-crystal composed of quarterthiophene donor molecules p-doped by (fluorinated)-tetracyanoquinodimethane. We find that the hybridization of the frontier electronic states is hindered along specific directions in the crystal cell, in favor of segregated states. We rationalize this behavior in terms of wave-function delocalization in the co-crystals competing and prevailing over the local interactions at the DA interfaces[1,2].

The anisotropic optical absorption spectra of the co-crystals are highly anisotropic and are dominated by a bright charge-transfer exciton at lowest-energy polarized along the direction of the DA stacks.

Our result contribute to rationalize the fundamental mechanisms ruling the formation of charge-transfer excitons in DA co-crystals.

[1] A M Valencia and C Cocchi, JPCC 2019, 123, 9617

[2] A M Valencia; M Guerrini and C Cocchi, PCCP 2020, 22, 3527

CPP 6.4 Mon 16:30 CPPp

Uncovering the enhancement mechanisms of thermoelectric performance of PEDOT: PSS films after physical-chemical dedoping — Suo Tu, Ting Tian, Anna-Lena Oechsle, and •Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

PEDOT: PSS is the most studied conducting polymer system due to their intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility in thermoelectric (TE) devices. The energy conversion efficiency of a TE material is evaluated by a dimensionless figure of merit ZT and defined as ZT = S2σT/k where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, k is the thermal conductivity, and S2σ is defined as the power factor (PF). Nevertheless, it is generally acknowledged that it is difficult to achieve a high ZT value of TE materials, due to the fact that the parameters S, σ, and k are interdependence as a function of carrier concentration and hard to be optimized simultaneously. In this work, we adopt a combination of DMSO addition and subsequent DMSO/salt mixture post-treatment to engineer TE performance of PEDOT: PSS thin films. Results show that the as-obtained PEDOT: PSS film presents a maximum PF of 105.2 *W(m-1K-2), which is ~1750-fold leap larger than that of pristine film. The origin and mechanism of the underlying improvement is systematically investigated by various characterizations to gain a more profound understanding of the fundamental nature of modified PEDOT: PSS films.

CPP 6.5 Mon 16:30 CPPp

Dependence of Electron and Ion Transport on the Intermolecular Coupling in Fluorinated Phthalocyanine Thin Films as Electrochromic Materials — •Thi Hai Quyen Nguyen[1], Marius Pelmus[2], Michael Schäfer[1], Sergiu M. Gorun[2] und Derck Schlettwein[1] — [1]Justus Liebig University Giessen, Institute of Applied Physics — [2]Seton Hall University, Department of Chemistry and Biochemistry

Phthalocyanines as organic ionic and electronic conductors are of great interest for the application in electrochromic devices. An influence of the degree of fluorination in copper phthalocyanines on the intermolecular coupling in the solid state and, thus, on the rate of electron and ion transport was observed: For $F_{16}PcCu$ the transport of electrons was faster than the diffusion of ions as opposed to $F_{64}PcCu$. In this work, thin films of a new type of fluorinated phthalocyanine ($F_{40}PcCu$) were prepared by physical vapor deposition. The dependence of the intermolecular coupling on the film thickness was analyzed by in situ UV/Vis spectroscopy. The electrochromic characteristics were studied by electrochemical and spectroelectrochemical measurements with an aqueous solution of KCl as electrolyte. The films provided a well-balanced, equally fast transport of electrons and ions. The optical absorption spectra revealed reversible changes of the films upon reduction with intercalation of the K^+ counterions and re-oxidation with extraction of the counterions. Fast and stable electrochromic switching of the films was achieved over at least 200 cycles. For a 1:1 mixed film of $F_{16}PcCu$ and $F_{64}PcCu$ a similar situation could be achieved.

CPP 6.6 Mon 16:30 CPPp

***In Situ* and *In Operando* KPFM Studies on Hexadecafluoro-Copper-Phthalocyanine ($F_{16}PcCu$) in OFET to Access Electrical Contact Resistance and Energy Level Alignment** — •Pascal Schweitzer, Clemens Geis, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen, GERMANY

Contact resistances are considered the major limiter of performance of organic field effect transistors (OFET). Perfluorinated copper-phthalocyanine ($F_{16}PcCu$) is a promising material as n-conductor to build complementary logical circuits. It is characterized by chemical stability under ambient conditions and a reasonably high charge carrier mobility. In this work, we used *in operando* Kelvin probe force microscopy under high vacuum to study the influence of contact resistances at the source and drain contacts on the OFET performance. Potentiometry at different applied external voltages revealed voltage drops at the interfaces to the source and drain metal contacts which allow for calculation of contact resistances. Thereby, the field-effect charge carrier mobility of $F_{16}PcCu$ was corrected for contact effects. Significantly higher values were obtained. *In situ* KPFM during film growth on polycrystalline gold visualizes film formation and corresponding shifts of energy levels confirming the existence of an injection barrier. We conclude, that tuning the energy level alignment and the interface effects to reduce contact resistances will lead to considerably improved performance of $F_{16}PcCu$ in OFET.

CPP 6.7 Mon 16:30 CPPp

Coupled organic-inorganic nanostructures (COINs) with mixed organic linker molecules — •Florian Grassl[1], Aladin Ullrich[1], Ahmed E. Mansour[3,4], Shaimaa Abdalbaqi[1], Norbert Koch[3,4], Andreas Opitz[3], Marcus Scheele[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, Germany — [2]Institute for Physical and Theoretical Chemistry, University of Tübingen, Germany — [3]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

COINs are composed of semiconducting inorganic nanoparticles and organic semiconductor molecules as ligands, which are covalently coupled to the surface of the nanoparticles [1]. A well-known organic ligand is 1,2-ethanedithiol (EDT) [2]; but it has the drawback of being very short as compared to the native oleic acid ligands. In this work we study the ligand Zinc β-tetraaminophthalocyanine (Zn4APc) [3], which has a desirable length comparable to oleic acid, but a low ligand exchange behaviour. To overcome this problem, a mixture of EDT and Zn4APc has been used. The binding of the ligands are compared by morphological, electronic, optical and electrical properties.

[1] M. Scheele, *Bunsen Magazin*, 2014, 4, 168

[2] J. Luther et al., *Nano Lett.*, 2008, 8, 3488

[3] J. Lauth et al., *Angew. Chem. Int. Ed.*, 2017, 56, 14061

CPP 6.8 Mon 16:30 CPPp

Impact of thermal treatment and humidity exposure on surface concentration and work function of PEDOT:PSS thin films — •Aman Anand[1,2], Jose Prince Madalaimuthu[1,2,3], Maximilian Schaal[4], Felix Otto[4], Marco Gruenewald[4], Shahidul Alam[1,2], Torsten Fritz[4], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — [3]Abbe School of Photonics, Friedrich Schiller University Jena, Albert-Einstein-Straße 6, 07745 Jena, Germany — [4]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Poly (3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is the most common and successful commercial conductive polyelectrolyte in the field of optoelectronics. In the present work, we have investigated the impact of the thermal treatments and relative humidity during film casting or storage on the work function of PEDOT:PSS films made from various commercial formulations. We find clear trends between the processing conditions and absolute work function which could be associated with the metal ions on the surface of the films. As a conclusion, we can suggest suitable processing parameters for a wide range of formulations and targeted electronic properties

CPP 6.9 Mon 16:30 CPPp

Compatible solution-processed interface materials for improving efficiency and prolonging the lifetime of organic solar cells — •Zhuo Xu[1,2], Jose Prince Madalaimuthu[1,2,3], Josef Bernd Slowik[1,2], Rico Meitzner[1,2], Shahidul Alam[1,2], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany. — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany. — [3]Abbe School of Photonics, Friedrich Schiller University Jena, Albert-Einstein-Straße 6, 07745 Jena, Germany

The electron transport layer (ETL) in an organic solar cell is one of the main components that play a crucial role in the separation of charges, improving effi-

ciency, and increasing the lifetime of the solar cells. Herein, solution-processed PBDTTT-CT: PC70BM based organic solar cells were fabricated using PDINO, Titanium Oxide (TiOx), and the mixture of PDINO and TiOx as an ETL. A power conversion efficiency (PCE) of 7.9% was achieved when a mixture of PDINO and TiOx was used as an ETL, which is one of the highest reported efficiency for halogen-free solvent processed PBDTTT-CT:PC70BM based polymer solar cells (PSCs). Furthermore, lower recombination, higher exciton dissociation probability, and longer lifetime were observed from the same device that indicates the selectivity of ETL can effectively improve the performance and stability of the solar cells.

CPP 6.10 Mon 16:30 CPPp

Observing Singlet Fission in Time-Energy-Momentum Space — •Alexander Neef[1], Sebastian Hammer[2], Samuel Beaulieu[1], Shuo Dong[1], Tommaso Pincelli[1], Julian Maklar[1], Martin Wolf[1], Laurenz Rettig[1], Jens Pflaum[2], and Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Experimental Physics VI, Julius- Maximilian University Wuerzburg, 97074 Wuerzburg, Germany

Under suitable conditions, the optically excited singlet exciton in organic crystals can split into two triplet excitons, a process known as singlet fission (SF) [Michl, 2010]. Though extensively studied, the proposed mechanisms for SF [Berkelbach, 2013] have not yet been unambiguously verified experimentally.

By means of XUV time- and angle-resolved photoemission spectroscopy (trARPES) performed on crystals of the archetypical SF compounds pentacene and tetracene, we are - for the first time - able to directly observe the transient behavior of the excited singlet and triplet states (S_1 and T_1) in momentum space. This allows us to compare the S_1 and T_1 energies with respect to the dispersing valence band within one measurement, implying that the T_1 energy is significantly smaller than previous estimates. Exploiting the multi-dimensionality of trARPES, we can furthermore decompose the excited states in pentacene by their unique signature in momentum space, thereby suggesting a strong mixing of charge-transfer (CT) states into S_1 and hence a CT-mediated superexchange mechanism of SF.

CPP 6.11 Mon 16:30 CPPp

Influence of solvent composition on optical and morphological properties of PTQ10:BTP-4F bulk heterojunctions — •Lukas Spanier, Xinyu Jiang, and Peter Müller-Buschbaum — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany

Organic solar cells have recently gained increasing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their production. However, their manufacture relies heavily on the use of halogenated solvents, as organic solar cells made with environmentally friendly solvents often suffer from major performance degradation. We investigate and compare the changes in morphology and the electro-optical behaviour of PTQ10:BTP-4F thin films processed from various solvents, utilising grazing-incidence X-ray scattering methods. We show the impact of solvent composition on the formation of polymer:non-fullerene acceptor bulk heterojunction films, affecting the resulting change in the performance of the organic solar cells.

CPP 6.12 Mon 16:30 CPPp

Qualification of Thieno-Quinoxaline Based Polymers for Application in Non-Fullerene Organic Solar Cells — •Md Moidul Islam[1,2], Shahidul Alam[1,2], Rico Meitzner[1,2], Christos L. Chochos[3,4], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldstrasse 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — [3]Institute of Chemical Biology, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece. — [4]Advent Technologies SA, Patras Science Park, Stadiou Street, Platani-Rio, 26504, Patra, Greece

Next-generation organic solar cells should not only be improved in performance but also should be environment-friendly throughout the production process. The processing of polymer-based solar cells with green solvents are highly desirable to make environmental friendly solar cells. In this study, we present bulk heterojunction polymer solar cells based on the thieno-quinoxaline based polymers blended with non-fullerene acceptor (NFA) in the non-halogenated solvent. Solar cells were prepared in conventional and inverted architecture, in order to investigate the material properties various spectroscopic measurements were performed in the pristine and blend films, as well as in the solutions. Finally, photovoltaic performances were investigated by different opto-electrical characterizations.

CPP 6.13 Mon 16:30 CPPp

Simulation of light-induced exciton diffusion and quenching on SWCNTs — •Manuel Rommel[1], Ralph Krupke[1,2], and Wolfgang Wenzel[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe — [2]Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt

The diffusion of excitons and charge carriers and the exciton loss processes like decay and quenching play an important role for the current characteristics in systems with light-induced charge carriers. A power-dependent photocurrent measurement on polymer-wrapped semiconducting single walled carbon nanotubes (SWCNT) has revealed a sublinear scaling of the electric current with laser power.

Here, we present a modified Monte-Carlo-based simulation with a fixed timestep and a pulsed laser. It models the stochastical generation, diffusion, collision and quenching of excitons, electrons and holes in 1D. Our results show that there are two regimes depending on laser power. At low laser power, current scales linearly with laser power. For high laser power (which coincides with the onset of exciton-exciton-quenching), the exponent of the power dependence becomes 0.63, which is very close to the experimental value of 0.59 ± 0.08. Furthermore, we can show that even a perfectly symmetric 1D system, where both electrodes favor the same charge carrier, exhibits a photocurrent if the illumination is asymmetric. We also show that power law characteristics depend on the SWCNT length.

This gives an insight into diffusion in SWCNTs and highlights the importance of exciton-exciton-quenching in SWCNT devices.

CPP 6.14 Mon 16:30 CPPp

In-situ sputter deposition of electrodes for non-fullerene organic photovoltaics application — •Xinyu Jiang[1], Simon J. Schaper[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], Jonas Drewes[4], Oleksandr Polonskyi[4], and Peter Müller-Buschbaum[1,5] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, Garching, Germany — [2]DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [4]Christian Albrechts-Universität zu Kiel, Materialverbunde Lehrstuhl, Materialwissenschaft Institut, Kaiserstr. 2, D-24143 Kiel, Germany — [5]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Electrode quality of photovoltaic devices plays a very important role in device performance. The metal growth process directly influences the material density, electrical conductivity and interface contact of the electrode. For understanding the mechanism of aluminium cluster growth on non-fullerene organic solar cells, we use in-situ grazing-incidence small-angle X-ray scattering (GISAXS) to observe detailed information during the sputtering process. We find that the early stages of Al cluster growth on the non-fullerene active layers determine the later stages and strongly influence the percolation threshold. Furthermore, the cluster growth varies for active layers with an additional electron blocking layer. These findings are of great importance for improving the performance of the photovoltaic devices.

CPP 6.15 Mon 16:30 CPPp

Sputter Deposition of Silver on Nanostructured PMMA-b-P3HT Copolymer Thin Films — •Marc Gensch[1,2], Matthias Schwartzkopf[1], Calvin Brett[1,3], Simon Schaper[2], Lucas Kreuzer[2], Nian Li[2], Wei Chen[2], Suzhe Liang[2], Jonas Drewes[4], Oleksandr Polonskyi[4], Thomas Strunskus[4], Franz Faupel[4], Peter Müller-Buschbaum[2,5], and Stephan Roth[1,3] — [1]DESY, Hamburg, Germany — [2]TUM, München, Germany — [3]KTH, Stockholm, Sweden — [4]CAU, Kiel, Germany — [5]MLZ, München, Germany

Nanostructured polymer-metal-composite films demonstrate great perspectives for optoelectronic applications, e.g. as sensors or organic photovoltaics (OPV). To enhance properties of such devices the metal cluster self-assembly process needs to be understood. We correlate the emerging nanoscale morphologies with electronic properties and quantify the difference in silver growth, comparing the diblock copolymer template with its corresponding homopolymer thin film counterparts. In this contribution, we investigate the silver cluster morphology during the growth on a PMMA-b-P3HT diblock copolymer template. We applied with grazing incidence small-angle X-ray scattering (GISAXS) to observe the cluster formation. Our study reveals the selective wetting of silver on one of the polymer blocks and the influence of the template on the percolation behavior of the silver layer, which is measured with resistance measurements during the sputter deposition.

CPP 6.16 Mon 16:30 CPPp

Memory effects in polymer brushes showing co-nonsolvency effects — •Simon Schubotz[1,2], Petra Uhlmann[1], Andreas Fery[1,2], Jens-Uwe Sommer[1,2], and Günter K. Auernhammer[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany

Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. Previous studies focused on the response of brushes which are entirely covered by a liquid. Here, we concentrate on partial wetting of co-nonsolvent polymer brushes, i.e., on the dynamics of a three-phase contact line moving over such brushes. We demonstrate that the wetting behavior depends on the wetting history of the polymer

brush. We use Poly(N-isopropylacrylamide) (PNiPAAm) brushes and water and ethanol as good solvents. In water/ethanol mixtures, the brush thickness is a non-monotonous function of the ethanol concentration. The memory of brushes is tested by consecutively depositing drops of increasing size at the same position. Previously deposited drops induce changes in the brush that modifies the wetting behavior (advancing contact angle) of subsequent drops. We believe that the change in the contact angels is induced by adaptation like swelling of or liquid exchange in the brush due to the drop on top.

CPP 6.17 Mon 16:30 CPPp

Quantification of Interfacial Fracture in Geometrically Confined Soft Elastomers by a Combined Analysis of Contact Force and Pressure — •Hares Wahdat and Alfred Crosby — Polymer Science and Engineering Department, University of Massachusetts Amherst, Amherst, MA, USA

Interfacial fracture occurs in many different situations ranging from the failure of polymer adhesives to the growth of wounds in human skin. Commonly, interfacial fracture can be studied by inserting a needle into a soft material and apply positive pressure while recording images. The combination of pressure and corresponding images has revealed insight into the interfacial fracture properties of gels or biological tissues. Still, the need for recording images can complicate the study of non-transparent samples or in-vivo studies. Here, we present experiments, in which the pressure-change and the corresponding contact between a rigid probe in contact with micrometer-thin soft elastomers, were analyzed to quantify the critical strain energy release rate for interfacial fracture. The modeling of interfacial fracture does not require image recording, making our experiment and analysis suitable for quantitative studies of interfacial facture in complicated systems such as biological tissues.

CPP 7: Perovskites - organized by Eva M. Herzig (University of Bayreuth, Bayreuth)

Time: Tuesday 9:00–16:30 Location: CPPa

CPP 7.1 Tue 9:00 CPPa

How do solvent molecules determine the electronic structure of halide perovskite precursors? — •Ana M. Valencia[1], Richard Schier[1], Oleksandra Shargaieva[2], Eva Unger[2], and Caterina Cocchi[1] — [1]Physics Dept., Humboldt-Universität zu Berlin und IRIS Adlershof — [2]Helmholtz-Zentrum Berlin, HySPRINT Innovation Lab, Berlin

Hybrid metal-halide perovskites have been demonstrated as excellent candidates for opto-electronic applications such as high-performing solar cells and light-emitting devices. The quality of the resulting materials, and hence their performance, strongly depends on the solution processing conditions. For this reason, it is of paramount importance to gain insight into their initial steps of formation of the solid-state materials. To do so, we investigate the inorganic building blocks of lead-iodide perovskites in DMSO solution. In order to mimic the initial steps of the perovskite nucleation, we consider PbI2(DMSO)4, Pb2I4(DMSO)6, and Pb3I6(DMSO)8, as model compounds treated fully atomistically and quantum-mechanically in the framework of density-functional theory and many-body perturbation theory. Through the analysis of the computed molecular orbitals, optical spectra, and electron and hole densities we discuss and rationalize the role of electronic hybridization between solute and solvent, and the mechanisms that are responsible for the absorption and emission peaks observed in the experiments.

CPP 7.2 Tue 9:20 CPPa

Solution-Processed Perovskite Solar Cells — Florian Mathies[1], Gopinath Paramasivam[1], Janardan Dagar[1], and •Eva Unger[1,2] — [1]Helmholtz Zentrum Berlin — [2]Lund University, Sweden

Metal halide perovskites (MHP) are being intensively researched for solar energy conversion applications and are the best solution-processable solar cell technology to date. For scaling the technology, high throughput and material-efficient printing and coating techniques can be utilised to make larger area devices. We will here present our systematic approach translating successful processing strategies developed for spin-coating to slot-die coating and inkjet printing through in-depth rationalisation of MHP formation gained from in-situ optical monitoring. Depending on the composition of MHP precursors and solvents as well as process conditions and process quenching by e.g. an antisolvent, thin film formation proceeds via crystalline intermediate phases or directly into the perovskite phase. Optimisation of MHP precursors composition and processing conditions enabled us to recently achieve 22% power conversion efficiency in small area devices by spin-coating and 15% on large are mini-modules that are being further optimised in the near future. We are currently working on translating process conditions to obtain high quality perovskite thin films to scalable solution based deposition methods such as slot-die coating and inkjet printing. To date, we have demonstrated slot-die coating and inkjet printed small area devices with power conversion efficiencies > 15%.

CPP 7.3 Tue 9:40 CPPa

In situ reflectometry and air flow control enables modeling of the drying process in blade coated hybrid perovskite solution films. — •Simon Ternes[1,2,3], Tobias Börnhorst[3], Jonas A. Schwenzer[1], Ihteaz M. Hossain[1,2], Uli Lemmer[1], Philip Scharfer[2,3], Wilhelm Schabel[3], Bryce S. Richards[1,2], and Ulrich W. Paetzold[1,2] — [1]Light Technology Institute, Karlsruhe, Germany — [2]Institute of Microstructure Technology, Eggenstein-Leopoldshafen, Germany — [3]Institute of Thermal Process Engineering, Karlsruhe, Germany

In recent years, hybrid perovskite solar cells (PCSs) have been introduced to the field of thin-film photovoltaics, exhibiting not only a steep increase in power conversion efficiencies from 3.8% in 2009 to above 25% to date, but also opening the perspective toward low-cost, large-scale solution processing. However, in order to design industrial-scale printing machines for PCSs in an efficient manner, general modeling of the dynamic drying and crystallization processes in perovskite solution films is required. This modeling must extend beyond trail-and-error optimization and beyond the commonly used, non-scalable spin coating technique. In the work presented here, we demonstrate simultaneous exact drying control by a laminar air flow and in situ film thickness measurements by reflectometry on blade coated perovskite solution films. In this way, we derive a general model of the drying process in these solution films and correlate it with the evolving morphology, providing a strategy of optimal process transfer from spin coating to any industrial coating and drying technique.

CPP 7.4 Tue 10:00 CPPa

Understanding the crystallization of solution processed, alloyed perovskites by multimodal characterization — •Shambhavi Pratap[1,2], Nobumichi Tamura[2], Zhenghao Yuan[3], Alastair MacDowell[2], Nicola Barchi[4], Jonathan Slack[2], Carolin Sutter-Fella[4], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, TU München, 85748 Garching, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA — [3]Eberly College of Science, The Pennsylvania State University, State College,16801, USA — [4]Chemical Sciences Division, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA

The crystallization behavior of solution processed hybrid plumbohalide perovskites is an ideal study to understand the formation of chemical alloys. Precursors corresponding to two different perovskites are mixed to serve as the precursor for an alloyed species. During crystallization, distinct crystalline species are isolated and characterized, as the equilibrium between the complex precursor intermediates and perovskites is transformed to the crystalline product by annealing the structure. The evolution of chemical structures is temporally resolved and the transient structures are studied for their optoelectronic transformation by photoluminescence.

40 min. meet the speakers - break

Invited Talk CPP 7.5 Tue 11:00 CPPa

Ultrafast spectroscopy of charge and structural dynamics in hybrid perovskites — •Felix Deschler — TU Munich

Metal-halide perovskites have emerged as promising semiconductors for optoelectronics, in which the soft-crystalline material structure leads to unexpected excitation dynamics, and for which the underlying physics remain unexplored. Unusually strong spin-orbit coupling was predicted to introduce Rashba-type state splitting in the electronic band structure of these materials, which is expected to affect recombination dynamics and spin-populations. It remains an open question, how dynamic changes in the material structure and electronic state populations control application-relevant electronic state nature and relaxation.

In my talk I will present how we use advanced optical spectroscopy to study the dynamics of optically-excited electronic state populations and crystal structure in functional hybrid perovskite semiconductors on ultrafast timescales. I will present results on mixed-cation mixed-halide bulk metal-halide perovskites, for which I will discuss how photodoping controls the properties and recombination of electronic states, and how these can enable highly-efficient optoelectronic devices and novel functionality. I will further discuss recent results on tracking the polaronic nature of excitation on ultrafast time-scales with ultrafast time-resolved diffraction experiments, from which we extract charge localization dynamics in real time.

CPP 7.6 Tue 11:40 CPPa

Investigating MAPbI_{3} Thin Film Formation during Spin Coating by Simultaneous in Situ Absorption and Photoluminescence Spectroscopy — Mihirsinh Chauhan[1,2], Yu Zhon[1], Konstantin Schötz[1], Brijesh Tripathi[2], Anna Köhler[1], Sven Huettner[1], and •Fabian Panzer[1] — [1]University of

Bayreuth, Bayreuth, Germany — [2]Pandit Deendayal Petroleum University, Gandhinagar, India

Until today, the two-step processing method represents an attractive route for the thin film formation of halide perovskites. However, a fundamental understanding about the film formation dynamics in case of spin coating methylammonium iodide (MAI) on PbI_{2} has not been established yet. Here we apply in-situ optical spectroscopy during the two-step film formation of the model halide perovskite MAPbI_{3} via spin coating. We identify and analyze in detail the optical features that occur in photoluminescence and corresponding absorption spectra during processing. We find that the film formation takes place in five consecutive steps, including the formation of a MAPbI3 capping layer via an interface crystallization and the occurrence of an intense dissolution-recrystallization process. Consideration of confinement and self-absorption effects in the PL spectra, together with consideration of the corresponding absorption spectra allows to quantify the growth rate of the initial interface crystallization to be 13 nm/s for our processing conditions. We find the main dissolution recrystallization process to happen with a rate of 445 nm/s, emphasizing its importance to the overall processing.

CPP 7.7 Tue 12:00 CPPa

Structural, optical and dielectric properties of $Cs_2AgBiBr_6$, a lead-free perovskite for photovoltaic applications — •Melina Armer[1], Maximilian Sirtl[2], Patrick Dörflinger[1], Julian Höcker[1], Thomas Bein[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Ludwigs Maximilian University München, 81377 München

As conventional perovskite solar cells contain lead and therefore suffer toxicity and stability issues, finding alternative and stable lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, lead-free $Cs_2AgBiBr_6$ single crystals have been synthesized using different solution based approaches, permitting a detailed characterization of the optical and structural properties of this material. The morphology and quality of the as grown crystals has been evaluated using scanning electron microscopy (SEM), energy dispersive X-ray microscopy (EDX) and X-ray diffraction (XRD). The crystals have been characterized using steady-state and time-resolved photoluminescence (PL) spectroscopy. We observed PL in the visible region characterized by large PL lifetimes. Furthermore, the dielectric constant of $Cs_2AgBiBr_6$ crystals has been measured at 9 GHz by time resolved microwave conductivity (TRMC). Using the obtained value of the dielectric constant the mobility of $Cs_2AgBiBr_6$ thin films could be estimated using TRMC.

CPP 7.8 Tue 12:20 CPPa

The Efficiency Potential of Neat Perovskite Films — •Martin Stolterfoht — Uni Potsdam

Perovskite photovoltaic (PV) cells have demonstrated power conversion efficiencies (PCE) that are close to those of monocrystalline silicon (m-Si) cells, however, in contrast to silicon PV, perovskites are not limited by Auger recombination. Nevertheless, compared to GaAs and m-Si devices, perovskite cells stand out by their significantly lower fill factors (FFs) which is due to a combination of resistive and non-radiative recombination losses. This necessitates a deeper understanding of the underlying loss mechanism and in particular the ideality factor of the cell. Here, by measuring the intensity (I) dependence of the external (V_OC) and internal voltage (i.e. the quasi-Fermi level splitting, QFLS), we can quantify the transport resistance-free efficiency of the complete cell as well as the efficiency potential of any neat perovskite films with and without attached transport layers (TLs). Moreover, QFLS(I) measurements on different perovskite compositions allow to disentangle the impact of the interfaces and the perovskite surface on the non-radiative FF and V_OC loss. We find that potassium passivated quadruple cation perovskite films stand out by their exceptionally high implied PCEs of above 28% which could be readily achieved if charge collection losses and energy alignment issues are overcome. Finally, strategies are presented to reduce both the ideality factor and transport losses to push the FF to the thermodynamic limits.

80 min. meet the speakers - break

Invited Talk CPP 7.9 Tue 14:00 CPPa

Structural dynamics of halide perovskites via in-situ electron microscopy — •Chen Li — Electron microscopy for Materials research (EMAT), University of Antwerp, Antwerp, Belgium

In-situ heating in electron microscopy is a powerful means of investigating phase changes in materials [1], and the focused electron probe in scanning transmission electron microscope (STEM) can also be used to stimulate the movement of atoms [2]. Here we apply such dynamic STEM to directly observe ion migration in both organic and inorganic halide perovskites. For instance, a phase transition from an orthorhombic δ-phase to a cubic α-phase in inorganic CsPbI3 perovskites has been tracked in atomic scale.

[1] C. Li, et. al., Secondary-phase-assisted grain boundary migration in CuInSe2. Phys. Rev. Lett. 2020, 124, 095702

[2] C. Li, et. al., Column-by-column observation of dislocation motion in CdTe: dynamic scanning transmission electron microscopy, Appl. Phys. Lett. 2016, 109, 143107

CPP 7.10 Tue 14:40 CPPa

The tetragonal to orthorhombic crystal phase transition in MAPI studied by time-resolved photoluminescence microscopy — •Alexander Biewald[1], Nadja Giesbrecht[1], Richard Ciesielski[1], Thomas Bein[1], Pablo Docampo[2], and Achim Hartschuh[1] — [1]LMU München, Butenandtstr. 11, 81377 Munich, GER — [2]Newcastle University, Newcastle upon Tyne, UK

Perovskite-based thin-film solar cells today reach power conversion efficiencies of more than 22% [1]. Methylammonium lead iodide (MAPI) is prototypical for this material class of hybrid halide perovskite semiconductors and at the focal point of interest for a growing community in research and engineering. We investigated the diffusion properties for the orthorhombic and tetragonal phase using time-resolved photoluminescence (PL) microscopy before [2]. Now we focus on the PL dynamics at the phase transition. First, the phase transition is observed in temperature dependent PL spectra, which show the correlated decrease and rise of two spectrally distinct bands. This indicates the coexistence of both phases in a limited temperature range. Second, at the phase transition, which is found to vary between grains, diffusive transport suddenly stops and only reappears upon further cooling or heating, respectively. Our spatio-temporal studies provide detailed microscopic insights into the phase transition and its influence on the carrier dynamics in large crystal MAPI thin films.

[1] M.A.Green et al.,Prog.Photovolt:Res.Appl.,26,427-436,2018

[2] A. Biewald et al.,ACS Appl.Mat.&Interfaces,11,20838-20844,2019

CPP 7.11 Tue 15:00 CPPa

Characterization of Perovskite Precursor Solutions in order to achieve High-Performance Solar Cells — •Marion Flatken[1], Nga Phung[1], Robert Wendt[1], Armin Hoell[1], and Antonio Abate[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) — [2]Department of Chemical, Materials and Production Engineering, University of Naples Federico II

Despite the current success of Perovskite Solar Cells, there are still open questions how to explain intrinsic parameters in terms of stability and general photovoltaic performance of varying perovskite compositions. Deeper knowledge in coordination chemistry of the perovskite itself is one key parameter to improve and control crystallization in the solution based fabrication. Using small angle scattering we can prove, that the coordination starts in the perovskite precursor solution and differs according to the perovskite composition. The observed colloidal structures are characterized via small angle neutron scattering (SANS) and is further compared to synchrotron based small angle x-ray scattering (SAXS). Based on nuclear magnetic resonsance spectroscopy the chemical composition of the complexes can be revealed, which leads us to a possible starting mechanism for nucleation and growth in perovskite precursor solutions. In our work we compare the precursor solutions of MAPbI3 and MAPbI3 x SrI2 to a cesium containing triple cation perovskite solution, which is known to be a highly efficient and stable perovskite. Observed differences and similarities might give one reason for the divergence in photovoltaic properties of the respective full device solar cells.

CPP 7.12 Tue 15:20 CPPa

Thermal decomposition dynamics of lead halide perovskite thin films — Thomas Burwig, Karl Heinze, Roland Scheer, and •Paul Pistor — MLU Martin-Luther-Universität Halle-Wittenberg

Despite the remarkable progress of lead halide perovskites, their low stability severely limits practical applications. To understand degradation pathways and pinpoint optimal compositions in terms of stability is therefore of utmost importance. Here we investigate the thermal stability of lead halide perovskite thin films grown by co-evaporation and analyze their thermal decomposition at elevated temperatures. Our approach allows to investigate the thermal decomposition by time-resolved in situ X-ray diffraction inside the vacuum growth chamber, without exposing the perovskite thin film to moisture or ambient air at any time. By applying fixed temperature ramps of 3-4 K/min. , we compare the onset of decomposition for a variety of different ABX_3 compositions and explore perovskites throughout the compositional space with A=MA,FA,Cs; B=Pb,Sn,(Ag,Bi) and X=I,Br,Cl. We find an increasing decomposition temperature for the series $MAPbCl_3$ - $MAPbI_3$ - $MAPbBr_3$, where the perovskite decomposes via degassing of MAX. The cation variation shows increased stability for $CsPbBr_3$ over $FAPbBr_3$ and $MAPbBr_3$, mainly due to the increased sublimation temperature of CsX, which is even higher than that of PbX_2. Finally, for the case of the most common and less stable $MAPbX_3$ perovskites, a series of time-resolved degradation experiments at constant temperatures provides detailed insights into the degradation kinetics of these materials.

50 min. meet the speakers - break

CPP 8: Complex Fluids - organized by Christine M. Papadakis (Technical University of Munich, Garching) (joint session CPP/DY)

Time: Tuesday 9:00–16:30 Location: CPPb

Invited Talk CPP 8.1 Tue 9:00 CPPb

Polymer Micelles with Crystalline Cores: confinement effects, molecular exchange kinetics and mechanical response — Nico Koenig[1], Lutz Willner[2], and •Reidar Lund[1] — [1]Department of Chemistry, University of Oslo, Postboks 1033 Blindern, 0315 Oslo, Norway. — [2]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS,

Partially crystalline, self-assembling systems with multiple components are omnipresent in nature with living cells as a prominent example. Here we study micelles formed by self-assembly of a series of well-defined n-alkyl-(polyethylene oxide) (Cn-PEO) polymers in aqueous solutions [1]. Using small-angle X-ray/neutron scattering (SAXS/SANS), densiometry and differential scanning calorimetry (DSC), we show that the n-alkane exhibit a first-order phase transition in the micellar cores, but with reduced melting points accurately described by the Gibbs-Thomson equation [2]. The effect of core crystallinity on the molecular exchange kinetics is investigated using time-resolved SANS (TR-SANS) [3-9]. We show that the melting transition is cooperative in the confined micellar core, whereas the exchange process is decoupled and unimeric in nature. [9] Telechelic polymers based on Cn-PEO-Cn forms clustered micelles and hydrogels composed of interconnected micelles at higher concentrations.[10] The results show that, contrary to regular micelles, the kinetics occurs in a multistep process involving a novel collision-induced single-molecule exchange mechanism.[11] Morever exchange kinetics directly controls the mechanical response of hydrogels through the bond life time [12]

CPP 8.2 Tue 9:40 CPPb

Foams stabilized by PNIPAM microgels — •Matthias Kühnhammer, Christian Appel, and Regine von Klitzing — Technical University of Darmstadt, Department of Physics, Soft Matter at Interfaces, 64287 Darmstadt, Germany

Cross-linked, short-chained poly-N-isopropylacrylamide (NIPAM) polymers have been in the focus of numerous studies in the past years and are still being discussed very actively in the context of multiple possible applications, because of their ability to respond to external stimuli. Because of their amphiphilic character, PNIPAM microgels can be used to stabilize dispersions like emulsions or foams.

In this contribution microgel stabilized foams are investigated. These foams are very stable at temperatures below the volume phase transition temperature (VPTT) of NIPAM and can be destabilized by increasing the temperature above the VPTT. The structure of the microgels inside the foam lamellae is investigated with neutron scattering. These results are compared to the organization of microgels at a single gas / water interface, which is studied with Langmuir isotherms and X-ray reflectivity.

Finally, these findings are related to macroscopic properties of the foams, namely foamability and foam stability.

CPP 8.3 Tue 10:00 CPPb

Functional, responsive microgels enlightened with super-resolution fluorescence microscopy — •Dominik Wöll, Laura Hoppe Alvarez, Eric Siemes, Ashvini Purohit, and Silvia Centeno Benigno — Institut für Physikalische Chemie, RWTH Aachen University, Landoltweg 2, 52074 Aachen

The elucidation of the structure and functionalization of materials in the submicron range is a key to their further development and application. Microgels are a class of such soft materials with high potential for multiple fields. Several groups have learnt to functionalize and structure microgels in sophisticated ways, but the evaluation of a successful functionalization or the envisioned properties are often limited by the ways of analysis and visualization. The development of modern super-resolved fluorescence microscopy methods opened up new ways of nanoscopic visualization that had not been possible previously due to the diffraction limit of light prohibiting spatial resolution beyond approx. 200 nm. In my contribution, the possibilities to elucidate shape and functionalization, to visualize single cross-linker positions and to address local polarity in microgels with 3D super-resolution fluorescence imaging will be discussed, and ways presented to address and answer scientific questions in soft matter science.

40 min. meet the speakers - break

Invited Talk CPP 8.4 Tue 11:00 CPPb

Dynamic behaviour of anisotropic magnetic particles in suspensions — •Sofia Kantorovich — University of Vienna — Ural Federal University

Stable dispersions of magnetic colloidal particles with sizes ranging from nanometers to couple of microns have been actively studied for several decades and the interest to them seems to keep growing. Such an attention to these systems is paid because of several reasons: they are biocompatible, can be remotely controlled by external magnetic fields and new synthesis techniques enable a rich variety of particle morphologies. In classical magnetic fluids with spherical polydisperse nanoparticles, dominating dipolar interactions typically limit the structural complexity of their aggregates to linear arrangements, namely chains, rings and branched structures. In this contribution I will show, how to either alter the shape of magnetic particles or their internal structure in order to extend dramatically the topology and properties of their suspensions. In particular I will focus on magnetic cubes, magnetic Janus particles, soft magnetic colloids and magnetically anisotropic nanoparticles. I will show how lattices, branched clusters of staggered chains, compact clusters, linear chains, and non aggregated configurations can be formed and interconverted reversibly in a controlled way. I will also discuss how adding an active component to magnetically anisotropic particles leads to unique properties. The results gathered in this presentation demonstrate that fundamentally new possibilities for responsive magnetic materials can arise when we step away from conventional dipolar hard spheres.

CPP 8.5 Tue 11:40 CPPb

Graphical Magnetogranulometry — •Ingo Rehberg, Reinhard Richter, and Stefan Hartung — Bayreuth University

The dipole strength of magnetic particles in a colloidal suspension can be obtained by a graphical rectification of the magnetization curves based on the inverse Langevin function. The method [1] yields the arithmetic and the harmonic mean of the particle distribution. It has an advantage compared to the fitting of magnetization curves to some appropriate mathematical model: It does not rely on assuming a particular distribution function of the particles.

[1] Measuring magnetic moments of polydisperse ferrofluids utilizing the inverse Langevin function, Ingo Rehberg, Reinhard Richter, Stefan Hartung, and Niklas Lucht, Birgit Hankiewicz, and Thomas Friedrich, Phys. Rev. B 100, 134425 (2019).

CPP 8.6 Tue 12:00 CPPb

Phase Behavior of Charged Magnetic Nanoplatelets — •Margaret Rosenberg[1] and Sofia Kantorovich[1,2] — [1]Department of Physics, University of Vienna, Austria — [2]2Department of Mathematical Physics, Ural Federal University, Russia

Recent decades have seen the emergence of a new branch of science, magnetic soft matter, fueled by the advances in synthesis techniques, which have also made a wide variety of anisotropic magnetic colloidal nanoparticles available. Colloidal anisometry can be used as an effective control parameter to tune both self-assembly scenarios and thermodynamic, rheological and phase behavior of dipolar (magnetic) soft matter. For instance, magnetic nanoplatelets can form macroscopic ferromagnetic phases at room temperature. Although the phase behavior of a system hard-core platelets is well known, the influence of the magnetic dipole moment and electrostatic repulsion on suspensions of magnetic platelets is not yet fully understood. We use MD simulations to recreate such a system. The colloidal particles are modelled by charged soft spheres, with a central dipole possessing a magnetic moment of a constant length, permanently oriented perpendicular to the platelet surface. In order to investigate the self-assembly and structural properties of the platelets, we vary the amplitude of an applied magnetic field and the magnetic dipole. We analyze at which electrostatic conditions the system exhibits self-assembly or/and field alignment, based on RDFs, structure factors parallel and perpendicular to the field and extensive cluster analysis.

CPP 8.7 Tue 12:20 CPPb

Magnetically Functionalized Star Polymers in Equilibrium and under Shear — •Gerhard Kahl[1], David Toneian[1], and Christos N. Likos[2] — [1]Institut für Theoretische Physik, TU Wien — [2]Fakultät für Physik, Universität Wien

Star polymers are macromolecules consisting of a central site, attached to which are a number f of linear polymer chains, called arms. Depending on the chemical composition of the arms, the polymer stars exhibit intriguing features, both in isolation and in concentrated solution.

We present star polymers with magnetically functionalized end groups as a novel polymeric system whose morphology, self-aggregation and orientation can easily be tuned by exposing these macromolecules simultaneously to an external magnetic field and to shear forces within a channel. Our investigations are based on a specialized simulation technique which faithfully takes into account the hydrodynamic interactions of the surrounding, Newtonian solvent. We find that the combination of magnetic field (including both strength and direction) and shear rate controls the mean number of magnetic clusters, which in turn is largely responsible for the static and dynamic behavior. While some properties are similar to comparable non-magnetic star polymers, others exhibit novel phenomena; examples of the latter include the breakup and reorganization of the clusters beyond a critical shear rate and a strong dependence of the efficiency

with which shear rate is translated into whole-body rotations on the direction of the magnetic field.

CPP 8.8 Tue 12:40 CPPb

Structural details of polymer grafted nanoparticles: Insights from coarse-grained molecular dynamics simulations — •Jiarul Midya[1], Michael Rubinstein[2], Sanat K. Kumar[3], and Arash Nikoubashman[1] — [1]Johannes Gutenberg University of Mainz, Mainz, Germany — [2]Duke University, Durham, United States — [3]Columbia University, New York, United States

Polymer grafted nanoparticles (GNPs) are promising materials with a wide range of applications in drug delivery, gas separation, photonic and electric materials. In this work, the structural properties of GNPs are studied via coarse-grained molecular dynamics simulations. We systematically vary the degree of polymerization at fixed grafting density, and study in detail the shape and size of the GNPs, the interpenetration between the grafted polymers and their conformations. We then compare these properties to the ones of pure polymer melts to assess the effect of confinement. We observe that the amount of chain-sections in the interpenetration zone is proportional to the length of the grafted chains, N_g, whereas, the brush height follows a power-law like behavior $h \sim N_g^{\alpha}$, where exponent α decreases from a value close to one to the limiting value of 1/3 with the increase of N_g. To understand the scaling behavior of h we provide an empirical form, involving the length of the grafted polymers and the core size of the GNPs, which explains our simulation results.

60 min. meet the speakers - break

CPP 8.9 Tue 14:00 CPPb

Charge regulation radically modifies electrostatics in membrane stacks — •Arghya Majee[1], Markus Bier[1,2], Ralf Blossey[3], and Rudolf Podgornik[4] — [1]MPI for Intelligent Systems, Stuttgart & University of Stuttgart, Germany — [2]University of Applied Sciences, Würzburg-Schweinfurt, Germany — [3]University of Lille, CNRS, UMR8576 UGSF, France — [4]CAS & KAVLI Institute of Theoretical Sciences, Beijing

Motivated by biological membrane-containing organelles in plants and photosynthetic bacteria, we study charge regulation in a model membrane stack [1]. Considering (de)protonation as the simplest mechanism of charge equilibration between the membranes and with the bathing environment [2], we uncover a symmetry-broken charge state in the stack with a quasiperiodic effective charge sequence. In the case of a monovalent bathing salt solution, our model predicts complex, inhomogeneous charge equilibria depending on the strength of the (de)protonation reaction, salt concentration, and membrane size. Our results shed light on the basic reorganization mechanism of thylakoid membrane stacks.

References:

[1] A. Majee, M. Bier, R. Blossey, and R. Podgornik, Phys. Rev. E **100**, 050601(R) (2019).

[2] A. Majee, M. Bier, and R. Podgornik, Soft Matter **14**, 985 (2018).

CPP 8.10 Tue 14:20 CPPb

Emulsion destabilisation by squeeze flow — •Riande Dekker, Antoine Deblais, and Daniel Bonn — Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

There is a large debate on the destabilisation mechanism of emulsions. We present a simple technique using mechanical compression to destabilise oil-in-water emulsions while at the same time confocal microscopy allows to visualise the mechanism directly. Upon compression of the emulsion, the continuous aqueous phase is squeezed out, while the dispersed oil phase progressively deforms from spherical to honeycomb-like shapes. The liquid films that separate the oil droplets are observed to thin and break at a critical oil/water ratio, leading to coalescence events that destabilise the emulsion. The destabilisation occurs like an avalanche propagating through the system. Local rearrangements occur after the fist destabilisation due to the fist coalescence event. The films participating in the cascade are the finest ones.

CPP 8.11 Tue 14:40 CPPb

Impact of hydrogen bonding strength on the structure and dynamics of supramolecular PEO — •Ana Brás[1], Ana Arizaga[1], Uxue Agirre[1], Marie Dorau[1], Patricia Bach[1], Judith E. Houston[2,3], Aurel Radulescu[3], Margarita Kruteva[4], and Annette M. Schmidt[1] — [1]UzK, Cologne, Germany — [2]ESS, Lund, Sweden — [3]FZJ, Garching, Germany — [4]FZJ, Jülich, Germany

In this work we investigate supramolecular poly(ethylene oxide) (PEO) oligomers at the entanglement molar mass (Me) with different hydrogen bonding end groups, such as diaminotriazine (Dat) and thymine-1- acetic acid (Thy), as well as 2-ureido-4[1H]-pyrimidinone (Upy). Small angle scattering and rheology were combined to study the influence of different end-groups association strength as Upy is highly self-associative in comparison to the heterocomplementary pair Thy/Dat. Results on the structure provide insight into the underlying molecular mechanisms and reveal that while Upy-terminated chains phase segregate, forming network-like systems, the Thy/Dat pair-terminated system self-assemble to linear chains, thereby increasing the effective chain length. Moreover, rheological measurements also reveal differences in the viscoelastic response as Upy-terminated chains exhibit an extended rubbery plateau, typical of networks, and the pair Thy/Dat presents a Newtonian fluid behaviour. Remarkably, albeit both systems show end-group association, different hydrogen bonding species influence the type of associates. Acknowledgements: DFG for a research grant (BR5303) and Prof. Dr. D. Richter, Prof. Dr. R. Strey and Dr. Wim Pyckhout-Hintzen for fruitful discussions.

CPP 8.12 Tue 15:00 CPPb

Structural characterization and rheology of biocompatible wormlike micelles - comparing experiment and theory — •Benjamin von Lospichl[1,2], Sabine H. L. Klapp[2], and Michael Gradzielski[1] — [1]Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin

Wormlike micelles exhibit a unique viscoelastic behaviour, which has been investigated intensely in the past decades by experimentalists and theoreticians [1,2]. Within our studies we explore the self-assembled structures and the flow behaviour of biocompatible wormlike micelles, which are a mixture of a short-chained C_8 cationic surfactant and the salts of long-chained C_{18} to C_{22} omega-9 fatty acids. The variation of the omega-9 fatty acids yields a change in thickness of the micelles, which strongly influences the flowing properties of the system. To characterize the size distribution and the relaxation time of the micellar solutions we use neutron scattering, rheology and electric birefringence. The obtained experimental results are then quantitatively compared to an established theoretical model describing the dynamics of micelles under shear. The model links mechanical properties such as stress to structural quantities like alignment or micellar length [3].

[1] C. Dreiss, Soft Matter **3**, 956, (2007)

[2] P. D. Olmsted, Rheo. Acta **47**, 283, (2008)

[3] B. v. Lospichl, S. H. L. Klapp, Phys. Rev. E **98**, 042605, (2018)

CPP 8.13 Tue 15:20 CPPb

Light driven passive and active motion of colloidal particles — •Pooja Arya, David Feldmann, and Svetlana Santer — University of Potsdam, Potsdam, Germany

We report on how one can manipulate an ensemble of colloidal particles trapped at a solid/liquid interface during irradiation with light of different wavelengths. The colloids are dispersed in an aqueous solution of photosensitive azobenzene containing cationic surfactant, which can photo-isomerize from trans to cis state under irradiation with light of appropriate wavelength. When focused light is applied, light-driven diffusioosmotic (LDDO) flow1 is generated at the solid/liquid interface resulting in a passive motion of particles within this flow. Utilizing the same LDDO mechanism one can also induce active motion of porous particles. Here the radially directed flow is generated by and around a single porous colloid when it is irradiated with either UV or blue light. This results in either mutual long-range diffusioosmotic repulsion of the particles or in even self-propelled motion when the colloids are turned into a Janus-like shape. Here, we discuss how to extend of passive and active motion of colloidal particles depends on the irradiation conditions such as wavelengths and intensities of light.

1.*Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova, O.I.; Santer, S., Scientific Reports 6 (2016) 36443

50 min. meet the speakers - break

CPP 9: Focus Phase Separation in Biological Systems I (joint session BP/CPP)

Time: Tuesday 9:00–11:00 Location: BPc

See BP 14 for details of this session.

CPP 10: Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)

Time: Tuesday 9:30–10:30 Location: DYa

See DY 21 for details of this session.

CPP 11: Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)

Time: Tuesday 11:00–13:00 Location: DYa

See DY 23 for details of this session.

CPP 12: Focus Phase Separation in Biological Systems II (joint session BP/CPP)

Time: Tuesday 14:00–16:00 Location: BPb

See BP 22 for details of this session.

CPP 13: Complex Fluids and Soft Matter 3 (joint session DY/CPP)

Time: Tuesday 14:30–16:30 Location: DYc

See DY 30 for details of this session.

CPP 14: Poster Session II - Complex Fluids and Perovskites

Time: Tuesday 16:30–18:30 Location: CPPp

CPP 14.1 Tue 16:30 CPPp

Direct Observation of the Time-dependent Dynamic Tube Dilation in Entangled Polymer Blends — •Paula Malo de Molina[1,2], Angel Alegría[1,3], Jürgen Allgeier[4], Margarita Kruteva[4], Ingo Hoffmann[5], Sylvain Prévost[5], Michael Monkenbusch[4], Dieter Richter[4], Arantxa Arbe[1], and Juan Colmenero[1,3,6] — [1]Materials Physics Center (CSIC-UPV/EHU), San Sebastian, Spain — [2]IKERBASQUE - Basque Foundation for Science, Bilbao, Spain — [3]Departamento de Física de Materiales (UPV/EHU), San Sebastian, Spain — [4]Forschungszentrum Jülich GmbH, Jülich, Germany — [5]Institut Laue-Langevin, Grenoble, France — [6]Donostia International Physics Center, San Sebastián, Spain

The viscoelastic properties of high molecular weight polymers are given by their entanglement dynamics. In asymmetric polymer blends, the finite lifetime of constraints leads to a dilation of the tube but how does the tube dilate? The effective terminal tube dilation of the long chains can be determined from macroscopic techniques such as dielectric spectroscopy (DS) and rheology, which cannot resolve the time evolution of the tube diameter at the nm-scale. Here, we exploit (i) the possibility of isotopic (H/D) labeling and (ii) the spatial and time resolution of neutron spin echo (NSE) to directly probe the time-dependent tube dilation for long linear entangled chains in model blends with smaller isofrictional linear chains and small star polymers. By combining NSE with rheology and DS on the additive, the characteristic time that governs tube dilation is identified as the terminal time of the additive.

CPP 14.2 Tue 16:30 CPPp

Spray-deposited anisotropic ferromagnetic hybrid polymer films of PS-b-PMMA and strontium hexaferrite magnetic nanoplatelets — •Wei Cao[1], Shanshan Yin[1], Andrei Chumakov[2], Matthias Opel[3], Markus Gallei[4], Matthias Schwartzkopf[2], Stephan V. Roth[2,5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, 85748 Garching — [2]DESY, 22607 Hamburg — [3]WMI, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — [5]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, 44 Stockholm, Sweden — [6]TU München, MLZ, 85748 Garching

Spray deposition is applied to fabricate anisotropic ferromagnetic hybrid polymer films by controlling the orientation of strontium hexaferrite nanoplatelets inside ultrahigh molecular weight diblock copolymer (DBC) polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) films. During spray deposition, the kinetics of structure evolution of the hybrid film is monitored in situ with grazing-incidence small-angle X-ray scattering. The obtained final hybrid film is then solvent annealed with tetrahydrofuran to study the influence of solvent vapor annealing (SVA). Due to the rearrangement of the nanoplatelets inside the DBC during SVA, an obvious change in the magnetic behavior of the hybrid film is observed. The hybrid film shows a perpendicular ferromagnetic anisotropy before SVA, which is strongly weakened after SVA. The spray deposited hybrid film appears highly promising for potential applications in magnetic data storage and sensors.

CPP 14.3 Tue 16:30 CPPp

Growth and morphology of sputtered iron layers on magnetic nanoparticle-containing diblock copolymer films — •Christopher Everett[1], Martina Plank[2], Markus Gallei[3], Matthias Schwartzkopf[4], Stephan Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — [2]TU Darmstadt, Ernst-Berl-Institute, Darmstadt, Germany — [3]Saarland University, Chair in Polymer Chemistry, Saarbrücken, Germany — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [5]KTH Royal Institute of Technology, Stockholm, Sweden — [6]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany

For highly functional magnetic sensors and high-density magnetic data storage, the exchange bias effect is of great technical importance. Exchange bias, typically observed at ferromagnetic/antiferromagnetic interfaces, has been reported in a variety of magnetic systems. In this investigation, ultra-high molecular weight polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) films with a large PS volume fraction are used as templates for ferrimagnetic magnetite (Fe3O4) nanoparticles (NPs). Through solvent vapor annealing, nanostructured hybrid films with up to 5 wt % of NPs are obtained. The sputtering of iron (Fe), which is ferromagnetic, on the polymer template is monitored in situ with grazing incidence small-angle X-ray scattering (GISAXS). An analysis reveals that the growth of Fe on nanoparticle-containing diblock copolymer films is a complex process and is important in understanding the resulting magnetic properties.

CPP 14.4 Tue 16:30 CPPp

Micellization of a Multi-Responsive Triblock Terpolymers — •Yanan Li[1], Chia-Hsin Ko[1], Athanasios Skandalis[2], Dmitry Molodenskiy[3], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Physik weicher Materie, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece — [3]EMBL at DESY, Hamburg, Germany

Triblock terpolymers having a hydrophobic, a thermo- and a pH- responsive block offer many possibilities for the formation of functional micelles and their manipulation by different environments. We investigate dual-stimuli-responsive micelles from poly(2-(dimethylamino) ethyl methacrylate)-b-poly(lauryl methacrylate)-b-poly(oligo(ethylene glycol) methyl ether methacrylate), PDMAEMA-b-PLMA-b-POEGMA [1]. The self-assembled micelles formed by these blocks can be applied in gene transfer and drug delivery applications. They consist of a strongly hydrophobic PLMA midblock, forming the core,

and two biocompatible hydrophilic blocks, forming the shell. PDMAEMA is a weak cationic polyelectrolyte, which is both pH- and temperature-responsive. To avoid precipitation of the triblock terpolymers upon heating at high pH values, a third, permanently water-soluble, biocompatible POEGMA block is included to form triblock terpolymers. We investigate the temperature- and pH-dependent micellar structures as a function of polymer concentration by dynamic light scattering and synchrotron small-angle X-ray scattering. [1] A. Skandalis, S. Pispas, Polym. Chem. 2017, 8, 4538.

CPP 14.5 Tue 16:30 CPPp

Multi-dimensional morphology control for PS-b-P4VP templated mesoporous iron (III) oxide thin films — •Shanshan Yin[1], Wei Cao[1], Qing Ji[2], Yajun Cheng[2], Lin Song[3], Nian Li[1], Christian L. Weindl[1], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, 315201, P. R. China — [3]Northwestern Polytechnical University, Xi'an 710072, China. — [4]DESY, Notkestr. 85, 22603 Hamburg, Germany — [5]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden — [6]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

We systematically investigate the synthesis of polystyrene-block-poly(4-vinylpyridine) templated Fe2O3 thin films by changing the solvent category (DMF or 1,4-dioxane) and the polymer-to-FeCl3 ratios. DMF/1,4-dioxane mixtures with different component ratios are also prepared for revealing the effect of the solvent selectivity on the thin film morphology. The structure transition mechanism of the thin films is explained by the preferential affinity and the small-molecule surfactant micelles theory.

CPP 14.6 Tue 16:30 CPPp

In-situ spraying of Colloids on Cellulose Nanofibers — •Constantin Harder[1,2], Marie Betker[1,3], Alexandros Alexakis[3], Andrei Chumakov[1], Elisabeth Erbes[1,4], Marc Gensch[1,2], Qing Chen[1], Jan Rubeck[1], Nils Le Coutre[5], Calvin J. Brett[1,3], Matthias Schwartzkopf[1], Eva Malmström[3], Daniel Söderberg[3], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany — [2]Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden — [4]Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Goettingen, Germany — [5]Universität Rostock, Universitätsplatz 1, 18055 Rostock, Germany

Layer formation and annealing of colloidal inks applied to porous materials is very relevant for printing and functional coatings. The goal is to distinguish and quantify the differences in structure formation during annealing of deposited colloidal inks on a porous and a solid material. As porous template we use a layer of cellulose nano fibers (CNF) with a charged surface. We use novel colloidal inks consisting of poly-butylmethacrylate (PBMA) and poly-sobrerolmethacrylate (PSobMA) with a charged shell in aqueous solution. We studied the deposition and the subsequent structural and morphological changes during annealing of the colloidal layers in real-time using grazing incidence small-angle X-ray scattering (GISAXS). During deposition, we expect that part of the liquid enters the CNF layer while part of the solvent and the colloids remain on top of the nanopaper surface, leading to a complex drying process. Subsequently, the structural changes in the colloidal layer are induced by annealing. With GISAXS we monitor these different processes and their effect on the CNF template.

CPP 14.7 Tue 16:30 CPPp

Observing the role of ß-lactoglobulin in biotemplating TiO_2 during spray deposition with in situ GIXS techniques: A route to green sol-gel chemistry — •Julian E. Heger[1], Wei Chen[1], Shanshan Yin[1], Christian L. Weindl[1], Christina Geiger[1], Calvin J. Brett[2,3], Wiebke Ohm[3], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany — [2]Royal Institute of Technology KTH, Teknikringen 34-35, 100 44 Stockholm, Sweden — [3]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Polymer directed sol-gel chemistry provides a powerful way for a morphological tailored synthesis of titania, which can be subsequently spray deposited to form functional films. For a green chemistry approach, synthetic polymers are substituted with water-soluble biopolymers. In this work, we investigate the templating effect of ß-lactoglobulin (ß-lg), which is known to form different aggregates as a function of net charge controlled by pH during denaturation. For this, ß-lg is mixed with an established titania precursor and denatured at a pH below its isoelectric point, to obtain hierarchical and crystalline titania at low-temperatures. Advanced in situ grazing incidence X-ray scattering (GIXS) synchrotron techniques identify the underlying kinetics of ß-lg biotemplated titania films during spray deposition.

CPP 14.8 Tue 16:30 CPPp

Water dynamics in a concentrated aqueous solution of perdeuterated poly(N-isopropylacrylamide) across the cloud point — •Bahar Yazdanshenas[1], Bart-Jan Niebuur[1], Dirk Schanzenbach[2], André Laschewsky[2,3], Michaela Zamponi[4], Daria Noferini[4], Alfons Schulte[5], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching — [2]Universität Potsdam, Institut für Chemie — [3]Fraunhofer IAP, Potsdam-Golm — [4]FZ Jülich, JCNS at MLZ, Garching — [5]University of Central Florida, Orlando, U.S.A.

In aqueous solutions of the thermoresponsive polymer poly(*N*-isopropylacrylamide) (PNIPAM), cooperative dehydration causes the polymer chains to collapse and aggregate at the demixing transition. Recent quasi-elastic neutron scattering (QENS) experiments have shown that the susceptibility spectra of hydration water occur at lower frequencies than those of bulk water and that their relative population decreases abruptly at the cloud point [1,2]. In the present study, we investigate the water dynamics on a perdeuterated PNIPAM sample in H_2O, down to ca. 0.08 GHz, using a combination of a high- and low-resolution QENS. Deuteration suppresses incoherent scattering from the polymer. In the observation window, we find two types of hydration water. 1. M. Philipp, C. M. Papadakis et al., J. Phys. Chem. B 2014, 118, 4253 2. B.-J. Niebuur, C. M. Papadakis et al., Macromolecules 2019, 52, 1942

CPP 14.9 Tue 16:30 CPPp

Co-nonsolvency induced collapse transition in thin PMMA-b-PNIPMAM films — •Julija Reitenbach[1], Christina Geiger[1], Gaetano Mangiapia[2], Cristiane Henschel[3], André Laschewsky[3], Christine Papadakis[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, 85748 Garching — [2]Helmholtz-Zentrum Geesthacht am Heinz Maier-Leibnitz Zentrum, Lichtenbergstr. 1, 85748 Garching — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm — [4]TU München, Physik-Department, Physik weicher Materie, James-Franck- Str. 1, 85748 Garching

Thin films of the thermoresponsive diblock copolymer PMMA-b-PNIPMAM exhibit a co-nonsolvency induced collapse transition when organic cosolvents, like acetone or methanol, are introduced in a certain ratio into the surrounding vapor atmosphere. The macroscopic changes during the swelling in aqueous vapor and the collapse transition in cosolvent vapor mixtures are investigated with spectral reflectance (SR) and time-of-flight neutron reflectometry (ToF-NR) measurements. We reveal the solvent/cosolvent exchange taking place at the polymer functional groups with in situ Fourier-transform infrared spectroscopy (FTIR) and attribute key changes in the local chemical environment to the macroscopic film collapse stages.

CPP 14.10 Tue 16:30 CPPp

ToF-NR swelling study on metal coated PNIPAM microgel thin films using a 3D-printed environmental chamber — •Tobias Widmann[1], Lucas P. Kreuzer[1], Christina Geiger[1], Julian E. Heger[1], Gaetano Mangiapia[2], Thomas Hellweg[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching — [2]HZG at MLZ, 85748 Garching — [3]Universität Bielefeld, Chemie Department, Physikalische und Biophysikalische Chemie, 33615 Bielefeld

Thermoresponsive microgels typically show a strong change in volume upon crossing the volume phase transition temperature (VPTT). For LCST type polymers, such as for example microgels based on N-isopropylacrylamide (NIPAM) which has an LCST of 32 °C, these microgels are in a hydrophilic state below the VPTT. In that temperature regime, they are highly sensitive to humidity, which makes them interesting candidates for humidity sensing applications on the nanoscale. Therefore, we investigate thin films of PNIPAM microgels cross linked with N,N*-methylenebisacrylamide under cyclic high and low humidity conditions. We follow the swelling and drying processes in situ using time-of-flight neutron reflectometry (ToF-NR). For that purpose, we used a custom made 3D-printed environmental chamber that was designed and built in the framework of the FlexiProb project, which aims for a quickly interchangeable sample environment for experiments at the European spallation source (ESS).

CPP 14.11 Tue 16:30 CPPp

Applications of Angular Cross-Correlation Analysis to Soft Matter — •Ivan Zaluzhnyy[1], Ruslan Kurta[2], Marcus Scheele[3], Frank Schreiber[1], Boris Ostrovskii[4], and Ivan Vartanyants[5,6] — [1]Institute of Applied Physics, University of Tübingen, Tübingen, Germany — [2]European XFEL, Schenefeld, Germany — [3]Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany — [4]Federal Scientific Research Center "Crystallography and photonics", Moscow, Russia — [5]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [6]National Research Nuclear University MEPhI, Moscow, Russia

An interesting feature of several soft matter systems is so-called orientational order, which can be referred to a specific orientation of anisotropic building blocks or bonds between these blocks. Angular x-ray cross-correlation analysis (AX-

CCA) is a method to analyze and interpret the anisotropy in x-ray scattering data in order to reveal the details of the orientational order [1]. In combination with scanning x-ray diffraction, AXCCA allows to study the spatial distribution of the orientational order across a large sample. After explaining the concepts of AXCCA, we will discuss the example of such a system, in which orientational order exists at several length scales, namely a superlattice of PbS nanocrystals coupled by organic linkers [2]. AXCCA allows to reveal the preferred orientation of nanoparticles with respect to the superlattice and the degree of angular disorder.

[1] I. Zaluzhnyy, et al., Materials 12 3464 (2019)
[2] I. Zaluzhnyy, et al., Nano Lett. 17 3511 (2017)

CPP 14.12 Tue 16:30 CPPp

Deformation and magnetic properties of clusters of supracolloidal magnetic polymers in microchannel under external field — •Vladimir Zverev[1], Ekaterina Novak[1], Sofia Kantorovich[2,1], and Pedro Sánchez[2,1] — [1]Ural Federal University, Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

Advances in synthesis technology in the field of magnetoreactive polymer supracolloid structures (magnetic filaments) have reduced their characteristic sizes from a few micrometers to a nanoscale. Magnetic filaments are actively studied theoretically, in particular their magnetic response, rheological properties, which is important for predicting behavior in closed geometries, such as microchannels used in microfluidic devices. Microchannels are tubes whose size does not exceed hundreds of microns, and has several advantages, for example, a high speed of heat and mass transfer.

This work is devoted to the study of the effect of liquid flow and an external magnetic field on the cluster placed in the microchannel. Clusters are made from magnetic filaments that have chain, ring, X, and Y-like structures. It was found that the external magnetic field enhances the deformation of the cluster in the microchannel in a flow. Clusters can significantly change their shape, and they can also demonstrate oscillating in time magnetic response. The use of magnetic filaments in microchannels makes it possible to control hydrodynamic interactions in the microfluidic system using an external magnetic field. The work was supported by RSF 19-72-10033.

CPP 14.13 Tue 16:30 CPPp

Rheological properties of clusters of supracolloidal magnetic polymers in a microchannel — •Ekaterina Novak[1], Vladimir Zverev[1], Marina Gupalo[1], and Sofia Kantorovich[1,2] — [1]Ural Federal University, Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

Construction of supracolloidal magnetic polymers (polymer-like structures in which magnetic nanoparticles are playing the role of monomers) has recently been made possible. The advantage of such magnetic polymers is that they keep their structure independently from the temperature and that is why they can be potentially used as an alternative to nanoparticles in magnetic fluids to obtain a desired and easily controlled magnetic or rheological response. In this contribution, using Langevin dynamics simulations, we focused on solutions of filaments, the magnetic nanoparticles in which are not only interacting via dipole-dipole potential but also via short-range attractive forces (Lennard-Jones type). Such filaments tend to aggregate in dense spherical droplet-like clusters. The resulting composite soft colloid is placed in the microchannel, where its behavior in the shear flow is investigated, varying a wide range of system parameters. We find that with time the cluster gets elongated. The higher is the shear rate the faster the flow can deform the cluster. The work was supported by RSF 19-72-10033.

CPP 14.14 Tue 16:30 CPPp

Influence of monomers on the self-assembly of supramolecular magnetic polymers — •Elena Pyanzina, Anna Akisheva, Egor Naumov, and Ekaterina Novak — Ural Federal University, Ekaterinburg, Russia

In this paper, an analysis of the qualitative change in equilibrium properties with temperature, at different lengths of the polymer and the parameters of the dipole-dipole interaction was carried out. As comparative characteristics were used: the radius of gyration, magnetic moment, form factor and anisotropy of the shape of the polymer. Both individual configurations were considered, and the best types of each filament were identified, and a general comparison of the filaments was made. The main objective of our work is to study the qualitative structural change in the behaviour of the filament when particle's size and shape are introduced in various polymer configurations.

This work was supported by RSF grant * 19-72-10033.

CPP 14.15 Tue 16:30 CPPp

Investigation of polymer templated Silicon-Germanium hybrid materials — •Christian L. Weindl[1], Christian Fajman[2], Michael A. Giebel[2], Matthias Schwarzkopf[3], Stephan V. Roth[3,4], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1,5] — [1]Technische Universität München, PhysikDepartment, Lehrstuhl für Funktionelle Materialien, James-FranckStraße 1, 85748 Garching, Germany — [2]Technische Universität München, Chemie-Department, Lehrstuhl für anorganische Chemie mit Schwerpunkt Neue Materialien, Lichtenbergstr. 4, 85748 Garching, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Noetkestraße 85, 22607 Hamburg, Germany — [4]Royal Institute of Technology KTH, Teknikringen 34-35, 10044 Stockholm, Sweden — [5]Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The latest research has revealed promising results for Silicon (Si) and Germanium (Ge) as anode materials for lithium-ion batteries. Owing to their high energy capacity these two semiconductors are considered auspicious alternatives to graphite anodes. In this study, we set the goal of synthesizing a porous silicon-germanium structure over a wet chemical sol-gel approach. Here, diblock copolymer polystyrene-block-polyethylene oxide is used as the structuring agent. Real-space data as SEM and microscopy images will be discussed with reciprocal-space analysis methods as grazing-incidence x-ray scattering in small and wide-angle mode.

CPP 14.16 Tue 16:30 CPPp

A Further Step Towards Space: Perovskite and Organic Solar Cells on a Rocket Flight — •Lennart Reb[1], Michael Böhmer[2], Benjamin Predeschly[1], Sebastian Grott[1], Christian Weindl[1], Goran Ivandekic[1], Renjun Guo[1], Christoph Dreissigacker[3], Roman Gernhäuser[2], Andreas Meyer[3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [2]TU München, Physik-Department, Zentrales Technologielabor, Garching, Germany — [3]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Köln, Germany — [4]Heinz Maier-Leibnitz-Zentrum, Garching, Germany

Perovskite and organic solar cells possess a revolutionary potential for space applications. The thin-film technologies enable an exceptional power per mass, exceeding herein their inorganic counterparts by magnitudes. However, research was mainly restricted to terrestrial conditions so far. We report the launch of two types of perovskite and organic solar cells on a suborbital rocket flight, possibly the first in-situ demonstration of these technologies in space conditions [1]. Both, planar and mesoscopic nip-type perovskite solar cell types exceeded an power per area of 14 mW cm-2, whereas both bulk heterojunction absorber PBDB-T:ITIC and PTB7-Th:PC71BM organic solar cell types reached more than 4 and 7 mW cm-2, respectively. Our results highlight both the suitability for near-Earth applications and the potential for deep space missions of these technologies. [1] L. Reb et al., Joule 4,1880-1892 (2020), doi.org/10.1016/j.joule.2020.07.004.

CPP 14.17 Tue 16:30 CPPp

Tuning ordered mesoporous titania films via introducing germanium nanocrystals for high-efficient photoanodes — •Nian Li[1], Renjun Guo[1], Wei Chen[1], Volker Körstgens[1], Julian E. Heger[1], Suzhe Liang[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg

With an aim of obtaining high-efficient titania photoanodes, we introduce germanium nanocrystals (GeNCs) into a diblock-copolymer template-assisted sol-gel synthesis. The surface and inner morphologies of the TiO2/GeNC films with different GeNC content after thermal annealing are investigated via scanning electron microscopy and grazing incidence small-angle X-ray scattering (GISAXS). We also probe the crystal phase, chemical composition and optical properties of the nanocomposite films via X-ray diffraction, transmission electron microscopy, X-ray photoelectron spectroscopy and ultraviolet-visible spectroscopy. These measurements show that even with GeNC addition, the nanocomposite films still have ordered nanostructures, good crystallinity and high transparency. We further study the charge-carrier dynamics of the nanocomposite films. Compared to pristine titania photoanodes, the GeNC addition enhances the electron transfer, resulting in an overall improvement in the short-circuit current density (Jsc) of the exemplary perovskite solar cells and thereby an enhanced solar cell efficiency.

CPP 14.18 Tue 16:30 CPPp

Degradation mechanisms of perovskite solar cells under different atmospheres — •Renjun Guo[1], Dan Han[2], Wei Chen[1], Linjie Dai[3], Kangyu Ji[3], Qiu Xiong[4], Saisai Li[5], Lennart K. Reb[1], Manuel A. Scheel[1], Shambhavi Pratap[1], Nian Li[1], Shanshan Yin[1], Tianxiao Xiao[1], Suzhe Liang[1], Anna-Lena Oechsle[1], Christian L. Weindl[1], Matthias Schwartzkopf[6], Hubert Ebert[2], Peng Gao[4], Mingjian Yuan[5], Neil C. Greenham[3], Samuel D. Stranks[3], Stephan V. Roth[6], Richard H. Friend[3], and Peter Müller-Buschbaum[1] — [1]TU München — [2]James-Franck-Str. 1 — [3]University of Cambridge — [4]Chinese Academy of Sciences — [5]Nankai University — [6]Deutsche Elektronen-Synchrotron

We investigate degradation mechanisms of perovskite solar cells under different atmospheres via in-situ grazing-incidence X-ray scattering methods. We reveal that the atmosphere has a significant influence on degradation mechanisms for materials. This results in the degradation of the performances of the relative perovskite solar cells. Compared with the performance evolution of perovskite solar cells under vacuum, they show better stability under nitrogen.

CPP 14.19 Tue 16:30 CPPp

Fabrication of Plasmonic Nanostructures for Perovskite Solar Cells — •Tianfu Guan, Renjun Guo, Suzhe Liang, Nian Li, Christian L. Weindl, Wei Cao, and Peter Müller-Buschbaum — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany

Plasmonic metal-dielectric composites have fascinated a great interest in various fields, owning to surface plasmon resonance (SPR) induced by incident radiation. The utilization of plasmonic metal nanoparticles (NPs) is frequently proposed as a means to further enhance the light absorption in the broad wavelength range as well as to facilitate charge collection and transport in the Perovskite solar cells (PSCs). To regulate the plasmonic spectral of Au NPs for maximizing the enhancement in light-absorption of the photoactive layer, we assembly the metal NPs onto the electron collecting layer to broaden the absorption band of the photoactive layer of optoelectronic devices as well as enhance the device performance. To meet the optimal results, we put effort into the plasmonic structure regulation, since the size, density, and morphology of the Au NPs will influence the crystallinity of the perovskite film and charge transportation of the device. Besides, grazing incidence small angle x-ray scattering (GISAXS) is used to study the quality of the plasmonic structure interface in terms of contact area between the perovskite film. Grazing incidence wide angle x-ray scattering (GIWAXS) is used to probe the crystalline structure of the perovskite active layers.

CPP 14.20 Tue 16:30 CPPp

Mesoporous ZnO thin films templated by diblock copolymer for photovoltaic applications — •Ting Tian and Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Mesoporous ZnO thin films have received tremendous attention in photovoltaic applications in view of their high electron mobility, high transparency, high surface area, and the superior ability to host the light-harvesting dyes and the organic molecular hole-transporters. Considering the morphology-dependent device performance, a precise control over the ZnO nanostructures is indispensable. Among the existing synthesis routes, the diblock copolymer assisted sol-gel approach has been corroborated to be powerful and promising in morphology tunability. Benefiting from the solution processability, this wet chemical method can be integrated into industry-based processes and thus achieve large-scale, high-throughput production. In the present work, an amphiphilic diblock copolymer is used as the structure-directing agent and slot-die coating is applied as the deposition technique to fabricate the mesoporous ZnO films. Effects of ZnO precursor variables on morphological evolution of mesoporous ZnO films are systematically investigated. The generated nanostructures on the film surface are detected by surface-sensitive scanning electron microscope (SEM), and the inner morphologies are probed by reciprocal-space Grazing-incidence small angle X-ray scattering (GISAXS) technique.

CPP 14.21 Tue 16:30 CPPp

The Role of CsBr in Crystal Orientation and Optoelectronic Properties of MAPbI3-based devices — Yuqin Zou and •Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany.

Orientations of crystal planes impact on the behavior of photogenerated charge carriers and are vital for developing electronic properties of the corresponding devices. Herein, we propose a facile approach to reveal the effect of crystal stacking on the charge carrier kinetics by doping CsBr to enable the formation of a mix-cations perovskite phase. We use grazing-incidence wide-angle X-ray scattering to probe the crystal structure and crystal orientation of the mixed perovskite thin films revealing the effect of the extrinsic CsBr doping on the stacking of the crystal planes. TPV, TPC and tDOS are also used to detect the recombination of the photo-generated charge carriers and the trap-state density. It is demonstrated that CsBr compositional engineering can effectively tune the crystallization orientation of crystal planes, reduce trap-state density and facilitate photocarriers transport across the absorber and pertaining interface simultaneously. This strategy provides a unique insight into the underlying relationship among the stacking pattern of crystal planes, the photo-generated charge carrier transport and the optoelectronic properties of solar cells.

CPP 14.22 Tue 16:30 CPPp

The Role of CsBr in Crystal Orientation and Optoelectronic Properties of MAPbI3-based devices — •Yuqin Zou and Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany.

Orientations of crystal planes impact on the behavior of photogenerated charge carriers and are vital for developing electronic properties of the corresponding devices. Herein, we propose a facile approach to reveal the effect of crystal stacking on the charge carrier kinetics by doping CsBr to enable the formation of a mix-cations perovskite phase. We use grazing-incidence wide-angle X-ray scattering to probe the crystal structure and crystal orientation of the mixed perovskite thin films revealing the effect of the extrinsic CsBr doping on the stacking of the crystal planes. TPV, TPC and tDOS are also used to detect the recombination of the photo-generated charge carriers and the trap-state density. It is demonstrated that CsBr compositional engineering can effectively tune the crystallization orientation of crystal planes, reduce trap-state density and facilitate photocarriers transport across the absorber and pertaining interface simultaneously. This strategy provides a unique insight into the underlying relationship among the stacking pattern of crystal planes, the photo-generated charge carrier transport and the optoelectronic properties of solar cells.

CPP 14.23 Tue 16:30 CPPp

Energetics of lead halide perovskite precursors in different solvents — •Richard Schier[1], Ana M. Valencia[2], and Caterina Cocchi[2] — [1]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin — [2]Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg

Lead halide perovskites (LHPs) are an emerging class of solution-processed materials with excellent photovoltaic performance. The characterization of LHP precursors in solution is a lively field of research [1,2]. The goal of this work is to understand the formation and stability of LHP precursors with chemical formula PbX_2M_4, where X = Cl, Br, I, and M = ACN, DMF, DMSO, GBL, NMP, PC are common solvents. In the framework of density functional theory coupled to the polarizable continuum model to implicitly simulate the solvent cavity, we calculate and analyze the energetics, the structural properties, and the charge distribution in all these systems. Our calculated formation energies are qualitatively in agreement with earlier reports in the literature [1]. With this systematic study we are able to capture general trends: heavier halide species lead to a lower formation energy; the explicit solvent exerts a clear influence on the energetics, on the Pb-X bond lengths and angle, and on the charge distribution within the complexes.

[1] Radicchi et al., ACS Appl. Energy Mater. 2, 3400 (2019)
[2] A.M. Valencia et al., arXiv2012.08440

CPP 14.24 Tue 16:30 CPPp

Imaging ferroelastic domains in MAPbI3 perovskite via dual frequency resonance tracking PFM — •Ilka Hermes[1] and Romain Stomp[2] — [1]Park Systems Europe, Mannheim, Germany — [2]Zuerich Instruments, Zuerich, Switzerland

Methylammonium lead iodide (MAPbI3)-based photovoltaics have seen an astonishing increase in efficiency due to their unique optoelectronic properties and charge carrier dynamics. Since MAPbI3 crystallizes in a tetragonal perovskite structure, researchers have long suggested that the material features ferroelectricity and -elasticity. These ferroic properties are thought to influence the charge carrier dynamics in MAPbI3 photovoltaics and, therefore, require accurate characterization on the nanoscale, available via piezoresponse force microscopy (PFM). On thin films, a weak piezoresponse often has to be enhanced by driving the electrical excitation of PFM close to the contact resonance of the cantilever. However, the contact resonance depends on a consistent tip-sample contact. Therefore, a high surface roughness or nanomechanical heterogeneities can introduce crosstalk, which exacerbates the data interpretation of the electromechanical sample response. Dual frequency resonance tracking (DFRT) improves the stability of the resonance enhancement via an additional frequency feedback that compensates for shifts in the contact resonance. Here, we demonstrate that DFRT-PFM, available by combining Park Systems atomic force microscopes with Zurich Instruments lock-in amplifiers, not only reduces crosstalk, but also resolves the mechanical contrast on ferroelastic MAPbI3 domains.

CPP 14.25 Tue 16:30 CPPp

In situ phase and texture evolution tracking of the formation of 2-step slot-die coated perovskite by GIWAXS — •Manuel A. Scheel[1], Lennart K. Reb[1], Renjun Guo[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department — [2]DESY, Notkestr. 85, 22607 Hamburg — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite slot-die coating is a particularly promising deposition technique for hybrid perovskite materials. With the perovskite absorber being the key material in a perovskite-based solar cell, structure and morphology control during thin-film formation is essential in achieving highly homogeneous and thus high-performing layers. To better understand morphology evolution and crystallization kinetics during film formation, we investigate the conversion of slot-die coated lead iodide and slot-die coated methylammonium iodide to perovskite by in situ grazing-incidence wide-angle X-ray scattering (GIWAXS). In this work we study the thin-film morphology and texture evolution during the conversion process triggered by thermal annealing. We track the phase evolution and their respective crystal orientations over time. As a reference, we investigate spin-cast PbI_2, MAI and $MAPbI_3$ thin-films and look into methodical differences that can influence the film quality.

CPP 14.26 Tue 16:30 CPPp

Optical properties and structure-property relations of lead halide perovskite building blocks in solution — •Giovanni Procida[1], Richard Schier[2], Ana Valencia[1,2], and Caterina Cocchi[1,2] — [1]Institut fur Physik, Carl von Ossietzky Universität Oldenburg — [2]Institut fur Physik and IRIS Adlershof, Humboldt- Universität zu Berlin

Hybrid metal-halide perovskites are among the best solution-processed currently available. Characterizing the optical properties of their building blocks in different solvents is of great relevance to link the behavior of the precursors to the final thin films. Here, we focus on $PbX_2(Sol)_4$ compounds in solution, where X=Cl, Br, and I, and Sol=DMSO, GBL, ACN, DMF, PC, NMP, and, in the first-principles framework of time dependent density functional theory coupled to the polarizable continuum model, we unravel their electronic and optical properties. We find that the energy of the frontier orbitals is modulated by the choice of the solvent. Specifically, electron-withdrawing groups lead to a downshift of both HOMO and LUMO while electron-donating groups give rise to the opposite effect. We also find dependence of the band-gap on the halide species, which in turns influences the energy of the absorption onset.

CPP 15: Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)

Time: Tuesday 17:45–18:30 Location: BPb

Details will be published in a programme update.

CPP 16: Charged Soft Matter - organized by Joachim Dzubiella (Albert Ludwigs University Freiburg, Freiburg)

Time: Wednesday 9:00–15:20 Location: CPPa

Invited Talk CPP 16.1 Wed 9:00 CPPa

Charging Dynamics and Structure of Ionic Liquids in Nanoporous Supercapacitors — •Christian Holm[1], Konrad Breitsprecher[1], and Svyatoslav Kondrat[2,3] — [1]University of Stuttgart, Institute for Computational Physics, Stuttgart, Germany — [2]Department of Complex Systems, Polish Academy of Sciences, Warsaw, Poland — [3]MPI for Intelligent Systems, Stuttgart, Germany

Ionic liquid based nanoporous supercapacitors have recently attracted much attention as energy storage devices with remarkable cyclability and high power and energy densities. However, their use in high-frequency applications might be limited by a relatively slow charging process. In this talk we will first discuss the fluid structure within a slit-pore capacitor system [1] and report on the physics and optimization of charge/discharge cycles [2,3]. We will see that step-voltage charging is slow because the coions become trapped in narrow pores of the supercapacitor electrodes. To avoid such trapping, a slow voltage-sweep charging is considered, which allows to accelerate the overall charging process substantially. We furthermore examine in detail the discharging process, as well. At the end we will report on the effect of nonlinear charging functions.

[1] K. Breitsprecher, M. Abele, S. Kondrat and C. Holm, J. Chem. Phys., 147, 104708 (2017).

[2] K. Breitsprecher, C. Holm, S. Kondrat, ACS nano 12 (10), 9733-9741 (2018) .

[3] K. Breitsprecher et al., Nature Communications 11, 6085 (2020)

CPP 16.2 Wed 9:40 CPPa

Structure and Relaxation Dynamics of an Ionic Liquid in Molecular Scale Confinement. — •Markus Mezger[1], Henning Weiss[1], Julian Mars[1], Hsiu-Wei Cheng[2], Markus Valtiner[2], and Veijo Honkimaeki[3] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]TU Wien, Institute for Applied Physics, Vienna, Austria — [3]ESRF-The European Synchrotron, Grenoble, France

Structure and dynamics of a confined ionic liquids were probed by an in-situ X-ray surface force apparatus in plane-cylinder geometry. Our novel device can shear, compress and decompress soft matter within a precisely controlled slit pore confinement. Complementary structural information is obtained by X-ray scattering and simultaneous force measurements. Here, we present results from the wet ionic liquid $C_{10}mim^+Cl^-$ in its columnar liquid crystalline mesophase. Defect-formation and structural relaxation processes in confinement were studied as reaction to external stimuli. The observed mesoscopic orientation induced by oscillatory shear is explained by the anisotropic mobility of the amphiphilic cations.

Reference: H. Weiss et al., Structure and Dynamics of Confined Liquids - Challenges and Perspectives for the X-Ray Surface Force Apparatus. Langmuir, DOI: 10.1021/acs.langmuir.9b01215 (2019).

CPP 16.3 Wed 10:00 CPPa

Hydrogen Bonding and Charge Transport in a Protic Polymerized Ionic Liquid — •Arthur Markus Anton[1,2], Falk Frenzel[2], Jiayin Yuan[3], Martin Tress[2,4], and Friedrich Kremer[2] — [1]The University of Sheffield, Department for Physics & Astronomy, Sheffield, UK — [2]Leipzig University, Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — [3]Stockholm University, Department of Materials and Environmental Chemistry, Stockholm, Sweden — [4]University of Tennessee Knoxville, Department of Chemistry, Knoxville, USA

Fourier transform infrared and broadband dielectric spectroscopy are combined in order to study hydrogen bonding and charge transport in the protic polymerized ionic liquid PAAPS in a wide temperature range from 170 to 300K. While the former allows to follow the formation of hydrogen bonds, the latter enables to record the complex conductivity in the spectral range from 10-2 to 10+9 Hz. On the one hand, the formation of the H-bond network exhibits a pronounced thermal hysteresis, whereas, on the other hand, the effective conductivity is reversibly affected by temperature. In combination with the fact that the conductivity changes with temperature by orders of magnitude, whereas the integrated absorbance of the N-H stretching vibration(being proportional to the number density of protons in the hydrogen bond network) changes only by a factor of 4, it is concluded that charge transport takes place predominantly due to dynamic glass transition assisted hopping conduction mechanism and is not significantly affected by the establishment of H-bonds.

40 min. meet the speakers - break

Invited Talk CPP 16.4 Wed 11:00 CPPa

Interaction of polyelectrolytes with proteins — •Matthias Ballauff — Institut für Chemie und Biochemie, Freie Universitaet Berlin

Highly charged natural polyelectrolytes as e.g. DNA or heparin play a central role in many biochemical processes and their interaction with proteins is of central importance as shown in a recent review [1]. In this lecture I shall review our studies of the interaction of well-defined synthetic polyelectrolytes with proteins that have been done mainly by calorimetry. There are two main factors that lead to the formation of a complex between a protein and a polyelectrolyte: i) The release of counterions condensed onto the highly charged polyelectrolyte, and ii) The release or uptake of water during complex formation. Systematic studies of the binding constant K_b as the function of temperature and salt concentration allow us to determine the contributions of both effects to the measured free energy of binding. This can be demonstrated by analyzing the binding of model proteins as lysozyme to well-characterized polyelectrolytes as e.g. heparin. The improved understanding of this complex formation may have direct medical implications as e.g. for virus binding to cell surfaces.

[1] K. Achazi, et al., Understanding the Interaction of Polyelectrolyte Architectures with Proteins and Biosystems, Angew. Chem. Int. Ed. 2020, 59, 2-25

CPP 16.5 Wed 11:40 CPPa

Identifying Mg^{2+} binding sites on RNA using MD simulations with accelerating force field parameters — •Kara K. Grotz, Sergio Cruz-León, and Nadine Schwierz — Department of Theoretical Biophysics, Max Planck Insitute of Biophysics, Frankfurt am Main, Germany

Mg^{2+} is one of the most abundant cations in living cells. The interaction between Mg^{2+} and RNA is essential for folding and function of the diverse macromolecule. Mg^{2+} binds specifically and often directly (inner-sphere configuration) to individual functional groups on the RNA. Localizing Mg^{2+} binding sites, however, is challenging as Mg^{2+} is silent in most experimental approaches. Computational studies can contribute molecular insight but often struggle with insufficiently accurate atomistic models (force fields) and time scale limitations due to the slow binding kinetics of Mg^{2+} (millisecond time scale). Herein, we use a recently developed Mg^{2+} force field that is based on ion-water and ion-ion properties of Mg^{2+}. In addition, the parameters are chosen such that they accelerate the water exchange kinetics (nanosecond time scale). Moreover, by incorporating experimental binding affinities towards specific RNA binding positions, we are able to find Mg^{2+} binding sites on RNA using unbiased simulations and observe outer-to-inner sphere transitions directly.

CPP 16.6 Wed 12:00 CPPa

Thermodynamics of Liquid-Liquid Phase Separation: Isothermal Titration Calorimetry of Hyaluronic Acid-Chitosan Coacervates — Fatma Akcay Ogur and •A. Basak Kayitmazer — Department of Chemistry, Bogazici University Istanbul, Turkey

Complex coacervation occurs between two oppositely charged macromolecules which undergo into macroscopic phase separation and form two liquid phases: polyelectrolyte-rich (coacervate) and polyelectrolyte-poor (dilute) liquid phases. Coacervation has several application areas including processed food, cosmetics, paper, textiles, pharmaceutical and food industries. For these industrial applications, coacervation is utilized as a microencapsulation platform for drugs, aromas, odors, and flavors. Recently, liquid-liquid phase separation has been shown to be the driving force for membraneless organelles such as P granulles and nucleoli. In our study, we have studied a model coacervate system composed of two oppositely charged polysaccharides, i.e. namely, hyaluronic acid (HA) and chitosan (CH). Isothermal titration calorimetry (ITC) was employed to understand the thermodynamic characteristics of complex coacervation between these semi-flexible biopolymers. Parameters (molecular weight of polyelectrolytes, pH and ionic strength of the medium, and temperature) that affect coacervation were studied to determine enthalpy change and binding constant of soluble complexes, stoichiometry of soluble complexes and coacervation, and molar heat capacity.

CPP 16.7 Wed 12:20 CPPa

The effects of ethanol and salt on the phase behavior and interactions of aqueous protein solutions — Rajeevann Uthayakumar, •Florian Platten, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

The addition of salts or organic solvents to aqueous protein solutions alters their optical and dielectric properties and the interactions between protein molecules in these mixtures change accordingly. Here, the effects of NaCl and ethanol on the phase behavior and interactions of protein solutions are studied in terms of the metastable liquid-liquid phase separation and second virial coefficient B_2 of lysozyme solutions. The cloud-point temperatures are reduced and raised by the addition of ethanol and salt, respectively. The extended law of corresponding states allows to interpret these trends as changes of B_2. Remarkably, the dependence of B_2 on both salt and ethanol content is quantitatively modelled by the DLVO theory.

CPP 16.8 Wed 12:40 CPPa

Surface morphology of polyelectrolyte multilayer films with short PSS chains in water and air. Determining the surface elasticity of nanofilms — •Amir Azinfar[1], Sven Neuber[1], Jiří Vaněček[2], Marie Vancová[2,3], Jan Sterba[2,3], Vítězslav Straňák[3], and Christiane A. Helm[1] — [1]Institute of Physics - Angewandte Physik, University of Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany — [2]Institute of Parasitology, Biology Centre, Czech Academy of Sciences, Branisovska 31, 37005 Ceske Budejovice, Czech Republic — [3]Faculty of Science, University of South Bohemia, Branisovska 1760, 37005 Ceske Budejovice, Czech Republic

We investigate the surface topology of polyelectrolyte multilayers made by sequential adsorption of polycations (PDADMA) and polyanions (low molecular weight PSS). We observed a buckling pattern of the film surface in air. The surface roughness σ(AFM) in air was always twice as high as in water. For PSS-terminated films, the periodicity of buckling patterns increased with the number of deposited layers from 185 nm to 225 nm. If the multilayer film was terminated with a PDADMA layer, the surface roughness σ(AFM) and the surface periodicity of buckling patterns were always bigger than for films terminated by a PSS layer. This is attributed to the larger surface coverage of PDADMA caused by its small linear charge density. We determined the surface elasticity of the film in non-linear and linear growth regimes by considering the surface strain and surface periodicity, and thus provide a model to explain the increase of periodicity with film thickness.

60 min. meet the speakers - break

CPP 16.9 Wed 14:00 CPPa

Ion Correlations in Polymer Electrolyte-Ionic Liquid Mixtures — •Diddo Diddens[1] and Andreas Heuer[1,2] — [1]Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster — [2]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster

Polymer electrolytes consist of a salt dissolved in a polymer matrix such as poly(ethylene oxide) (PEO). Even though they are safer than conventional liquid battery electrolytes due to their reduced flammability and mechanical stability, their conductivity is still too low for an efficient technological use. To overcome this issue, the use of small molecular shuttles has been proposed [1], in which the cation of an ionic liquid (IL) is functionalized by a small oligoether side chain that can detach the lithium ions from the slow PEO chains. Additionally, dynamically coupling the lithium ions to the IL cations in this way, it is expected that IL and lithium cations move cooperatively in an electric field, giving rise to enhanced transference numbers. In this contribution, we explicitly check this assumption by focusing on dynamical ion correlations within the electrolyte, and on their impact on the lithium transference number as well as the overall conductivity.

[1] D. Diddens *et al.*, *J. Electrochem. Soc.* **2017**, 164, E3225

CPP 16.10 Wed 14:20 CPPa

Local dynamics of ionic liquids studied by ^{2}H NMR — •Elisa Steinrücken, Manuel Becher, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Room Temperature Ionic Liquids (RTIL) are molten salts at ambient temperatures with a low vapour pressure. They are usually glass forming systems with complex and heterogeneous molecular dynamics. The combination of different cations and anions opens wide ranges of chemical and physical applications. Hence, a fundamental understanding of molecular dynamics is of crucial importance. Here, RTILs consisting of imidazole-based cations and $[Tf2N]^-$ or $[BF_4]^-$ anions are in the experimental focus. Nuclear Magnetic Resonance (NMR) provides access to dynamics in wide ranges of time and length scales [M. Becher, E. Steinrücken, M. Vogel, J. Chem. Phys., 2019]. Due to its isotope selectivity the dynamical behaviour of the two components can be distinguished. Performing ^{2}H NMR experiments on selectively deuterated cations, we gain deep insights into their microscopic rotational dynamics. When combining ^{2}H spin-lattice relaxation (SLR) and stimulated-echo (STE) experiments, rotational correlation times of the cation are accessible from the fast motion in the liquid to slow glassy dynamics. Furthermore, we exploit that STE experiments and ^{2}H line-shape analysis provide information about the mechanism for rotational motion. Altogether, we show that application of ^{2}H NMR to RTIL has a high potential for the characterization of time scales and motional mechanisms of the molecular dynamics.

CPP 16.11 Wed 14:40 CPPa

Chain length dependent structure and dynamics of imidazolium based ionic liquids mixtures with water. — •Sebastian Kloth and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

With the huge amount of possible combinations, ionic liquids can be tailored to different properties and applications. In particular, the application as a "green" solvent is of high interest. For this a fundamental understanding of structure and dynamics on the composition of the ionic liquid is needed. Moreover it is important to analyze of the properties in mixtures with other substances, in particular water. To obtain a better understanding of these properties we perform molecular dynamics simulations. The studied ionic liquids are made of 1-alkyl-3-methylimidazolium cations and BF_4 or NO_3 anions and contain water. As in previous studies [1,2] we analyze structure and dynamics on various length scales, but this time for different alkyl chain lengths and water mole fractions. Of special interest are two properties of the mixtures. First, the existence of structural inhomogeneity and second, the transport between different clusters. Thus, our approach enables detailed insights into structure-dynamics relations in ionic liquids.

[1] Pal, T. et al., ChemPhysChem, 18 (16), **2017**
[2] Pal, T. et al., J. Chem. Phys., 150 (12), **2019**

CPP 16.12 Wed 15:00 CPPa

Correlation Length in Concentrated Electrolytes: Insights from All-Atom Molecular Dynamics Simulations — Samuel W. Coles[1], •Chanbum Park[2,3], Rohit Nikam[2,3], Matej Kanduč[2,4], Joachim Dzubiella[2,5], and Benjamin Rotenberg[1] — [1]Sorbonne Université, CNRS, Physicochimie des électrolytes et nanosystèmes interfaciaux, UMR PHENIX, 4 pl. Jussieu, F-75005, Paris, France — [2]Research Group for Simulations of Energy Materials, Hahn-Meitner-Platz 1, D-14109, Berlin, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489, Berlin, Germany — [4]Jožef Stefan Institute, Jamova 39, SI-1000, Ljubljana, Slovenia — [5]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104, Freiburg, Germany

We study the correlations length of the charge-charge pair correlations in concentrated electrolyte solutions by means of all-atom, explicit-solvent molecular dynamics simulations. We investigate LiCl and NaI in water, as well as two more complex, molecular electrolyte systems of LiTFSI, in water and in DME/DOL. We observe a Debye-Hückel like regime at low concentration, followed by a minimum reached when $d/\lambda_D \simeq 1$, where λ_D is the Debye correlation length and d the effective ionic diameter, and an increasing correlation length with salt concentration in very concentrated electrolytes. As in the experiments, we find that the screening length in the concentrated regime follows a universal scaling law as a function d/λ_D for all studied salts. However, the scaling exponent is significantly lower than the experiments.

CPP 17: Theorie and Simulation - organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden) (joint session CPP/DY)

Time: Wednesday 9:00–14:40 Location: CPPb

Invited Talk CPP 17.1 Wed 9:00 CPPb

Data-driven methods in polymer physics: exploring the sequence space of copolymers — •Marco Werner — Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Germany

Automated experiments and computer simulation on highly parallel machines push the limits of available data in the field of soft matter. For long polymer chains, however, any data set can cover only a marginal fraction of the giant chemical space and conformation space involved. In this talk, data-driven strategies are discussed that allow to trace hidden physical patterns in both giant spaces by machine learning algorithms. The discussion is centered on the example of hydrophilic / hydrophobic copolymers and their interaction with lipid membranes. A neural network has been trained to predict the free energy landscape near a membrane as a function of the copolymer sequence. The information learned in the hidden neural layers showed that the neural network compressed the sequence space into physically meaningful latent variables. The learned semantics was transferable between simulation data with different levels of coarse-graining, and allowed for a physics-informed inverse search for the copolymer sequence leading to the smallest translocation time through the membrane.

CPP 17.2 Wed 9:40 CPPb

Prediction of iSCFT chemical potentials via machine learning — •Lucia Milena Wesenberg, Ludwig Schneider, and Marcus Müller — Institute for Theoretical Physics, Georg-August University Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

We explore the use of machine learning to enhance the simulation of polymeric nanostructures. Self-assembly of symmetric diblock copolymers is the chosen testing system for this purpose. Such polymers consist of two equally long blocks of different monomer types. As the two monomer types are incompatible but linked in the center of each polymer, microphase separation occurs.

Simulations of such systems often pose a challenge for particle-based models as large systems and concomitantly long time scales need to be simulated. Thus, continuum models are employed, where the dynamics can be conceived as the relaxation towards the local minimum of a free-energy basin and jumps between such basins. These models reduce the degrees of freedom by integrating out the molecular degrees of freedom. The most detailed continuum model investigated here is the Self-Consistent Field Theory (SCFT). Unfortunately, dynamic SCFT requires the chemical potential of a non-equilibrium morphology that is computationally expensive to obtain. The SCFT potential calculation is an iterative process, and the stability of the algorithm depends heavily on the starting conditions. Our machine learning approach provides suitable initial conditions for the algorithm. The predicted starting conditions reduce the computational effort considerably.

CPP 17.3 Wed 10:00 CPPb

Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning: A Case Study for Amorphous and Liquid Hafnium dioxide — •Anand Narayanan Krishnamoorthy[1,2], Ganesh Sivaraman[3], Matthias Baur[1], Christian Holm[1], Chris Benmore[6], Marius Stan[4], Gabor Csanyi[5], and Álvaro Vázquez–Mayagoitia[7] — [1]Institute for Computational Physics, University of Stuttgart — [2]Helmholtz Institute Muenster — [3]Leadership Computing Facility, Argonne National Laboratory - USA — [4]Applied Materials Division, Argonne National Laboratory, USA — [5]Department of Engineering, University of Cambridge, UK — [6]X-ray Science Division, Argonne National Laboratory, USA — [7]Computational Science Division, Argonne National Laboratory, USA

We propose a novel active learning scheme for automatically sampling a minimum number of uncorrelated configurations for fitting the Gaussian Approximation Potential (GAP). We apply this scheme to a Hafnium dioxide (HfO2) dataset generated from a melt-quench ab initio molecular dynamics (AIMD) protocol. Our results show that the active learning scheme, with no prior knowledge of the dataset is able to extract a configuration that reaches the required energy fit tolerance. Further, molecular dynamics (MD) simulations performed using this active learned GAP model on 6144-atom systems of amorphous and liquid state elucidate the structural properties of HfO2 with near ab initio precision and quench rates (ie 1.0 K/ps) not accessible via AIMD.

40 min. meet the speakers - break

CPP 17.4 Wed 11:00 CPPb

BoltzmaNN: Heuristic inverse design of pair potentials using neural networks — •Fabian Berressem, Mihir Khadilkar, and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University Mainz, Germany

In this work, we investigate the use of neural networks (NNs) to devise effective equations of state from a given isotropic pair potential using the virial expansion of the pressure. We train the NNs with data from molecular dynamics simulations, sampled in the NVT ensemble at densities covering both the gas- and liquid-like regime. We find that the NNs provide much more accurate results compared to the analytic estimate of the second virial coefficient derived in the low density limit. Further, we design and train NNs for computing the potential of mean force from the radial pair distribution function, g(r), a procedure which is often performed for coarse-graining applications. Here, we find that a good choice for the loss function is crucial for an accurate prediction of the pair potentials. In both use cases, we study in detail how providing additional information about forces and the density impacts the performance of the NNs. We find that including this additional information greatly increases the quality of the predictions, since more correlations are taken into account. Further, the predicted potentials become smoother and are in general much closer to the target potential.

CPP 17.5 Wed 11:20 CPPb

PolyEC - an event-chain framework — •Tobias A. Kampmann, David Müller, and Jan Kierfeld — TU Dortmund University, Germany

PolyEC is a MC event chain framework suitable for simulation of various colloidal systems. We focus on modularity and extensibility to simulate heterogenous systems. In event-chain simulations only one particle is active and interactions can be treated independently by factorization, which allows for a highly modular approach for particlebased simulations. Albeit ECMC is a montecarlo method, a single event-chain is deterministic (although there are modifications where this is not true). One crucial feature of this method is that each state a piece-wise deterministic event-chain visits between events are properly (Boltzmann-) weighted. This opens the possibility to measure observables like pressure or the distribution of energy on the fly. As examples we show needle-colloid mixtures and an active particle system.

Invited Talk CPP 17.6 Wed 11:40 CPPb

Structure formation in drying films and droplets — •Arash Nikoubashman[1], Michael Howard[2], Michael Kappl[3], and Hans-Jürgen Butt[3] — [1]Johannes Gutenberg University Mainz, Mainz, Germany — [2]Auburn University, Auburn (AL), USA — [3]Max Planck Institute for Polymer Research, Mainz, Germany

Drying complex liquids are encountered in many technologies, including painting, manufacturing polymer LED displays, and spraying pesticides. Here, colloids and/or polymers are typically initially dispersed in a solvent such as water, which then evaporates, leaving behind a dried residue. Our recent simulations and experiments of drying bidisperse suspensions revealed that sufficiently fast evaporation could induce spatial segregation of the two species, with the smaller ones accumulating at the liquid-air interface followed by a homogeneously mixed region of small and big particles. To understand this counter-intuitive behavior, we conducted particle-based simulations and dynamic density functional theory calculations, with and without hydrodynamic interactions. According to our model calculations, this drying-induced segregation occurs due to a local increase of the solute concentration near the film-air interface, resulting in a chemical potential gradient for both species; typically, this gradient is steeper for the larger particles, leading to a stronger force pushing them away from the liquid-air interface. Segregation then occurs if the mobility of the larger particles decreases slower than the driving force increases. Comparing the various simulations and experiments, we found that including hydrodynamics can decrease or even completely suppress the segregation.

CPP 17.7 Wed 12:20 CPPb

Structure of bottlebrush polymers end-grafted to a planar surface — •Jaroslaw Paturej[1], Paul Jungmann[2], Jens-Uwe Sommer[3], and Torsten Kreer[2] — [1]University of Silesia, Katowice, Poland — [2]IPF, Dresden, Germany — [3]Johannes Gutenberg Universität, Mainz, Germany

Polymer brush is a hybrid material composed of a solid substrate coated with end-grafted polymers. We conducted coarse-grained molecular dynamics simulations and scaling theory of the equilibrium structure of planar brushes formed by bottlebrush polymers. Bottlebrushes are branched macromolecules consisting of densely spaced linear side chains grafted along a central (linear) backbone. We elucidate the relationship between bottlebrush architecture, surface coverage σ and polymer brush thickness H. We study the impact of three length scales on the brush height H: D_0 , the cross-section radius of bottlebrushes determined by the degree of polymerization of side chains N_{sc} , R_0 the (overall) size of bottlebrushes controlled by the degree of polymerization of backbone N_{bb} and d the distance between nearest-neighbor tethering sites. The latter quantity provides a measure of molecular coverage σ of a substrate defined as the number of bottlebrush polymers per unit surface area $\sigma \propto 1/d^2$. Our theoretical anal-

ysis identifies three conformational regimes for the height H, which gradually establish upon increasing substrate coverage and stem from interplay between relevant length scales: d, D_0 and R_0.

CPP 17.8 Wed 12:40 CPPb

Thermal conductivity of commodity plastics: From conventional to smart polymers — •Debashish Mukherji — Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver Canada

Polymers are an important class of soft matter whose properties are dictated by large fluctuations. Because of this reason commodity polymers are ideal for the flexible design of advanced materials. However, applications of polymers are often hindered by their low thermal conductivity κ. While low κ values are desirable for thermoelectric materials, they create severe problems when used under the high temperature conditions. Going from the polymers dictated by weak Van der Waals to hydrogen-bonded interactions, κ varies between 0.1-0.4 W/Km. Using molecular dynamics simulations we study thermal transport and its links to the elastic response of polymers. We find that there exists a maximum attainable stiffness, thus limiting an upper bound of κ. The specific chemical details and the glass transition temperature play no role in controlling κ, especially when the microscopic interaction is hydrogen bonded. These results are consistent with the minimum thermal conductivity model and experiments.

[1] D. Mukherji, C. M. Marques, K. Kremer, Annual Review of Condensed Matter Physics 11, 271 (2020). [2] D. Bruns, T. E. de Oliveira, J. Rottler, D. Mukherji, Macromolecules 52, 5510 (2019). [3] C. Ruscher, J. Rottler, C. Boott, M. J. MacLachlan, D. Mukherji, Physical Review Materials (accepted) (2019).

60 min. meet the speakers - break

CPP 17.9 Wed 14:00 CPPb

Polymer Architectures by Chain Walking Catalysis - Theory, Simulations, and Experiments — •Ron Dockhorn[1], Laura Plüschke[1,2], Albena Lederer[1,2], Jan Merna[3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]University of Chemistry and Technology Prague, CZ-16628 Praha, Czech Republic

Recently developed chain walking catalysis is an elegant approach to synthesize branched polyethylenes (CWPE) with controllable structure and properties. The catalyst is able to walk along the polymer and to polymerize ethylene and α-olefines into complex topologies depending on pressure, temperature, and olefine concentration introducing branch-on-branch structures. Coarse-grained Monte Carlo simulations utilizing the bond fluctuation model of the CWPE are performed to investigate the influence of the walking mechanism on the polymer architecture. For slow walking rates the structure growths with linear chain extensions, whereas fast walking rates promote dendritic growth of the polymer. The crossover regime is characterized by linear global features and dendritic local substructures contrary to randomly hyperbranched systems. Indeed, the obtained CWPE systems have characteristics of dendritic bottle brushes and the degree of branching can be adjusted by the walking rate of the catalyst. These findings are aimed to understand the physical properties of the CWPE structures and to improve the synthesis of a new class of hyperbranched molecules.

CPP 17.10 Wed 14:20 CPPb

Mechanics of shape-shifting droplets — •Ireth Garcia-Aguilar[1], Piermarco Fonda[1], Eli Sloutskin[2], and Luca Giomi[1] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Department of Physics and Institute of Nanotechnology & Advanced Materials, Bar-Ilan University, Ramat-Gan, Israel

It has been long understood that dispersed liquid droplets are spherical in order to minimize the tension at their interface. Surprisingly, oil emulsion droplets in water have been observed to spontaneously deform into polyhedral shapes when cooling down the system. The equilibrium shape of a droplet at some temperature depends on its initial volume but all deformations take place below the freezing point of the surfactant monolayer, while the bulk oil and water remain liquid. The frozen interface forms an hexagonal lattice which is topologically constrained to accommodate defects. These produce large stresses that induce in and out-of-plane deformations in the crystal which in turn are opposed by the interfacial tension between oil and water. Initially, it was thought that this competition determines the droplet shape; however, this alone can not explain the size dependence of the deformations. By modeling the interface as a 2D elastic surface and studying its equilibrium geometry, we found a mechanism that explains the size-scaling behaviour. Interestingly, crystalline defects are not the only peculiarity playing a role in shaping the droplets.

CPP 18: Complex Fluids and Soft Matter 1 (joint session DY/CPP)

Time: Wednesday 9:00–10:30 Location: DYa

See DY 35 for details of this session.

CPP 19: Glasses and Glass Transition 1 (joint session DY/CPP)

Time: Wednesday 9:30–10:30 Location: DYc

See DY 39 for details of this session.

CPP 20: Complex Fluids and Soft Matter 2 (joint session DY/CPP)

Time: Wednesday 11:00–13:00 Location: DYa

See DY 40 for details of this session.

CPP 21: Glasses and Glass Transition 2 (joint session DY/CPP)

Time: Wednesday 11:00–13:00 Location: DYc

See DY 42 for details of this session.

CPP 22: Poster Session III - Charged Soft Matter and Theory and Simulation

Time: Wednesday 16:30–18:30 Location: CPPp

CPP 22.1 Wed 16:30 CPPp

In-situ investigation of the thermal stability of thermoelectric thin films based on ionic liquid post-treated PEDOT:PSS — •Anna Lena Oechsle[1], Julian E. Heger[1], Nian Li[1], Shanshan Yin[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]ELETTRA Sincrotrone Trieste S. C. p. A., 34149 Basovizza TS, Italy — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

In total around 66% of the global produced primary energy is lost as waste heat, for example from industrial or everyday life processes. Thermoelectric generators, as they enable the direct conversion of a temperature gradient into electrical power, are therefore considered a promising technique to recycle these large amounts of heat waste. Especially, organic thermoelectric polymers are attractive, owning some advantages like low cost, lightness and high mechanical flexibility, low or no toxicity, as well as a usually low thermal conductivity. In our work we research the positive effect of ionic liquid (IL) treatment on the

thermoelectric properties of semi-conducting PEDOT:PSS thin films. Therefore, we measure parameters, like the Seebeck coefficient, electrical conductivity, and furthermore examine the inner film morphology with scattering techniques like grazing incidence small angle x-ray scattering (GISAXS). In addition to find the influence of ILs treatment on the morphology-function relation of the PEDOT:PSS thin films, we also investigate the thermoelectric performance stability these films under operation at elevated temperatures.

CPP 22.2 Wed 16:30 CPPp

Structural and Dynamic Insights in the Conduction of Lithium-Ionic-Liquid Mixtures in Nanoporous MOFs as Solid-State Electrolyte — Micaela Vazquez[1], •Modan Liu[2], Zejun Zhang[1], Abhinav Chandresh[1], Anemar Bruno Kanj[1], Wolfgang Wenzel[2], and Lars Heinke[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Metal-organic framework (MOF) based separators in Li-ion-battery (LIB) help stabilize the solid electrolyte interphase and strongly affect the battery performance. The mobility and conduction of the Lithium-ion and organic ionic liquids (ILs) in these materials is crucially dependent on the MOF structures and the IL loading factors.

Here, via both experiments and all-atom molecular dynamics (MD) simulations, we observe complex conduction behaviors of Li-IL in the MOF with loading and composition dependence, particularly the presence of Li-ion prevents the conductivity collapse at high IL loading. MD reveals a vehicular transport for the IL and a Grotthuss-like conduction for Li-ions. At small pore fillings, the Li conduction is limited by the large separation between anions. At high pore fillings, the conduction is governed by the bunching of IL. In contrast to the Li-free IL, the bunching effect is attenuated by the formation of charge-neutral Li-anion complexes, which results in a tremendously increased conductivity at maximum filling. This tuning mechanism may contribute to development of advanced batteries.

CPP 22.3 Wed 16:30 CPPp

Quantitative prediction of charge regulation in peptides and model ampholytes — •Peter Košovan, Raju Lunkad, Anastasiia Murmiliuk, Pascal Hebbeker, Zdeněk Tošner, and Miroslav Štěpánek — Department of Physical and Macromolecular Chemistry, Charles University

Weak ampholytes are ubiquitous in nature and commonly found in artificial pH-responsive systems. However, our limited understanding of their charge regulation and the lack of predictive capabilities hinder the bottom-up design of such systems. Here, we used a coarse-grained model of a flexible polymer with weakly ionisable monomer units to quantitatively analyse the ionisation behaviour of two oligopeptidesmodel ampholytes. Our simulations predict differences in the charge states between oligopeptides and monomeric amino acids, showing that not only electrostatic interactions between charged groups but also conformational flexibility plays a key role in the charge regulation. By comparing our simulations with experimental results from potentiometric titration, capillary zone electrophoresis and NMR, we demonstrated that our model reliably predicts the charge state of various peptide sequences. Ultimately, our simulation model is the first step towards understanding the charge regulation in flexible ampholytes, and towards predictive bottom-up design of charge-regulating systems.

CPP 22.4 Wed 16:30 CPPp

Investigating the surface charge of microplastic particles with Colloidal Probe-Atomic Force Microscopy — •Thomas Witzmann and Andreas Fery — Leibniz-Institute of Polymer Research Dresden, Germany

To date, plastic particles have mainly been categorized by polymer type, shape, and size. But there is another important issue arising when investigating microplastic and its interaction with cells. With decreasing size, the surface-volume ratio increases which makes surface properties more important to consider. It is generally believed that the surface properties of the particles influence the cell interaction. Therefore, we investigated un-functionalized polystyrene particles with the size of 3 micrometer with different surface properties of two different manufactures. We found out that the cellular interaction and uptake of microplastic particles (polystyrene) differs for the two particle types. Using Colloidal Probe-Atomic Force Microscopy (CP-AFM) we could show a significant difference in the electric surface properties: homogeneously charged particles vs. heterogeneously charged particles. The heterogeneous surface charge manifests itself in an electrostatic interaction of the particles that depends on the mutual orientation of the particles. CP-AFM is therefore a magnificent tool to obtain additional information*s about surface charge and its distribution on microplastic particles.

CPP 22.5 Wed 16:30 CPPp

Investigation of Cononsolvency Phase Transition of Poly(sulfobetaine)-based Diblock Copolymer Thin Films — •Peixi Wang[1], Christina Geiger[1], Lucas P. Kreuzer[1], Tobias Widmann[1], Suzhe Liang[1], Robert Cubitt[2], André Laschewsky[3], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]Technische Universität München, Garching, Germany — [2]Institut-Laue-Langevin, Grenoble, France — [3]Universität Potsdam, Potsdam-Golm, Germany

Co-nonsolvency occurs if a mixture of two good solvents causes the collapse or demixing of polymers into a polymer-rich phase in a certain range of compositions of these two solvents. The nonionic thermo-responsive polymer, poly(N-isopropylmethacrylamide) (PNIPMAM), has been widely used to investigate its collapse transition behavior in a mixture of two competing good solvents. However, co-nonsolvency response of its block copolymer containing the zwitterionic poly(sulfobetaine)s, especially poly(4-((3-methacrylamidopropyl)dimethyllammonio)butane-1-sulfonate)) (PSBP), shows a strong swelling transition in aqueous media, is newly studied. We focus on the co-nonsolvency behavior of PSBP-b-PNIPMAM thin films in water/acetone mixtures by in situ time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance (SR). Furthermore, Fourier transform infra-red (FTIR) spectroscopy is applied to investigate the interactions between the polymer thin film and water/co-solvent, which strongly alters dependend on their deuteration level.

CPP 22.6 Wed 16:30 CPPp

ToF-NR investigation of cononsolvency in PNIPAM-based block-copolymer thin films — •Christina Geiger[1], Julija Reitenbach[1], Lucas P. Kreuzer[1], Tobias Widmann[1], Peixi Wang[1], Robert Cubitt[2], Cristiane Henschel[3], André Laschewsky[3], Christine M. Papadakis[4], and Christina Geiger[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Institut Laue-Langevin, 38000 Grenoble, France — [3]Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam, Germany — [4]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

The diblock copolymer PMMA-b-PNIPAM forms micelles in aqueous solution that exhibit a reversible shell collapse transition at the lower critical solution temperature (LCST). Apart from a temperature stimulus, the collapse can be induced by the addition of organic co-solvents due to the competitive attachment and detachment of water and co-solvent to the PNIPAM chains. We demonstrate that the co-nonsolvency effect is transferrable from solutions to thin film systems. The film swelling and contraction kinetics due to the uptake of water and co-solvent via solvent vapors are investigated with a focus on time-of-flight neutron reflectometry (ToF-NR). Sequential contrasting experiments using protonated and deuterated compounds are performed to differentiate between the distributions of water and co-solvent within the polymer films.

CPP 22.7 Wed 16:30 CPPp

Layer-by-layer Spray-oating of Cellulose Nanofibrils and Silver Nanoparticles for Hydrophilic Interfaces — •qing chen[1,2], calvin brett[1,3], andrei chumakov[1], marc gensch[1,4], matthias schwartzkopf[1], volker körstgens[4], daniel söderberg[3], anton plech[5], peng zhang[6], peter müller-buschbaum[4], and stephan roth[1,3] — [1]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [2]University of Science and Technology of China, 230026 Hefei, China — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [4]Technische Universität München, 85748 Garching, Germany — [5]Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [6]Sun Yat-sen University, 510275 Guangzhou, China

Silver nanoparticles (AgNPs) and AgNP-based composite materials have attracted growing interest due to their structure-dependent optical, electrical, catalytic and stimuli-responsive properties. In this work, the fabrication of AgNP/cellulose nanofibril (CNF) thin-films via layer-by-layer (LBL) spray-coating is reported. The CNF substrate contributes to a more uniform distribution of AgNPs by its network structure, and by absorbing the partially dissolved AgNP agglomerates. Our approach provides a platform for a scalable production of AgNP/CNF films with low agglomeration rate by two different methods: (1) multi-step layer-by-layer (LBL) spray coating; and (2) direct spray coating of the AgNP/ CNF mixture. We also obtained a uniform AgNP layer with tailorable wettability and plasmonic properties, suggesting their potential applications in anti-fouling coatings and label-free biosensors.

CPP 22.8 Wed 16:30 CPPp

Charge-Dependent Microphase Separation in Thin Films from a Multiresponsive Pentablock Quaterpolymer — •Florian A. Jung[1], Dorthe Posselt[2], Detlef-M. Smilgies[3], Panayiota A. Panteli[4], Constantinos Tsitsilianis[5], Costas S. Patrickios[4], and Christine M. Papadakis[1] — [1]Physics Department, Soft Matter Group, Technical University of Munich, Garching, Germany — [2]Department of Science and Environment, Roskilde University, Roskilde, Denmark — [3]Wilson Laboratory, Cornell University, Ithaca, USA — [4]Department of Chemistry, University of Cyprus, Nicosia, Cyprus — [5]Department of Chemical Engineering, University of Patras, Greece

Multiblock copolymers and block copolymers with charged segments are attractive candidates for tunable self-assembly of complex morphologies, but their understanding is still at an early stage. In this contribution, we present an investigation of the self-assembly behavior of a pentablock quaterpolymer with (C- *co*-D)-

A-B-A-(C- *co*-D) architecture containing ionizable A blocks in thin films using grazing-incidence small-angle X-ray scattering (GISAXS). The two-dimensional scattering patterns were analyzed using simulations combined with a multi-step fitting procedure. Furthermore, we performed in-situ swelling experiments to explore the impact of solvents with different selectivities and polarities on the morphology. We find that varying the degree of ionization of the ionizable blocks allows altering of the segregation strength between the blocks. The nature of the solvent used for swelling gives the opportunity to tune the structures in a wide range.

CPP 22.9 Wed 16:30 CPPp

Hybrid Energy Harvester based on Triboelectric Nanogenerator and Solar Cell — •Tianxiao Xiao[1], Wei Chen[1], Wei Cao[1], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TUM, Garching, Germany — [2]DESY, Hamburg, Germany — [3]KTH, Stockholm, Sweden — [4]MLZ, Garching, Germany

Developing clean energy lies the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easily fabricated, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dots (QDs) based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 22.10 Wed 16:30 CPPp

Dynamics in polymer-fullerene blends for photovoltaic applications — •Dominik Schwaiger[1], Wiebke Lohstroh[2], and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien James-Franck-Straße 1, 85748 Garching — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed and excitons are created. After diffusion to a donor-acceptor interface, the excitons are dissipated and charge carriers can be extracted from the electrodes. A promising low-bandgap electron donor material is the conjugated polymer PTB7. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited. We investigated films of PTB7, the fullerene derivate PCBM and different blends of these two, prepared out of chlorobenzene solutions. Quasielastic neutron scattering experiments were done at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching). Hydrogen dynamics of pure compounds as well as the blend films are investigated on a pico- to nanosecond timescale in a temperature range from 150 K to 400 K. Results are set into context of photovoltaic performance studies and increase the knowledge base, which is needed for the design of new materials to push the field of organic photovoltaics.

CPP 22.11 Wed 16:30 CPPp

CNF thin films as sustainable carrier material and their functionalization for energy applications — •Marie Betker[1,2], Constantin Harder[1,3], Marc Gensch[1,3], Calvin Brett[1,2], Matthias Schwartzkopf[1], Andrei Chumakov[1], Qing Chen[1], Daniel Söderberg[2], and Stephan Roth[1,2] — [1]Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, Teknikringen 8, 10044 Stockholm, Sweden — [3]Physik-Department E13, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Sustainable carrier materials will play an important role in the design of future functional items. One matching candidate for that purpose are cellulose nanofibrils (CNF) with their many beneficial properties: It is lightweight, transparent, flexible and recyclable, and can therefore be used as template for thin-film applications. Spray deposition is a suitable technique to fabricated thin, homogeneous films of large scale and with a ultra-low roughness, which make it fitting for industrial applications. It can also be used to functionalize and thus to implement functional, nanostructured films and multi-component systems. The deposition of conductive silver nanowires as flexible electrodes, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate as blocking layer and of the photoactive layer poly(3-hexylthiophene) and [6,6]-phenyl C61-butyric acid methylester on nanostructured CNF thin films was studied in situ using GISAXS. Important insights into possible templating effects of CNF and into the interactions between the CNF-layers and the functional materials could be gained.

CPP 22.12 Wed 16:30 CPPp

Oxygen plasma effects on the nanoscale morphology of polyzwitterion-gold interfaces during gold sputtering — •Apostolos Vagias[1,2], Simon J. Schaper[1], Julian E. Heger[1], Yuqin Zou[1], Shanshan Yin[1], Christina Geiger[1], Matthias Schwartzkopf[3], Marc Gensch[1,3], André Laschewsky[4,5], Stephan V. Roth[3,6], and Peter Müller-Buschbaum[1,2] — [1]Fachgebiet Physik weicher Materie/Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), D-22607 Hamburg, Germany — [4]Institut für Chemie, Universität Potsdam,14476 Potsdam-Golm, Germany — [5]Fraunhofer Institut für Angewandte Polymerforschung IAP, 14476 Potsdam-Golm, Germany — [6]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Sulfobetaine-based polyzwitterions are efficient interlayers for organic photovoltaics, but their polymer-metal interfacial morphology remains elusive. Moreover, plasma pretreatment of organic solar cells can bypass operational degradation from prolonged light exposure. By in-situ grazing incidence small angle X-ray scattering, we probe the evolution of gold cluster growth on thin polysulfobetaine films during metal sputtering, the latter being an industrially-relevant metal deposition technique. We present differences on the sputtered gold nanostructural morphology with and without oxygen plasma pretreatment.

CPP 22.13 Wed 16:30 CPPp

Morphology investigation of the active layer of hybrid solar cells with TOF-GISANS — •Volker Körstgens[1], Lautaro Diaz Piola[1], Christina Geiger[1], Julian Heger[1], Lucas Kreuzer[1], Anna-Lena Oechsle[1], Tobias Widmann[1], Matthias Nuber[2], Klara Stallhofer[2], Gaetano Mangiapia[3], Hristo Iglev[2], Reinhard Kienberger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Physik Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching — [3]Helmholtz-Zentrum Geesthacht am Heinz Maier- Leibnitz Zentrum, Lichtenbergstr. 1, 85747 Garching

One aspect for the development of non-conventional solar cells should be the sustainability of the production process of devices. Following this idea, we developed hybrid solar cells which can be processed out of aqueous solution. The active layer of these devices is based on laser-processed titania nanoparticles dispersed in a water-soluble thiophene-based polyelectrolyte. The active layers were produced with two of the most common deposition techniques: spray deposition and slot die coating. With these techniques the thickness of layers can be easily controlled and the scale-up toward the coating of large areas is done with low effort. We investigated the morphology of the deposited active layers with time of flight - grazing incidence small angle neutron scattering (TOF-GISANS). The difference of the morphology of these layers is presented and its impact on the performance of devices is discussed.

CPP 22.14 Wed 16:30 CPPp

In-situ GISAXS Investigation of Sprayed Drugs on a Cellulose Based Matrix — •Elisabeth Erbes[1,2], Naireeta Biswas[1,2], Stephan V. Roth[1,3], Simone Techert[1,2], Matthias Schwartzkopf[1], Calvin Brett[1,6], Jose Velazquez Garcia[1], Sreevidya Thekku Veedu[1], Korneliya Goordeyeva[3], Andrei Chumakov[1], and Peter Müller-Buschbaum[4,5] — [1]DESY, 22607 Hamburg, Germany — [2]Institute for X-ray Physics, Goettingen University, 37077 Goettingen, Germany — [3]Department of Fibre and Polymer Technology, KTH, 100 44 Stockholm, Sweden — [4]Department of Physics, Technical University Munich, 85748 Garching, Germany — [5]MLZ, Technical University Munich, 85748 Garching, Germany — [6]Department of Mechanics, KTH, 100 44 Stockholm, Sweden

These experiments show the first steps to a novel drug carrier strategy for a controlled dosage of anti-COVID-19 drugs. The drugs were embedded into a matrix made of a mixture of hydrophilic carboxymethylated nanocellulose (CMC) hydrogel and disordered hydrophobic peptide hydrogel (P). This gives the opportunity to vary the local uptake in hydrophobic or hydrophilic compartments in the matrix. The structural intercalation and the time-resolved process were investigated with in-situ grazing incidence small angle X-ray scattering (GISAXS) experiments. By using the spraying technique the drug concentration can be tuned for a personalized treatment of the patients. This poster focuses only on the structural change analysis of the CMC fibers. For the analysis of the peptide part please see the poster of Naireeta Biswas.

CPP 22.15 Wed 16:30 CPPp

Wrinkled Functional Hybrid Multilayers Between Order and Disorder — •Lukas Wolfram[1], Regine Frank[1,2], and Thomas Fuhrmann-Lieker[1] — [1]Institute of Chemistry, University of Kassel, Germany — [2]Department of Physics and Astronomy, Rutgers, the State University of New Jersey, USA

Multilayer systems of thin films give the opportunity to produce self-structured surfaces via thermal annealing. The corrugations build, so-called wrinkles, are

directional isotropic. Wrinkles can be compared to the surface structure of raisins, compressed tissues, or mountain ranges. A possible application for these structures in thin film technology is the use as a periodic random resonator [1] or previously shown by N.M. Hoinka with spiro compounds.

This Poster will present the first results in testing for a proper mate-rial system. So far, experiments with spiro bilayers showed wrinkling over a wide range of surface area. The use of a metallic layer sputtered in a magnetic field can be used to align wrinkles parallel in sucha system.My work concentrates on the conditions causing random lasing in these systems and whether there is any systematic correlation existing between the sample morphology and the spectrum observed. For this purpose, python scripts were written to analyse the shape of the corrugation and their directionality to correlate them with imaged spectra in the future.

[1] Shen, Z. *et al.*, Appl. Phys. Lett. 105, 021106, **(2014)**.
[2] N. M. Hoinka, Doctoral Thesis, **2020**.

CPP 22.16 Wed 16:30 CPPp

Co-nonsolvency-type behavior of a poly(sulfobetaine) and a poly(N-isopropylmethacrylamide) thin film in water / methanol vapor — •Lucas P. Kreuzer[1], Christoph Lindenmeier[1], Christina Geiger[1], Tobias Widmann[1], Viet Hildebrand[2], André Laschewsky[2], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik- Department, LS Funktionelle Materialien, 85748 Garching — [2]Universität Potsdam, Institut für Chemie, 14476 Potsdam Golm

The behavior of a poly(sulfobetaine) (PSPE) and a poly(Nisopropylmethacrylamide)(PNIPMAM) thin film in pure water and in mixed water/methanol vapor is studied in-situ with spectral reflectance and Fourier-transform infrared spectroscopy. While PSPE is insoluble in methanol, PNIPMAM is soluble but exhibits a co-nonsolvency behavior in water/methanol mixtures. In thin film geometry, both the PSPE and PNIPMAM swell in pure water vapor, while upon methanol addition, they contract. Their behavior differs significantly regarding the amount of absorbed water in pure water vapor, and the contraction mechanism in mixed water/methanol vapor. The PSPE thin film shows an abrupt one-step contraction, while the PNIPMAM contraction occurs in two steps. When changing to a pure methanol vapor, both, the PSPE and PNIPMAM thin film, show a higher swelling degree than in mixed water/methanol vapor, which indicates a co-nonsolvency-type behavior in polymer thin films.

CPP 22.17 Wed 16:30 CPPp

Pore-network model for polymer electrolyte membranes — •Peter Berg and Philippe Nadon — Department of Science, University of Alberta

A random pore-network model for polymer electrolyte membranes (PEM) is presented that couples the flow of protons and water through cylindrical channels (bonds) to the swelling of the membrane. While the flows are determined by closed-form solutions of the Poisson-Nernst-Planck-Stokes equations, the fluid-structure interaction is described by a pressure balance at the channel walls. Macroscopic membrane properties, such as the conductivity, permeability and electro-osmotic coefficient, are computed and compared to experimental data in the literature. In light of the model simplifications, the results compare favourably to data but they also point to the importance of describing proton diffusion in PEM nanopores accurately

CPP 22.18 Wed 16:30 CPPp

Coarse-grained MD simulations of nanoplastic particles interacting with a non-polar environment in aqueous solution — •Lorenz Dettmann, Ashour Ahmed, and Oliver Kühn — University of Rostock, Albert-Einstein-Str. 23-24, 18059 Rostock

Plastic waste in form of small particles is an emerging threat for marine and terrestrial ecosystems. Little is known about the fate and potential impacts of plastic nanoparticles in the environment. In this work, an attempt for understanding the molecular level interaction behavior between nanoplastics (NPs) and non-polar environments in aqueous solution is introduced. Here, NPs are simulated with different polymers, namely polyethylene oxide (PEO), polyethylene (PE), polypropylene (PP) and polystyrene (PS). On the other hand, carbon nanotubes (CNTs) are used to mimic non-polar environmental molecular systems. Moreover, hydrophobicity of CNTs is modified by introducing different hydrophobic and hydrophilic functional groups into the inner surface of CNTs. The interaction of the modeled NPs with bare and modified CNTs in the presence of water is investigated via MARTINI force field based coarse-grained molecular dynamics simulations. The results show that hydrophobic polymers have a relatively strong affinity to CNTs, especially PE. The hydrophobic functional groups introduced into CNTs increased the interaction between hydrophobic polymers and CNTs. In contrast, PEO showed the lowest affinity towards CNTs. Therefore, one can expect that hydrophobic polymers have a higher tendency to accumulate at non-polar environmental molecular systems.

CPP 22.19 Wed 16:30 CPPp

A mesoscopic approach to magnetostriction of magnetic gels and elastomers — •Lukas Fischer and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Our focus is on magnetic gels and elastomers, consisting of rigid magnetizable particles embedded in an elastic polymeric environment. While the particles are discrete objects on the mesoscopic scale, the polymeric body represents an elastic continuum. When magnetized, the particles are subject to magnetic forces and push against the polymeric environment, inducing macroscopic magnetostrictive distortions.

Using analytical theory and numerical evaluations, we determine the overall distortion resulting for different discrete particle arrangements enclosed by a finite-sized, linearly elastic sphere [1–3]. Overall changes in volume and shape are evaluated. In contrast to many other approaches, our formalism includes the basically infinite number of internal degrees of freedom of deformation of the elastic environment.

We assume well-separated particles, all identically magnetized from outside. Depending on the particle arrangement and the compressibility of the elastic material, overall contraction or elongation along the magnetization axis results [1]. Twisted particle structures can lead to overall twist deformations [2], while targeted positioning of particles of different size can tune the overall response [3]. We presume that our approach can support the design of magnetostrictive actuation devices.

[1] L. Fischer and A. M. Menzel, *J. Chem. Phys.* **151**, 114906 (2019).
[2] L. Fischer and A. M. Menzel, *Phys. Rev. Research* **2**, 023383 (2021).
[3] L. Fischer and A. M. Menzel, *Smart Mat. Struct.* **30**, 014003 (2021).

CPP 22.20 Wed 16:30 CPPp

In situ GISAXS Observation of Sputter-Deposited Gold Nanostructure on Mesoporous Titanium Dioxide Template — •Suzhe Liang[1], Wei Chen[1], Shanshan Yin[1], Simon J. Schaper[1], Thomas Strunskus[2], Matthias Schwartzkopf[3], Stenphan V. Roth[3,4], and Peter Müller-Buschbaum[1,5] — [1]TU München, Garching, Germany — [2]CAU,Kiel, Germany — [3]DESY, Hamburg, Germany — [4]KTH, Stockholm, Sweden — [5]Heinz Maier-Leibniz Zentrum (MLZ), TU München, Garching, Germany

Gold/titanium dioxide (Au/TiO_2) nanohybrid materials have attracted significant attention due to the outstanding optical, photocatalytic and photovoltaic performance. Compared to chemical synthesis and lithography, sputter deposition is a facile and scalable method to produce metallic thin films and nanoparticles on substrates in precise controllability. Using nanostructured templates, ordered metal nanostructures were achieved through the sputter deposition approach. Herein, we propose a strategy to fabricate nanostructured Au/TiO_2 hybrid thin films by sputter-depositing Au on mesoporous TiO_2 template. The mesoporous TiO_2 template is prepared by a typical sol-gel synthesis approach with the assistance of diblock copolymer (PS-b-PEO). In order to investigate the kinetics of the sputter-deposited Au growth on the TiO_2 template, in situ grazing-incidence small-angle X-ray scattering (GISAXS) during sputter deposition is measured.

CPP 22.21 Wed 16:30 CPPp

Modeling and molecular dynamics studies on induced helical polymers — •Montserrat Penaloza-Amion and Wolfgang Wenzel — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Helical conformation plays an important role in biological functions, such as recognition, catalysis and structural support of superstructures. Synthetic helical polymers depend on their inversion barrier and obtaining structural information of dynamic helical polymers requires advanced experimental techniques. Yashima et.al. showed that chiral amines can induce one-handed helical structure in stereoregular cis-transoid poly((4-carboxyphenyl)acetylene) (poly-1), showing intense bands of circular dichroism (CD). Helical models were created based on poly-1. Scan calculations over the dihedral backbone using density functional theory (DFT) on dimers and tetramers of poly-1 backbone were performed to understand the helicity. From these results, Counterclockwise twist with values of -41 and 130 degrees (CCW), and Clockwise twist with values of 42 and -134 degrees (CW) for backbone dihedral were obtained. Molecular Dynamics simulations were performed for 20 ns for both helical models of 20mer with chiral amines and DMSO. Our results show lowest values for RMSD for complexes polymer-R2(CCW) with 0.942 Å, and polymer-S3(CW) with 1.654 Å corresponding to the systems with higher CD intensity in the work of Yashima et.al and indicating that R2 chiral amines could induce a CCW conformation and S3 chiral amines a CW conformation on poly-1.

CPP 22.22 Wed 16:30 CPPp

Co-nonsolvency effect on phase segregation of polymer solution — •Zahra Mohammadyarloo and Jens-uwe Sommer — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

Phase segregation of polymer solution in the presence of cosolvent (CNS) is studied by molecular dynamics simulations, where CNS particles are preferential solvent for the polymers. Simulation results for different attraction strengths are compared with the prediction of the adsorption-attraction mean-field theory under constant osmotic pressure. The osmotic pressure has been simulated by a semi-permeable wall in the simulation box. The polymer solution without cosolvent was prepared in the semi-dilute state. Polymer concentration increases

until reach a peak by adding more CNS particles, then decreases in higher concentrations of CNS. The radius of gyration of individual chains also display as non-monotonic behavior which in part be explained by the scaling law in semi-dilute solutions, and with the increasing effective excluded due to adsorption of cosolvent. At higher attraction strengths a jump-like collapse of the polymer volume can be observed which corresponds to a type-II phase transition of the polymer solution. For interaction strengths greater than critical, two states of polymer solution coexists. Furthermore we have calculated the single-chain and collective structure factors. The dynamics was studied and the monomer diffusion coefficient was presented as a function of attraction strength.

CPP 22.23 Wed 16:30 CPPp

Challenges and limits of Mechanical Stability in 3D Direct Laser Writing — •Elaheh Sedghamiz, Modan Liu, and Wolfgang Wenzel — Karlsruhe Institute of Technology, Karlsruhe, Germany

Direct laser writing is an effective technique for the fabrication of complex polymeric 3D polymer networks using ultrashort laser pulses. Practically, it remains a challenge to design and fabricate high-performance materials with different functions that possess a combination of high strength, substantial ductility, and tailored functionality, in particular for small feature sizes. To date, it is difficult to obtain a time-resolved microscopic picture of the printing process in operando. To close this gap, we have developed a molecular dynamics simulation approach to model direct laser writing and investigate the effect of writing condition and aspect ratio on the mechanical properties of the printed polymer network. We show that writing condition provides a possibility to tune the mechanical properties and an optimum writing condition can be applied to fabricate structures with improved mechanical properties. We reveal that beyond the writing parameters, aspect ratio plays an important role to tune the stiffness of the printed structures.

CPP 22.24 Wed 16:30 CPPp

Periodic Boundary Calculations of photosensitive Ru(bpy)$_3$ complexes attached to polymer chains — •Miftahussurur Hamidi Putra and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Polymers are considered as potential candidate materials for the photocathodes of p-type dye sensitized solar cells (p-DSSCs), as they can be easily synthesized and are robust under operation conditions [1]. To optimize the performance of such solar cells, a better understanding of the structural and electronic coupling between the dyes and the polymer matrix is necessary which can be obtained through first-principles total energy calculations. However, dyes attached to polymer chains represent a challenge for quantum chemistry calculations because of their large system size. Here we present a first-principles computational study based on density functional theory of a Ru(bpy)$_3$ dye, one of the common dyes in p-DSSCs, attached to a polymer chain using a periodic boundary approach [2].

We will particularly address the geometrical and electronic coupling between the dye and the polymer chain and elucidate the changes in the optical properties of the dye upon the attachment to the polymer chain.

[1] Y. Pellegrin, L. Le Pleux, E. Blart, A. Renaud, B. Chavillon, N. Szuwarski, M. Boujtita, L. Cario, S. Jobic, D. Jacquemin, and F. Odobel, J. Photochem. PhotobiolA: Chem. **219**, 235 (2011).

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CPP 22.25 Wed 16:30 CPPp

Machine learning approach to long time step molecular dynamics for hard sphere systems — •ka chun chan and wolfgang wenzel — Institute of Nanotechnology Technology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

Atomistic simulation techniques such as molecular dynamics (MD) provide an accurate and precise description of atomic motion, molecular structure and permit the prediction of the physical and chemical properties of molecular system. However, MD requires expensive computation of energy and force which leads to significant computational effort. This severely limits MD applications to biological system and soft matter physics on long time scales.

The usual MD time step is approximately 1/10 of the fastest frequency of the molecular system. In order to accelerate the MD computation, we propose a machine learning approach to propagate the molecular system instead of the usual MD time step. As a first step we developed a machine learning (ML) propagator for hard-sphere systems that propagates the molecular system with each atomic collision as a new time step. The proposed algorithm learns the time evolution of the atomic motion and the collision between atoms, such that the neural network are able to predict the system trajectory, identify the collided atomic pairs and correct the trajectory of the collided pairs for each collision time step. We will discuss the perspective of this newly ML propagator for the acceleration of MD simulations and further application to the molecular system with long time scales.

CPP 22.26 Wed 16:30 CPPp

Kinetic Monte Carlo modeling of graphene growth on chemical vapor deposition. — •Meysam Esmaeilpour, Mariana Kozlowska, and Wolfgang Wenzel — Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany

Chemical vapor deposition (CVD) is the most promising method for high quality, large area graphene synthesis. Optimization of this chemical process will enable control over crucial properties, such as graphene quality and domain size. This requires the development of a detailed atomistic understanding of the underlying processes guiding the growth mechanism. In particular there is a need to understand the mechanism behind graphene nucleation and growth during CVD and its dependence on the synthetic parameters: temperature, CVD pressure, catalyst type, facet etc.

The complexity of CVD prohibits a complete description of all reaction mechanisms at the DFT level. Using the library of surface reaction rates, we have developed a Kinetic Monte Carlo (KMC) method to study the process of CVD of graphene from methane on Cu(111) under different synthesis conditions. It explains how synthesis parameters *affect the quality and domains size of graphene. The results are compared with experimental measurements, enabling better understanding of the CVD mechanism.

CPP 22.27 Wed 16:30 CPPp

A theoretical and computational study of ionic liquid mixtures in front of charged surfaces — •Takeshi Kobayashi, Maria Fyta, and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The properties of the electric double layer formed in front of charged surfaces in room temperature ionic liquids (RTILs) solutions are studied by means of atomistic Molecular Dynamics simulations and the theory of the Lattice Boltzmann Gas model. We study 1-Ethyl-3-methylimidazolium dicyanamide ([EMIm]+[DCA]-) with water or dimethyl sulfoxide (DMSO) mixtures at different concentrations in order to investigate the solvent effects on the IL structuring in front of the surfaces. Our results reveal clear differences between water and DMSO mixtures at the interfaces. By applying the Lattice Boltzmann Gas model, the entropic and enthalpic contributions to the accumulation of the solvent molecules are discussed. The differences mainly appear in front of the positively charged interface where water accumulation but DMSO depletion occurs. Such outcomes are assigned to the combination of size and polarity of water or DMSO and the corresponding interactions with the cations or the anions in the solution. Overall, our results provide a deep understanding of the ionic liquid (IL) behavior close to interfaces and links to a proper selection of IL-based mixtures in order to optimize specific technological applications.

CPP 22.28 Wed 16:30 CPPp

A computational model for the study of catalysts in the Supported Ionic Liquid Phase in mesoporous media — •Takeshi Kobayashi[1], Hamzeh Kraus[2], Niels Hansen[2], and Takeshi Kobayashi[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart, Germany

We set-up a model for the investigation of a linker-free immobilization of catalysts in confined media in an ionic liquid (IL)-mixture. Specifically, we study the mixture of n-heptane and 1-Butyl-3-methylimidazolium trifluoromethanesulfonate ([BMIm]+[Otf]-) in a closed pore geometry with a pore diameter of 5nm. The inner walls of the pore are functionalized in order to tune the polarity of the pore and its interaction with the solvent. The immobilization of the catalyst is expected to lead to higher turnover rates in the catalysis. Using Molecular Dynamics simulations, we model the catalyst in the IL-heptane mixture within the nanopore. Our simulations reveal that the IL accumulates within the pore, while we also follow the dynamics of all molecules involved in the system. Using quantum mechanical calculations, we parameterize a force-field for the catalyst, which is being further used for a more accurate model of the catalyst within the IL-mixture. Our results provide important information on the influence of steric and IL-specific effects, the structuring of a varying solvent environment, the pore functionality, and their interactions with the catalytic center. These aspects promote a rational design of the catalyst immobilization and point to the relevant conditions.

CPP 22.29 Wed 16:30 CPPp

Self-assembly of silica nanoparticles guided by directional crystallization of grafted polymers — •Aswathy Muttathukattil[1], Afshin Nabiyan[2], Federico Tomazic[1], Felix Helmut Schacher[2], and Michael Engel[1] — [1]Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg, Cauerstrasse 3, 91058 Erlangen, Germany — [2]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich-Schiller University Jena, Lessingstraße 8, 07743 Jena, Germany

Self-assembly of nanoparticles (NP) is an efficient bottom-up approach to produce nanostructures with complex architectures. Here, we report the formation of an inorganic-organic hybrid network by self-assembly of silica NPs grafted by poly(2-iso-propyl-2-oxazoline)(PIPOX) at elevated temperatures. To resolve the

underlying molecular mechanism, we utilize coarse-grained molecular dynamics simulations. Earlier reports stated that PIPOX polymers crystallize into long fibers guided by directional dipolar interactions between amide groups. Building on this information, we represent PIPOX monomers by spherical, patchy beads. Chains of patchy beads represent polymer is attached to NP sphere. Our simulations of this NP-polymer system characterize the two steps of the self-assembly process: (1) rapid formation of amorphous aggregates via gelation, mediated by interaction between NPs through grafted polymers; (2) slower formation of diverging fibers via directional crystallization of unbound polymers with the grafted polymer matrix. The understanding of the molecular mechanism is a step towards targeted self-assembly for catalysis and other applications.

CPP 22.30 Wed 16:30 CPPp

Low-symmetry phases in attraction-driven assembly of nanotriangles — •Marco Klement and Michael Engel — Institute for Multiscale Simulation, IZNF, FAU Erlangen, Erlangen, Germany

Hard triangles at high packing density spontaneously order into high-symmetry phases [1,2] with wallpaper groups p6 and p6mm. Recent experiments with coated nanotriangles [3] observed additional phases with wall paper groups pmg and p2. The appearance of these low-symmetry phases depends on the contour length and grafting density of surfactant polymer ligand molecules. We develop a novel simulation algorithm for anisotropic interacting nanoparticles, which attribute a majority of the observations to effective rounding of triangle vertices. The remaining observation, a p2 symmetric phase for the shortest molecules in use is a consequence of a soft attractive interaction of surfactant molecules.

[1] Gantapara, A. P., Qi, W., and Dijkstra, M. "A novel chiral phase of achiral hard triangles and an entropy-driven demixing of enantiomers". Soft Matter 11, 8684-8691 (2015).

[2] Walker, D. A., Browne, K. P., Kowalczyk, B., and Grzybowski, B. A. "Self-Assembly of Nanotriangle Superlattices Facilitated by Repulsive Electrostatic Interactions." Angewandte Chemie International Edition 49, 6760*6763 (2010).

[3] Liu, Yang and Klement, Marco and Zhong, Yaxu and Chen, Jun and Engel, Michael and Ye, Xingchen, "Using Ligand Engineering to Control Self-Assembly of Polysterol Coated Nano Triangles", in preparation (2021)

CPP 22.31 Wed 16:30 CPPp

Pendant drop tensiometry: A machine learning approach — •Felix Kratz and Jan Kierfeld — Department of Physics, TU Dortmund University, Dortmund, Germany

Modern pendant drop tensiometry relies on the numerical solution of the Young-Laplace equation and allows us to determine the surface tension from a single picture of a pendant drop with high precision. Most of these techniques solve the Young-Laplace equation many times over to find the material parameters that provide a fit to a supplied image of a real droplet. Here, we introduce a machine learning approach to solve this problem in a computationally more efficient way. We train a deep neural network to determine the surface tension of a given droplet shape using a large training set of numerically generated droplet shapes. We show that the deep learning approach is superior to the current state of the art shape fitting approach in speed and precision, in particular if shapes in the training set reflect the sensitivity of the droplet shape with respect to surface tension. In order to derive such an optimized training set, we clarify the role of the Worthington number as a quality indicator in conventional shape fitting and in the machine learning approach. Our approach demonstrates the capabilities of deep neural networks in the material parameter determination from rheological deformation experiments, in general.

CPP 22.32 Wed 16:30 CPPp

Magneto-mechanical response of nanoscale magnetic filaments — Deniz Mostarac[1], Pedro A. Sánchez[1,2], and •Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria. — [2]Ural Federal University, Ekaterinburg, Russia.

Nanoscopic magnetic filaments (MFs) are magnetic, nano-sized colloids, crosslinked into polymer-like linear chains. They are a promising platform for engineering new magnetically controlled filtering and flow control elements in micro-fluidic devices. Recent advances, advocating an assembly mechanism where the structure building instructions are embedded into nanoparticles via DNA origami frames, synthesis of MFs with desirable mechanical properties.[2,3] Using MD simulations we have studied how possible crosslinking scenarios and magnetic nature of monomers (ferromagnetic or superparamagnetic) influence equilibrium properties of MFs.[4] In this contribution, we elucidate an interesting phenomenology of MFs, by examining their behaviour in a Langevin thermostat (equilibrium properties) and explicit solvent representations using the Lattice Boltzmann method (dynamics in rotating magnetic fields). Magnetization of super-paramagnetic monomers is taken into account in an accurate manner, inclusive of non-linear contributions. [1] Sánchez, P. A., et al. Macromolecules 48.20 (2015): 7658-7669. [2] Liu, W., et al. Nature chemistry 8.9 (2016): 867. [3] Tian, Y., et al. Nature mate- rials 15.6 (2016): 654. [4] Mostarac, D., et al. Nanoscale (2020).

CPP 22.33 Wed 16:30 CPPp

Directing the Diffusion of a Nonmagnetic Nanosized Active Particle with External Magnetic Fields — •Martin Kaiser[1] and Sofia Kantorovich[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Ural Federal University, Lenin Av. 51, Ekaterinburg 620000, Russian Federation

With the help of molecular dynamics simulations we show that an arbitrary non-magnetic active particle with a size below one micrometer, being immersed in a polydisperse system of magnetic nanoparticles, can diffuse twice faster along the direction of the applied field than perpendicular to the latter, whereas, for a monodisperse system, the ratio between diffusion coefficients parallel and perpendicular to the field approaches two orders of magnitude, even for magnetic fields of moderate strength. The ability to direct a non-magnetic active particle along the magnetic field stems from the formation of chains of magnetic nanoparticles aligned with the field direction. Such chains form effective channels through which the active particle can diffuse. We find that the ability to direct an active particle of a given size can be maximised by changing magnetic particle concentration so that the tunnels formed by the change have a mean width of approximately the active particle size.

CPP 22.34 Wed 16:30 CPPp

Deformation of Azo-Polymer Droplets by Light: Modeling the Effects of Light on Glassy Azobenzene Materials — •Markus Koch, Marina Saphiannikova, and Olga Guskova — Institute Theory of Polymers, IPF Dresden, Germany

Azobenzene (azo) is the most widespread light-responsive molecule due to its well-studied trans-cis photoisomerization mechanism. This compound has gained prominence due to the possibility to create surface relief gratings in azo-polymer materials using light interference patterns. However, it remains an open question how light induces mechanical stresses in the material. To study this process we consider a model system: A droplet composed of PMMA with azobenzene side chains is exposed to linearly polarized UV-Vis light. Experiments demonstrate, that such droplets deform along the polarization direction [1]. Here, using all-atom MD simulations two different approaches are applied: In the first case, the angle-dependent photoisomerization of azobenzene is simulated explicitly. In the second case, an effective orientation potential acts on the azo groups [2]. We demonstrate that both approaches lead to the reorientation of azobenzene in the polymer matrix and discuss the induced deformation of the droplet.

We thank the German Research Foundation (DFG) for financial support, project GU 1510/5-1.

[1] Loebner, S. et al., J. Phys. Chem. B, 122 (6), 2001-2009 (2018)

[2] Toshchevikov, V. et al. J. Phys. Chem. Lett., 8 (5), 1094-1098 (2017)

CPP 22.35 Wed 16:30 CPPp

End-Adsorbing Chains in Polymer Brushes: Pathway to Highly Metastable Switchable Surfaces — •Markus Koch[1], Dirk Romeis[1], and Jens-Uwe Sommer[1,2] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute Theory of Physics, TU Dresden, Germany

Polymer brushes are promising systems for the design of stimulus-responsive surfaces. In addition, it is often highly desirable to controllably hide or expose functional groups. To this end, we investigate monodisperse polymer brushes, which contain a small fraction of end-modified minority chains [1]. The length of these chains is variable and their end groups can adsorb to the grafting surface. We study these systems using Scheutjens-Fleer SCF calculations [2], MD simulations, and analytical theory. The conformational changes of the admixed chains are explored, which depend on their length and the attraction between their end groups and the surface. Based on the free energy profiles of the adsorption transition, free energy barriers are extracted, which are in good agreement with our theoretical predictions. The barriers are strongly reduced upon the collapse of the brush and can be tuned to attain reversible or irreversible switching behavior.

Financial support by the DFG, project SO 277/17-1, is gratefully acknowledged.

[1] Koch, M., Romeis, D., Sommer, J.-U., Macromolecules, 53 (17), 7356-7368 (2021)

[2] Fleer, G. J., et al. Polymers at Interfaces. London, Chapman and Hall, 1993

CPP 22.36 Wed 16:30 CPPp

Fast high-accuracy optimization of delocalized Gaussian sets for eigenfunctions — Mohammadreza Eidi, •Benjamin Rabe, and Jan-Michael Rost — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Gaussian basis sets are widely used to represent the wave function of atomic and molecular systems due to their great advantage that matrix elements with Gaussians at different locations can often be calculated analytically [1]. However, it is not trivial to optimize for a large set of Gaussians $\{exp(-\alpha_i(x-x_i)^2 | i = 1, ..., N\}$ the parameters $\{\alpha_i, x_i\}$. Procedures with predefined positions following a geometric series, so called even tempered basis sets (e.g. [2]), have been put forward. Here we introduce an iterative scheme which optimizes positions and widths simultaneously for a given number N of s-type Gaussians. To this end we use only

during the optimization process auxiliary Gaussians which have in 3D angular momentum p and d character. This way one gets highly accurate results at low computational cost, even for small numbers of Gaussians. We will demonstrate how the method works with explicit 1D examples for various potentials representing atomic and molecular scenarios. [1] Mitroy, Jim, et al., Rev. Mod. Phys. 85.2 (2013): 693. [2] Cherkes, I., Klaiman, S., and Moiseyev, N., Int. J. Quantum Chem. 109, 2996 (2009).

CPP 22.37 Wed 16:30 CPPp

Phase behavior of polymeric microemulsion in ternary A+B+AB blends — •Russell Spencer[1] and Mark Matsen[2] — [1]Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — [2]Department of Chemical Engineering, Department of Physics & Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

Ternary blends of AB diblock copolymers with A and B homopolymers microphase segregate into lamellae (LAM) for copolymer-rich blends and macrophase segregate into A- and B-rich regions for homopolymer-rich blends. Mean-field theory predicts that these regions are separated by three-phase coexistence of the LAM, A-rich, and B-rich phases, which terminates at a Lifshitz critical point. Experiments, however, report that the Lifshitz point is destroyed by fluctuations and that the three-phase coexistence is replaced by a channel of bicontinuous microemulsion (BμE). Using field-theoretic simulations, we show that fluctuations do indeed destroy the Lifshitz point, but that three-phase coexistence continues to exist. However, at high temperatures, the LAM+A+B coexistence predicted by mean-field theory is replaced by BμE+A+B coexistence. We speculate that the single-phase BμE observed in experiments is a result of kinetic trapping as the blend is cooled from the mixed state.

CPP 22.38 Wed 16:30 CPPp

Understanding the static and dynamic behaviour of stars forming reversible networks — •Kiran Suresh Kumar[1,2], Toni Müller[1,2], Jens-Uwe Sommer[1,2], and Michael Lang[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Strasse 6, 01069 Dresden, Germany — [2]nstitute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

Reversible networks break and reform continously allowing the material to flow and self-heal on long time scales while being a solid on short times. Recent experiments and simulation studies find an apparent anomalous superdiffusive regime in reversible networks by analyzing Forced Rayleigh Scattering (FRS) data [1-3]. The molecular origin of this superdiffusive regime is not yet fully understood. In our contribution, we approach this problem by computer simulations of FRS experiments in reversible networks using the Bond Fluctuation Model. We analyze the static properties and the connectivity of individual stars and develop an analytic model for the statistics of connections. We analyze dynamic properties of individual stars and compute the collective relaxation as accessible in FRS. Our goal is to develop a model based upon the molecular statistics that allows to quantitatively predict the collective dynamics of the reversible network.

[1] Tang, S.; Wang, M.; Olsen , B. D. J. Am. Chem. Soc. 2015, 137, 3946-3957. [2] Tang, S.; Habicht, A.; Li, S.; Seiffert, S.; Olsen, B. D. Macromolecules 2016, 49, 5599-5608. [3] Ramirez, J.; Dursch, T. J.; Olsen , B. D. Macromolecules 2018, 51, 2517-2525.

CPP 22.39 Wed 16:30 CPPp

Self-Assembly of Copolymers in Presence of Solvent Evaporation — •Gregor Ibbeken and Marcus Müller — Institut für Theoretische Physik, Georg August Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Integral asymmetric block copolymer membranes constitute a fascinating new technology for ultrafiltration. Solvent evaporation aligns and facilitates the long-range order of microphase separating diblock copolymers, which is exploited to form monodisperse pores. More specifically, we are interested in the emergence of perpendicularly oriented, cylindric morphologies. We investigate a system consisting of a diblock copolymer, a solvent and air by use of a continuum model in which the concentrations act as order parameters. This allows us to explore the high-dimensional parameter space with a parameter study. Four parameters turn out to have a dominant influence on emergent morphologies, namely the polymer volume fraction, the surface preference, the incompatibility of polymer blocks and the evaporation rate. Kinetically, the orientation of cylinders is determined immediately after the onset of microphase separation. If cylinders become stable when the evolution zone is wide enough, initially developed spheres elongate vertically. Most notably, this occurs for high evaporation rates. Additionally, we are able to demonstrate that the kinetic pathways taken are describable as paths in a two-dimensional parameter space consisting of effective block ratio f^{eff} and effective segregation strength χN_{ab}^{eff}.

CPP 22.40 Wed 16:30 CPPp

Magnetic nanogels in magnetic field — •Ivan Novikau[1], Pedro Sanchez[1], and Sofia Kantorovich[1,2] — [1]University of Vienna — [2]Ural Federal University

Nanogels (NGs) with multifunctionalized magnetic nanoparticles (MNPs) have demonstrated the ability to effectively destroy cancer cells in vivo, without causing visible damage to healthy organs [1]. The presence of MNPs inside the NGs also offers an additional mechanism to control their properties by means of applied magnetic fields.

Our study of a suspension of NGs loaded with MNPs in zero-field case showed that the structural properties of a single gel, and the self-assembly in the given system, strongly depend on the strength of the dipole-dipole interaction (dipolar coupling parameter) between the MNPs [2].

Here, we investigate a suspension of magnetic NGs in a constant external magnetic field by means of molecular dynamics computer simulations [3]. Each NG is initially modeled as a system of bead-spring polymer chains randomly crosslinked into a polymer network. MNPs are arbitrary incorporated into this network.

We find that even weak fields lead to drastic changes in the structure factors of both, the embedded MNPs and of whole NGs. But what is even more curious, is that the polymer matrix of nanogels enhances the magnetization of free MNPs.

[1] Qing Wu et al., Nat. Commun., 10 (240), 2019.
[2] Novikau et al., JMMM, 498, 2020.
[3] Novikau et al., J. Mol. Liq., 307, 2020.

CPP 22.41 Wed 16:30 CPPp

Water purification with pvdf membrane — •René Hafner[1,2] and Peter Klein[1] — [1]Fraunhofer ITWM, Kaiserslautern, Deutschland — [2]TUK, Kaiserslautern, Deutschland

We investigate the interaction of crystal and amorphous Polyvinylidenfluorid (PVDF) membranes with the pharmaceutical diclofenac, i.e. an inflammatory pain killer, as a surrogate of a wider class of charged drug molecules via the potential of mean force (PMF) method. While the crystal membrane is in polar beta zigzag form of PVDF, both are created by a structure generator of our own. We further highlight the features of our structure generator. For both membrane and diclofenac the Charmm force field is used. Simulations were conducted using the simulation software NAMD. The PMFs between drug and membrane are obtained via the adaptive biasing force method ABF and its extended version. Comparism is drawn between amorphous and crystal PVDF membranes and their adsorption capabilities are discussed.

CPP 22.42 Wed 16:30 CPPp

Separable intermolecular force fields from first principles — •Manuel Konrad and Wolfgang Wenzel — Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

The decomposition of intermolecular interactions into physically meaningful components can be a useful tool to gain a deeper understanding about non-covalently bonded complexes. However, separable ab initio methods, such as symmetry adapted perturbation theory (SAPT), are limited to small systems. Here we present a systematic approach to derive an analytical force field from a finite number of SAPT calculations while preserving the energy decomposition of the reference method. For several small organic molecules, we apply this model in molecular dynamics simulations to compute thermodynamic properties. The comparison against experimental values shows promising prediction capabilities. Together with the additional insight from the energy decomposition, this makes our method a potentially versatile tool for the in silico discovery of new molecular materials, where force field parametrizations can't rely on experimental target data.

CPP 22.43 Wed 16:30 CPPp

Structure formation in 2D-Copolymer Networks — •Gaoyuan Wang and Marcus Müller — Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

Two-dimensional polymer networks, characterized by a planar geometry, open new possibilities for the design of polymer molecules with novel properties. Using large-scale simulations, we study microphase separation in two-dimensional, defect-free, interpenetrating phantom networks, obtained by crosslinking symmetric diblock copolymers. The system exhibits a complex interplay between the network structure, characterized by the length (geometry) of a unit cell, and the lamellar microphase with its periodicity that depends on the incompatibility between the blocks. We investigate the incompatibility at which system microphase separates as a function of the size of the (unperturbed) unit cell of the network and quantify the network structure in the microphase-separated state. Our findings are compared to the microphase separation linear diblock, triblock and multiblock copolymers as well as to the mechanical properties of networks.

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Overview of Invited Talks and Sessions

Invited Talks

DY 4.1	Mon	9:00– 9:30	DYc	**X-ray tomography investigation of cyclically sheared granular materials** — •Yujie Wang
DY 7.1	Mon	10:00–10:30	DYa	**Can convective heat transport be more efficient than the so-called 'ultimate' regime?** — •Basile Gallet
DY 15.1	Mon	16:00–16:30	DYb	**Glassy physics: from liquids to living cells** — •Liesbeth Janssen
DY 18.1	Tue	9:00– 9:30	DYa	**Reinforcement learning of microswimmer chemotaxis using genetic algorithms** — •Andreas Zöttl, Benedikt Hartl, Maximilian Hübl, Gerhard Kahl
DY 22.1	Tue	10:00–10:30	DYc	**Stability and dynamics of convection in dry salt lakes** — •Lucas Goehring, Jana Lasser, Marcel Ernst, Matthew Threadgold, Cédric Beaume, Steven Tobias
DY 27.1	Tue	14:00–14:30	DYa	**Human exhaled particles from nanometres to millimetres** — •Gholamhossein Bagheri
DY 29.1	Tue	14:00–14:30	DYc	**Fingers, fractals, and flow in liquid metals** — •Karen Daniels
DY 31.1	Tue	15:40–16:10	DYb	**Fixation and ancestry of competing species growing on a rugged front** — •Mehran Kardar
DY 35.4	Wed	10:00–10:30	DYa	**When surface viscosities rule: Bubble relaxation and thin film wrinkling** — •Kirsten Harth
DY 37.1	Wed	9:00– 9:30	DYc	**Physical properties of ultrastable computer-generated glasses** — •Ludovic Berthier
DY 44.1	Wed	14:00–14:30	DYb	**Life in a tight spot: How bacteria swim in complex spaces** — •Sujit Datta
DY 45.1	Wed	14:00–14:30	DYc	**Small diffusive systems warm up faster than they cool down** — Alessio Lapolla, •Aljaz Godec

Sessions

DY 1.1–1.14	Mon	9:00–16:30	CPPb	**Wetting - organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen) (joint session CPP/DY)**
DY 2.1–2.3	Mon	9:00–10:00	DYa	**Fluid Physics 1 - organized by Stephan Weiss and Michael Wilczek (Göttingen)**
DY 3.1–3.5	Mon	9:00–10:40	DYb	**Statistical Physics 1 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)**
DY 4.1–4.1	Mon	9:00– 9:30	DYc	**Invited Talk: Yujie Wang (Shanghai)**
DY 5.1–5.4	Mon	9:00–11:00	BPb	**Active Biological Matter I (joint session BP/DY/CPP)**
DY 6.1–6.3	Mon	9:30–10:30	DYc	**Granular Physics 1 - organized by Matthias Sperl (Köln)**
DY 7.1–7.1	Mon	10:00–10:30	DYa	**Invited Talk: Basile Gallet (Saclay)**
DY 8.1–8.6	Mon	11:00–13:00	DYa	**Fluid Physics 2 - organized by Stephan Weiss and Michael Wilczek (Göttingen)**
DY 9.1–9.6	Mon	11:00–13:00	DYb	**Statistical Physics 2 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) und Thomas Speck (Mainz)**
DY 10.1–10.6	Mon	11:00–13:00	DYc	**Granular Physics 2 - organized by Matthias Sperl (Köln)**
DY 11.1–11.6	Mon	11:00–13:30	BPb	**Active Biological Matter II (joint session BP/CPP/DY)**
DY 12.1–12.22	Mon	14:00–16:30	DYp	**Posters DY - Fluid Physics, Active Matter, Complex Fluids, Soft Matter and Glasses (joint session DY/BP)**
DY 13.1–13.7	Mon	15:00–17:20	DYc	**Granular Physics 3 - organized by Matthias Sperl (Köln)**
DY 14.1–14.6	Mon	16:00–18:00	DYa	**Microfluidics and Droplets - organized by Uwe Thiele (Münster)**
DY 15.1–15.1	Mon	16:00–16:30	DYb	**Invited Talk: Liesbeth Janssen (Eindhoven)**
DY 16.1–16.4	Mon	16:30–17:50	DYb	**Statistical Physics 3 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)**
DY 17.1–17.13	Tue	9:00–16:30	CPPb	**Complex Fluids - organized by Christine M. Papadakis (Technical University of Munich, Garching) (joint session CPP/DY)**

DY 18.1–18.1	Tue	9:00– 9:30	DYa	**Invited Talk: Andreas Zöttl (Vienna)**
DY 19.1–19.5	Tue	9:00–10:40	DYb	**Statistical Physics 4 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)**
DY 20.1–20.3	Tue	9:00–10:00	DYc	**Nonlinear Dynamics 1 - organized by Azam Gholami (Göttingen)**
DY 21.1–21.3	Tue	9:30–10:30	DYa	**Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)**
DY 22.1–22.1	Tue	10:00–10:30	DYc	**Invited Talk: Lucas Goehring (Nottingham)**
DY 23.1–23.6	Tue	11:00–13:00	DYa	**Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)**
DY 24.1–24.6	Tue	11:00–13:00	DYb	**Dynamics and Statistical Physics - Open Session**
DY 25.1–25.6	Tue	11:00–13:00	DYc	**Nonlinear Dynamics 2 - organized by Azam Gholami (Göttingen)**
DY 26.1–26.5	Tue	11:00–12:40	SOEa	**Data Analytics for Complex Dynamical Systems (joint SOE/DY Focus Session) (joint session SOE/DY)**
DY 27.1–27.9	Tue	14:00–17:10	DYa	**Fluid Physics 3 - organized by Stephan Weiss and Michael Wilczek (Göttingen)**
DY 28.1–28.5	Tue	14:00–15:40	DYb	**Statistical Physics 5 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)**
DY 29.1–29.1	Tue	14:00–14:30	DYc	**Invited Talk: Karen Daniels (Raleigh)**
DY 30.1–30.6	Tue	14:30–16:30	DYc	**Complex Fluids and Soft Matter 1 - organized by Uwe Thiele (Münster) (joint session DY/CPP)**
DY 31.1–31.1	Tue	15:40–16:10	DYb	**Invited Talk: Mehran Kardar (Boston)**
DY 32.1–32.24	Tue	16:30–19:00	DYp	**Posters DY - Statistical Physics, Brownian Motion and Nonlinear Dynamics**
DY 33	Tue	17:45–18:30	BPb	**Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)**
DY 34.1–34.10	Wed	9:00–14:40	CPPb	**Theorie and Simulation - organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden) (joint session CPP/DY)**
DY 35.1–35.4	Wed	9:00–10:30	DYa	**Complex Fluids and Soft Matter 2 - organized by Uwe Thiele (Münster) (joint session DY/CPP)**
DY 36.1–36.5	Wed	9:00–10:40	DYb	**Active Matter 3 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)**
DY 37.1–37.1	Wed	9:00– 9:30	DYc	**Invited Talk: Ludovic Berthier (Montpellier)**
DY 38.1–38.3	Wed	9:00–10:00	SOEa	**Partial Synchronization in Networks (Focus Session joint with DY and BP) (joint session SOE/DY)**
DY 39.1–39.3	Wed	9:30–10:30	DYc	**Glasses and Glass Transition 1 - organized by Andreas Heuer (Münster) (joint session DY/CPP)**
DY 40.1–40.6	Wed	11:00–13:00	DYa	**Complex Fluids and Soft Matter 3 - organized by Uwe Thiele (Münster) (joint session DY/CPP)**
DY 41.1–41.6	Wed	11:00–13:00	DYb	**Active Matter 4 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)**
DY 42.1–42.6	Wed	11:00–13:00	DYc	**Glasses and Glass Transition 2 - organized by Andreas Heuer (Münster) (joint session DY/CPP)**
DY 43.1–43.6	Wed	14:00–16:00	DYa	**Pattern Formation - organized by Azam Gholami (Göttingen)**
DY 44.1–44.1	Wed	14:00–14:30	DYb	**Invited Talk Sujit S. Datta (Princeton)**
DY 45.1–45.7	Wed	14:00–16:30	DYc	**Brownian Motion and Anomalous Transport - organized by Ralf Metzler (Potsdam)**
DY 46.1–46.4	Wed	14:30–15:50	DYb	**Active Matter 5 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)**

Sessions

– Invited Talks, Contributed Talks, and Posters –

DY 1: Wetting - organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen) (joint session CPP/DY)

Time: Monday 9:00–16:30 Location: CPPb

See CPP 3 for details of this session.

DY 2: Fluid Physics 1 - organized by Stephan Weiss and Michael Wilczek (Göttingen)

Time: Monday 9:00–10:00 Location: DYa

DY 2.1 Mon 9:00 DYa

Transition to the ultimate regime in a stochastic model for radiatively driven turbulent convection — •Marten Klein[1], Heiko Schmidt[1], and Alan R. Kerstein[2] — [1]Lehrstuhl Numerische Strömungs- und Gasdynamik, Brandenburgische Technische Universität Cottbus-Senftenberg, Germany — [2]Consultant, Danville, California, USA

Heat transfer in thermal convection is investigated using the stochastic one-dimensional-turbulence model (ODT). A Boussinesq fluid of Prandtl number 1 is confined between two horizontal adiabatic no-slip walls (located at $z = 0$ and H) and exposed to constant gravity that points in vertical ($-z$) direction. A flow is driven by radiative heating from below yielding the local heating rate $Q(z) = (P/\ell)\ \exp(-z/\ell)$, where P is the prescribed heat flux and ℓ the absorption length. ODT resolves all relevant scales of the flow, including molecular-diffusive scales, along a vertical one-dimensional domain, whereas stochastically sampled eddy events represent the effects of turbulent advection. ODT results reproduce and extrapolate available reference experiments direct numerical simulations of Lepot *et al.* (*Proc. Natl. Acad. Sci. USA*, **115**, 2018, pp. 8937–8941) and Bouillaut *et al.* (*J. Fluid Mech.*, **861**, 2019, R5) in particular capturing the turbulent transition from the classical to the 'ultimate' regime. For these regimes, the exponent values in $Nu \sim Ra^p$ scaling are found to be $p \approx 0.3$ and $p \approx 0.55$, respectively, in agreement with measured values. Joint probabilities of eddy size and location indicate that the regime transition is accompanied by a relative increase of bulk turbulence.

DY 2.2 Mon 9:20 DYa

Reservoir Computing of Dry and Moist Turbulent Rayleigh- Bénard Convection — •Florian Heyder, Sandeep Pandey, and Jörg Schumacher — TU Ilmenau, Ilmenau, Germany

Reservoir Computing (RC) is one efficient implementation of a recurrent neural network that can describe the evolution of a dynamical system by supervised machine learning without solving the underlying nonlinear partial differential equations. We apply such a neural network to approximate the large-scale evolution and the resulting low-order turbulence statistics of two-dimensional dry and moist Rayleigh-Bénard convection. We acquire training and test data by long-term direct numerical simulations (DNS). They are postprocessed by a Proper Orthogonal Decomposition (POD) with the snapshot method. The training data comprise time series of the first 150 POD modes, which are associated with the largest total energy amplitudes and thus the large-scale structure of the flows. Feeding the data to the Reservoir Computing model and optimizing the reservoir parameters results in predictions for the evolution of the dry and moist convection flows. The prediction capabilities of our model are comprehensively tested by a comparison with DNS and test data, the latter of which are reconstructed from the most energetic POD modes. Vertical profiles of mean thermodynamic fields and their mean vertical transport show good agreement. We find that RC is capable to model the large-scale structure and low-order statistics of dry and moist turbulent convection. This shows potential for subgrid-scale turbulence parameterization in large-scale atmospheric circulation models.

DY 2.3 Mon 9:40 DYa

Generation of zonal flows in convective systems by travelling thermal waves — •Philipp Reiter[1], Rodion Stepanov[2], and Olga Shishkina[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Götttingen, DE — [2]Institute of Continuous Media Mechanics, Russian Academy of Science, Perm, RU

In this work we study the effects of travelling thermal waves which are applied at the fluid layer, specifically on the formation of global mean horizontal (zonal) flow. Earlier studies suggest that the periodic heating of the Earth's, due to Earth's rotation, could cause zonal winds in the atmosphere. Additionally, the 4-day retrograde rotation in the Venus' atmosphere might be driven by such a periodic thermal forcing. In this work we revisited an existing theoretical model and validated it by means of direct numerical simulations (DNS). Furthermore, we expanded the analysis above the limits of the theory and studied travelling thermal waves in strongly convective flows.

Our results can be summarized as follows. The 2D simulations show excellent agreement with the theoretical model for low Rayleigh numbers (Ra). For larger Ra, the theory overestimates the magnitude of the zonal flows. However, the asymptotic scalings are still valid. The 3D system shows very similar characteristics than the 2D flows, therefore we provide further evidence for the relevance of this problem to natural systems. Finally, we show that the direction of the induced mean zonal flows can change. While it is always directed opposite to the travelling wave (retrograde) for low Ra flows, as the Ra increases the zonal flow is often found in a prograde state.

DY 3: Statistical Physics 1 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)

Time: Monday 9:00–10:40 Location: DYb

DY 3.1 Mon 9:00 DYb

The Five Problems of Irreversibility* — •Michael te Vrugt — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149, Münster, Germany

Macroscopic thermodynamics has a clear arrow of time: Systems irreversibly approach equilibrium accompanied by a monotonous increase of entropy. This stands in contrast to the laws of microscopic theories, which are invariant under time-reversal. The question how this difference can be explained has created a long debate, with suggestions involving coarse-graining methods as well as cosmological considerations about the entropy of the early universe. In this talk, I will show that a part of the difficulty in solving the problem of irreversibility arises from the fact that it actually consists of five different sub-problems [1], which are mixed in most discussions. Understanding why these problems have to be distinguished and how they are related to each other then allows to solve them on the basis of modern nonequilibrium statistical mechanics. The general approach is illustrated using the example of dynamical density functional theory (DDFT) [2].

[1] M. te Vrugt, arXiv:2004.01276 (2020)

[2] M. te Vrugt, H. Löwen, and R. Wittkowski, Advances in Physics 69, 121-247 (2020)

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DY 3.2 Mon 9:20 DYb

Thermodynamic Uncertainty Relation for Time-Dependent Driving — •Timur Koyuk and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Thermodynamic uncertainty relations yield a lower bound on entropy production in terms of the mean and fluctuations of a current. In this talk we will present the general form of the thermodynamic uncertainty relation for systems under arbitrary time-dependent driving from arbitrary initial states [1]. This approach

unifies earlier derived relations valid for discrete Markovian systems or continuous overdamped Langevin systems. One powerful application of the TUR is to infer entropy production by observing an arbitrary current and its fluctuations without knowing the details of the interactions or underlying topology of the network. In this context we will extend the TUR beyond currents to state variables, which allows one to estimate entropy production by only observing, e.g., a binary observable. We will illustrate the quality of the bounds for various types of observables for the dynamical unfolding of a small protein, which is based on extant experimental data. As another important application of the TUR we will show how to bound the efficiency of cyclic heat engines by using the TUR for periodically driven systems [2]. This bound on the efficiency involves the output power, its fluctuations as well as its response with respect to the driving frequency. It thus imposes fundamental constraints on every cyclic stochastic heat engine for reaching Carnot efficiency.

[1] T. Koyuk and U. Seifert, Phys. Rev. Lett. 125, 260604 (2020).
[2] T. Koyuk and U. Seifert, Phys. Rev. Lett. 122, 230601 (2019).

DY 3.3 Mon 9:40 DYb

Thermodynamic Uncertainty Relation for a Stochastic Field Theory – KPZ-Equation as a Paradigmatic Example — •Oliver Niggemann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

Recently, a thermodynamic uncertainty relation (TUR) for a generic stochastic field theory has been proposed [1]. In this talk, I will first formulate a framework which describes the constituents of the field-theoretic TUR, namely current, entropy production and diffusivity. This general setting is then applied to the (1+1)-dimensional Kardar-Parisi-Zhang (KPZ) equation, a paradigmatic example of a non-linear field-theoretic Langevin equation. In particular, I will treat the dimensionless KPZ-equation with an effective coupling parameter, λ_{eff}, measuring the strength of the non-linearity. It will be shown that the field-theoretic TUR holds both in the weak and strong coupling regimes and that its value depends on λ_{eff} [2]. For $\lambda_{\text{eff}} \downarrow 0$, the TUR product is equal to 5, whereas for $\lambda_{\text{eff}} \gg 1$ it grows linearly with λ_{eff}. There is no value for λ_{eff} with the TUR product being saturated. Furthermore, I will present numerical simulations of the TUR constituents and the TUR product itself. These simulations display good agreement with the theoretical results for both the weak and strong coupling regime.

[1] Niggemann, O. and Seifert, U. *J Stat Phys* 178, 1142–1174 (2020). https://doi.org/10.1007/s10955-019-02479-x
[2] Niggemann, O. and Seifert, U. *J Stat Phys* 182, 25 (2021). https://doi.org/10.1007/s10955-020-02692-z

DY 3.4 Mon 10:00 DYb

Entropy Production in Open Systems: The Predominant Role of Intraenvironment Correlations — •Krzysztof Ptaszyński[1] and Massimiliano Esposito[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland — [2]Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We show [1] that the entropy production in small open systems coupled to environments made of extended baths is predominantly caused by the displacement of the environment from equilibrium rather than, as often assumed, the mutual information between the system and the environment. The latter contribution is strongly bounded from above by the Araki-Lieb inequality, and therefore is not time-extensive, in contrast to the entropy production itself. Furthermore, we show that in the thermodynamic limit the entropy production is associated mainly with generation of the mutual information between initially uncorrelated environmental degrees of freedom. We confirm our results with exact numerical calculations of the system-environment dynamics.

[1] K. Ptaszyński, M. Esposito, Phys. Rev. Lett. 123, 200603 (2019)

DY 3.5 Mon 10:20 DYb

Negative entropy production rates in Drude-Sommerfeld metals — Marcus V. S. Bonança[1], •Pierre Nazé[1], and Sebastian Deffner[2,1] — [1]Universidade Estadual de Campinas, Campinas, Brazil — [2]University of Maryland, Baltimore County, Baltimore, USA

It is a commonly accepted creed that in typical situations the rate of entropy production is non-negative. We show that this assertion is not entirely correct if a time-dependent, external perturbation is not compensated by a rapid enough decay of the response function. This is demonstrated for three variants of the Drude model to describe electrical conduction in noble metals, namely the classical free electron gas, the Drude-Sommerfeld model, and the Extended Drude-Sommerfeld model. The analysis is concluded with a discussion of potential experimental verifications and ramifications of negative entropy production rates.

[1] Marcus V. S. Bonança, Pierre Nazé, and Sebastian Deffner, Phys. Rev. E 103, 012109 (2021)

DY 4: Invited Talk: Yujie Wang (Shanghai)

Time: Monday 9:00–9:30 Location: DYc

Invited Talk DY 4.1 Mon 9:00 DYc

X-ray tomography investigation of cyclically sheared granular materials — •Yujie Wang — School of Physics and Astronomy, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, China

We perform combined x-ray tomography and shear force measurements on a cyclically sheared granular system with highly transient behaviors, and obtain the evolution of microscopic structures and the macroscopic shear force during the shear cycle.We explain the macroscopic behaviors of the system based on microscopic processes, including the particle level structural rearrangement and frictional contact variation. Specifically, we show how contact friction can induce large structural fluctuations and cause significant shear dilatancy effect for granular materials, and we also construct an empirical constitutive relationship for the macroscopic shear force.

DY 5: Active Biological Matter I (joint session BP/DY/CPP)

Time: Monday 9:00–11:00 Location: BPb

See BP 2 for details of this session.

DY 6: Granular Physics 1 - organized by Matthias Sperl (Köln)

Time: Monday 9:30–10:30 Location: DYc

DY 6.1 Mon 9:30 DYc

Flow study for poly-dispersed dense granular suspension in Non-Newtonian media, mimicking concrete flow — •Himanshu P Patel, Peyman Rostami, and Günter K Auernhammer — Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Straße 6, D-01069 Dresden, Germany

The study of internal flow dynamics and associated particle migration for polydispersed dense granular suspension, e.g., flowing concrete, still lacks quantification on a single particle level.

We use a macroscopically highly transparent model system for concrete and cement paste [1] that is a dense granular suspension of particles suspended in non-Newtonian media (particle volume fractions of 42% to 48%). The model system mimics the rheology behavior of cement paste (yield stress and plastic viscosity) and is completely index matched. The rheological characteristics of the model system is tunable through its composition of additives.

We analyze gravity-assisted continuous flow for the model system through a cylindrical pipe. Our setup allows tracking of polydisperse tracer particles at different sections of the pipe and near its wall using diffused back-light illumination. The flow analysis revels a flow profile similar to a plug flow and a migration of larger towards the central region of the flow. Sliding and rolling motion of the particles is observable. The lubrication layer thickness is also evaluated in the study.

[1] Auernhammer, Günter K., et al., Materials & Design (2020): 108673.

DY 6.2 Mon 9:50 DYc

Uncertainty relations for mesoscopic coherent light — •Ohad Shpielberg — University of Haifa, Haifa, Israel

Thermodynamic uncertainty relations unveil useful connections between fluctuations in thermal systems and entropy production. This talk extends these ideas

to the disparate field of zero temperature quantum mesoscopic physics where fluctuations are due to coherent effects and entropy production is replaced by a cost function defined using a novel disorder reversal operator. A simple expression is obtained for the average cost function, which depends on the dimensionless conductance g and on a geometrical factor B controlled by boundary conditions. Contrary to thermodynamic machines aimed at minimising fluctuations to increase precision, it is desirable in mesoscopic devices to increase coherent effects. The cost function indicates that increasing coherent effects can be achieved by playing with the geometry and boundary conditions through B and not only by decreasing the bulk conductance g.

DY 6.3 Mon 10:10 DYc

Coupling between rotational and translational motions of a vibrated polygonal disk — •Simeon Voelkel[1] and Kai Huang[1,2] — [1]Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Institute of Applied Physical Sciences and Engineering, Division of Natural and Applied Sciences, Duke Kunshan University, No. 8 Duke Avenue, Kunshan, Jiangsu, China 215316

We investigate experimentally the dynamics of a single polygonal disk (regular n-gon with $3 \leq n \leq 8$) under vertical vibrations against gravity. The disks tend to precess continuously upon vibrations, transferring the mechanical energy injection into the rotational as well as the translational degrees of freedom (DoF) spontaneously. An analysis of the velocity distribution functions in both DoF suggests that the mobility in both DoF are coupled with each other with a preferred angular velocity that depends on the confinement, the geometry of the disk as well as the driving condition. The favored angular velocity can be captured with a model considering sustainable precession due to continuous driving. We also find a regime in the parameter space where the kinetic energy in both DoF agree with each other, despite of the strong energy dissipation and fluctuations in the system upon frequent collisions of the disk with the vibrating plates.

DY 7: Invited Talk: Basile Gallet (Saclay)

Time: Monday 10:00–10:30 Location: DYa

Invited Talk DY 7.1 Mon 10:00 DYa

Can convective heat transport be more efficient than the so-called 'ultimate' regime? — •Basile Gallet — CEA Saclay, Gif-sur-Yvette, France.

Decades of investigation of the Rayleigh-Bénard (RB) thermal convection setup indicate that the heat transport is restricted by boundary layers near the hot and cold solid plates. This prevents the unambiguous observation of the 'ultimate' scaling-regime of thermal convection, where bulk turbulence controls the convective heat flux independently of molecular diffusivities. In contrast to the RB setup, many geophysical and astrophysical convective flows are driven radiatively: absorption of light by a body of fluid induces local internal heating. We have developed a laboratory experiment that reproduces such radiative heating: heat is directly input inside the bulk turbulent flow and away from the boundary layers.

After providing experimental and numerical evidence that this setup leads to the ultimate regime of thermal convection, I will discuss the maximum theoretical Nusselt number that can be achieved by such internally heated and cooled convection. I will show that there exist steady laminar solutions that transport heat more efficiently than the ultimate regime, with a scaling behavior Nu~Ra. These solutions can be stable in 2D, but they are unstable in 3D and quickly evolve into a turbulent state. I will show that a maximization of the heat transport over turbulent flows only leads to an upper bound on the Nusselt number that is proportional to the square root of the Rayleigh number, in line with the experimental data.

DY 8: Fluid Physics 2 - organized by Stephan Weiss and Michael Wilczek (Göttingen)

Time: Monday 11:00–13:00 Location: DYa

DY 8.1 Mon 11:00 DYa

Interpreted machine learning: Explaining relaminarisation events in wall-bounded shear flows — Martin Lellep[1], Jonathan Prexl[2], Bruno Eckhardt[3], and •Moritz Linkmann[4] — [1]School of Physics and Astronomy, University of Edinburgh, UK — [2]Dept. of Civil, Geo and Environmental Engineering, Technical University of Munich, Germany — [3]Dept. Physics, Philipps-University of Marburg, Germany — [4]School of Mathematics and Maxwell Institute for Mathematical Sciences, University of Edinburgh, UK

Machine Learning (ML) is becoming increasingly popular in fluid dynamics. Powerful ML algorithms such as neural networks or ensemble methods are notoriously difficult to interpret. Here, we use the novel Shapley Additive Explanations (SHAP) algorithm (Lundberg & Lee, 2017), a game-theoretic approach that explains the output of a given ML model, to ascertain which physical processes are significant in the prediction of relaminarisation events in wall-bounded parallel shear flows. The flow is described by an established low-dimensional model whose variables have a clear physical and dynamical interpretation in terms of known representative features of the near-wall dynamics, i.e. streamwise vortices, streaks and linear streak instabilities. We consistently find only three modes to play a major role in the prediction: the laminar profile, the streamwise vortex, and a specific streak instability. SHAP thus distinguishes representative from significant features, hence we demonstrate that it is an explainable AI method which can provide useful and human-interpretable insight for fluid dynamics.

DY 8.2 Mon 11:20 DYa

Small scale structures of turbulence in terms of entropy and fluctuation theorems — André Fuchs[1], •Joachim Peinke[1], Matthias Wächter[1], Silvio M Durate Queiros[2], Alain Girard[3], and Pedro G Lind[4] — [1]ForWind, Inst Physik , University of Oldenburg, — [2]Centro Brasileiro de Pesquisas Fisicas and National Institute of Science and Technology for Complex Systems, Rio de Janeiro - RJ, Brazil — [3]INAC-SBT, UMR CEA-Grenoble, 38054 Grenoble, France — [4]Department of Computer Science, OsloMet - University, N-0130 Oslo, Norway

Experimental evidence that the integral fluctuation theorem as well as a detailed-like fluctuation theorem holds for large entropy values of the turbulent cascade processes. Stochastic equations describing the scale-dependent cascade process are derived. From individual cascade trajectories an entropy term can be determined. The statistical fluctuation theorems set the occurrence of positive and negative entropy events in strict relation, which is consistent with a stochastic description of the turbulence by a Fokker-Planck equation. Most interestingly the entropy concept of cascade trajectories is linked to turbulent structures: Whereas trajectories with entropy- production show expected decreasing behavior; trajectories with entropy-consumption end at small scale at velocity increments with finite size and show a lower bound for small scale increments. This indicates a tendency to local discontinuities in the velocity field. Our current research indicates that the velocity increment dynamics through scales in the cascade process can be described by applying an instanton approach.

DY 8.3 Mon 11:40 DYa

Statistical geometry of material loops in turbulence — Lukas Bentkamp[1], Theodore D. Drivas[2], Cristian C. Lalescu[3], and •Michael Wilczek[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Stony Brook University, Stony Brook, USA — [3]Max Planck Computing and Data Facility, Garching, Germany

Turbulent mixing is often characterized by the statistics of one- or two-particle dispersion. An even more comprehensive characterization of the complexity of turbulent mixing can be achieved by capturing the evolution of extended material lines and surfaces. Here, we investigate the statistical geometry of material loops, i.e. closed material lines, by combining simulations, statistical turbulence theory, and dynamical systems theory. Tracking these structures in direct numerical simulations of homogeneous isotropic turbulence reveals that, while the loops develop convoluted shapes over time, their statistical geometry approaches a stationary state. In particular, their curvature distribution forms clear power-law tails, which we analytically determine in the framework of the Kraichnan model. Dynamically, we show that the high-curvature regime is dominated by the formation of isolated folds and that the power-law exponent can be related quantitatively to finite-time Lyapunov exponents. Thereby, the statistical geometry of material lines can be traced back to their dynamical evolution.

DY 8.4 Mon 12:00 DYa

Velocity measurements in rotating Rayleigh-Bénard convection and the Boundary Zonal Flow — Marcel Wedi[1], •Denis Funfschilling[2], and Stephan Weiss[1] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Université Strasbourg, France

Rotating turbulent thermal convection is of great importance in various astro- and geophysical systems, where the buoyancy driven flow strongly influenced by Coriolis forces due to rotation of the celestial bodies. It has been studied for decades in the so-called Rayleigh-Bénard setup, where a horizontal fluid layer is heated at the bottom and cooled at the top and rotated around the vertical axis. We investigate the horizontal velocity field using 2D-particle image velocimetry (PIV) in a cylindrical cell (H = 196 mm high) with aspect ratio $\Gamma = D/H = 1$. We use water and various water-glycerol mixtures as working fluid resulting in a Prandtl number (Pr) in the range $6 \leq Pr \leq 70$ and Rayleigh numbers (Ra) $10^8 < Ra < 2 \times 10^9$. With our rotating table we reach Ek as low as 10^{-5}. We are mainly interested in studying the recently discovered *Boundary Zonal Flow* (BZF, see Zhang et al., Phys.Rev.Lett. 2020). The BZF is observed in a region close to the lateral sidewall with a cyclonic flow, i.e, a positive mean azimuthal velocity that is separated from and anticyclonic bulk, with negative mean azimuthal velocity. We measure the size of the BZF as a function of Ek and Ra, and compare the results with DNS (Zhang and Shishkina, 2020).

DY 8.5 Mon 12:20 DYa

Transport and rotation statistics of self–propelled ellipsoids in turbulence — •Jose-Agustin Arguedas-Leiva and Michael Wilczek — Max Planck Institute for Dynamics and Self–Organisation, Am Fassberg 17, 37077, Goettingen, Germany

Many plankton species are motile. Motility is, for example, key for grazing and evading predation. Apart from the swimming speed, shape is a critical parameter in defining the response to hydrodynamic flows. A comprehensive understanding of the relation between the relevant particle parameters, shape and motility, and their transport properties and encounter rates in turbulent flows is still missing. Here, we study self–propelled ellipsoids in turbulence as a simple model for motile microorganisms in aquatic environments. Using direct numerical simulations we find non–trivial dispersion properties and rotation statistics as a result of a complex interplay between turbulent advection, motility, and particle spinning and tumbling rates. We show that one important aspect is the effect of rotation on particle transport. In contrast to spinning, tumbling constantly changes particle orientation. As tumbling rates are shape–dependent, this leads to intrinsically different transport properties for differently shaped particles. Our investigation thus helps to characterize the intricate dynamics of self–motile ellipsoids in turbulent flows and sheds light on the role played by shape and motility.

DY 8.6 Mon 12:40 DYa

Lagrangian Turbulence at Unprecedented Reynolds Numbers — •Christian Küchler[1,2], Antonio Ibanez Landeta[1,2], Jan Molacek[1], and Eberhard Bodenschatz[1,2,3] — [1]Max-Planck-Institute for Dynamics and Self-Organisation, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems of the University of Göttingen, Germany — [3]Cornell University, Ithaca, USA

The Lagrangian reference frame, in which turbulence is viewed by tracking fluid elements over time, is the natural framework for studying transport and mixing phenomena (Sawford (2001)) and previously unexplored properties of turbulence (Toschi & Bodenschatz (2009)). Particularly important Lagrangian dynamics occur at large Reynolds numbers, e.g. the formation of clouds and precipitation. To our knowledge, the Variable Density Turbulence Tunnel (Bodenschatz et al. (2014)) is the only apparatus capable of generating turbulence at Taylor-scale Reynolds numbers up to 6000, while permitting Lagrangian measurements. In addition, the turbulence generation is highly adjustable through a uniquely flexible active grid (Griffin et al. (2019)) and by tuning the pressure of the working fluid SF6 up to 15 bar. Here we present the first measurements of Lagrangian particle tracking in this high-pressure environment. We describe the particle injection mechanism, the high-speed camera setup, and the illumination system. We present initial results of particle accelerations at Reynolds numbers greater than 3000, marking the highest Reynolds numbers at which such statistics have ever been recorded. Finally, we provide an outlook on the overall capabilities of the setup.

DY 9: Statistical Physics 2 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) und Thomas Speck (Mainz)

Time: Monday 11:00–13:00 Location: DYb

DY 9.1 Mon 11:00 DYb

Path integral approach to strong fluctuations in chemical reaction network dynamics using the Plefka expansion — •Moshir Harsh and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany

Biochemical reaction networks such as *gene* regulation, *protein* interaction and signalling pathways involve the participation of just a few copies of some key molecular species. With the advent of modern capabilities in live quantitative fluorescence microscopy and spectroscopy, the dynamics of a number of molecular species in these networks can be observed experimentally. However, inferring dynamical parameters from such data remains a challenge as the trajectories of low copy number species show large fluctuations, causing approximate approaches like the Fokker-Planck equation and moment closure to fail in this regime, while the in principle exact master equation has no general analytical solution.

Here we present an alternative method based on constructing the path integral for the dynamics of a generic reaction network, which is then treated within a Gaussian approximation by constraining the first and the second order statistics of the field variables using the systematic Plefka expansion of the dynamical free energy. We develop the method to treat any system of reactions in full generality and show its applicability and accuracy across a range of example systems. The approximate path integral can also form the basis for making inferences from experimentally measured dynamics.

DY 9.2 Mon 11:20 DYb

Negative dissipation and instability in systems with distributed delay — •Sarah A.M. Loos[1], Simon Hermann[2], and Sabine H.L. Klapp[3] — [1]Universität Leipzig — [2]Humboldt-Universität zu Berlin — [3]Technische Universität Berlin

Many natural and artificial systems are subject to some sort of delay, which can be in the form of a single discrete delay or distributed over a range of times. Here, we discuss the impact of this distribution on (thermo-)dynamical properties of time-delayed stochastic systems. To this end, we study a simple model with white and colored noise, and focus on the class of Gamma-distributed delays which includes a variety of distinct delay distributions typical for feedback experiments and biological systems. A physical application is a colloid subject to time-delayed feedback control, which is, in principle, experimentally realizable by co-moving optical traps. We uncover several unexpected phenomena in regard to the system's linear stability and its thermodynamic properties. First, increasing the mean delay time can destabilize, or stabilize the process, depending on the distribution of the delay. Second, for all considered distributions, the heat dissipation of the controlled system (e.g., the colloidal particle) can become negative, which implies that the delay force extracts energy of the heat bath. This refrigerating effect is particularly pronounced for exponential delay. The exponential delay further yields the largest stable parameter regions. In this sense, exponential delay represents the most effective and robust type of delayed feedback.

DY 9.3 Mon 11:40 DYb

On the fluctuation-dissipation theorem of a buckminster fullerene — •Andreas Baer[1], David Smith[2], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Institute for Theoretical Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Division of Physical Chemistry, Ruđer Bošković Institute, Zagreb, Croatia

The fluctuation-dissipation theorem goes back to the first half of the last century with a lot of work in statistical physics sharpening the limits of applicability [1]. The Stokes-Einstein relation is a direct consequence of the fluctuation-dissipation theorem and was recently, within an experimental study, argued to be valid for dissolved buckminster fullerenes [2], while theoretical and simulation studies deny the applicability at such small scales [3]. We perform both equilibrium and constrained molecular dynamics studies of a buckminster fullerene dissolved in toluene. Retrieving velocity and force autocorrelation functions, we can directly show the failure of the fluctuation-dissipation theorem. Additionally, transport coefficients obtained via the Green-Kubo formalism can be compared to the friction coefficient retrieved from the ratio of pulling force and resulting velocity to test the Stokes-Einstein relation. We outline the most important assumptions of the theory not fulfilled and provide a solution to the apparent contradiction with experimental studies.

[1] Zwanzig, R., *Annu. Rev. Phys.* 1965, **16**, 67-102
[2] Pearson, J. et al., *J. Phys. Chem. Lett.* 2018, **9**, 6345-6349
[3] Schmidt J. R. et al., *J. Phys. Chem. B* 2004, **108**, 21, 6767-6771

DY 9.4 Mon 12:00 DYb

Quantifying configurational information for a stochastic particle in a flow-field — •Evelyn Tang[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Flow-fields are ubiquitous systems that are able to transport vital signaling molecules necessary for system function. While information regarding the location and transport of such particles is often crucial, it is not well-understood how to quantify the information in such stochastic systems. Using the framework of nonequilibrium statistical physics, we develop theoretical tools to address this question. We observe that rotation in a flow-field does not explicitly appear in the generalized potential that governs the rate of system entropy production. Specifically, in the neighborhood of a flow-field, rotation contributes to the information content only in the presence of strain – and then with a comparatively weaker contribution than strain and at higher orders in time. Indeed, strain and especially the flow divergence, contribute most strongly to transport properties such as particle residence time and the rate of information change. These results shed light on how information can be analyzed and controlled in complex artificial and living flow-based systems.

DY 9.5 Mon 12:20 DYb

Asymmetric nascent Dirac delta functions and their application to probability and mechanics — •Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham, UK

The Dirac delta distribution is ubiquitious from quantum mechanics and statistical physics to Fourier analysis. In theoretical physics lectures, a commonly presented approach uses a series of nascent delta functions which are normalized and localized and converge point-wise to zero except at the origin. For simplicity, nascent delta functions are usually chosen to be even, i.e. $\delta_n(x) = \delta_n(x)$. However, this is not a necessary assumption, and in physical interactions as the inelastic collision of two rigid bodies, the force between the particles as a function of time may follow an asymmetric profile; nevertheless with the total momentum transferred in a Dirac delta pulse in the limit of an infinesimal short interaction time.

Here I discuss asymmetric nascent Dirac delta functions and their implications in probability and physics. The gross advantage of asymmetric nascent delta functions is found in their application to probability theory. By introduction of totally asymmetric nascent delta functions, the inconsistencies of using the Dirac delta in mixed discrete-continuous probability spaces when arriving at the cumulative distribution function are resolved. It is anticipated that asymmetric nascent delta functions find further applications in mathematical physics and the theory of measurement.

DY 9.6 Mon 12:40 DYb

Hilbert space average of transition probabilities — •Nico Hahn, Thomas Guhr, and Daniel Waltner — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The typicality approach and the Hilbert space averaging method as its technical manifestation are important concepts of quantum statistical mechanics. Extensively used for expectation values we will extend them to transition probabilities. We find that the transition probability of two random uniformly distributed states is connected to the spectral statistics of the considered operator. We will demonstrate our quite general result for a kicked spin chain.

DY 10: Granular Physics 2 - organized by Matthias Sperl (Köln)

Time: Monday 11:00–13:00 Location: DYc

DY 10.1 Mon 11:00 DYc

Particle shape-dependence of the stability properties of granular piles — •Steffen Richters-Finger and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Germany

It is well known that the shape of particles has a major influence on the behavior of densely packed granular matter making it an important subject of interest for various applications. Multiple schemes for the numerical simulation of non-spherical particles have previously been proposed in the literature [1].

Applying a discrete function representation (DFR) approach for collision detection, we investigate the shape-dependence of the stability properties (e.g. critical angle of stability) of a granular pile in a two-dimensional discrete element model for a wide range of polar geometries generated by the so-called superformula [2].

[1] G. Lu, J.R. Third, C.R. Müller, Chem. Eng. Sci. **127**, 425-465 (2015).
[2] J. Gielis, Am. J. Bot. **90**, 333-338 (2003).

DY 10.2 Mon 11:20 DYc

Machine learning aided tracking of rod-like particles in 3D microgravity experiments on granular gases — •Dmitry Puzyrev, Kirsten Harth, Torsten Trittel, and Ralf Stannarius — Institute of Physics, Otto von Guericke University, Magdeburg, Germany

Granular gases are nonlinear systems which exhibit fascinating dynamical behavior far from equilibrium, including unusual cooling properties, clustering and violation of energy equipartition. Our investigation is focused on 3D microgravity experiments with dilute ensembles of rod-like particles, where the mean free path is substantially reduced as compared to gases of spherical grains of identical volume fraction [1]. Moreover, elongated particles provide the possibility to efficiently study the energy transfer between the translational and rotational degrees of freedom.

One particular problem is the reliable detection and tracking of the rods in 3D, especially at volume fractions beyond the very dilute limit. We have developed a Machine Learning aided approach [2] to the experimental data analysis which allows to recognize and track individual particles in ensemble.

[1] K. Harth et al., Free cooling of a granular gas of rodlike particles in microgravity, Phys. Rev. Lett., 120 (2018), 214301

[2] Puzyrev et al., Machine learning for 3D particle tracking in granular gases, Microgravity Sci. Technol., 32 (2020), 897

DY 10.3 Mon 11:40 DYc

Particle size dynamics in abrading pebble populations — •Janos Török[1,2], Andras Sipos[1,3], and Gabor Domokos[1,3] — [1]MTA-BME Morphodynamics Research Group, Budapest University of Technology and Economics — [2]Department of Theoretical Physics, Budapest University of Technology and Economics — [3]Department of Mechanics, Materials and Structures, Budapest University of Technology and Economics

Abrasion of sedimentary particles in fluvial and aeolian environments is widely associated with collisions encountered by the particle. Although the physics of abrasion is complex, purely geometric models recover the course of mass and shape evolution of individual particles in low and middle energy environments (in the absence of fragmentation) remarkably well. In this paper, utilizing results of this individual, geometric abrasion theory as a collision kernel, following techniques adopted in the statistical theory of coagulation and fragmentation, we construct the corresponding Fokker-Planck equation as the first model for the collision-driven collective mass evolution of sedimentary particles. Our model uncovers a startling fundamental feature of collective particle size dynamics: collisional abrasion may, depending on the energy level, either focus size distributions, thus enhancing the effects of size selective transport or it may act in the opposite direction by dispersing the distribution. This complex behaviour does not contradict existing geological observations on mass distributions.

DY 10.4 Mon 12:00 DYc

Applying Edwards' theory for a $2+\epsilon$ dimensional frustrated granular system — •Sára Lévay[1], David Fischer[2], Ralf Stannarius[2], Ellák Somfai[3], Tamás Börzsönyi[3], Lothar Brendel[4], and János Török[1,5] — [1]Budapest University of Technology and Economics — [2]Otto von Guericke University — [3]Wigner Research Centre for Physics — [4]University of Duisburg-Essen — [5]MTA-BME Morphodynamics Research Group

Despite the inherent athermal features of granular materials, treating jammed granular systems in analogy to thermal equilibrium statistical mechanics was proposed by Edwards by using a volume ensemble of equiprobable jammed states. We introduce a simple system to analyze statistical properties of jammed granular ensembles to test Edwards' theory.

Identical spheres packed in a nearly two-dimensional thin geometrical confinement were studied in experiments and numerical simulations. When tapped, it evolves towards a ground state, but due to incompatible domain structures it gets trapped. Analytical calculations of the Edwards ensemble reproduce well our simulation results, which allows us to test Edwards' theory on a coupled system of two subsystems with different properties. We find that the joint system can only be described by a common compactivity if the stress equilibrium is also taken into account and the system is treated as a whole. The results show some counterintuitive effects, as the side with more order compactifies.

DY 10.5 Mon 12:20 DYc

Can machine learning help to identify variables of a granular theory? — •Ansgar Kühn, Song-Chuan Zhao, and Matthias Schröter — Max Planck Institute for Dynamics and Self-Organization, Göttingen

Presently, the best theory for predicting the number of contacts in a granular packing is using the local package fraction as its independent variable [1]. In order to go beyond this one-parameter approach, a more detailed description of the local geometry is given in the form of Minkowski tensors of the Voronoi cell.

With this data as features, machine learning provides a more accurate prediction of contact numbers than [1]. Feature selection can be used to identify new variables most relevant for the prediction in order to expand the theory.

[1] Song et al. Nature, 453, 629–632 (2008)

DY 10.6 Mon 12:40 DYc

Flow in an hourglass: particle friction and stiffness matter — •Tamás Börzsönyi[1], Tivadar Pongó[1,2], Viktória Stiga[1], János Török[3], Sára Lévay[3], Balázs Szabó[1], Raúl Cruz Hidalgo[2], and Ralf Stannarius[4] — [1]Wigner Research Centre for Physics, H-1525 Budapest, Hungary — [2]Universidad de Navarra, Pamplona, Spain — [3]Institute of Physics BME, Budapest, Hungary — [4]Otto-von-Guericke-University, D-39106 Magdeburg, Germany

For usual granular materials the discharge rate from a silo is known to be time independent (constant flow rate). This is opposed to the case of a liquid for which the decreasing height leads to decreasing pressure, resulting in gradually decreasing flow rate during a discharge process. We performed laboratory experiments and numerical simulations with traditional (frictional hard) granular materials and grains with reduced surface friction and hardness. We show, that particle stiffness has a strong effect on the qualitative features of silo discharge. For deformable grains lowering the friction coefficient leads to a gradual change in the discharge curve: the flow rate becomes filling height dependent, it decreases during the discharge process. For hard grains the flow rate is much less sensitive to the value of the friction coefficient. For more details see Pongó et al., New J. Phys., (2021)

DY 11: Active Biological Matter II (joint session BP/CPP/DY)

Time: Monday 11:00–13:30 Location: BPb

See BP 5 for details of this session.

DY 12: Posters DY - Fluid Physics, Active Matter, Complex Fluids, Soft Matter and Glasses (joint session DY/BP)

Time: Monday 14:00–16:30 Location: DYp

DY 12.1 Mon 14:00 DYp

Jerky active matter: a phase field crystal model with translational and orientational memory* — •Michael te Vrugt, Julian Jeggle, and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149, Münster, Germany

Most field theories for active matter neglect effects of memory and inertia. However, recent experiments have found inertial delay to be important for the motion of self-propelled particles. A major challenge in the theoretical description of these effects, which makes the application of standard methods very difficult, is the fact that orientable particles have both translational and orientational degrees of freedom which do not necessarily relax on the same time scale. In this work, we combine modern mathematical methods from particle physics and nonlinear dynamics to derive the general mathematical form of a field theory for soft-matter systems with two different time scales. This allows to obtain a phase field crystal model for polar (i.e., nonspherical or active) particles with translational and orientational memory. Notably, this theory is of third order in temporal derivatives and can thus be seen as a spatiotemporal jerky dynamics. An analysis of the model reveals interesting effects of memory on the dynamics of active systems.

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

DY 12.2 Mon 14:00 DYp

Dynamic role of coherent structures in two-dimensional Navier-Stokes turbulence — •Jiahan Wang[1], Wolf-Christian Müller[1], and Jörn Sesterhenn[2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Universität Bayreuth, Bayreuth, Germany

Turbulent coherent structures can phenomenologically be described as regions in a flow exhibiting a high level of spatio-temporal correlation. Although these structures are ubiquitously observed in nature, providing a universal and rigorous definition of them is not a straightforward task. Therefore the choice of a suitable structure detection method is generally not unique and problem-dependent. We are interested in structures appearing in statistically isotropic Navier-Stokes turbulence. For this purpose, direct numerical simulations (DNS) of a two-dimensional flow, forced at small spatial scales, are employed to compare different definitions of structural coherence. This setup inherently forms large scale structures due to the inverse cascade of energy. Detection methods such as the identification of Lagrangian coherent structures (LCS), dynamic mode decomposition (DMD) and wavelet denoising are all capable of splitting physical fields into coherent and incoherent contributions. Based on that, the analysis of the scale-to-scale decomposed energy flux yields a physical interpretation for the influence of those structures onto the overall inverse cascade dynamics. As a result, the decomposed fluxes gained from LCS and DMD are related, whereas the wavelet decomposition shows no similarity at all.

DY 12.3 Mon 14:00 DYp

Magnetic helicity inverse transfer in supersonic isothermal MHD turbulence — •Jean-Mathieu Teissier[1,2] and Wolf-Christian Müller[1,2,3] — [1]Technische Universität Berlin, ER3-2, Hardenbergstr. 36a, D-10623 Berlin, Germany — [2]Max-Planck/Princeton Center for Plasma Physics — [3]Berlin International Graduate School in Model and Simulation Based Research

Magnetic helicity is an ideal invariant of the magnetohydrodynamic (MHD) equations which exhibits an inverse transfer in spectral space. Up to the present day, its transport has been studied in direct numerical simulations only in incompressible or in subsonic or transonic flows. Inspired by typical values of the turbulent root mean square (RMS) Mach number in the interstellar medium, this work presents some aspects of the magnetic helicity inverse transfer in high Mach number isothermal compressible turbulence, with RMS Mach numbers up to the order of ten:

1) a clear Mach-number dependence of the spectral magnetic helicity scaling but an invariant scaling exponent of the co-spectrum of the Alfvén velocity and its curl,

2) the approximate validity of a dynamical balance relation found by incompressible turbulence closure theory,

3) a characteristic structuring of helically-decomposed nonlinear shell-to-shell fluxes that can be disentangled into different spectrally local and non-local transfer processes.

DY 12.4 Mon 14:00 DYp

Molecular dynamics of janus polynorbornenes: glass transitions and nanophase separation — •Mohamed A Kolmangadi, Paulina Szymoniak, Martin Böhning, and Andreas Schönhals — Bundesantalt für Materialforschung und -prüfung (BAM), Berlin, Germany

For the first time, dielectric and calorimetric investigations of a homologous series of Janus polynorbornenes with rigid main backbones and flexible Si(OR)3 side groups of differing length alkyl chains (R = propyl, butyl, hexyl, octyl, and decyl) is reported.Two dielectrically active processes are observed at low temperatures, denoted as β- and α-relaxation. The former can be assigned to localized fluctuations, while the latter is related to the glassy dynamics of the flexible Si(OR)3 side groups, creating a nanophase separation in both the alkyl chain-rich and backbone-rich domains. This is confirmed through temperature-modulated differential scanning calorimetry (TMDSC) measurements and X-ray scattering experiments. The glass transition temperatures of the backbone rich domains, which are beyond or near to their degradation temperatures in terms of conventional DSC, are determined for the first time using fast scanning calorimetry employing both fast heating and cooling rates. This is complemented with scattering experiments that show how the size of the alkyl chain-rich domains increases with the side chain length. Alongside these results, a significant conductivity contribution was observed for all poly(tricyclononenes) with Si(OR)3 side groups, which is interpreted in terms of a percolation model

DY 12.5 Mon 14:00 DYp

Classical Density Functional Theory for Particles with Hard Cores and Soft Square Shoulders — •Markus Hoffmann, Robert F. B. Weigel, and Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Classical density functional theory is an excellent tool to investigate classical many-body systems from fundamental principles, in particular soft matter systems. We consider particles with hard cores and soft square shoulders in two dimensions. The hard-core is implemented by using a variant of the Fundamental Measure Theory that probably is the best mean field approach to hard particles.

The hard core-square shoulder interaction possesses two independent length scales namely the diameter of the hard core and the diameter of the square shoul-

ders. We observe the expected crystallization transitions into a triangular phase for both very weak shoulders where the hard cores dominate and for strong shoulders effectively leading to a soft sphere system.

However, the most interesting cases are expected when the two length scales of the systems are competing. As a result, not only square patterns are observed but we also want to explore quasicrystals. Note that previous mean field descriptions of quasicrystals (like Phase Field Crystal approaches) usually consider cluster crystals and so far have not been able to explain the formation of quasicrystals for particles with hard cores.

DY 12.6 Mon 14:00 DYp

Organizing bacterial vortex lattices by periodic obstacle arrays — •Henning Reinken[1], Sebastian Heidenreich[2], Markus Bär[2], and Sabine H. L. Klapp[1] — [1]Technische Universität Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Berlin, Germany

Recent experimental studies have shown that the turbulent vortex structures emerging in bacterial active fluids can be organized into regular vortex lattices by weak geometrical constraints such as small pillars [1]. Using a continuum-theoretical approach [2,3], we show how these artificial obstacles reorganize self-induced topological defects which guides the flow profile of the active fluid and enables the stabilization of vortex patterns with tunable properties. Beyond the stabilization of square and hexagonal lattices, we also provide a striking example of a chiral, antiferromagnetic lattice induced by arranging the obstacles in a Kagome-like array [3]. In this setup, the interplay of lattice topology, activity and length-scale selection generates a net rotational flow. Further, we explore the connections between the stabilized non-equilibrium vortex patterns and equilibrium phase transitions in classical spin lattice models, e.g., the Ising model.

[1] D. Nishiguchi, I. S. Aranson, A. Snezhko, and A. Sokolov, Nat. Commun. **9**, 4486 (2018)
[2] H. Reinken, S. H. L. Klapp, M. Bär, and S. Heidenreich, Phys. Rev. E **97**, 022613 (2018)
[3] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, Commun. Phys. **3**, 76 (2020)

DY 12.7 Mon 14:00 DYp

Active mobile oscillators: Density fluctuations and phase ordering — Astik Haldar[1], •Swarnajit Chatterjee[2], Apurba Sarkar[3], Raja Paul[3], and Abhik Basu[1] — [1]Saha Institute of Nuclear Physics, Kolkata, India — [2]Center for Biophysics & Department for Theoretical Physics, Saarland University, Saarbrücken, Germany — [3]Indian Association for the Cultivation Of Science, Kolkata, India

We consider the collective motion of nearly phase-ordered active oscillators on a substrate. The dynamics include activity-induced couplings between the local phase with the concentration of the mobile oscillators on the interface. We show that such a system can be stable over a wide range of model parameters. When stable, the system can also show a variety of orders. In different regions of the phase space, the system can show phase ordering that is stronger than the conventional quasi long-range order (QLRO) together with hyperuniform number fluctuations, or phase ordering weaker than QLRO together with giant number fluctuations, or even QLRO with uniform density fluctuations. In other parameter regimes, the system becomes unstable with the eventual loss of any phase ordering beyond a finite (small) system size. We have also constructed an appropriate agent-based lattice-gas model. Numerical simulations of this model corroborate the analytical predictions and validate the results on the phase fluctuations.

DY 12.8 Mon 14:00 DYp

Structural and dynamical properties of gel networks — •Matthias Gimperlein and Michael Schmiedeberg — Institut für theoretische Physik 1, FAU Erlangen-Nürnberg

Gelation is connected to a slow-down in dynamics, the onset of percolation and an increasing number of neighboring particles. The slow-down occurs on different time scales depending on the studied length scales.

Using Brownian Dynamics simulation for a system of colloidal particles interacting due to a modified square well and Yukawa potential we investigate the structural properties of gel networks on different time and length scales depending on system parameters as the strength of attraction or repulsion respectively.

The square well potential is modified by introducing an interaction range α to flatten the walls of the square well. The phase diagram was determined by fitting the vapour-liquid binodal. In the square well limit ($\alpha \to 0$) results from the literature are recovered. Structural properties as node distribution or link lengths are extracted from minimal networks which allow an easier analysis of the underlying network structure.

Further research includes distinguishing dynamic regimes or structures on different length and time scales, investigating the history/protocol dependency of the development (i. e. starting from different initial configuration) and finding stable or metastable structures to describe the evolution of gel networks not on the particle level anymore, but on a coarse grained level.

DY 12.9 Mon 14:00 DYp

Simple model for drops on elastic substrates — •Christopher Henkel[1], Uwe Thiele[1], and Jacco Snoeijer[2] — [1]Institut für Theoretische Physik, WWU-Münster, Germany — [2]Fac. of Science and Technologie, University Twente, Netherlands

The investigation of the wetting behavior on viscoelastic or elastic substrates is of great interest. In this talk we present a simple model for steady liquid drops on fully compressible elastic substrates and show that a double transition of contact angles appears under variation of the substrate softness, similar to the one described in [1]. We further discuss whether these angles agree with the Neumann and Young-Laplace conditions in the liquid-liquid and liquid-solid limit respectively and how the transitions depend on drop size. Finally, we employ a gradient dynamics model in the long-wave limit and show first results of direct time simulations.

[1] Lubbers, L. A., Weijs, J. H., Botto, L., Das, S., Andreotti, B., and Snoeijer, J. H., (2014). Drops on soft solids: free energy and double transition of contact angles. *Journal of fluid mechanics*, 747.

DY 12.10 Mon 14:00 DYp

Flocking and reorientation transition in the q-state active Potts model — •Matthieu Mangeat[1], Swarnajit Chatterjee[1,2], Raja Paul[2], and Heiko Rieger[1] — [1]Saarland University, Saarbrücken, Germany — [2]IACS, Kolkata, India

We study the q-state active Potts model (APM) on a two-dimensional lattice in which active particles have q internal states corresponding to the q directions of motion. A local alignment rule inspired by the ferromagnetic q-state Potts model and self-propulsion via biased diffusion according to the internal particle states leads to a collective motion at high densities and low noise. We formulate a coarse-grained hydrodynamic theory with which we compute the phase diagram of the APM and explore the flocking dynamics in the region, in which the high-density (polar liquid) phase coexists with the low-density (gas) phase and forms a fluctuating band of coherently moving particles. As a function of the particle self-propulsion velocity, a novel reorientation transition of the phase-separated profiles from transversal to longitudinal band motion is found, which is absent in the Vicsek model [1] and the active Ising model [2]. The origin of this reorientation transition is revealed by a stability analysis: for large velocities the transverse diffusion constant approaches zero and then stabilizes longitudinal band motion. Computer simulations corroborate the analytical predictions of the flocking and reorientation transitions and validate the phase diagrams of the APM.

[1] T. Vicsek *et al.*, Phys. Rev. Lett. **75**, 1226 (1995).
[2] A. P. Solon and J. Tailleur, Phys. Rev. Lett. **111**, 078101 (2013).

DY 12.11 Mon 14:00 DYp

Cell fitness in growth driven active matter: decoupling turnover rate and homeostatic pressure predictors — •Yoav G. Pollack[1], Philip Bittihn[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, 37077, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, OX1 3PU, UK

In growth-driven dense cellular active matter, cell dynamics and competition are governed by the intricate relations between growth, proliferation, removal (e.g. death, extrusion) and mechanical interactions. Though the rates at which a cell proliferates or dies have already been established as a significant factor for fitness, homeostatic pressure was recently suggested as an equivalent predictor of fitness and one that can be more easily measured. Here we show that this equivalence in not universal and can be broken. By introducing an additional time-scale that governs the duration of the single-cell removal process in a simple growing dumbbell model of cells, the homeostatic pressure is partially decoupled from the turnover rate, leading to a distinct prediction for each. When the two factors are modulated in this way in a simulated competition assay of a mixture of two cell species in a closed 1D channel, we show that while the homeostatic pressure does not predict well which species triumphs, the turnover rate does. A good fitness measure is important in studies of tumor growth, bacterial evolution, etc. and this result is a first step in understanding for which scenarios is the homeostatic pressure a valid predictor.

DY 12.12 Mon 14:00 DYp

Unjamming of Active Rotators — •Linda Ravazzano[1], Silvia Bonfanti[1], Maria C. Lionetti[1], Maria R. Fumagalli[1], Roberto Guerra[1], Oleksandr Chepizhko[2], Caterina A. M. La Porta[1], and Stefano Zapperi[1] — [1]Center for Complexity and Biosystems, University of Milan, Italy — [2]Leopold-Franzens-Universität Innsbruck, Austria

Active particles assemblies are of peculiar interest thanks to the richness of dynamical phases they can undergo varying internal parameters such as density, adhesion strength or self-propulsion. Most theoretical studies of active matter consider self-propelled particles driven by active forces. The observation of the motion of Chlamydomonas reinhardtii algae, in which the active particles have also the ability to self-rotate, suggests, however, that active torques may also play an important role. Inspired by this example, we simulate the dynam-

ics of a system of interacting active 2D disks endowed with active torques and self-propulsive forces. We studied this model system of active rotators in different conditions: at low packing fractions, where adhesion causes the formation of small rotating clusters, at higher densities, where our simulations show a jamming to unjamming transition promoted by active torques and hindered by adhesion, and in presence of both self-propulsion and self-rotation, studying the interplay between those quantities and deriving a phase diagram. Our results yield a comprehensive picture of the dynamics of active rotators, highlighting the importance of the internal degrees of freedom of active particles in determining the collective behavior of the system.

DY 12.13 Mon 14:00 DYp

The thermodynamics and kinetics of protein crystallization probed by isothermal microcalorimetry — Lorena Hentschel, •Jan Hansen, Florian Platten, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

During a first-order phase transition, a thermodynamic system releases or absorbs latent heat. Despite their fundamental importance, the heat or enthalpy change occurring during protein crystallization has been directly measured only in a few cases, and the associated entropy change can only be determined indirectly. Here, the thermodynamics and kinetics of tetragonal lysozyme crystallization are studied for various physicochemical solution parameters. Direct microcalorimetric and indirect van't Hoff enthalpy determinations quantitatively agree, suggesting a two-state crystallization process. Assuming that crystals are electrostatically neutral, the weak dependences of the crystallization enthalphy and entropy on salt concentration and pH value are explained by a Poisson-Boltzmann model. Furthermore, the calorimetric signal is related to the concentration change during nucleation and growth, from which the induction time and the growth rate are inferred. Their dependences on the chemical potential are in line with previous findings and can be modelled by classical nucleation theory and 2D growth models, respectively.

DY 12.14 Mon 14:00 DYp

Real-Time Investigations during Sputter Deposition on Polymer Thin Films — •Matthias Schwartzkopf[1], Marc Gensch[1,2], Thomas Strunskus[3], Franz Faupel[3], Peter Müller-Buschbaum[2] und Stephan V. Roth[1,4] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]CAU zu Kiel, Kaiserstr.2, 24143 Kiel — [3]TUM, James-Franck-Str. 1, D-85748 Garching — [4]KTH, Teknikringen 56-58,SE-100 44 Stockholm

The reproducible low-cost fabrication of functional metal-polymer-nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the evolution at the nanogranular metal-polymer interface, we employed time-resolved surface sensitive X-ray scattering during sputter deposition of gold on thin polystyrene films [1] and SiOx [2]. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of atomic deposition rate on the growth regimes with their specific thresholds. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015); [2] Schwartzkopf et al., Nanoscale 5, 5053 (2013).

DY 12.15 Mon 14:00 DYp

Fluid transport by metachronal waves of model cilia — •Albert von Kenne, Thomas Niedermayer, and Markus Bär — Department of Mathematical Modelling and Data Analysis, Physikalisch-Technische Bundesanstalt Berlin, Abbestraße 2-12, Berlin 10587, Germany

Motile cilia are hair-like cell extensions that undergo a cyclic motion with the purpose to transport the extracellular fluid at a low Reynolds number, providing crucial functionality of living matter such as cell locomotion and molecular transport in tissue. A striking feature of populations of cilia is a state of collective motion known as metachronal wave.

To investigate these collective states we generalize a simple phase oscillator model for the elastohydrodynamic coupling in ciliated systems [1], to include the effects due to the confined flow in proximity of a cell substrate. Our model encompasses spontaneous creation of waves as well as directed cycle-average fluid flow, yet it's simple enough to be solved analytically. We obtain analytical results for the linear stability of metachronal waves in presence of long-range hydrodynamic interactions, illustrate their properties by numerical simulations and relate the change in transport efficiency to the specific properties of metachronal waves.

[1] . Niedermayer, B. Eckhardt, and P. Lenz, Chaos **18**, 037128 (2008)

DY 12.16 Mon 14:00 DYp

Athermal Jamming for particles with exponentially decreasing repulsions — •Nicolas Wohlleben and Michael Schmiedeberg — Institut für Theoretische Physik I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstraße 7, 91058 Erlangen, Germany

We study the jamming of a colloidal system where the particles interact according to a Yukawa potential, i.e., the repulsion decreases exponentially with the distance as expected for screened Coulomb interactions of charged colloids in solution. The decay occurs on a length scale given by the screening length and in addition we consider a cutoff length where the potential is set to zero in a smooth way as often used in simulation.

By determining the athermal jamming transition by trying to remove overlaps we find that the transition packing fraction only depends on the cutoff length but hardly on the screening length. We also explore the radial distribution function and again confirm the importance of the cutoff length.

The picture that emerges is that the influence of a cutoff length on athermal jamming is superior to that of the screening length, although the screening length is expected to control the slowdown of the dynamics (i.e., the dynamical glass transition). As a consequence, athermal jamming (as defined by overlaps) and the glass transition obviously are unrelated in the considered system.

DY 12.17 Mon 14:00 DYp

Detection of defects in soft quasicrystals with neural networks — •Ali Döner and Michael Schmiedeberg — Institut für Theoretische Physik I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudstr. 7, 91058 Erlangen, Germany

The aim of this work is to construct and employ a neural network for the detection of topological defects in dodecagonal quasicystalline patterns. Even though quasircrystals are aperiodic, they exhibit a longe-range order. Furthermore, in principle any discrete rotational symmetry can occur.

In this work, dodecagonal quasicrystalline patterns in two-dimensions with a built-in dislocation are generated and employed as input images of the neural network. The network then should figure out not only the position but also the type of the Burgers vector of the defect.

Our trained neural network is able to recognize the type of the Burgers vector perfectly. The position of the dislocation is recognized up to a mean deviation from the real position that is much smaller than the small length scale in the quasicrystals. In future, we want to train the network with patterns that contain multiple dislocations as well as phasonic excitations.

DY 12.18 Mon 14:00 DYp

Bistable vortices formed by active particles with retarded interactions - Theory — Xiangzun Wang[1], •Pin-Chuan Chen[2], Viktor Holubec[2,3], Klaus Kroy[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University of Leipzig, 04103 Leipzig — [2]Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany — [3]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, 18000 Prague, Czech Republic

In a recent experiment (see the companion contribution "Experiment", serial number DY193), thermophoretic microswimmers were observed to self-assemble into a bistable mode of circular collective motion. We explain the underlying mechanism qualitatively by deriving a coarse-grained Langevin model for active Brownian particles with retarded interactions. For a single microswimmer attracted to an immobile attractive sphere, it can be broken down to an effective model for the angular degree of freedom. The reduced one-dimensional overdamped Langevin equation features a virtual potential for the angular velocity, self-generated by the retarded propagation of the interaction. We work out the quantitative analytical predictions for the delay-dependent bifurcation scenario and the Kramers rates and numerical results for spontaneous transitions between the degenerate chiral modes of angular motion, beyond the bifurcation point. Our theoretical predictions are found to agree well with the experimental observations and simulations.

DY 12.19 Mon 14:00 DYp

Bistable vortices formed by active particles with retarded interactions - Experiment — •Xiangzun Wang[1], Pin-Chuan Chen[2], Viktor Holubec[2,3], Klaus Kroy[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, 04103 Leipzig, Germany — [2]Institute for Theoretical Physics, Universität Leipzig, 04103 Leipzig, Germany — [3]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, 18000 Prague, Czech Republic

Rotating formations of living species are frequently observed in nature from bacterial systems and insects to larger animals like fish or birds. The ubiquity of this behavior suggests universal underlying principles. One could be related to inevitable delays caused by sensimotoric feedback. We explore experimentally the influence of a delayed interaction between individual self-thermophoretic microswimmers on their collective behaviour. Our microswimmers are gold nanoparticle decorated melamine resin colloids, which are propelled by self-thermophoresis due to a local heating of the gold nanoparticles with a focused laser. Using a feedback algorithm we are able to introduce time-delayed virtual interactions with other particles or targets. We find for a single swimmer attracted to an immobilized particle, a transition from a diffusive to a rotating state with two possible rotation directions. This behavior is captured by a simple theoretical model (see companion contribution). This bifurcation is also observed in ensembles of multiple particles where the rotational phase of the ensemble is synchronized by particle collisions.

DY 12.20 Mon 14:00 DYp

Effect of Alignment Activity on the Collapse Kinetics of a Flexible Polymer — •Subhajit Paul[1], Suman Majumder[1], Subir K Das[2], and Wolfhard Janke[1] — [1]Institut fuer Theoretische Physik, Universitaet Leipzig, Bruederstr. 16, D-04103, Leipzig, Germany — [2]Theoretical Sciences Unit, JNCASR, Bangalore-560064, India.

Dynamics of various biological filaments can be understood within the framework of active polymer models. Keeping this in mind, we construct a bead-spring flexible polymer chain in which the active interaction among the beads is introduced via an Vicsek-like alignment rule. Following a quench from the high-temperature coil phase to a low-temperature state, we study the non-equilibrium coarsening kinetics of this model via molecular dynamics (MD) simulations. For the passive polymer case the low-temperature equilibrium state is a compact globule. Results from our MD simulations reveal that though the globular state is also expected to be the typical final state in the active case as well, the non-equilibrium pathways change due to the alignment interaction among the beads. We observe that the probability of deviation from the intermediate *pearl-necklace*-like arrangement and the formation of more elongated dumbbell- like structures increases with increasing activity. Also, there exists nonmonotonicity in coarsening with the variation of the strength of activity. In this work, our focus is on such non-equilibrium dynamics results for which we compare with those of the passive case. These are concerning scaling laws related to collapse time and growth of clusters.

DY 12.21 Mon 14:00 DYp

The parameter space of thermohaline stairs — •Axel Rosenthal and Andreas Tilgner — Institut für Geophysik, Georg-August-Universität Göttingen, Deutschland

Convection and diffusion in water can be observed when a gradient in temperature or in salinity takes effect on density in presence of gravity. Both gradients can force or stabilize the process. We conducted experiments where the salt gradient is the driving force and simultaneously the temperature gradient is stabilizing in opposite direction, observed by particle image velocimetry. The question is at which gradients, expressed by Rayleigh numbers, does the transport occure in stable so called "thermohaline stairs"? Thermohaline stairs are a sequence of two flow systems, a finger regime and a large scale circulation.

DY 12.22 Mon 14:00 DYp

Fluctuations of a driven tracer in a viscoelastic bath — •Juliana Caspers — Institut für Theoretische Physik, Göttingen

Recently, viscoelastic fluids have attracted attention as their large structural relaxation times induce a variety of new phenomena such as nontrivial back reactions of the bath on a driven probe particle. Berner *et al* [1] found particle oscillations in the linear response regime, both in theory and experiment. Moreover, Müller *et al* [2] investigated effects of nonlinear baths in equilibrium. They observed inter-dependencies entering the coefficients in an effective linear generalized Langevin equation. For example, the friction memory kernel depends on properties of the external trap [3] or on the bare tracer friction in the case of an overdamped setting. In [1,2], the simple model of a confined tracer particle interacting via a stochastic Prandtl-Tomlinson model with a bath particle was found to be a good candidate to mimick the properties of a nonlinear viscoelastic bath. This work focuses on the interplay of the external trap that confines the tracer particle and the nonlinearity of the bath. In a nonequilibrium situation we made a first observation of shear thickening, an increase in the microrheological friciton coefficient for a certain regime of driving velocities.

[1] J. Berner, B. Müller, J. R. Gomez-Solano, M. Krüger, and C. Bechinger. *Nat. Commun.*, 9(1):999, 2018

[2] B. Müller, J. Berner, C. Bechinger, and M. Krüger. *New J. Phys.*, 22:023014, 2020

[3] J. O. Daldrop, B. G. Kowalik, and R. R. Netz. *Phys. Rev. X*, 7:041065, 2017

DY 13: Granular Physics 3 - organized by Matthias Sperl (Köln)

Time: Monday 15:00–17:20 Location: DYc

DY 13.1 Mon 15:00 DYc

Monitoring granular drag with non-invasive particle tracking techniques — •Kai Huang[1,2], Jinchen Zhao[1], Chen Lyu[1], Valentin Dichtl[2], and Simeon Voelkel[2] — [1]Institute of Applied Physical Sciences and Engineering, Division of Natural and Applied Sciences, Duke Kunshan University, No. 8 Duke Avenue, Kunshan, Jiangsu, China 215316 — [2]Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Considering granular materials as a complex fluid with a finite yield stress, an object moving inside has to locally unjam and mobilize the surrounding particles in order to step forward. Consequently, granular drag depends strongly on the local rheological behavior and it is essential to have an 'insider' view on granular dynamics. Experimentally, this is achieved using microwave radar and embedded IMU sensor techniques. Our results are in align with discrete element simulations equipped with coarse-graining techniques, which provide additional information on response of the granular bed. Our results of the intruder dynamics are in congruent with existing phenomenological model on granular drag. Interestingly, we find that the macroscopic profiles of the granular bed ahead of the intruder decays exponentially in the co-moving system of the intruder, giving rise to a characteristic length scale on the order of intruder size. Stepping further, we explore the influence of gravity on granular drag by means of microgravity environment in order to shed light on challenges arising from space exploration.

DY 13.2 Mon 15:20 DYc

Granular Rheology from First Principles — •Till Kranz[1], Olfa Lopez[2], Olivier Coquand[2], and Matthias Sperl[2,1] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

We have recently demonstrated that the *Granular Integration Through Transients* (GITT) formalism allows to derive a constitutive equation for the shear stress σ as a function of the shear rate $\dot{\gamma}$ for arbitrary shear rates and high densities [1] of a granular fluid. Here we extend the formalism to derive a constitutive equation for the pressure $p(\dot{\gamma})$. This allows us to discuss flow curves at constant pressure and the *effective friction* $\mu = \sigma/p$. The phenomenological $\mu(I)$ rheology [2] relates the friction μ to the dimensionless inertial number I. We will discuss the relation between the GITT expressions and $\mu(I)$ rheology. In addition, we will present experimental stress measurements on fluidised glass beads covering several orders of magnitude in shear rate and displaying all the rheologigcal regimes predicted by GITT, namely, Newtonian rheology, as well as shear thinning and shear thickening behaviour.

[1] W. T. Kranz, F. Frahsa, A. Zippelius, M. Fuchs and M. Sperl, PRL **121**, 148002 (2018); PRF **5** 024305 (2020)

[2] GDR Midi, EPJ E **14**, 341 (2004)

DY 13.3 Mon 15:40 DYc

Aeolian structure formation in a laboratory wind tunnel — •Merve Seckin[1], Philip Born[1], and Matthias Sperl[1,2] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Institut für Theoretische Physik, Uni Köln

Aeolian transport causes structure formation in beds of granular particles. The length scale of structures formed by aeolian transport is fundamentally connected to the saturation length of the particle flux. Achieving structures on length scales suitable for laboratory experiments by minimizing this saturation length is challenging, but would allow testing and calibrating models of aeolian transport.

Here we show results obtained with very fine particles with an additional surface treatment to minimize cohesion. Saturation lengths of a centimeter can be obtained with this particle system. Consequently, we can show that self-initiated and sustained structure formation from particle beds by aeolian transport is possible at ambient conditions in a benchtop wind tunnel. Barchan-like structures emerge from flat particle beds and from particles heaps, which migrate downwind even without particle influx. We compare the experimental results with the existing theory and discuss open questions.

DY 13.4 Mon 16:00 DYc

Numerical investigation of the rheology of elongated particles — •Ellák Somfai[1], Dániel Nagy[1], Philippe Claudin[2], and Tamás Börzsönyi[1] — [1]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Budapest, Hungary — [2]Physique et Mécanique des Milieux Hétérogènes, PMMH UMR 7636 CNRS, ESPCI Paris, PSL University Sorbonne Université, Université de Paris, Paris, France

We performed discrete element model simulations to investigate the rheology of a realistic 3-dimensional frictional granular material consisting of elongated particles. Such systems develop orientational ordering when exposed to shear flow. The degree of this ordering depends on the interparticle friction and particle elongation in a nontrivial manner. Namely, the shear induced orientational ordering is in principle increasing with particle elongation, but the characteristics of collisional and frictional interactions between neighbours (which hinder each others rotation) changes with the interparticle friction coefficient. We measured how key rheological quantities, including effective friction and normal stress differences depend on these two key parameters. We found that the aspect ratio dependence of the effective friction is non-monotonic not only for frictionless particles as we saw earlier, but also for frictional particles up to interparticle friction coefficient $\mu_p \lesssim 0.4$, – a range already relevant for every day materials. For higher μ_p the effective friction is monotonically increasing. We can explain the microscopic origins of both the non-monotonic behaviour for small and intermediate μ_p and the monotonic one for large μ_p.

DY 13.5 Mon 16:20 DYc

Migrating shear bands in shaken granular matter — Joelle Claussen[1], Stefan Gerth[1], Jonathan E. Kollmer[2,3,4], Thorsten Pöschel[3], Michael Salamon[1], •Matthias Schröter[3,5], Tara Shreve[3,6], and Norman Uhlmann[1] — [1]Fraunhofer-Entwicklungszentrum Röntgentechnik, Flugplatzstr. 75, 90768 Fürth, Germany — [2]Experimentelle Astrophysik, Universität Duisburg-Essen, Lotharstr. 1-21, 47057 Duisburg, Germany — [3]Institute for Multiscale Simulation of Particulate Systems, Cauerstr. 3, 91058 Erlangen, Germany — [4]Dept. of Physics, 2401 Stinson Drive, North Carolina State University, Raleigh, NC 27695, USA — [5]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [6]Université de Paris, Institut de physique du globe de Paris, CNRS, F-75005, Paris, France

When dense granular matter is sheared, the strain is often localized in shear bands. After some initial transient these shear bands become stationary. Here we introduce a setup that periodically creates horizontally aligned shear bands which then migrate upwards through the sample. Using X-Ray radiography we demonstrate that this effect is caused by dilatancy, the reduction in volume fraction occurring in sheared dense granular media. Further on, we argue that these migrating shear bands are responsible for the previously reported periodic inflating and collapsing of the material.

Ref.: Kollmer *et al.* Phys. Rev. Lett. 125, 048001 (2020)

DY 13.6 Mon 16:40 DYc

Force chains in granular packings visualized by stress-birefringent spheres — •David Fischer[1], Karsten Tell[2], Peidong Yu[2], Matthias Sperl[2], and Ralf Stannarius[1] — [1]Otto-von-Guericke-Universität, Institut für Physik, Abteilung Nichtlineare Phänomene, Magdeburg — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Köln

Force networks play an important role in the stability of granular packings. These networks are able to redirect part of the particle weight inside a container to the side walls, leading to pressure saturation in a certain depth below the granular surface. We employ monodisperse stress-birefringent spheres embedded in an immersion fluid to visualize the contact forces and force network structure of spheres in a quasi-2D and a nearly-2D cuboid cell. A load at the top prevents floating of the spheres caused by buoyancy. In both cell types, an "inverse" Janssen effect is observed, with the pressure decreasing from the top to the bottom of the container.

DY 13.7 Mon 17:00 DYc

Intermittent flow and transient congestions of soft low-friction spheres in silo discharge — •Jing Wang[1], Kirsten Harth[1], Ralf Stannarius[1], and Tamas Börzsönyi[2] — [1]Institute of Physics, Otto von Guericke University, Magdeburg, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest, Hungary

During discharge of hard particles from a silo with a small orifice at the bottom, grains flow freely only when the orifice size at least 5 times the particle diameter. The outflow rate is practically independent of the fill level. Below a certain outlet diameter, hard particles reach stable clogs, which can only be destroyed by external forcing. We study soft, low-friction particles (hydrogel beads) that show very different, peculiar features during discharge: They flow freely even when the orifice is only slightly larger than two particle diameters. At small orifice sizes, strong fluctuations of the flow velocity set in. Non-permanent congestions are characteristic that have previously been described only for lifestock or pedestrians passing narrow gates or exits, but never for inanimate hard granular material. We present experimental data recorded in a 2D silo.

This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 812638 and DFG Grant HA8467/2-1. [1] K. Harth et al., Soft Matter 16 8013 (2020).

DY 14: Microfluidics and Droplets - organized by Uwe Thiele (Münster)

Time: Monday 16:00–18:00 Location: DYa

DY 14.1 Mon 16:00 DYa

Near-field acoustic manipulation in a confined evanescent Bessel beam — •Pierre-Yves Gires[1,2] and Cédric Poulain[2,3] — [1]University Grenoble Alpes, CEA LETI — [2]University of Bayreuth, Experimental Physics I — [3]University Grenoble Alpes, CNRS, Grenoble INP, Institut Néel

Microparticles such as cells can be manipulated in a suspension by the application of an ultrasonic acoustic field. Following the path taken in the development of optical tweezers, we demonstrate the potential of working in the evanescent regime, with both sub-wavelength confinements and resonators [1]. We generate an evanescent acoustic Bessel beam in liquid above a thin, circular, axisymmetrically excited plate. In the sub-MHz domain, the resulting radiation force causes the particles to assemble at the pressure antinodes along concentric circles corresponding to the Bessel profile. By imposing an axial confinement in the evanescent region, the sub-wavelength two-plate sandwich system becomes resonant, increasing the radiation force magnitude. Resonances occur for some well-defined gaps for which whole numbers of antinodal circles are observed. Through fine tuning, particles as small as bacteria can be patterned. Further amplification can be obtained by trapping a microbubble in the Bessel beam axis.
[1] Pierre-Yves Gires and Cédric Poulain. Near-field acoustic manipulation in a confined evanescent bessel beam. Communications Physics, 2(1):1-8, 2019

DY 14.2 Mon 16:20 DYa

Actuation of soft particles in oscillating Poiseuille flow — •Winfried Schmidt[1], Sebastian W. Krauss[2], Andre Förtsch[1], Matthias Laumann[1], Matthias Weiss[2], and Walter Zimmermann[1] — [1]Theoretische Physik 1, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Experimentalphysik 1, Universität Bayreuth, 95440 Bayreuth, Germany

What is the dynamical behavior of soft particles in oscillatory (pulsating) Poiseuille flow at low Reynolds number? By investigating the overdamped motion of 2D bead-spring models, as well as 3D capsules and red blood cells, we predict particle actuation in the case of vanishing mean flow. This effect is generic as it does not depend on the model. We show that symmetric particles propagate for asymmetric flow oscillations with non-equal flow sections. The mean actuation (swim) velocity of a particle is caused by its varying shape in both parts of the flow period. Since the actuation steps depend also on the size and the rigidity of soft particles, this novel actuation (passive swimming) mechanism is also appropriate for particle sorting.

DY 14.3 Mon 16:40 DYa

Two orders of magnitude boost in the detection limit of droplet-based micro-magnetofluidics — •Julian Schütt[1], Rico Illing[1], Oleksii Volkov[1], Tobias Kosub[1], Pablo Nicolás Granell[1,2], Hariharan Nhalil[3], Jürgen Fassbender[1], Lior Klein[3], Asaf Grosz[4], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany — [2]Escuela de Ciencia y Tecnología, UNSAM, Buenos Aires, Argentina — [3]Department of Physics & Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel — [4]Department of Electrical and Computer Engineering, Ben-Gurion University of the Negev, Israel

The detection of magnetic nanoparticles is of major importance in biomedical and biological applications. Here, the trend goes towards improvements of state-of-the-art methods in the spirit of high-throughput analysis at ultra-low volumes. Microfluidics addresses these requirements as it deals with the control and manipulation of liquids in confined microchannels. Sensor elements utilizing the planar Hall Effect (PHE) are exceptionally suited for this conjunction and were already applied in continuous flow microfluidics. We present a sensing strategy relying on PHE sensors in digital microfluidics for the detection of a multiphase liquid flow. We show the detection of nanoliter-sized superparamagnetic droplets with a concentration of 0.58mg/cm3, biased in a geomagnetic field, down to 0.04mg/cm3 in a magnetic field of 5mT. We are convinced that the tracking of microfluidic droplets can greatly contribute to state-of-the-art magnetoresistive sensing with dramatic downscaling of the analyzed volume.

DY 14.4 Mon 17:00 DYa

Theoretical and numerical investigation of an EWOD-driven micro pump — •Sebastian Bohm and Erich Runge — Technische Universität Ilmenau, Theoretische Physik 1, Weimarer Straße 25, 98693 Ilmenau

We show how the EWOD (electrowetting-on-dielectric) effect can be used to realize a micro pump that uses no moveable components at all, as described in [1]. The flow is generated due to the periodic movement of liquid-vapor interfaces in a large number ($\approx 10^6$) of microcavities ($\Delta V \approx 1pl$ per cavity). The total flow resulting from all microcavities adds up to a few hundred nanolitres per cycle. Tesla-Diodes are used as valves to completely forgo on moving parts.
The theoretical description of the pumping mechanism is a challenge due to the coupling of the fluid- and electrodynamics and the intrinsic multi-scale character of the system. The flow in each microcavity can be modelled as multiphase flow with time-dependent wetting properties as boundary conditions. The optimization of the Tesla diodes is also a challenge, as they must produce a reasonable valve action even at small Reynold numbers, which are typical for microfluidics. A novel time-efficient simulation method for the calculation of the static interface shapes of a liquid-vapor interface in electric fields is presented. With

this method, the voltage-dependent volume stroke can be determined efficiently. Topological optimization methods for the design of the Tesla-Diodes are shown. Finally, possibilities for the time-resolved simulation of the entire pumping system are discussed.
[1] Hoffmann, M., Dittrich, L., Bertko, M.; DE11 2011 104 467 (2012)

DY 14.5 Mon 17:20 DYa

Anchoring-dependent flow bifurcation in nematic microflows within circular capillaries — •Paul Steffen[1], Eric Stellamanns[2], and Anupam Sengupta[1] — [1]Physics of Living Matter, Dept. of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany
Capillary microflows of liquid crystal (LC) phases are fundamental to biological and bio-inspired systems. Here we investigate stationary flows of nematic LC within circular capillaries under homeotropic (normal) and uniform planar anchoring conditions, using numerical simulations based on the continuum theory of Leslie, Ericksen and Parodi for the material parameters of 5CB, a single component flow-aligning nematic LC. Instead of the expected unique solution with a director field monotonously approaching the alignment angle for increasing Ericksen numbers, we report a second anomalous solution that emerges above a threshold flow rate, leading to an anchoring-dependent flow bifurcation. For homeotropic surface anchoring, the anomalous director field orients against the alignment angle in the vicinity of the pipe center; while in the uniform planar case, the anomalous director field extends throughout the capillary volume, leading to reduction of the flow speed for increasing pressure gradients. Experimental signatures of the second solutions in each case are found in authors's experimental results, reported previously in Phys. Rev. Lett. 110, 048303, 2013 (homeotropic) and Int. J. Mol. Sci. 14, 22826, 2013 (planar case).

DY 14.6 Mon 17:40 DYa

Characterizing the speed, size and shape of droplets during their flight from an ultrasonic spray coater — •Pieter Verding[1,2], Wim Deferme[1,2], and Werner Steffen[3] — [1]Hasselt University Institute for Materials Research, Diepenbeek, Belgium — [2]IMEC, Diepenbeek,Belgium — [3]Max-Planck-Institut for Polymer research, Mainz, Germany
Ultrasonic spray coating - USSC is a technology offering numerous possibilities, such as depositing ultrathin homogeneous layers up to 20 nm on large scale. However, its application is limited due to the many process parameters which have a large impact on the quality of the coating. For this reason, measuring the droplet size, speed and concentration during the flight from the ultrasonically generated droplet to the substrate, gives insight in how to tune these parameters. Because thousands of droplets are created at the same time, measuring the properties of the droplets during flight is a complicated task. Three different measurement techniques have been developed in and around an USSC setup. Dynamic Light Scattering (DLS) shows, after Fourier transformation, shifted peaks, representing the speed of the droplets. By applying Turbidimetry, it is possible to determine the size of the droplets. Droplets size and speed could be measured and gave comparable results as measured with a High Speed Camera (HSC). Furthermore, it was shown that the size and velocity of the droplets depend on the process parameters. It is therefore concluded from this work that a combination of DLS and Turbidimetry is a valuable alternative to measure droplets during their flight from an USSC.

DY 15: Invited Talk: Liesbeth Janssen (Eindhoven)

Time: Monday 16:00–16:30 Location: DYb

Invited Talk DY 15.1 Mon 16:00 DYb

Glassy physics: from liquids to living cells — •Liesbeth Janssen — Eindhoven University of Technology, The Netherlands
The liquid-to-glass transition is a ubiquitous yet highly complex phenomenon, which still lacks a universal physical understanding. In this talk I will share some recent progress on the development and application of so-called Generalized Mode-Coupling Theory–a framework that aims to predict glassy dynamics purely from first principles. I will demonstrate that the theory can be applied not only to ordinary glass-forming materials, but also to more complex systems such as dense collectives of living cells.

DY 16: Statistical Physics 3 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)

Time: Monday 16:30–17:50 Location: DYb

DY 16.1 Mon 16:30 DYb

Aging in the Long-Range Ising Model — •Henrik Christiansen[1], Suman Majumder[1], Malte Henkel[2,3,4], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]Laboratoire de Physique et Chimie Théoriques (CNRS UMR 7019), Université de Lorraine Nancy, 54506 Vandœuvre-lès-Nancy Cedex, France — [3]Centro de Física Teórica e Computacional, Universidade de Lisboa, 1749-016 Lisboa, Portugal — [4]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany
The current understanding of aging phenomena is mainly confined to the study of systems with short-ranged interactions. Little is known about the aging of long-ranged systems. Here, the aging in the phase-ordering kinetics of the two-dimensional Ising model with power-law long-range interactions is studied via Monte Carlo simulations. The dynamical scaling of the two-time spin-spin autocorrelator is well described by simple aging for all interaction ranges studied. The autocorrelation exponents are consistent with $\lambda = 1.25$ in the effectively short-range regime, while for stronger long-range interactions the data are consistent with $\lambda = d/2 = 1$. For very long-ranged interactions, strong finite-size effects are observed. We discuss whether such finite-size effects could be misinterpreted phenomenologically as sub-aging.
[1] H Christiansen, S Majumder, W Janke, Phys. Rev. E 99, 011301(R) (2019)
[2] H Christiansen, S Majumder, M Henkel, W Janke, Phys. Rev. Lett. 125, 180601 (2020)

DY 16.2 Mon 16:50 DYb

Ageing and linear response in a mean field elastoplastic model — •Jack T. Parley[1], Suzanne M. Fielding[2], and Peter Sollich[1,3] — [1]Institut für Theoretische Physik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Science Laboratories, Department of Physics, Durham University, South Road, Durham DH1 3LE, United Kingdom — [3]Department of Mathematics, King's College London, London WC2R 2LS, United Kingdom
Elastoplastic descriptions, based on the alternating elastic/plastic deformation of mesoscopic regions, provide key insights into the complex dynamics of athermal amorphous solids. These systems have recently also been found to display non-trivial ageing dynamics, driven by plastic events and the ensuing Eshelby (quadrupolar) stress redistribution. Here we construct a mean-field elastoplastic model for studying time-dependent perturbations and ageing dynamics, building on the work of Lin and Wyart (2016) for steady shear. Local stresses are driven by power-law distributed mechanical noise, characterised by the exponent μ. We study the ageing behaviour in the glassy regime, where the form of the yield rate decay varies for different values of the exponent μ, reflecting the relative importance of far-field and near-field events as the range of the stress propagator is varied. Moreover, a comparison of the mean-field predictions with ageing simulations of a lattice elastoplastic model shows excellent agreement. Finally, we obtain expressions for the linear stress response in the ageing regime, which will allow to test the theoretical predictions against stress measurements from experiments or simulations of model athermal systems.

DY 16.3 Mon 17:10 DYb

Evaluation of memory effects at phase transitions — •Hugues Meyer — Department of Theoretical Physics and Center for Biophysics, Universität des Saarlandes, Saarbrücken, Germany
Modeling the dynamics of order parameters at phase transitions is often done in terms of stochastic equations of motion but there is to this day no consensus about a systematic strategy to tackle this problem. In particular, the detailed structure of the equations that needs to be used is still debated. Motivated by recent works on crystal nucleation, we propose to describe the dynamics of phase transitions in terms of a non-stationary Generalized Langevin Equation for the order parameter. By construction, this equation is non-local in time, i.e. it involves memory effects whose intensity is governed by a memory kernel. Here we do not aim at investigating the physical origin of memory effects at phase transitions in general, but rather to relate the extent of the memory kernel to quantities that are experimentally observed such as the induction time and the duration of the phase transformation process. Using a simple kinematic model

and a recently developed numerical procedure, we show that the extent of the memory kernel is positively correlated with the duration of the transition and of the same order of magnitude, while the distribution of induction times does not have an effect. This theoretical observation is finally tested at the example of several model systems.

DY 16.4 Mon 17:30 DYb

Emergent memory and kinetic hysteresis in strongly driven networks — •David Hartich and Aljaz Godec — MPI BPC, Göttingen, Germany

Stochastic network-dynamics are typically assumed to be memory-less. Involving prolonged dwells interrupted by instantaneous transitions between nodes such Markov networks stand as a coarse-graining paradigm for chemical reactions, gene expression, molecular machines, spreading of diseases, protein dynamics, diffusion in energy landscapes, epigenetics and many others. However, as soon as transitions cease to be negligibly short, as often observed in experiments, the dynamics develops a memory. That is, state-changes depend not only on the present state but also on the past. Here, we establish the first thermodynamically consistent mapping of continuous dynamics onto a network, which reveals ingrained dynamical symmetries and an unforeseen kinetic hysteresis [1]. These symmetries impose three independent sources of fluctuations in state-to-state kinetics that determine the 'flavor of memory'. The hysteresis between the forward/backward in time coarse-graining of continuous trajectories implies a paradigm shift for the thermodynamics of active molecular processes beyond the assumption of local detailed balance. Our results provide a new understanding of fluctuations in the operation of molecular machines as well as catch-bonds involved in cellular adhesion.

[1] DH, A Godec, arXiv:2011.04628 (2020).

DY 17: Complex Fluids - organized by Christine M. Papadakis (Technical University of Munich, Garching) (joint session CPP/DY)

Time: Tuesday 9:00–16:30 Location: CPPb

See CPP 8 for details of this session.

DY 18: Invited Talk: Andreas Zöttl (Vienna)

Time: Tuesday 9:00–9:30 Location: DYa

Invited Talk DY 18.1 Tue 9:00 DYa

Reinforcement learning of microswimmer chemotaxis using genetic algorithms — •Andreas Zöttl, Benedikt Hartl, Maximilian Hübl, and Gerhard Kahl — TU Wien

Many bacteria and eukaryotic cells are able to move in viscous fluids by performing nonreciprocal body deformations, such as rotating attached flagella or by distorting their entire body. In order to perform chemotaxis, i.e. to move towards and to stay at high concentrations of nutrients, they adapt their swimming gaits in a nontrivial manner.

We propose a model how microswimmers are able to autonomously adapt their shape in order to swim towards high field concentrations using an internal decision making machinery modeled by an artificial neural network. We present two methods to measure chemical gradients, spatial and temporal sensing. Surprisingly simple neural networks evolve by using the NEAT genetic algorithm which control the shape deformations of the microswimmer and allows them to navigate in static and complex time-dependent chemical environments [1]. By including noisy signal transmission in the neural network the well-known biased run-and-tumble motion emerges. Our work demonstrates that the evolution of a simple internal decision-making machinery, which we can fully interpret and is coupled to the environment, allows navigation in diverse chemical landscapes. These findings are of relevance for sensing mechanisms of single cells, or for the simple nervous system of small multicellular organisms such as C. elegans.

[1] B. Hartl, M. Hübl, G. Kahl, and A. Zöttl, under review (2021).

DY 19: Statistical Physics 4 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)

Time: Tuesday 9:00–10:40 Location: DYb

DY 19.1 Tue 9:00 DYb

Universal properties of creep flow — •Marko Popovic[1,2], Tom de Geus[1], Wencheng Ji[1], Alberto Rosso[3], and Matthieu Wyart[1] — [1]Institute of Physics, EPFL, Lausanne — [2]MPI-PKS, Dresden — [3]LPTMS, CNRS, Univ. Paris-Sud, Universite-Saclay, 91405 Orsay, France

Amorphous solids, such as atomic glasses, colloidal suspensions, granular matter or foams, begin to deform plastically when exposed to external stress Σ. Steady state flow of these materials in absence of thermal fluctuations is usually described as $\dot{\epsilon} \sim (\Sigma - \Sigma_c)^\beta$ for stresses above critical stress Σ_c and vanishes below. In presence of thermal fluctuations flow persists below Σ_c but is exponentially suppressed. The transient plastic deformation, called creep flow, is much less understood despite its importance in practical applications. Creep flow often displays a power-law decay in time $\dot{\epsilon} \sim t^{-\mu}$ after which it can either arrest or yield at fluidisation time τ_f. Recently, various numerical values and laws have been suggested for μ and τ_f in experimental or numerical studies. We propose that the creep flow parameters μ and τ can be expressed in terms of the steady state flow parameters, both in athermal and thermally activated systems. We successfully tested all our predictions using different mesoscopic elasto-plastic models of amorphous solids and found them to be consistent with published experimental results.

DY 19.2 Tue 9:20 DYb

Universality of photon counting below a local bifurcation threshold — •Lisa Arndt and Fabian Hassler — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

At a bifurcation point, a small change of a parameter causes a qualitative change in the dynamics of the system. Quantum fluctuations wash out this abrupt transition and enable the emission of photons below the classical bifurcation threshold. Close to the bifurcation point, the resulting photon counting statistics is determined by the instability. This talk discusses a generic method to derive a characteristic function of photon counting close to a bifurcation threshold that only depends on the dynamics and the type of bifurcation, based on the universality of the Martin-Siggia-Rose action. The method is exemplified for the cusp catastrophe without conservation laws, which can be implemented by an experimental setup using driven Josephson junctions.

DY 19.3 Tue 9:40 DYb

Fermionic Criticality Out-of-Equilibrium — •Bernhard Frank and Francesco Piazza — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Coupling critical bosons to a Fermi surface provides a standard route for the formation of a non-Fermi liquid: Its correlation functions do not show features of Landau quasiparticles but exhibit anomalous power laws, which give rise to substantial deviations from Fermi liquid results. So far these systems have been extensively studied in thermal equilibrium, for instance in the context of strange metals. However, recent experiments combine semi-conductor devices with optical cavities and therefore mandatorily require a theoretical formulation that takes into account the intrinsically open nature of the photonic sector in order to understand the electronic many-body physics. In particular, associating the photon with the critical bosonic mode leads to non-Fermi liquids out-of-equilibrium. Here, we use Keldysh field theory to study the paradigmatic Ising-nematic model in two-dimensions within a simple driven-dissipative setup. Compared to the situation in the ground state one observes increased decay rates in the low-energy sector of the fermionic spectrum as well as a violation of the thermal fluctuation dissipation relation caused by the enhanced bosonic fluctuations generated by the drive.

DY 19.4 Tue 10:00 DYb

On the dynamics of the Forest Fire Model — •Diego Rybski[1,2] and Jan W. Kantelhardt[3] — [1]Potsdam Institute for Climate Impact Research – PIK, Member of Leibniz Association, P.O. Box 601203, 14412 Potsdam, Germany — [2]Department of Environmental Science Policy and Management, University of California Berkeley, 130 Mulford Hall #3114, Berkeley, CA 94720, USA — [3]Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany.

We investigate the Forest Fire Model in its version proposed by Henley (PRL 1993). Extracting the time series of shares of trees in the system, we investigate the temporal dynamics. For large tree growth probabilities p we find stable regions in which the system reaches a periodic attractor. With decreasing p the period of the attractor increments and for small values the system enters a chaotic regime as found in a Feigenbaum-Diagram. However, this chaotic regime also exhibits (quasi-)periodic fluctuations where the frequency is equal to p. On larger time-scales we observe a random walk behavior ($\approx 1/f^2$ scaling) which approaches white noise (approximately flat spectrum) for very long simulations, but $1/f$ noise only appears as a transition. The standard deviation of the fluctuations is proportional to $p^{1/2}$. Our results call for a new view on forest fire dynamics.

DY 19.5 Tue 10:20 DYb

Minority games played by arbitrageurs on the energy market — •Tim Ritmeester and Hildegard Meyer-Ortmanns — Jacobs University, Bremen, Germany

Along with the energy transition, the energy markets change their organization toward more decentralized and self-organized structures, striving for locally optimal profits. These tendencies may endanger the physical grid stability. One realistic option is the exhaustion of reserve energy due to an abuse by arbitrageurs. We map the energy market to different versions of a minority game and determine the expected amount of arbitrage as well as its fluctuations as a function of the model parameters. Of particular interest are the impact of heterogeneous contributions of arbitrageurs, the interplay between external stochastic events and nonlinear price functions of reserve power, and the effect of risk aversion due to suspected penalties. As conclusions from our results we propose economic and statutory measures to counteract a detrimental effect of arbitrage.

DY 20: Nonlinear Dynamics 1 - organized by Azam Gholami (Göttingen)

Time: Tuesday 9:00–10:00 Location: DYc

DY 20.1 Tue 9:00 DYc

Discrete light bullets in passively mode-locked semiconductor lasers — •Thomas Seidel[1,2], Svetlana V. Gurevich[2], and Julien Javaloyes[1] — [1]Dpt. de Física, Universitat de les Illes Balears & IAC-3, Campus UIB, E-07122 Palma de Mallorca, Spain — [2]Institute for Theoretical Physics & Center for Nonlinear Science (CeNoS), University of Münster, Schlossplatz 2, 48149 Münster, Germany

We study the emergence and stability of discrete light bullets in the output of a passively mode-locked semiconductor laser array coupled to a distant saturable absorber. First, we investigate the dynamics of the tranverse field which can be modeled by a discretised version of the generalised Rosanov equation and next, we also include the longitudinal direction and thus, show the existence of three-dimensional dissipative localized structures with one discrete (transverse) and two continuous (longitudinal) directions. In both situations, we observe multistability between solution branches consisting of a different number of lasing lasers by numerical time integration. For the transverse case, a detailed bifurcation analysis by means of path continuation was conducted in order to study the transition between different solution branches. Further, the existence of drifting solitons is demonstrated for both bright and dark localized structures.

DY 20.2 Tue 9:20 DYc

Laminar Chaos in Experiments: Nonlinear Systems with Time-Varying Delays and Noise — •David Müller-Bender[1], Andreas Otto[1], Günter Radons[1], Joseph D. Hart[2,3], and Rajarshi Roy[2,3,4] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, Maryland 20742, USA — [3]Department of Physics, University of Maryland, College Park, Maryland 20742, USA — [4]Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742, USA

A new type of dynamics called laminar chaos was discovered in systems with time-varying delay [1]. It is a low-dimensional dynamics characterized by laminar phases of nearly constant intensity with periodic durations and a chaotic variation of the intensity from phase to phase. This is in contrast to the typically observed higher-dimensional turbulent chaos, which is characterized by strong fluctuations. In this work [2], we demonstrate experimentally and theoretically that laminar chaos is a robust phenomenon. Therefore, we provide the first experimental observation of laminar chaos by studying an optoelectronic feedback loop with time-varying delay and provide a time-series analysis toolbox for its detection. The toolbox is benchmarked by experimental data and by time-series of a delayed Langevin equation.

[1] Müller, Otto, and Radons, Phys. Rev. Lett. 120, 084102 (2018).

[2] Hart, Roy, Müller-Bender, Otto, and Radons, Phys. Rev. Lett. 123, 154101 (2019).

DY 20.3 Tue 9:40 DYc

Non-local effects in external cavity passively mode-locked lasers — •Jan Hausen[1], Christian Schelte[2], Julien Javaloyes[2], Svetlana V. Gurevich[2,3], and Kathy Lüdge[1] — [1]TU Berlin, Hardenbergstrasse 36, 10623 Berlin — [2]Universitat de les Illes Balears & Institute of Applied Computing and Community Code, Cra. de Valldemossa, km 7.5. Palma (Illes Balears) — [3]WWU Münster, Wilhelm-Klemm-Strasse 9, 48149 Münster

Asymetrical cavity geometries can improve the performances of passively mode-locked vertical external-cavity surface-emitting lasers and give rise to non-equidistant pulse patterns. We show that these geometries create non-local effects; by analysing a previously developed delay differential equation model, we derive rigorously a master partial differential equation from the pulse evolution that contains such non-local terms. We extend our analysis to the dynamics of non-equidistant pulse patterns in the long cavity regime, in which the pulses become temporal localized structures. We study the influence of the non-locality stemming from the asymmetric position of the elements in the cavity on the pulse distance within these patterns and deduce an analytic framework. By performing a Floquet-analysis, we find that with increasing cavity round-trip times there is a continuous transition from bound pulse patterns to pulses which are globally bound by the non-local effects, but locally independent, similar to catenane molecules.

DY 21: Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)

Time: Tuesday 9:30–10:30 Location: DYa

DY 21.1 Tue 9:30 DYa

Swirl formation of active colloids near criticality — •Robert C. Löffler[1], Tobias Bäuerle[1], Mehran Kardar[2], Christian M. Rohwer[3], and Clemens Bechinger[1] — [1]FB Physik, Universität Konstanz, Germany — [2]Dep. Physics, MIT, Cambridge, MA, USA — [3]Dep. Mathematics, University of Cape Town, South Africa

Animal groups like flocks of birds or schools of fish normally show a high degree of order. Yet they are also responsive to external factors in order to optimize nutrition and avoid predation. Various observations of such responsiveness have let to the assumption that those systems represent a state of order close to a critical point.

In our experiments, we use light-responsive active Brownian particles (ABPs) to which we can apply individual torques in a feedback controlled system to study such behavioral rules. Through the variation of a single parameter in our interaction model based on information about a particles local neighbors, we observe a continuous phase transition in the collective motion of the group: The ABPs transition from a disordered swarm to a stable swirl (i.e. milling, vortex-like state). Being able to continuously change our control parameter we observe a critical point with explicit bifurcation dynamics in the rotational order parameter and critical slowing down, as well as hysteresis in the symmetry-breaking regime of the control parameter. Observation of such critical behavior in simple models not only allows for more insight in complex animal behavior but also helps with designing future rules for collective tasks in robotic or other autonomous systems.

Bäuerle *et al.*, Nat. Comm. **11**, 2547 (2020); Löffler *et al.* (in review).

DY 21.2 Tue 9:50 DYa

A particle-field approach bridges phase separation and collective motion in active matter — •Robert Grossmann[1], Igor Aranson[2], and Fernando Peruani[3] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Department of Chemistry, Pennsylvania State University, University Park (PA), United States of America — [3]Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université, Cergy-Pontoise, France

Linking seemingly disconnected realms of active matter – active phase-separation of repulsive discs and collective motion of self-propelled rods – is a major contemporary challenge. We present a theoretical framework based on the representation of active particles by smoothed continuum fields which brings the simplicity of alignment-based models, enabling an analytical analysis, together with more realistic models for self-propelled objects including their steric, repulsive interactions. We demonstrate on the basis of the collision kinetics how nonequilibrium stresses acting among self-driven, anisotropic objects hinder the emergence of motility-induced phase separation and facilitate orientational ordering. Moreover, we report that impenetrable, anisotropic rods are found to form polar, moving clusters, whereas large-scale nematic structures emerge for soft rods, notably separated by a bistable coexistence regime. Thus, the symmetry of the ordered state is not dictated by the symmetry of the interaction potential but is rather a dynamical, emergent property of active systems. This theoretical framework can represent a variety of active systems: cell tissues, bacterial colonies, cytoskeletal extracts or shaken granular media.

DY 21.3 Tue 10:10 DYa

A Quantitative Kinetic Theory of Flocking in Dry Active Matter Including a Three Particle Closure — •Rüdiger Kürsten and Thomas Ihle — Institut für Physik, Universität Greifswald, Germany

We consider aligning self-propelled point particles in two dimensions. Their motion is given by generalized Langevin equations, however, the qualitative behavior is as for the famous Vicsek model. We develop a kinetic theory of flocking beyond mean field. In particular, we take into account the full pair correlation function. We find excellent quantitative agreement of those pair correlations with direct agent-based simulations within the disordered regime. Furthermore we use a closure relation to incorporate the spatial correlations of three particles. In that way we achieve good quantitative agreement of the onset of flocking with direct simulations. Compared to mean field theory, the flocking transition is shifted significantly towards lower noise because angular correlations favor disorder.

DY 22: Invited Talk: Lucas Goehring (Nottingham)

Time: Tuesday 10:00–10:30 Location: DYc

Invited Talk DY 22.1 Tue 10:00 DYc

Stability and dynamics of convection in dry salt lakes — •Lucas Goehring[1], Jana Lasser[2], Marcel Ernst[3], Matthew Threadgold[4], Cédric Beaume[4], and Steven Tobias[4] — [1]Nottingham Trent University — [2]Complexity Science Hub Vienna — [3]University of Kassel — [4]University of Leeds

Dry lakes covered with a salt crust organised into beautifully patterned networks of narrow ridges are common in arid regions. This talk will consider the possible origins of this pattern as the surface expression of buoyancy-driven convection in the porous soil beneath a salt crust. Specifically, we look at convection in a deep porous medium with a constant through-flow boundary condition on a horizontal surface, which resembles the situation found below an evaporating salt lake. Solving the linear stability problem, we show that typical field conditions will be unstable to subsurface convection. Further exploring the non-linear regime of this model, we demonstrate how the growth of small downwelling plumes is itself unstable to coarsening, as the system develops into a dynamic steady state. Interestingly, a robust length-scale emerges for the pattern wavelength, which is largely independent of the driving parameters, and consistent with the size of typical salt crust patterns (arXiv:2004.10578). Finally, we will show how these results can be extended into three-dimensions and more realistic boundary conditions, and include comparisons to field observations.

DY 23: Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/CPP)

Time: Tuesday 11:00–13:00 Location: DYa

DY 23.1 Tue 11:00 DYa

Mesoscale turbulence and dynamical clustering in active polar fluids — •Vasco Marius Worlitzer[1], Gil Ariel[2], Avraham Be'er[3], Holger Stark[4], Markus Bär[1], and Sebastian Heidenreich[1] — [1]Department of Mathematical Modelling and Data Analysis, Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, 10587 Berlin — [2]Department of Mathematics, Bar-Illan University, Ramat Gan 52000, Israel — [3]Zuckerberg Institute for Water Research of the Negev, Sede Boqer Campus 84900 Midreshet Ben-Gurion, Israel — [4]Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

Bacterial suspensions are fascinating examples for active polar fluids which exhibit large scale collective behavior ranging from polar and disordered states to so-called mesoscale turbulence and vortex lattices. Previous approaches take into account the self-propulsion of bacteria and an effective polar-alignment interaction but assume for simplicity a constant density. Comparison with experiments showed that this modelling approach is successful, to some extent, in a relatively narrow regime corresponding to wild-type swarms in which density is indeed approximately constant and velocity distributions are Gaussian. We seek a unified model that can explain the observed phenomena across the entire phase space of swarming bacteria. To this end, we present a continuum model that allows variations in density. The model predicts new dynamical regimes, such as mixed states with coexisting vortex patterns and dynamical clusters, obeying anomalous statistics, similar to experimental observations.

DY 23.2 Tue 11:20 DYa

Rewarding cargo-carrier interactions: cell-mediated particle transport — •Valentino Lepro[1,2], Robert Grossmann[1], Oliver Nagel[1], Stefan Klumpp[3], Reinhard Lipowsky[2], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, 37077 Göttingen, Germany

As society paves its way towards devices miniaturization and precision medicine, micro-scale actuation and guided transport become increasingly prominent research fields, with high potential impact in both technological and clinical contexts. To accomplish directed motion of micron-sized cargos towards specific target sites, a promising strategy is the usage of living cells as smart biochemically-powered carriers, developing so-called bio-hybrid systems. In this talk, we discuss eukaryotic active particle transport, using Dictyostelium discoideum as a model organism. We shed light on the underlying mechanics and the emerging dynamics governing such cell-mediated transport. A simple yet powerful model is proposed which reproduces the observed phenomenology and, moreover, elucidates the role of cell-cargo interactions for the long-time mass transport efficiency.

DY 23.3 Tue 11:40 DYa

Predictive local field theories for interacting active Brownian spheres* — Jens Bickmann and •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

We present predictive local field theories for the dynamics of interacting spherical active Brownian particles in two and three spatial dimensions. Alongside the general theories, which include configurational order parameters and derivatives up to infinite order, we present reduced models that are easier to apply. We show that our theories contain popular models such as Active Model B + as special cases and that they provide explicit expressions for the coefficients occurring in these models. As further outcomes, the theories yield analytical expressions, e.g., for the density-dependent mean swimming speed and the spinodal corresponding to motility-induced phase separation of the particles. The analytical predictions are found to be in very good agreement with results of Brownian dynamics simulations and results from the literature.

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DY 23.4 Tue 12:00 DYa

Dynamical States in Underdamped Active Matter with Anti-alignment Interaction — •Dominic Arold[1] and Michael Schmiedeberg[2] — [1]TransDeNLab, UKD, Dresden, Germany — [2]Institut für Theoretische Physik 1, FAU, Erlangen, Germany

Many active matter systems, especially on the microscopic scale, are well approximated as overdamped, meaning that any inertial momentum is immediately dissipated by the environment. On the other hand, for macroscopic active systems, the time scale of inertial motion can become large enough to be relevant for the dynamics already on the single-particle level [1]. This raises the question of how collective dynamics and the resulting states in active matter are influenced by inertia. We propose a coarse-grained continuum model for underdamped active matter based on a dynamical density functional theory for passive systems [2]. Further, we apply the model to a system with short-range alignment and distant anti-alignment interaction known from the context of pattern formation. Our simulations of under- and overdamped dynamics both predict a structured laning state. However, activity-induced convective flows only present in the underdamped model destabilize this state when the anti-alignment is weakened, leading to a collective motion state which is not predicted in the overdamped limit. A turbulent transition regime between the two states is distinguished by strong density fluctuations and the absence of global ordering.

[1] Scholz C *et al.* 2018 *Nature communications* **9** 5156
[2] Archer A J 2009 *The Journal of chemical physics* **130** 014509

DY 23.5 Tue 12:20 DYa

Chemokinesis causes trapping and avoidance by dynamic scattering — •Justus Kromer[1] and Benjamin Friedrich[2,3] — [1]Stanford University, Stanford, United States of America — [2]cfaed TU Dresden, Dresden, Germany — [3]PoL TU Dresden, Dresden, Germany

A minimal control strategy for artificial microswimmers with limited information processing capabilities is chemokinesis: the regulation of random directional fluctuations or speed as function of local, non-directional cues. In contrast to chemotaxis, it is not well understood whether chemokinesis is beneficial for the search for hidden targets.

We present a general theory of chemokinetic search agents that regulate directional fluctuations according to distance to a target. We characterize a dynamic scattering effect that reduces the probability to penetrate regions with strong directional fluctuations. If the target is surrounded by such a region, dynamic scattering causes beneficial inward-scattering of agents that had just missed the target, but also disadvantageous outward-scattering of agents approaching the target for the first time. If agents respond instantaneously to positional cues, outward-scattering dominates and chemokinetic agents perform worse than simple ballistic search. Yet, agents with just two internal states can decouple both effects and increase the probability to find the target significantly. We apply our analytical theory to the biological example of sperm chemotaxis of marine invertebrates. Sperm cells need to pass a 'noise zone' surrounding the egg, where chemokinesis masks chemotaxis. Kromer et al., PRL 124, 118101 (2020)

DY 23.6 Tue 12:40 DYa

Magnetic microswimmers exhibit Bose-Einstein-like condensation — Fanlong Meng[1], Daiki Matsunaga[2], •Benoît Mahault[3], and Ramin Golestanian[3] — [1]CAS Key Laboratory for Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences — [2]Graduate School of Engineering Science, Osaka University — [3]Max Planck Institute for Dynamics and Self-Organization

We study an active matter system comprised of magnetic microswimmers confined in a microfluidic channel and show that it exhibits a new type of self-organized behavior. Combining analytical techniques and Brownian dynamics simulations, we demonstrate how the interplay of non-equilibrium activity, external driving, and magnetic interactions leads to the condensation of swimmers at the center of the channel via a non-equilibrium phase transition that is formally akin to Bose-Einstein condensation. We find that the effective dynamics of the microswimmers can be mapped onto a diffusivity-edge problem, and use the mapping to build a generalized thermodynamic framework, which is verified by a parameter-free comparison with our simulations. Our work reveals how driven active matter has the potential to generate exotic classical non-equilibrium phases of matter with traits that are analogous to those observed in quantum systems.

DY 24: Dynamics and Statistical Physics - Open Session

Time: Tuesday 11:00–13:00 Location: DYb

DY 24.1 Tue 11:00 DYb

Analysing and Optimizing Nonlinear Memory Capacity of Photonic Reservoir Computing — •Felix Köster[1], Serhiy Yanchuk[2], and Kathy Lüdge[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, 10623 Berlin — [2]Institut für Mathematik, TU Berlin, Hardenbergstraße 36, 10623 Berlin

Reservoir computing is a neuromorphic inspired machine learning paradigm that utilizes the naturally occurring computational capabilites of dynamical systems. In this work, we investigate the linear and nonlinear memory capacity of a delay-based class-A and class-B-laser reservoir computer via eigenvalue analysis and numerical simulations. We show that these two quantities are deeply connected, and thus the reservoir computing performance is predictable by analyzing the eigenvalue spectrum. We introduce two new quantities to describe the influence of the eigenvalue spectrum on the reservoir computer performance. The insight won by the eigenvalue analysis yields understanding and thus helps applying better performing reservoir systems for a broader range of tasks.

DY 24.2 Tue 11:20 DYb

Dissipative nonequilibrium synchronization of topological edge states via self-oscillation — •Christopher W. Wächtler[1,2,3], Victor M. Bastidas[3], Gernot Schaller[1], and William J. Munro[3,4] — [1]Institut für Theoretische Physik, Berlin, Germany — [2]Max-Planck Institut für Physik komplexer Systeme, Dresden, Germany — [3]NTT Basic Research Laboratories, Atsugi, Japan — [4]National Institute of Informatics, Tokyo, Japan

The interplay of synchronization and topological band structures with symmetry protected midgap states under the influence of driving and dissipation is largely unexplored. Here we consider a trimer chain of electron shuttles, each consisting of a harmonic oscillator coupled to a quantum dot positioned between two electronic leads. Each shuttle is subject to thermal dissipation and undergoes a bifurcation towards self-oscillation with a stable limit cycle if driven by a bias voltage between the leads [1]. By mechanically coupling the oscillators together, we observe synchronized motion at the ends of the chain, which can be explained using a linear stability analysis. Because of the inversion symmetry of the trimer chain, these synchronized states are topologically protected against local disorder [2]. Furthermore, with current experimental feasibility, the synchronized motion can be observed by measuring the dot occupation of each shuttle. Our results open another avenue to enhance the robustness of synchronized motion by exploiting topology.

[1] C. W. Wächtler et al., NJP 21, 073009 (2019).
[2] C. W. Wächtler et al, PRB 102, 014309 (2020).

DY 24.3 Tue 11:40 DYb

Athermal Clustering and Jamming of Active Particles — •Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

In simulations of overdamped, repulsive, active particles in two dimensions at zero temperature the formation of clusters is observed. Note that it is not the temperature (as for mobility-induced phase transitions in thermal systems) but the unjamming dynamics that competes with the activity.

To be specific, large clusters that are even jammed in the inside only occur for intermediate activities. Decreasing the activity unjams the system and increasing the activity breaks up the clusters. Our simulations are in agreement with our results in [1], where athermal clustering has been studied in three dimensions in a simplified model system.

Our results demonstrate that even in the absence of thermal fluctuations a complex clustering behavior can be observed in active systems. An interesting task for future works will be to further compare the relation between the athermal clustering and mobility-induced phase transitions in thermal systems to the relation between athermal jamming and thermal jamming.

[1] M. Maiti and M. Schmiedeberg, EPL 126, 46002 (2019).

DY 24.4 Tue 12:00 DYb

Unravel the rotational properties of a squirmer in viscoelastic fluids — •Kai Qi[1], Marco De Corato[2], and Ignacio Pagonabarraga[1] — [1]CECAM, EPFL, Lausanne, Switzerland — [2]IBEC, BIST, Barcelona, Spain

We investigate the rotational motion of a single swimmer in viscoelastic fluids via Lattice Boltzmann (LB) simulations. Here, the generic squirmer model is employed and fluid viscoelasticity is achieved by added flexible polymer chains. The interplay of activity and boundary conditions between the squirmer and polymers on the squirmer's rotational motion is addressed. For Reynolds number close to unity, the rotational diffusion of a pusher/puller that employs the no-split boundary condition is enhanced over an order of magnitude. This is mainly due to the asymmetric torques generated during the heterogeneous collisions between the squirmer and polymers. However, this enhancement is about 5 times weaker when a short-range repulsion between squirmer's surface and monomers is used. By increasing system viscosity, we decrease the Reynolds number by an order of magnitude. Consequently, polymer's motility is suppressed profoundly. We find that the rotational diffusion coefficients of a pusher/neutral swimmer obtained from two boundary conditions are nearly identical. But the rotational enhancement of a puller with a no-slip boundary condition is twice stronger compared with the one exploiting short-range repulsion. This is because collisions occur mainly in the front of a puller due to its special swimming scheme.

DY 24.5 Tue 12:20 DYb

Transport coefficients of active particles: reverse perturbations and response theory — •Thomas Ihle[1], Arash Nikoubashman[2], Sven Stroteich[1], and Rüdiger Kürsten[1] — [1]Greifswald University — [2]Johannes-Gutenberg-University Mainz

The reverse perturbation method [1] for shearing simple liquids is extended to the Vicsek model (VM) of self-propelled particles. The sheared systems exhibit a skin effect: Momentum that is fed into the boundaries of a layer decays mostly exponentially toward the center of the layer. It is shown how the shear viscosity and the momentum amplification coefficient can be obtained by fitting this decay with an analytical solution of the hydrodynamic equations for the VM. The viscosity of the VM consists of two parts, a kinetic and a collisional contribution. Here, a novel expression for the collisional part is derived by an Enskog-like kinetic theory [2]. In agent-based simulations, using several methods to measure transport coefficients, we find excellent agreement between these different methods and also good agreement with the theoretical predictions. In addition, we introduce a response theory that allows us to verify the analytical predictions of kinetic theory and to obtain expressions for non-local transport coefficients. [1] F. Müller-Plathe, Phys. Rev. E 59, 4894 (1999), [2] A. Nikoubashman, T. Ihle, Phys. Rev. E 100, 042603 (2019)

DY 24.6 Tue 12:40 DYb

Long-time diffusion and energy transfer in mixtures of particles with different temperatures — •Efe Ilker[1,2], Michele Castellana[1], and Jean-François Joanny[1,3] — [1]Institut Curie, Paris, France — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Collège de France, Paris, France

In biological systems, crowding and composition are key factors affecting the rates of material transport while nonequilibrium aspects of active systems enrich this dynamics from molecular scales to cell populations. Transport properties of solute particles at long timescales differ from their short-timescale behavior due to interactions between the constituent particles. The collisions generate additional friction on a particle, while on top of that, for nonequilibrium (active) systems, the collisions can also lead to an exchange of energy between different constituents. Thus, the long-time diffusion coefficient of a tagged particle is shaped by the interplay between the effective friction and the energy transfer. Using the multiple temperature model, we probe these effects in dilute solutions and derive long-time friction and self-diffusion coefficients as a function of volume fractions, sizes and temperatures of particles. At these long timescales, we show that the tagged particle experiences a size-dependent "bath" temperature which stems from the interparticle energy transfer.

DY 25: Nonlinear Dynamics 2 - organized by Azam Gholami (Göttingen)

Time: Tuesday 11:00–13:00 Location: DYc

DY 25.1 Tue 11:00 DYc

Social distancing in pedestrian dynamics and its effect on disease spreading — Sina Sajjadi, Alireza Hashemi, and •Fakhteh Ghanbarnejad — Physics Department, Sharif University of Technology, Tehran, Iran

Non-pharmaceutical measures such as social distancing, can play an important role to control an epidemic. In this paper, we study the impact of social distancing on epidemics for which it is executable. We use a mathematical model combining human mobility and disease spreading. For the mobility dynamics, we design an agent based model consisting of pedestrian dynamics with a novel type of force to resemble social distancing in crowded sites. For the spreading dynamics, we consider the compartmental SEI dynamics plus an indirect transmission with the footprints of the infectious pedestrians being the contagion factor. We show that the increase in the intensity of social distancing has a significant effect on the exposure risk. By classifying the population into social distancing abiders and non-abiders, we conclude that the practice of social distancing, even by a minority of potentially infectious agents, results in a drastic change on the population exposure risk, but reduces the effectiveness of the protocols when practiced by the rest of the population. Furthermore, we observe that for contagions which the indirect transmission is more significant, the effectiveness of social distancing would be reduced. This study can provide a quantitative guideline for policy-making on exposure risk reduction.

arXiv preprint: arXiv:2010.12839

DY 25.2 Tue 11:20 DYc

Damage-Resilient Computation in Spiking Neural Networks — •Fabio Schittler Neves, Georg Börner, and Marc Timme — Chair for Network Dynamics, Institute for Theoretical Physics & Center for Advancing Electronics Dresden (cfaed), TU Dresden, Dresden, Germany

Networks of spiking neurons with inhibitory coupling exhibit reconfigurable k-winner-take-all computations via changes to a single parameter [1], robustly determining the k strongest out of N analog inputs. Such partial rank ordering of signals provides a natural basis for computing arbitrary functions. Moreover, computations are completed within a few spikes (~k), thus requiring low power. Here we show that such networks are strongly resilient with respect to failure or removal of neural units. We develop strategies for immediate function recovery that work even after damage to an extremely large number of units. These networks exhibit two forms of resilience: first, the loss of less than N-k units do not translate in any change in dynamics, as the N-k neurons receiving the weaker inputs never spike, thus never contribute to any collective network dynamics; second, the systems provide great flexibility through symmetric coupling, because any unit in the network can functionally replace any other. Suitably interacting inhibitory neural networks may provide resilient and flexible analogue computations at low power and offer attractive solutions where unit repair or replacements are economically or practically infeasible, for example in autonomous and remote computing.

[1] F. S. Neves & M. Timme, IEEE Access 8:179648 (2020).

DY 25.3 Tue 11:40 DYc

Localization in the Kicked Ising Chain from a Dual Perspective — •Daniel Waltner[1], Petr Braun[1], Maram Akila[2], Boris Gutkin[3], and Thomas Guhr[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Fraunhofer IAIS, Schloss Birlinghoven, 53757 Sankt Augustin, Germany — [3]Department of Applied Mathematics, Holon Institute of Technology, 58102 Holon, Israel

Determining the border between ergodic and localized behavior is of central interest for interacting many-body systems. We consider here the recently very popular spin-chain model that is periodically excited. A convenient description of such a many-body system is achieved by the dual operator that evolves the system in contrast to the time-evolution operator not in time but in particle direction. We identify by various methods the largest eigenvalue of the dual operator as a convenient tool to identify if the system shows ergodic or many-body localized features.

DY 25.4 Tue 12:00 DYc

Understanding the origin of line defects in heart tissue. — •Marcel Hörning[1], Alessandro Loppini[2], Alessio Gizzi[2], Flavio H Fenton[3], and Simonetta Filippi[2] — [1]Institute of Biomaterials and Biomolecular Systems, University of Stuttgart, Stuttgart, Germany — [2]University Campus Bio-Medico of Rome, Rome, Italy — [3]School of Physics, Georgia Institute of Technology, Atlanta, Georgia, USA

Spatiotemporal patterns are observed in a wide range of excitable systems. They have important and diverse regulatory functions. In the heart, excitable waves can form complex oscillatory and chaotic patterns even at an abnormally higher frequency than normal heart beats, which increase the risk of fatal heart conditions by inhibiting normal blood circulation. Previous studies suggested that the occurrence of line defects in alternans play a critical role in the stabilizion of those undesirable patterns. However, this nonlinear phenomenon is still poorly understood. It remains to be elucidated, how nodal lines form, what their origin is, and how they stabilise. Here we show new insights in the stability of those by observing and analysing nodal line dynamics in spiral waves (in-vitro) and entrained high-frequency waves (ex-vivo).

DY 25.5 Tue 12:20 DYc

Effects of social distancing and isolation modeled via dynamical density functional theory* — •Michael te Vrugt, Jens Bickmann, and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149, Münster, Germany

For preventing the spread of epidemics such as the coronavirus disease COVID-19, social distancing and the isolation of infected persons are crucial. However, existing reaction-diffusion equations for epidemic spreading are incapable of describing these effects. In this talk, we present an extended model for disease spread based on combining a susceptible-infected-recovered model with a dynamical density functional theory where social distancing and isolation of infected persons are explicitly taken into account [1]. We show that the model exhibits interesting transient phase separation associated with a reduction of the number of infections, and provides new insights into the control of pandemics. An extension of the model [2] allows for an investigation of adaptive containment strategies. Here, a variety of phases with different numbers of shutdowns and deaths are found, an effect that is of crucial importance for public health policy.

[1] M. te Vrugt, J. Bickmann and R. Wittkowski, Nature Communications 11, 5576 (2020)

[2] M. te Vrugt, J. Bickmann and R. Wittkowski, arXiv:2010.00962 (2020)

*Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1

DY 25.6 Tue 12:40 DYc

Information spread enhanced by criticality in high-responsive groups of fish — •Luis Gómez Nava[1,3], Robert T. Lange[2,3], Pascal P. Klamser[1,2], Henning Sprekeler[2,3], and Pawel Romanczuk[1,3] — [1]Institute for Theoretical Biology, Philippstrasse 13, Humboldt University of Berlin, 10115 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience, 10115 Berlin, Germany — [3]Science of Intelligence (SCIoI), Marchstrasse 23, Technical University of Berlin, 10587 Berlin, Germany

Collective dynamics in animal groups has been studied in recent years intensively. Recent works have suggested that such multi-agent systems should operate in a special parameter region, close to critical points. This is relevant because critical systems exhibit unique properties like maximal responsiveness to external stimuli and optimal propagation of information within the group. In our work, we study a high-density system of sulphur mollies in their natural habitat. We measure the surface activity of the fish and characterize their response to external fluctuations. This surface activity results to be similar to the one observed in critical systems (we observe power law-distributed observables, as well as separation of time scales of the activity). We model the system dynamics using cellular automata and we conclude that this natural system operates indeed in a special parameter region. We provide as well a biological interpretation of the characteristic features of such a critical system.

DY 26: Data Analytics for Complex Dynamical Systems (joint SOE/DY Focus Session) (joint session SOE/DY)

Time: Tuesday 11:00–12:40 Location: SOEa

See SOE 4 for details of this session.

DY 27: Fluid Physics 3 - organized by Stephan Weiss and Michael Wilczek (Göttingen)

Time: Tuesday 14:00–17:10 Location: DYa

Invited Talk DY 27.1 Tue 14:00 DYa

Human exhaled particles from nanometres to millimetres — •Gholamhossein Bagheri — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

COVID-19 and other airborne diseases are transmitted to healthy individuals by inhalation of pathogen-containing particles exhaled by infectious persons. Here I provide an overview of the mechanisms involved in formation of these particles and the flow physics of the exhaled air. I will present results of our comprehensive experimental study to characterise the size distribution of exhaled particles from more than 125 subjects aged 5-88 years using aerosol size spectrometers and in-line holography. I will also discuss the physics of the exhalation flows during different respiratory manoeuvres by presenting results from our size-resolved three-dimensional particle tracking imaged at 10-15 kHz, which are furthermore complemented by two-dimensional optical flow measurements. In total, we have collected and analysed 200 h of exhalation samples with the spectrometers, 9000 holograms, and more than three million images from the high-speed cameras. With this database, we are now able to predict risk of infection from human exhaled particles in indoor environments using conventional infection models as shown in our multilingual web application (https://aerosol.ds.mpg.de). Finally, we have further improved risk assessment models to account for particles containing multiple pathogens. This research is funded by the Max Planck Society, Universitätsmedizin Göttingen and Bundesweites Forschungsnetz Angewandte Surveillance und Testung project.

DY 27.2 Tue 14:30 DYa

Emergent transport in growing bacterial colonies — •Anupam Sengupta — Physics of Living Matter, Dept. of Physics and Materials Science, University of Luxembourg

Bacteria are known to mediate vital processes in ecology, medicine and industry. Morphology, a key bacterial trait, has been long studied for its biophysical functions. Yet, only recently we have started to uncover the role of morphology in tuning the emergent properties in active cellular micro-environments[1]. Here, I will present recent results that elucidate how non-motile bacteria harness morphology to regulate transport properties over colony scales. We examine the geometric and mechanical properties of growing colonies, with a particular focus on the emergence of topological defects that act as active hydrodynamic sites. Our experimental results indicate that the number of topological defects depends on the cell geometry and colony dimensions, which in turn regulate the emergent transport properties within the bacterial colonies. Our results are supported by MD simulations and continuous modelling [2, 3], suggesting that defect mediated mechanics can potentially lead to biological functions, owing to the active hydrodynamics at scales that are orders of magnitude larger than individual cells. [1] A. Sengupta, Microbial Active Matter: A Topological Perspective, Front. Phys. 8, 184, 2020; [2] You, Pearce, Sengupta, Giomi, Phys. Rev. X. 8 (2018); [3] You, Pearce, Sengupta, Giomi, Phys. Rev. Lett. 123 (2019).

DY 27.3 Tue 14:50 DYa

Hydrodynamically coupled cilia: synchronization and noise — •Anton Solovev and Benjamin M. Friedrich — TU Dresden, Germany

Motile cilia on ciliated epithelia in mammalian airways, brain ventricles and oviduct can display coordinated beating in the form of metachronal (=traveling) waves [1]. Past research proposed hydrodynamic coupling as a mechanism of synchronization, yet if such synchronization is stable in the presence of noise (corresponding to active fluctuations of cilia beating) has been addressed only for $n = 2$ cilia [2], while the question of multi-stable synchronization in cilia carpets ($n >> 1$) remains open.

Using multi-scale simulations [3] that map hydrodynamic interactions between cilia on a generalized Kuramoto model of phase oscillators with local coupling, we predict many multi-stable metachronal wave states, yet only one or two of them have considerable basins of attraction.

In the presence of noise, we observe stochastic transitions between different waves [4]. Active noise excites long-wavelength perturbations (which take relatively long time to decay). Strong noise impedes global synchronization and causes a break-up into smaller synchronized patches (similar to a chimera state).

[1] W. Gilpin, M.S. Bull, and M. Prakash, Nat Rev Phys 2, 74 (2020)
[2] R. Ma et al., Phys. Rev. Lett. 113, 048101 (2014)
[3] A. Solovev, B.M. Friedrich, preprint arXiv:2010.08111 (2020)
[4] A. Solovev, B.M. Friedrich, preprint arXiv:2012.11741 (2020)

DY 27.4 Tue 15:10 DYa

Boundary conditions for polar active fluids exhibiting mesoscale turbulence — •Sebastian Heidenreich[1], Henning Reinken[2], Daiki Nishiguchi[3], Andrey Sololov[4], Igor S. Aranson[5], and Sabine H. L. Klapp[2] — [1]Physikalisch Technische Bundesanstalt Braunschweig und Berlin, Germany — [2]Technische Universität Berlin, Germany — [3]University of Tokyo, Japan — [4]Argonne National Laboratory, USA — [5]Pennsylvania State University, USA

Bacterial suspensions are intriguing examples for active polar fluids which exhibit large-scale collective behaviour from mesoscale turbu- lence to vortex lattices. The bulk collective motion is well described by a continuum equation with derivatives up to the fourth order [1]. That simple model reproduces experimental findings of mesoscale turbulence and was recently derived from a minimal micro-swimmer model. How- ever, the treatment of boundaries to describe the collective motion in a confinement or near walls remains so far unknown. In the talk, we propose boundary conditions for active polar fluids suitable to de- scribe recent experiments of Bacillus subtilis bacteria moving in an array of lithographic designed pillars [2]. Furthermore, we describe the collective motion of bacteria around single pillars of different sizes in experiments and show that the model with the mentioned boundary conditions reproduces this behavior faithfully.

[1] J. Dunkel, S. Heidenreich, M. Bär and R. E. Goldstein, New. J. Phys. 15, 040516 (2013). [2] D. Nishiguchi, I. S. Aranson, A. Snezhko and A. Sokolov Nat. Comm. 9, 4486 (2018).

DY 27.5 Tue 15:30 DYa

Non-equilibrium phase transitions in bacterial vortex lattices — •Henning Reinken[1], Sebastian Heidenreich[2], Markus Bär[2], and Sabine H. L. Klapp[1] — [1]Technische Universität Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Berlin, Germany

Recent theoretical and experimental studies have shown that the turbulent vortex structures emerging in bacterial active fluids can be organized into regular vortex lattices by weak geometrical constraints such as small pillars [1,2].

Using a deterministic continuum-theoretical approach for the effective microswimmer velocity [3], we show that the emergence and disappearance of these non-equilibrium structures shares many similarities with second-order equilibrium phase transitions including critical behavior, e.g., long-range correlations and divergent susceptibility at the critical point. The exponents are very close to those of the 2D Ising model with nearest-neighbor interactions. A mapping to

the Onager solution allows us to identify an effective temperature linear in the strength of nonlinear advection.

[1] D. Nishiguchi, I. S. Aranson, A. Snezhko, and A. Sokolov, Nat. Commun. **9**, 4486 (2018)
[2] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, Commun. Phys. **3**, 76 (2020)
[3] H. Reinken, S. H. L. Klapp, M. Bär, and S. Heidenreich, Phys. Rev. E **97**, 022613 (2018)

DY 27.6 Tue 15:50 DYa

Impact of the gut motility on nutrient absorption and bacterial growth — •Agnese Codutti[1,2] and Karen Alim[1,2] — [1]MPIDS, Goettingen, Germany — [2]TUM Physics, Munich, Germany

The small intestine malfunctioning and its microbiome have been linked to serious diseases (from obesity, diabetes, Crohn disease to depression and anxiety). Therefore, the study of the physics underlaying such malfunctioning and the healthy gut behavior is of vital importance. In our work, we aim to theoretically model the tight link between gut motility, fluid flows, nutrients absorption and bacterial growth. We extend the Taylor dispersion approach to the case of an absorbing tube with moving walls, and we use a system of coupled equations to model nutrients and bacteria. We show that the gut motility deeply impacts the nutrient absorption: motility patterns with slow flows such as segmentation increase the nutrient absorption due to the long permanence times, while motility patterns with strong flows such as peristalsis reduce the absorption. On the contrary, segmentation favours the bacterial growth, while peristalsis reduces it. Therefore, we prove that the gut alternates such patterns to maximize nutrient absorption and minimise bacterial growth.

DY 27.7 Tue 16:10 DYa

Wet-tip versus dry-tip regimes of osmotically driven bile flow in the liver — Oleksandr Ostrenko, Michael Kücken, and •Lutz Brusch — Center for Information Services and High Perfor- mance Computing (ZIH), Technische Universität Dresden, Germany

The secretion of osmolites into a lumen and thereby caused osmotic water inflow drive fluid flows like saliva, sweat and bile in organs without a mechanical pump, as opposed to the heart in blood circulation. The effects of elevated fluid pressure and the associated mechanical limitations of organ function remain largely unknown. We consider the pressure profile of the coupled osmolite-flow problem with combined velocity and pressure boundary conditions. Notably, the entire lateral boundary acts as a fluid source, the strength of which is determined by feedback from the emergent pressure solution itself. Hence, the pressure difference between the boundaries is not imposed but self-organises. Our theoretical results reveal fundamental parameter dependencies and a phase boundary separating the commonly considered "wet-tip" regime with steady flow out of the very tip of a channel from a "dry-tip" regime suffering stalled flow and a self-organised block of osmotic water inflow [1]. We validate model predictions against intravital video microscopy data from mouse liver [2] and propose a relation between the predicted phase boundary and the onset of zonated cholestasis, a pathological liver condition [3].

[1] Ostrenko et al. (2019) Scientific Reports 9, 4528. [2] Meyer et al. (2017) Cell Systems 4, 277. [3] Segovia-Miranda et al. (2019) Nature Medicine 25, 1885.

DY 27.8 Tue 16:30 DYa

Resistive force theory and wave dynamics in swimming flagellar apparatus isolated from C. reinhardtii — Samira Goli Pozveh[1], Albert Bae[2], and •Azam Gholami[1] — [1]MPI for Dynamics and Self-organization, Göttingen, Germany — [2]Department of Biomedical Engineering, Univ. of Rochester, USA

The-biflagellated micro-swimmer Chlamydomonas reinhardtii is a model organism to study dynamics of flagellar synchronization. Hydrodynamic interactions, intracellular mechanical coupling or cell body rocking are believed to play crucial role in synchronization of flag- ellar beating in green algae. Here, we use freely swimming intact flagellar apparatus isolated from wall-less strain of Chlamydomonas to investigate wave dynamics. Our analysis in phase coordinates show that, when the frequency difference between the flagella is high (10-41% of the mean), neither mechanical coupling via basal body nor hydrodynamics interactions are strong enough to synchronize two flagella, indicating that beating frequency is perhaps controlled internally by the cell. We also examined the validity of resistive force theory for a flagellar apparatus swimming freely in the vicinity of a substrate and found a quantitative agreement between experimental data and simulations with drag anisotropy of ratio 2. Finally, using a simplified wave form, we investigated the influence of phase and frequency differences, intrinsic curvature and wave amplitude on the swimming trajectory of flagellar apparatus. Our analysis shows that by controlling phase or frequency differences between two flagella, steering can occur.

DY 27.9 Tue 16:50 DYa

Rectified Diffusion of *E. coli* in Microfluidic Labyrinths — •Ariane Weber[1,2,3], Marco Bahrs[4], Zahra Alirezaeizanjani[4], Xingyu Zhang[1,2], Carsten Beta[4], and Vasily Zaburdaev[1,2] — [1]Department Biologie, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen — [3]Max-Planck-Institut für Menschheitsgeschichte, Jena — [4]Institut für Physik und Astronomie, Universität Potsdam

In many natural environments such as tissue or soil, bacteria have to orient through and interact with complex surroundings. To describe the bacterial dispersal in such environments, the movement of bacteria in the presence of spatial restrictions has to be understood qualitatively and quantitatively. In the present work, we take a first step in this direction by studying the spreading of *E. coli* in labyrinths of square and hexagonal geometry, both experimentally and theoretically. Using a microscopic tracking system, we first generate experimental data quantifying the dispersal of the bacteria in quasi-two-dimensional microfluidic labyrinths. Second, we formulate a two-dimensional random walk model of the bacterial movement within the labyrinths to (i) find theoretical expressions quantifying the diffusive motion and (ii) produce numerical results by implementing it in computer simulations. We then verify the analytical results by comparing them with the simulation statistics and the experimental data. Taken together, we are able to quantify the bacterial dispersal on short time scales and model it on large time scales, predicting faster dispersal and a prolonged time of non-Gaussian diffusion within the labyrinths.

DY 28: Statistical Physics 5 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)

Time: Tuesday 14:00–15:40 Location: DYb

DY 28.1 Tue 14:00 DYb

Non-Reversible Monte Carlo Simulations of Long-Range Interacting Molecular Systems — •Philipp Höllmer[1], Liang Qin[2], Michael F. Faulkner[3], A. C. Maggs[4], and Werner Krauth[2] — [1]University of Bonn, Germany — [2]École normale supérieure de Paris, France — [3]University of Bristol, United Kingdom — [4]ESPCI Paris, France

We present current progress of developing non-reversible Markov-chain Monte Carlo (MCMC) algorithms for efficient simulations of atom-based models of molecules that include long-ranged interactions. The event-chain Monte Carlo (ECMC) algorithm samples the Boltzmann distribution exactly without computing energy changes, which removes the computational bottleneck of traditional reversible MCMC simulations. Also, in contrast to molecular dynamics, the mixing and autocorrelation times of MCMC are not locked to the physical dynamics.

We introduce our open-source JeLLyFysh (JF) application that implements ECMC in a general way by demonstrating number of worked out molecular-simulation examples that include, e.g., liquid water. We then highlight recent improvements of the application and ECMC itself. This includes, in particular, the concept of fast sequential Markov chains where ECMC's direction of motion is sequentially chosen from a set. Choosing a large direction set leads to much shorter mixing times of the rotational degree of freedom, and may thus greatly accelerate ECMC simulations of molecular systems.

DY 28.2 Tue 14:20 DYb

What can kinetic Monte Carlo do for active Matter? — •Juliane U. Klamser[1], Olivier Dauchot[1], and Julien Tailleur[2] — [1]Gulliver UMR CNRS 7083, ESPCI Paris, Université PSL, 75005 Paris, France — [2]Laboratoire Matiere et Systemes Complexes, UMR 7057 CNRS/P7, Université Paris Diderot, 10 rue Alice Domon et Leonie Duquet, 75205 Paris cedex 13, France

As an efficient numerical method, discrete-time, continuous-space Monte Carlo (MC) is wildly used in physics. While constructing an active matter version is straightforward, the question remains to what extent it faithfully captures real-world active systems. We focus on a kinetic MC version for the simplest kind of active matter: persistently moving, non-polar, interacting particles. On the multi-particle level, the MC dynamics captures not only Motility-induced phase separation but also features a non-equilibrium extension of the celebrated two-dimensional melting. An attempt to characterize these phases and their transitions relies on the existence of a thermodynamic pressure, which is not guaranteed outside equilibrium. For a soundly chosen version of the MC dynamics, we show that pressure is a thermodynamic state variable over a robust parameter range. This is demonstrated by deriving the corresponding Langevin description and the associated expression for pressure, which is confirmed by large scale many-particle simulations. Last but not least, our work culminates in a prescription for extending kinetic MC to the standard active matter models, namely active Brownian particles and active Ornstein-Uhlenbeck particles.

DY 28.3 Tue 14:40 DYb

General solution to the one-dimensional connectivity problem — •Fabian Coupette, Andreas Härtel, and Tanja Schilling — Institut of Physics, University of Freiburg, Germany

We present a general method to obtain the connectivity properties of an arbitrary one-dimensional pairwise interacting n-body system in thermal equilibrium. As input, solely the pair density distribution associated to the equilibrium state is required. Accordingly, if exact analytic results exist for the pair density distribution, the pair connectivity can be determined equally exactly. This is illustrated for fully penetrable and impenetrable rods as well as a repulsive $1/r^2$ nearest-neighbor interaction potential. We also discuss implications of our work for long-ranged interactions, systems in external fields and higher dimensions.

DY 28.4 Tue 15:00 DYb

Criticality in the mechanical regulation of cell adhesion — •Kristian Blom and Aljaz Godec — Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Cell adhesion, the process by which cells physically attach to their environment, is established through binding of cellular adhesion molecules located at the outer cell membrane. While on the single molecule level adhesive strength is set by the intrinsic-binding affinity alone, on the many-body level an effective interaction between neighboring adhesion molecules arises through fluctuations of the anchoring cell membrane. Changes in the membrane stiffness, observed in e.g. tumor and muscle cells, alter the effective interaction strength and in turn facilitate mechanical regulation of adhesion. In this talk we will explain how mechanical regulation affects the equilibrium binding state and (un)binding kinetics of adhesion clusters. Ranging from small to large clusters, we show that there always exists an optimal membrane stiffness at which the (un)binding rates are largest. In the thermodynamic limit we observe a dynamical phase transition at which the dominant (un)binding pathway undergoes a qualitative change.

[1] K. Blom, A. Godec, arXiv:2011.05310 (2020)

DY 28.5 Tue 15:20 DYb

Complex routes towards a fully-grown monolayer of "sticky" hard rods — •Miriam Klopotek, Hans Joachim Schöpe, and Martin Oettel — University of Tübingen, Tübingen, Germany

We study "sticky" hard rods confined to maximally one monolayer, i.e. "(2+1)D" confinement, in a basic, on-lattice model system for thin film growth with anisotropic particles at early stages [1]. We execute a large array of kinetic Monte Carlo (KMC) simulations of the nonequilibrium dynamics [2]. The physics of monolayer growth with "sticky" hard rods is extremely rich. The bounty of phenomena on metastable phases and complex phase transition kinetics we find has not been addressed before by comparable simulation or analytical models. We identify at least five different phase transition scenarios; the different dynamical regimes are traceable in the 2D plane ("map") spanned by the reduced temperature (or attraction strength) and deposition-flux–to–diffusion ratio. The rod-length as well as simple substrate potentials further shift these regimes and alter the topology of the "map", i.e. the set of phase transition scenarios. The specific model choice for microscopic rotational dynamics of rods is another, surprisingly important factor altering the kinetics and, therewith, the morphological evolution.

[1] G. Hlawacek and C. Teichert, *J. Phys.: Condens. Matter* 25 (2013), p. 143202.
[2] M. Klopotek *et al.*, *J. Chem. Phys.* 146.8 (2017), p. 084903.

DY 29: Invited Talk: Karen Daniels (Raleigh)

Time: Tuesday 14:00–14:30 Location: DYc

Invited Talk DY 29.1 Tue 14:00 DYc

Fingers, fractals, and flow in liquid metals — •Karen Daniels — North Carolina State University, USA

A droplet of pure water placed on a clean glass surface will spread axisymmetrically, and a droplet of mercury will bead up into a spherical droplet. In both cases, the droplet is minimizing its surface energy – creating an object with a minimized surface area – and there is nothing to break the symmetry. Remarkably, droplets of the room-temperature liquid gallium-indium (EGaIn), which like all metals have an enormous surface tension, can nonetheless undergo fingering instabilities in the presence of an oxidizing voltage. I will describe how this oxide acts like a reversible surfactant, generating fingering instabilities, tip-splitting, and even fractals, through Marangoni instabilities. Remarkably, we find that EGaIn droplets placed in an electrolyte under an applied voltage can achieve near-zero surface tension. This effect can in turn be used to suppress the Rayleigh-Plateau instability in falling streams. Quantitative control of these effects provides a new route for the development of reconfigurable electronic, electromagnetic, and optical devices that take advantage of the metallic properties of liquid metals.

DY 30: Complex Fluids and Soft Matter 1 - organized by Uwe Thiele (Münster) (joint session DY/CPP)

Time: Tuesday 14:30–16:30 Location: DYc

DY 30.1 Tue 14:30 DYc

How Frost Forms and Grows on Lubricant Impregnated Surfaces — •Lukas Hauer[1], William S.Y. Wong[1], Lou Kondic[2], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Mathematical Sciences, NJIT, Newark, USA

In many technical applications the formation of frost and ice displays a hazard to the steady functionality of devices. This motivates the development of new materials to tackle the reduction of frosting and icing on surfaces. While icing on surfaces is commonly studied by localized nucleation mechanisms, the formation of frost is comparable more complicated: Formation of condensate droplets, freezing, and frost front propagation are multi-physical processes on multiple time and length scales. Lubricant impregnated surfaces are known for improved anti-icing properties. They experience lower ice drop adhesion and allegedly delayed surface frost formation. We show that frost formation can induce immensely strong capillary forces that could result in surface damage, lubricant depletion and the loss of anti-icing properties. Laser scanning confocal microscopy enables us to monitor the dynamic lubricant migration during condensation frosting on micro-structured surfaces. We present a quantitative model of the lubricant migration, utilizing lubrication theory. This work serves to improve understanding of lubricant dynamics during condensation frosting, providing roadmaps towards the future design of anti-icing surfaces.

DY 30.2 Tue 14:50 DYc

Hydraulic and electric control of cell spheroids — •Charlie Duclut[1], Jacques Prost[2], and Frank Jülicher[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Laboratoire Physico Chimie Curie, Institut Curie, Paris, France — [3]Center for Systems Biology Dresden, Germany

In addition to generating forces and reacting to mechanical cues, tissues are capable to actively pump fluid and create electric current. In this talk, we will discuss how a hydraulic or electrical perturbation, imposed for instance by a drain of micrometric diameter, can be used to perturb tissue growth dynamics. We address this issue in a continuum description of a spherical cell assembly that includes the mechanical, electrical and hydraulic properties of the tissue. This approach allows us to discuss and quantify the effect of electrohydraulic perturbations on the long-time states of the tissue. We highlight that a sufficiently strong external flow or electric current can drive a proliferating spheroid to decay. We propose that this could have applications in medicine.

DY 30.3 Tue 15:10 DYc

Controlling Elastic Turbulence — •Reinier van Buel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Controlling the flow patterns of viscoelastic fluids is extremely challenging due to their inherent non-linear and time-dependent properties. These complex fluids exhibit transitions from laminar to turbulent flows, which is useful for heat and mass transport in liquids at the micron scale [1], whereas in Newtonian fluids transport is dominated by diffusion. Turbulent viscoelastic flows show similar properties as their counterparts in Newtonian fluids [1,2] and consequently the observed flow pattern is called *elastic turbulence* [1]. It occurs in shear flow for increasing Weissenberg number Wi, the product of polymer relaxation time and shear rate.

Numerically solving the Oldroyd-B model in a two-dimensional Taylor-Couette geometry, we have identified and described the supercritical transition to turbulent flow at a critical Weissenberg number [2]. Here, we demonstrate that elastic turbulence can be controlled by a time-modulated shear rate. The order

parameter measuring the strength of turbulence continuously goes to zero with increasing modulation frequency or Deborah number De. It ultimately vanishes via a supercritical transition, where flow then becomes laminar. Moving closer to the critical Weissenberg number, smaller modulation frequencies are sufficient to induce laminar flow.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).
[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).

DY 30.4 Tue 15:30 DYc

Hydrodynamics of a Pair of Soft Capsules in Inertial Microfluidics — •Kuntal Patel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

In recent years, inertial microfluidics has emerged as a robust technique to precisely manipulate solid particles and biological cells. Also, the fact that inertial microfluidics operates at finite Reynolds numbers enables to achieve high throughput. In the present work, we perform 3D numerical simulations to study the hydrodynamic interaction and inertial migration of two soft capsules in a microchannel with quadratic cross section. We employ the lattice Boltzmann method to determine fluid flow and the finite element method to model capsule dynamics. The coupling between bulk fluid and capsules is realized using the immersed boundary method.

We investigate the effect of different starting positions for mono- and bi-dispersed pairs of varying softness and capsule shape. Based on the temporal evolution of interparticle distance, we characterize the dynamics of various mono- and bi-dispersed pairs into four types: stable pair, stable pair with damped oscillations, stable pair with bounded oscillations, and unstable pair. We observe that stable pairs become unstable when increasing the particle stiffness. Furthermore, a pair with both capsules in the same channel half is more prone to become unstable than a pair with capsules in the opposite channel halves.

DY 30.5 Tue 15:50 DYc

Hydrodynamics of immiscible binary fluids with viscosity contrast: A Multiparticle Collision Dynamics approach — •Zihan Tan[1], Vania Calandrini[2], Jan Dhont[1], Gerhard Nägele[1], and Roland Winkler[3] — [1]Biomacromolecular Systems and Processes, Institute of Biological Information Processing, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Computational Biomedicine, Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany — [3]Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

By coupling distinct collision steps in each fluid domain, immiscible binary fluids with different viscosities connected by coarse-grained planer interfaces are realized by multiparticle collision dynamics (MPC). The flow and the stress-viscosity relation of the system are investigated under shear flow, excellently agree with continuum hydrodynamics solution and the analytical theory of MPC. Later, the hydrodynamic mobility coefficients of an embedded colloid close to the fluid-fluid interface are measured, which coincide with hydrodynamic multipole expansion calculations. To validate the length and time scales of hydrodynamics in this model, we explore the corresponding transverse velocity correlations. It is found that the correlations for the fluid regions occupied by one phase are identical to single-phase MPC fluid. In contrast, the transverse modes at the interfacial region can be interpreted by the superposition of both viscous components.

DY 30.6 Tue 16:10 DYc

Optimal hematocrit for ATP release by red blood cell in microcirculation — •Zhe Gou and Chaouqi Misbah — Laboratoire Interdisciplinaire de Physique, Grenoble, France

ATP release by red blood cells (RBCs) acts as an important signaling molecule for various physiological functions, such as vasodilation. When flowing in microcirculation, RBCs experience a cascade of branching vessels, from arterioles to capillaries, and finally to venules, which affects not just flow behavior of blood but also ATP release. In a previous study, we have proposed a model of ATP release by RBCs through two pathways of cell membrane: pannexin 1 channel (Px1), sensitive to shear stress, and cystic fibrosis transmembrane conductance regulator (CFTR) which responds to cell deformation. As a continuation, present work further investigates the effect of flow strength, hematocrit, and vascular diameter by numerical simulations. We found a nontrivial spatial RBC organization and ATP patterns due to application of shear stress on the RBC suspension. Conditions for optimal ATP release per cell are identified, which depend on vessel size and hematocrit Ht. Increasing further Ht beyond optimum enhances the total ATP release but should degrade oxygen transport capacity, a compromise between an efficient ATP release and minimal blood dissipation. Moreover, ATP is boosted in capillaries suggesting a vasomotor activity coordination throughout the resistance network. Further studies of vascular network may help to explore the whole signaling cascade of ATP.

DY 31: Invited Talk: Mehran Kardar (Boston)

Time: Tuesday 15:40–16:10 Location: DYb

Invited Talk DY 31.1 Tue 15:40 DYb

Fixation and ancestry of competing species growing on a rugged front — •Mehran Kardar — Physics Department, MIT, Cambridge, MA 02139, USA

When competing species expand into new territory the population is dominated by descendants of a few successful ancestors at the expansion front. Successful ancestry is stochastic, but biased by fitness of the individual, as well as favorable geographic location. We consider a simple model of range expansion of competing bacteria, in which reproduction and competition only take place at the growing front. Based on symmetry considerations we construct a pair of nonlinear stochastic partial differential equations that describe the coevolution of the profile of the growing surface and the composition of the bacterial species on the front. Macroscopic manifestations (phenomenology) of these equations on growth patterns and genealogical tracks of range expansion will be presented.

DY 32: Posters DY - Statistical Physics, Brownian Motion and Nonlinear Dynamics

Time: Tuesday 16:30–19:00 Location: DYp

DY 32.1 Tue 16:30 DYp

Jarzynski equality for conditional stochastic work — •Akira Sone[1] and Sebastian Deffner[2] — [1]Aliro Technologies, Inc, Boston, MA 02135, USA — [2]University of Maryland, Baltimore County, Baltimore, Maryland 21250, USA

We present our recent work on the fluctuation theorems of conditional stochastic work for classical Hamiltonian dynamics. The notion of conditional stochastic work is inspired by the one-time measurement paradigm, and built upon the change of energy expectation value, which is conditioned on the surface of the initial energy. This notion leads to the generalized Jarzynski equality and a modified second law of thermodynamics, whose sharper bound characterizes the adiabaticity of the thermodynamic process of interest.

DY 32.2 Tue 16:30 DYp

Anharmonic lattice dynamics in large thermodynamic ensembles with machine-learning force fields: the breakdown of the phonon quasipartic le picture in CsPbBr3 — •Jonathan Lahnsteiner and Menno Bokdam — University of Twente, Enschede, Netherlands

The harmonic approximation is a very powerful method for describing phonon dispersion relations. However, when the temperature is raised and the potential energy landscape exhibits more anharmonicity, the approximation fails to capture all crystal lattice dynamics properly. Here we study, for the first time, the phonon dispersion of a complex "Dynamic Solid" with machine-learning force fields, by simulating the dynamic structure factor (DSF) S(q,omega) and the projected velocity autocorrelation function (PVACF) trough large-scale molecular dynamics. These force fields have near first-principles accuracy and the linear scaling computational cost of classical potentials. To asses the strengths and weaknesses of the three methods we start with an analysis based on the classical Morse potential. Hereafter, the methods are applied to the inorganic perovskite: CsPbBr3. This perovskite serves as an archetypal example of a wider class of novel perovskite solar-cell materials. Imaginary modes in the harmonic picture of the CsPbBr3 structure are absent in the calculated DSF and PVACF, indicating a dynamic stabilization of the crystal. The anharmonic nature of the potential and the presence of rattling Cs+ cations, result in the breakdown of the phonon quasi-particle picture.

DY 32.3 Tue 16:30 DYp

Long-range correlations in musical time-series? — •Corentin Nelias and Theo Geisel — MPI for Dynamics and Self-Organization, Goettingen, Germany

Musical pitch time-series seem to present long-range correlations reflected in 1/f-type power-spectral densities. The existence, nature, and shape of these correlations have remained unclear as conflicting results were reported in the literature. The present work is clarifying the existing controversy by a careful analysis of power-spectral densities on a corpus 256 compositions and improvised pieces. Generally we do find 1/f-type spectra, but they show up on limited spectral scales only, corresponding to time scales typically up to a few musical bars.

DY 32.4 Tue 16:30 DYp

Voltage Dynamics in Power Grids — •Hannes Vogel — Stockholm University, Stockholm, Sweden

Understanding the stability of voltage dynamics in power grids is essential to the development of decentralized power networks for renewable energy sources. Current voltage dynamics models are motivated by physics and control theory. We formulate the power grid dynamics in terms of complex voltages, which combine the dynamics of rotor angle, frequency and voltage amplitude. To get a better overview of the properties of different models and to find criteria for classification, a common general formulation is needed.

Indeed, such a formulation is obtained by writing the differential equations in a complex power series. Therefore, the mathematical structure of the Stuart-Landau equation functions as a prototype.

DY 32.5 Tue 16:30 DYp

Satellite instability in Passively Mode-Locked Integrated External-Cavity Surface Emitting Lasers — Christian Schelte[1,2], •Denis Hessel[2], Julien Javaloyes[1], and Svetlana Gurevich[2,3] — [1]Departament de Física, Universitat de les Illes Balears & Institute of Applied Computing and Community Code (IAC-3), Cra. de Valldemossa, km 7.5, E-07122 Palma de Mallorca, Spain — [2]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, D-48149 Münster, Germany

We are interested in a pulse instability appearing in passively modelocked integrated external-cavity surface-emitting lasers (MIXSELs) modelled by delayed algebraic differential equations (DADEs). The micro-cavity geometry induces third order dispersion (TOD) that can lead to a train of satellites on the leading edge of a pulse. We show that those can become unstable due to carrier interaction. The resulting limit cycle is born in a global bifurcation of the saddle-node infinite period (SNIPER) type and exhibits behavior characteristic of excitable systems.

DY 32.6 Tue 16:30 DYp

Spectral theory of fluctuations in time-average statistical mechanics of reversible and driven systems — •Alessio Lapolla, David Hartich, and Aljaz Godec — Mathematical BioPhysics group, Max Plack Institute for Biophysical Chemistry, Goettingen, Germany

Time-averaged observables are one of the building blocks for the analysis of both theoretical and experimental systems. We present a spectral-theoretic approach to derive exact results for the mean, fluctuations, and correlations of time-average observables for ergodic stochastic processes, with continuous or discrete dynamics and with reversible or irreversible dynamics. The emergence of the universal central limit law is shown explicitly on large- deviation timescales. Our results are directly applicable to a diverse range of phenomena underpinned by time-average observables and additive functionals in physical, chemical, biological, and economical systems.

[1] Alessio Lapolla, David Hartich, and Aljaž Godec Phys. Rev. Research 2, 043084 (2020)

DY 32.7 Tue 16:30 DYp

Near and far field of coupled microresonators — •Julia Unterhinninghofen and Lasse Rosskamp — Hochschule Koblenz, Konradd-Zuse-Str. 1, 56075 Koblenz

Wavelength-scale microresonators have various applications as sensors, in nonlinear optics, as filters and micro-laser cavities. Multiple interference effects can be seen in microresonator ensembles, both concerning the far (change in far field emission directions, directional emission [1]) and the near field (formation of new cavity modes [2,3]). We compare microresonator arrays of different geometries and their far field emission properties both in a wave and a ray model as well as the near field of strongly coupled ensembles. The effects of surface roughness on the near and far fields is also investigated.

[1] J. Kreismann et al., Superdirectional light emission and emission reversal from microcavity arrays, Phys. Rev. Research 1 (2019) [2] J. Unterhinninghofen et al., Interplay of Goos-Hänchen shift and boundary curvature in deformed microdisks, Phys. Rev. E 82 (2010) [3] J.-W. Ryu et al., Abnormal high-Q modes of coupled stadium-shaped microcavities, Opt. Lett. 39 (2014)

DY 32.8 Tue 16:30 DYp

Critical exponent ν of the Ising model in three dimensions with long-range correlated site disorder analyzed with Monte Carlo techniques — •Stanislav Kazmin[1,2] and Wolfhard Janke[2] — [1]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — [2]Universität Leipzig, Institute for Theoretical Physics, Leipzig, Germany

We study the critical behavior of the Ising model in three dimensions on a lattice with site disorder by using Monte Carlo simulations [1]. The disorder is either uncorrelated or long-range correlated with correlation function that decays according to a power law r^{-a}. We derive the critical exponent of the correlation length ν and the confluent correction exponent ω in dependence of a by combining different concentrations of defects $0.05 \leq p_d \leq 0.4$ into one global fit ansatz and applying finite-size scaling techniques. We simulate and study a wide range of different correlation exponents $1.5 \leq a \leq 3.5$ as well as the uncorrelated case $a = \infty$ and are able to provide a comprehensive picture not yet known from previous works. Additionally, we perform a dedicated analysis of our long-range correlated disorder ensembles and provide estimates for the critical temperatures of the system in dependence of the correlation exponent a and the concentrations of defects p_d. We compare our results to known results from other works and to the conjecture of Weinrib and Halperin: $\nu = 2/a$ and discuss the occurring deviations.

[1] S. Kazmin and W. Janke, Phys. Rev. B 102, 174206 (2020)

DY 32.9 Tue 16:30 DYp

Haldane Insulator in the 1D Nearest-Neighbor Extended Bose-Hubbard Model with Cavity-Mediated Long-Range Interactions — •Johannes Sicks and Heiko Rieger — Theoretical Physics, Saarland University, Campus E2.6, 66123 Saarbrücken, Germany

In the one-dimensional Bose-Hubbard model with on-site and nearest neighbor interactions, a gapped phase characterized by an exotic non-local order parameter emerges, the Haldane insulator. Bose- Hubbard models with cavity-mediated global range interactions display phase diagrams, which are very similar to those with nearest neighbor repulsive interactions, but the Haldane phase remains elusive there. Here we study the one-dimensional Bose-Hubbard model with nearest-neighbor and cavity-mediated global- range interactions and scrutinize the existence of a Haldane Insulator phase. With the help of extensive quantum Monte-Carlo simulations we find that in the Bose-Hubbard model with only cavity-mediated global-range interactions no Haldane phase exists. For a combination of both interactions, the Haldane Insulator phase shrinks rapidly with increasing strength of the cavity-mediated global-range interactions. Thus, in spite of the otherwise very similar behavior the mean-field like cavity-mediated interactions strongly suppress the non-local order favored by nearest neighbor repulsion in some regions of the phase diagram.

DY 32.10 Tue 16:30 DYp

Depinning of confined colloidal dispersions under oscillatory shear — •Marcel Hülsberg and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Strongly confined colloidal dispersions under shear exhibit a variety of dynamical phenomena, including a depinning transition similar to single particles that are driven over a periodic substrate potential [1]. Here, we investigate the depinning behavior of these systems under pure oscillatory shearing with shear rate $\dot{\gamma}(t) = \dot{\gamma}_0 \cos(\omega t)$, as it is a common scenario in rheological experiments [2]. The colloid's depinning behavior is assessed from a microscopic level based on particle trajectories, which are obtained from overdamped Brownian Dynamics simulations. The numerical approach is complemented by an analytic one based on a single-particle model in the limit of weak driving. We determine the frequency-dependent critical shear rate amplitude $\dot{\gamma}_{0,crit}(\omega)$, which marks the onset of the depinning transition. Furthermore, we identify the dominant system-intrinsic time scale that dictates the scaling behavior of $\dot{\gamma}_{0,crit}$ with driving frequency ω. Finally, we discuss potential consequences of the depinning behavior on the system's rheological properties [2].

[1] S. Gerloff and S.H.L. Klapp, Phys. Rev. E **94**(6), 062605 (2016)
[2] J.M. Brader, et al., Phys. Rev. E **82**(6), 061401 (2010)

DY 32.11 Tue 16:30 DYp

Subharmonic oscillations in stochastic systems under periodic driving — •Lukas Oberreiter[1], Andre Cardoso Barato[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Department of Physics, University of Houston, Houston, Texas 77204, USA

We investigate the conditions under which subharmonic oscillations can persist for a long time in open systems with stochastic dynamics due to thermal fluctuations. In contrast to stochastic autonomous systems in a stationary state, for which the number of coherent oscillations is fundamentally bounded by the number of states in the underlying network [1], we demonstrate that in periodically driven systems, subharmonic oscillations can in principle remain coherent forever, even in networks with a small number of states [2]. By interpreting our finite state model as a single subharmonically oscillating spin, we construct an interacting spin system [3]. The mean-field model displays the phenomenon of subharmonic synchronization, which corresponds to collective subharmonic oscillations of the individual units. The 2D model does not display synchronization but it does show a time-crystalline phase, which is characterized by a power-law behavior of the number of coherent subharmonic oscillations with system size.

[1] A. C. Barato and U. Seifert *Phys. Rev. E* **95**, 062409, (2017)
[2] L. Oberreiter, U. Seifert, and A. C. Barato *Phys. Rev. E* **100**, 012135, (2019)
[3] L. Oberreiter, U. Seifert, and A. C. Barato *Phys. Rev. Lett.* **126**, 020603, (2021)

DY 32.12 Tue 16:30 DYp

Propagator for a driven Brownian particle in step potentials — •Volker Weissmann, Matthias Uhl, and Udo Seifert — II. Institute for Theoretical Physics , University of Stuttgart

Although driven Brownian particles are ubiquitous in stochastic dy- namics and often serve as paradigmatic model systems for many as- pects of stochastic thermodynamics, fully analytically solvable models are few and far between. In [1], we introduce an iterative calculation scheme, similar to the method of images in electrostatics, that enables one to obtain the propagator if the potential consists of a finite number of steps. For the special case of a single potential step, this method con- verges after one iteration, thus providing an expression for the prop- agator in closed form. In all other cases, the iteration results in an approximation that holds for times smaller than some characteristic timescale that depends on the number of iterations performed. This method can also be applied to a related class of systems like Brow- nian ratchets, which do not formally contain step potentials in their definition, but impose the same kind of boundary conditions that are caused by potential steps.

[1]: Matthias Uhl et al 2021 J. Phys. A: Math. Theor. 54 065002 https://doi.org/10.1088/1751-8121/abc21f

DY 32.13 Tue 16:30 DYp

Phase separation: from colloids to biological mixtures — •Filipe C. Thewes — Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Understanding the dynamics of phase separation in complex mixtures remains a profound challenge. In this work, we aim to build a bridge between the well-studied area of phase separation in colloidal systems and its intriguing and complex biological counterpart. We first introduce a model that interpolates between the two limiting cases and investigate the phase diagram using techniques of random matrix theory. Second, in order to understand the competing mechanisms leading to phase separation, we perform lattice simulations within a mean-field approximation and analyse the time evolution of the system in different regions of the parameter space. In the colloidal limit the model reproduces known results from the existing literature. On the biological side, our simulations provide new insights into the competing scaling obtained by early and late time analysis in the random interaction model. The intermediate regime shows new crossovers between condensation and demixing-dominated kinetics. Time permitting, results will be shown from further exploration of the model with a focus on crowding effects.

DY 32.14 Tue 16:30 DYp

The narrow escape problem in two-shell circular domains — •Matthieu Mangeat and Heiko Rieger — Saarland University, Saarbrücken, Germany

The stochastic motion of particles in living cells is often spatially inhomogeneous with a higher effective diffusivity in a region close to the cell boundary due to active transport along actin filaments [1,2]. As a first step to understand the consequence of the existence of two compartments for stochastic search problems we consider here a Brownian particle in a circular domain with different diffusivities and potentials in the inner and the outer shell. We focus on the narrow escape problem and compute the mean first passage time (MFPT) for Brownian particles starting at some pre-defined position to find a small region on the outer reflecting boundary (cell membrane). We find that the MFPT can be minimized for a specific value of the width of the outer shell only if the particle is sufficiently attracted in the outer shell whereas the MFPT depends monotonously on all model parameters without attraction. A criterion on the difference of potential between the two shells can be calculated analytically with respect to the escape region size and the ratio of diffusivities. Moreover we show that the limit of small width of the outer shell is equivalent to the surface-mediated diffusion problem [3].

[1] K. Schwarz *et al.*, Phys. Rev. Lett. **117**, 068101 (2016).
[2] A. E. Hafner and H. Rieger, Phys. Biol. **13**, 066003 (2016); Biophys. J **114**, 1420-1432 (2018).
[3] J.-F. Rupprecht *et al.*, Phys. Rev. E **86**, 041135 (2012).

DY 32.15 Tue 16:30 DYp

Clustering and emergence of collective motion in two dimensional colloidal systems with delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback in colloidal systems has become an active and promising field of study [1,2], key topics being history dependence and the manipulation of transport properties.

Here we study the dynamics of a two-dimensional colloidal suspension, subject to time-delayed feedback. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen (WCA) potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential [1], that depends on the difference of the particle position at the current time, $x(t)$ and the particle position at an earlier time, $x(t - \tau_{\mathrm{delay}})$.

We show that the introduction of this type of delayed feedback leads to clustering and the emergence of collective motion in Brownian WCA systems. Depending on the particle density, the cluster size and the propagation speed can be tuned by adjusting the delay time, the strength and the range of the repulsive feedback potential.

We also analyze the effects of time-delayed feedback on the mean-squared displacement (MSD) and, thus, the diffusion of one particle, as well as the effects on the MSD in the two-dimensional many-particle system described above.

[1] S. Tarama, S. U. Egelhaaf, and H. Löwen, Phys. Rev. E 100, 022609 (2019).
[2] R. Gernert and S. H. L. Klapp, Phys. Rev. E 92, 022132 (2015).

DY 32.16 Tue 16:30 DYp

The Role of Resampling in Population Annealing — •Denis Gessert[1,2] and Martin Weigel[1,3] — [1]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, United Kingdom — [2]Institut für Theoretische Physik, Leipzig University, Postfach 100920, D-04009 Leipzig, Germany — [3]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Population Annealing (PA) is a population-based Monte Carlo algorithm that can be used for equilibrium simulations of thermodynamic systems with a rough free energy landscape. The algorithm has a number of parameters that can be fine-tuned to improve performance. While there is some theoretical and numerical work relating the parameters, little is known to date about the effect of choosing specific resampling protocols.

The 2d Ising model is used as a benchmarking system for this study. At first various resampling methods are implemented and numerically compared using a PA implementation on GPUs. In a second part the exact solution of the Ising model is utilized to create an artificial PA setting with effectively infinite Monte Carlo updates at each temperature as well as an infinite population. This allows one to look at resampling in isolation from other parameters and draw some general conclusions about the effects of the choice of resampling scheme.

DY 32.17 Tue 16:30 DYp

A Mapping between the Spin and Fermion Algebra — •Felix Meier, Daniel Waltner, Petr Braun, and Thomas Guhr — University Duisburg-Essen, Duisburg, Germany

We derive a formalism to express the spin algebra $\mathfrak{su}(2)$ in a spin s representation in terms of the algebra of L fermionic operators that obey the Canonical Anti-commutation Relations. We also give the reverse direction expressing the fermionic operators of many-body systems as non-linear expressions in the spin operators of a single spin. We extend here to further spin values the previous investigations by Dobrov [J.Phys.A: Math. Gen 36 L503, (2003)] who in turn clarified on an inconsistency within a similar formalism in the works of Batista and Ortiz [Phys. Rev. Lett. 86, 1082 (2001)]. Then we consider a system of L fermion flavors and apply our mapping in order to express it in terms of the spin algebra. Furthermore we investigate a possibility to simplify certain Hamiltonian operators by means of the mapping [1].

[1] arXiv:2101.10119 (2021)

DY 32.18 Tue 16:30 DYp

Percolation Properties of Spin Glasses — •Lambert Münster and Martin Weigel — TU Chemnitz, Institute of Physics, Chemnitz, Germany

In the Ising model there exists a direct interrelation between percolation of Fortuin-Kasteleyn clusters and the ferromagnetic phase transition. Percolation of Fortuin-Kasteleyn clusters in spin glasses occurs at a higher temperature than the spin-glass transition [1,2]. Even when looking at the Fortuin-Kasteleyn percolation in two replicas simultaneously the percolation temperature remains above the critical one [3].

In this work we consider Fortuin-Kasteleyn percolation also in more than two replicas. Since the utilization of multiple replicas shifts the percolation transition to lower temperatures this can possibly provide an Ansatz to develop new cluster algorithms for spin glasses. To adress the question of how the percolation threshold behaves as a function of the number of replicas we perform Monte Carlo simulations of the two-dimensional Ising spin glass.

[1] L. de Arcangelis, A. Coniglio, and F. Peruggi, Europhys. Lett. **14** 515 (1991).
[2] H. Fajen, A. K. Hartmann, and A. P. Young, Phys. Rev. E **102**, 012131 (2020).
[3] J. Machta, C. M. Newman, and D. L. Stein, J. Stat. Phys. **130**, 113 (2008).

DY 32.19 Tue 16:30 DYp

How to control a cooperative co-infection dynamics — Adib Khazaee[1] and •Fakhteh Ghanbarnejad[1,2] — [1]Sharif University of Technology, Tehran, Iran — [2]Technische Universität Dresden, Dresden, Germany

In previous studies, it has been shown that the cooperation between pathogens in co-infection spreading dynamics may lead to a discontinuous transition. Here, we are investigating how interventions like quarantine or vaccination with certain rates can turn the discontinuous transitions into continuous ones while in-

creasing the threshold. We have used symmetric coupled Susceptible-Infectious-Recovered (SIR) equations to model the dynamics of co-infection spreading in a well-mixed population. Then we have intervened the epidemic dynamics by decreasing the susceptible population at a given rate, which means that the decreased susceptible compartment will be either quarantined or immunized at the same rate. Firstly, we have solved the equations numerically for a wide range of parameters and different initial conditions. We have illustrated how these interventions can change the type of the transition when the outflow rate gets large enough. Secondly, we have also solved the equations analytically for a special case in which the outflow rate varies with the size of the infectious compartment. Using the exact results for this special case, we can show how the characteristics of the fixed points change when the parameters change. Thirdly, we have explored the same dynamics on metapopulations and also agent based networks to examine how the topology of networks affects the effectiveness of interventions on the co-infection spread.

DY 32.20 Tue 16:30 DYp

In search for defining structural measures of real-world complex networks — •Máté Józsa[1], Alpár Sándor Lázár[2], and Zsolt Iosif Lázár[1] — [1]Department of Physics, Babeș-Bolyai University, M. Kogălniceanu nr. 1, 400084, Cluj-Napoca, Romania — [2]Faculty of Medicine and Health Sciences, University of East Anglia, NR4 7TJ, Norwich, UK

Based on a large dataset containing thousands of real-world networks ranging from genetic, protein interaction, and metabolic networks to brain, language, ecology, and social networks we search for defining structural measures of the different complex network domains (CND). We calculate 208 measures for all networks and investigate the limitations and possibilities of identifying the key graph measures of CNDs. Relevant features are identified based on their role in classifying CNDs by machine learning algorithms. The approach presented here managed to identify well distinguishable groups of network domains and confer their relevant features. Instead of being universal these feature spaces turn out to be specific to each CND and not unique, i.e., depeding on the CND several network measures can be substituted for another. Based on: Józsa et al. Opportunities and challenges in partitioning the graph measure space of real-world networks. accepted for publication in Journal of Complex Networks.

DY 32.21 Tue 16:30 DYp

Kauffman NK models interpolated between K=2 and K=3 — •James Sullivan, Dmitry Nerukh, and Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham, UK

The NK model was introduced by Stuart Kauffman and coworkers [1] as a model for fitness landscapes with tunable ruggedness, to understand epistasis and pleiotropy in evolutionary biology. In the original formulation, fitness is defined as a sum of fitness functions for each locus, each depending on the locus itself and K other loci. Varying K from $K = 0$ to $K = N - 1$ leads to different ruggedness of the landscape. In previous work we introduced a generalization that allows to interpolate between integer values of K by allowing K_i to assume different values for each locus. We focus on the interpolation between the most widely studied cases of $K = 2$ and $K = 3$ and characterize the landscapes by study of their local minima. Here we transfer this approach to Random Boolean Networks and investigate attractor basins and limit cycles where the average K assumes integer and noninteger values. Relaxing the assumption of degree-homogeneity is an important step towards more realistic boolean network models, relevant to a broad range of applications in the dynamics of social systems and in systems biology.

[1] Kauffman, S.; Levin, S., Journal of Theoretical Biology. 128, 11 (1987); Kauffman, S.; Weinberger, E., Journal of Theoretical Biology. 141, 211 (1989).

DY 32.22 Tue 16:30 DYp

Multiple Singularities of the Equilibrium Free Energy in a One-Dimensional Model of Soft Rods — •Juliane U. Klamser[1], Sushant Saryal[2], Tridib Sadhu[3], and Deepak Dhar[2] — [1]Gulliver UMR CNRS 7083, ESPCI Paris, Université PSL, 75005 Paris, France — [2]Indian Institute of Science Research and Education, Pashan, Pune 411008, India — [3]Tata Institute of Fundamental Research, Mumbai 400005, India

The Landau-Peierls argument and the Perron-Frobenius theorem are frequently used to argue against the existence of equilibrium phase transitions in one dimension. We present a new mechanism for the emergence of singularities in the thermodynamic free energy even in one dimension. This mechanism is observed in an instructive model of thin, rigid, linear rods of equal length 2ℓ whose centers lie on a one-dimensional lattice, of lattice spacing a. The interaction between rods is a soft-core interaction, having a finite energy U per overlap of rods. By solving the model analytically, we show that the equilibrium free energy per rod $\mathscr{F}(\frac{\ell}{a}, \beta)$, at inverse temperature β, has an infinite number of singularities, as a function of $\frac{\ell}{a}$. A two-dimensional extension of this model shows an interesting combination of two kinds of phase transitions, which we understand by an exact solution on the Bethe lattice.

DY 32.23 Tue 16:30 DYp

Interfaces beyond the elastic approximation — •Nirvana Caballero and Thierry Giamarchi — Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva, Switzerland

The framework of disordered elastic systems is widely used to describe the physics of very diverse systems with typical scales ranging from nanometers to kilometers. However, this approach has the limitation that is only applicable to univalued and smooth interfaces, thus inducing uncontrolled approximations. Solving interface dynamics and statics in more realistic systems beyond the elastic approximation is still a largely open theoretical/analytical problem. We propose to address this problem by analyzing a Ginzburg-Landau model that allows us to extend the theory of disordered elastic systems. We show the connection of our approach with the disordered elastic systems theory [1]. In addition, we show how through this connection it is possible to explain otherwise not-understood experimental results in ferromagnetic interfaces [2]. [1] N. Caballero, E. Agoritsas, V. Lecomte, T. Giamarchi. PRB 102, 104204 (2020) [2] N.Caballero. arXiv:2009.14205 (cond-mat).

DY 32.24 Tue 16:30 DYp

Dynamical Casimir interactions with a body in uniform motion and the connection to nonreciprocal media — •Philip Rauch and Matthias Krüger — Institute for Theoretical Physics, Georg-August-Universität, 37077 Göttingen, Germany

The field of the dynamical Casimir effect opened up with the discovery of the phenomenon of vacuum friction acting on accelerated objects in a quantum electrodynamic vacuum. It was later shown that a cold body in vacuum, rotating along it's axis of symmetry, experiences a frictional force and spontaneously radiates energy.

However, the dynamical Casimir effect is not limited to setups with accelerated bodies. Even two parallel plates in relative lateral constant motion experience a frictional force without being in direct contact. The described phenomenas can be explained through the appearance of fluctuating electromagnetic fields, of thermal and quantum nature, in the respective system.

In the context of this work, we intend to extend and generalize the configuration of two parallel plates in relative motion. We study the setup of a translationally invariant body in uniform motion, relative to a body of arbitrary geometry and of reciprocal or nonreciprocal media. The goal is to compute the frictional force between the bodies, which is of relevance for recently developed Casimir engines [1]. As a framework we choose the Rytov formalism, complemented with scattering theory.

[1] David Gelbwaser-Klimovsky, Noah Graham, Mehran Kardar and Matthias Krüger, arXiv preprint arXiv:2012.12768 (2020)

DY 33: Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)

Time: Tuesday 17:45–18:30 Location: BPb

Details will be published in a programme update.

DY 34: Theorie and Simulation - organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden) (joint session CPP/DY)

Time: Wednesday 9:00–14:40 Location: CPPb

See CPP 17 for details of this session.

DY 35: Complex Fluids and Soft Matter 2 - organized by Uwe Thiele (Münster) (joint session DY/CPP)

Time: Wednesday 9:00–10:30 Location: DYa

DY 35.1 Wed 9:00 DYa

Flow structure of marangoni-contracted sessile droplets — O. Ramirez[1], M.A. Hack[2], W. Kwiecinski[3], E.S. Kooij[3], T.J. Seegers[2], J.H. Snoeijer[2], and •S. Karpitschka[1] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Physics of Fluids Group, University of Twente, Enschede, Netherlands — [3]Physics of Interfaces Group, University of Twente, Enschede, Netherlands

A droplet of two miscible liquids should spread over a high-energy surface until complete wetting. However, if one component is more volatile and has a higher surface tension, a quasi-stationary non-vanishing apparent contact angle can be observed. This is caused by the enrichment of the residual component near the contact line and the associated surface tension gradient. A hydrodynamic-evaporative model, using a long-wave approximation for the droplet coupled to diffusion limited evaporation predicts a balance between Marangoni and capillary flows and a power law between the apparent contact angle and the ambient humidity [Karpitschka et al., Langmuir (2017)]. This explanation differs from a recent model, where the low surface tension of a precursor around the droplet is held responsible [Benusiglio et al., Soft Matter (2018)]. A discrimination between possible mechanisms requires experimental resolution of the flow in the drop. We present uPIV measurements and relate them to the apparent shape of the drop, for aqueous solutions of various short chain carbon diols. Depending on the surface activity of the diol, its concentration, and the ambient humidity, we observe different regimes, indicating that multiple mechanisms lead to the observed angles.

DY 35.2 Wed 9:20 DYa

Coalescence of liquid droplets in a quasi 2D liquid film — •Christoph Klopp, Ralf Stannarius, and Eremin Alexey — Institute of Physics, Otto von Guericke University, Department of Nonlinear Phenomena, 39106 Magdeburg

Coalescence of droplets plays a crucial role in nature and modern technology. Various experimental and theoretical studies explored droplet dynamics in 3D and on 2D solid or liquid substrates [1-3].

Here, we demonstrate coalescence of isotropic droplets in thin quasi 2D liquids, an overheated smectic A films. We investigated their dynamics experimentally and measured the shape deformation during the whole merging process using high-speed imaging. This system is a unique example, where the lubrication approximation can be directly applied, and the smectic membrane plays the role of the precursor film. Our studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared our results with existing models for liquid lens coalescence on liquid and solid surfaces.

[1] J. D. Paulsen et al., Coalescence of bubbles and drops in an outer fluid, Nat. Commun. 5, 3182 (2014)

[2] D. G. A. L Aarts et al., Hydrodynamics of Droplet Coalescence, Phys. Rev. Lett. 95, 164503 (2005)

[3] N. S. Shuravin et al., Coalescence of viscous two-dimensional smectic islands, Phys. Rev. E 99, 062702 (2019)

DY 35.3 Wed 9:40 DYa

Designing Pickering Emulsions for Catalysis: Influence of Nanoscale Particle Properties on Microscale Droplets — •Sebastian Stock[1], Annika Schlander[1], Kai Spanheimer[1], Maresa Kempin[2], Ariane Weber[3], Reinhard Schomäcker[3], Anja Drews[2], Marcus Gallei[4], and Regine von Klitzing[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]HTW Berlin, Berlin, Germany — [3]TU Berlin, Berlin, Germany — [4]Saarland University, Saarbrücken, Germany

Pickering Emulsions (PEs) describe emulsions stabilized by (nano) particles. The aim of the work was to design PEs as a reaction environment for catalytic reactions. As a model reaction the hydroformylation of 1-dodecene was investigated. Due to the PEs high stability separation methods with outstanding energy efficiency are applicable e. g. the separation of the oil phase by nanofiltration. Many microscopic and macroscopic PE properties are determined in a large degree by the nanoscale properties of the particles. In order to distinguish the impact of particle surface charge both positively and negatively charged silica spheres were produced. This was achieved by adequate surface modification. The resulting nanoscale particle properties concerning size, shape, charge, and hydrophobicity were investigated via Transmission Electron Microscopy (TEM), ζ-potential and sessile drop measurements, the effect on the microscopic emulsion properties were studied with microscopy and the PEs reaction behavior including yield and stability was evaluated.

Invited Talk DY 35.4 Wed 10:00 DYa

When surface viscosities rule: Bubble relaxation and thin film wrinkling — •Kirsten Harth — Institut für Physik, Otto von Guericke Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

The dynamics of liquid drops and gas bubbles in a surrounding fluid is a classic field of fluid mechanics, studied for over a century. The mathematical problem can be complex already for the case of clean fluid-fluid interfaces, characterized solely by a constant surface tension. However, applications such as ink-jet printing, emulsion characterization or typical biologically inspired systems usually deal with more complex interfacial properties, e.g., adsorbed fluid or contaminant films. Those can completely dominate the overall shape dynamics.

Merged centimeter-sized soap bubbles or rupturing micrometer-thick soap films are a simple yet ideal model system for surface-tension based relaxation. Replacing the soap film by a more complex membrane, nanometer-thin liquid crystalline films in our case, introduces qualitatively new effects due to reorganization of the membrane upon surface area reduction. The talk highlights two aspects: First, the consequences of an effective interfacial viscosity for the relaxation dynamics, known also from interfacial fluid films or adsorbed surfactant layers. Second, out-of-plane bulging and dynamic wrinkling of the interfacial membrane in response to external stress. Experiments will be accompanied by a theoretical / numerical analysis.

DY 36: Active Matter 3 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)

Time: Wednesday 9:00–10:40 Location: DYb

DY 36.1 Wed 9:00 DYb

Localized States in active Phase-Field-Crystal models — •Max Philipp Holl[1], Lukas Ophaus[1,2], Svetlana Gurevich[1,2], and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, Münster, Germany — [2]Center for Nonlinear Science, Münster, Germany

The phase-field-crystal (PFC) model represents a gradient dynamics of a single order parameter field related to density and is able to describe crystallisation processes. The model describes a variety of spatially extended periodic and localized steady structures. In an active PFC model, encoding for instance the active motion of self-propelled colloidal particles, the PFC model's gradient dynamics structure is broken by a nonreciprocal coupling of density and an additional polarization field. Then, resting and traveling localized states exist with transitions characterized by parity-breaking drift bifurcations. We briefly review the snaking behavior of localized states in passive and active PFC models before discussing the bifurcation behaviour of localized states in systems of (i) two passive PFC with nonreciprocal coupling and (ii) coupled passive and active PFCs.

DY 36.2 Wed 9:20 DYb

Cooling by Heating in Inertial Active Brownian Particles — •Lukas Hecht and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

The active Brownian particle (ABP) model is commonly used to model active matter consisting of particles which extract energy from their environment to generate directed motion. For both overdamped and inertial ABPs, motility-induced phase separation occurs in a certain parameter regime. Remarkably, inertial ABPs show a coexistence of different effective temperatures of the dilute and the dense phase whereas overdamped ABPs have a uniform effective temperature even in the phase-separated state [1].

The coexistence of different temperatures brings us to the cooling-by-heating idea: Increasing the self-propulsion speed locally could lead to a locally decreased temperature. We investigate the cooling-by-heating idea with numerical simulations of ABPs with translational and rotational inertia. Since a locally increased self-propulsion speed causes a decrease of the local particle density, detailed knowledge about the phase diagram is essential to determine appropri-

ate parameters for which cooling by heating is possible. Therefore, we analyze the phase transition behavior of inertial ABPs and the corresponding phase diagram.

[1] S. Mandal, B. Liebchen, and H. Löwen, "Motility-Induced Temperature Difference in Coexisting Phases", Phys. Rev. Lett. 123, 228001 (2019).

DY 36.3 Wed 9:40 DYb

Active dynamics of microalgae in an anisotropic porous environment — •Florian von Rüling and Alexey Eremin — Otto von Guericke University Magdeburg

Understanding the motion of active colloids in porous media is essential for fundamental physics and a wide range of biological and medical applications. Cell growth and motion is often restricted by complex environments such as the cytoskeleton. Here, we report experimental studies on the motion of the unicellular microalgae Chlamydomonas reinhardtii through a flexible anisotropic lattice of chains formed by magnetic particles. In a thin cell or capillary, the microalgae interact with chain-like aggregates that form in a magnetic field. Shape-anisotropic structures guide the swimmers or initiate tumbling. They affect the persistence time of the microswimmer's motion. As the chains of magnetic particles disintegrate quickly after turning off the magnetic field, the system transforms into an unperturbed state. We investigate the effect of the chains on the orientational velocity correlations in the active dynamics of the algae.

DY 36.4 Wed 10:00 DYb

Effective Langevin equations for a polar tracer in an active bath — •Milos Knezevic and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We study the motion of a polar tracer, having a concave surface, immersed in a two-dimensional suspension of active particles. Using Brownian dynamics simulations, we measure the distributions and auto-correlation functions of force and torque exerted by active particles on the tracer.The tracer experiences a finite average force along its polar axis, while all the correlation functions show exponential decay in time. Using these insights we construct the full coarse-grained Langevin description for tracer position and orientation, where the active particles are subsumed into an effective self-propulsion force and exponentially correlated noise for both translations and rotations. The ensuing mesoscopic dynamics can be described in terms of five dimensionless parameters. We perform a thorough parameter study of the mean squared displacement, which illustrates how the different parameters influence the tracer dynamics, which crosses over from a ballistic to diffusive motion. We also demonstrate that the distribution of tracer displacements evolves from a non-Gaussian shape at early stages to a Gaussian behavior for sufficiently long times. Finally, for a given set of microscopic parameters, we establish a procedure to estimate the matching parameters of our effective model, and show that the resulting dynamics is in a very good quantitative agreement with the one obtained in Brownian dynamics simulations.

DY 36.5 Wed 10:20 DYb

Collective behaviour of self-propelled elliptical particles — •Ashreya Jayaram, Andreas Fischer, and Thomas Speck — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

Ensembles of anisotropic self-propelled particles exhibit a rich variety of emergent phases. A combination of short-ranged excluded volume interactions, which induce inter-particle forces and torques, and self-propulsion determines the resulting macroscopic structure. Starting from a point in parameter-space which displays motility-induced phase separation (MIPS) for isotropic particles, we systematically increase the aspect ratio of the constituent ellipses. On doing so, first, MIPS breaks down paving way to a spatially homogeneous state comprising polar domains. Secondly, at sufficiently large aspect ratios, particles aggregate into polar bands. We rationalize these observations from simulations by extracting two effective parameters, *viz.*, the force imbalance coefficient and the coupling to the local polarization, that enter the mean-field description of the system.

DY 37: Invited Talk: Ludovic Berthier (Montpellier)

Time: Wednesday 9:00–9:30 Location: DYc

Invited Talk DY 37.1 Wed 9:00 DYc

Physical properties of ultrastable computer-generated glasses — •Ludovic Berthier — Laboratoire Charles Coulomb, University of Montpellier and CNRS

Computer simulations give unique insights into the microscopic behavior of amorphous materials. It became recently possible to generate ultrastable glass configurations using a simple Monte Carlo algorithm for a broad variety of model glass-formers. In this talk, I will show that this discovery has allowed a deeper understanding of the rheological, thermodynamic and dynamic aspects of glasses and supercooled liquids.

DY 38: Partial Synchronization in Networks (Focus Session joint with DY and BP) (joint session SOE/DY)

Time: Wednesday 9:00–10:00 Location: SOEa

See SOE 8 for details of this session.

DY 39: Glasses and Glass Transition 1 - organized by Andreas Heuer (Münster) (joint session DY/CPP)

Time: Wednesday 9:30–10:30 Location: DYc

DY 39.1 Wed 9:30 DYc

Molecular dynamics study of 1,4-polybutadiene supported films — •Fedir Demydiuk[1], Hendrik Meyer[1], Joerg Baschnagel[1], Mathieu Solar[1], and Wolfgang Paul[2] — [1]Institute Charles Sadron, University of Strasbourg, UPR22 CNRS 67034 Strasbourg, France — [2]Institut für Physik, University of Halle, 06120 Halle (Saale), Germany

Our work is dedicated to studying the influence of realistic intrachain constraints imposed due to the presence of torsional barriers on the glass transition in thin polymer films of supported geometry by means of classical molecular dynamics simulations. In order to do so, we use the well-established united-atom model of 1,4-polybutadiene, that has been developed by W. Paul and coworkers (G. D. Smith and W. Paul, *J. Phys. Chem. A*, 102, 1200 (1998)) and studied in confined systems (M. Solar, K. Binder and W. Paul, *J. Chem. Phys*, 146, 203308 (2017)). In our case, the model had to be adapted for usage in systems with free surface.

Focusing on dynamics of united atoms and shear-stress relaxation, we first discuss our results for bulk polybutadiene and then present first extensions of bulk simulations to supported films. First analysis of the supported films shows that dynamics is enhanced at the free surface and slowed down at the substrate.

DY 39.2 Wed 9:50 DYc

Glassy dynamics, glass transition and electrical conductivity of Guanidinium based ILCs: Influence of the cation headgroup configuration — •Mohamed A Kolmangadi, Arda Yildirim, and Andreas Schönhals — Bundesantalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Molecular mobility and conductivity of four bent shaped tetramethylated guanidinium based ionic liquid crystals (ILCs) with varying head group configuration (cyclic or acyclic) and alkyl chain length is investigated by a combination of broadband dielectric spectroscopy (BDS) and specific heat spectroscopy (SHS). BDS investigation reveals two relaxation processes: a localized γ process and $\alpha 1$ process corresponding to the glassy dynamics. SHS investigations show one calorimetrically active $\alpha 2$ relaxation process also corresponding to the glassy dynamics of the system. The temperature dependencies of the relaxation rates of two different glassy dynamics are similar for the cyclic ILC while for the acyclic counterpart they are different. Possible molecular assignments for the $\alpha 1$ and $\alpha 2$ relaxation are discussed in detail. Alongside relaxation processes, a significant conductivity contribution was observed for all ILCs, where the absolute value of DC conductivity increases by 4 orders of magnitude at the transition from

the crystalline to the hexagonal columnar phase. The increase is traced to the change in the underlying conduction mechanism from the delocalized electrical conduction in the Cry phase to ionic conduction in the quasi 1D ion columns formed in the hexagonal columnar mesophase.

DY 39.3 Wed 10:10 DYc

A new approach to probe the plastic rearrangements inside a shear band. — •Moumita Maiti and Andreas Heuer — University of Münster, Münster, Germany

We follow a single particle trajectory of a system subjected to a uniform shear by calculating it's instantaneous displacement with time. There are intermittent hops in the trajectory, which are treated as plastic events, and the particles which have performed hops, are called active. In the steady state, the number of events per particle of the whole system increases initially by increasing system size, and by further increment the number almost saturates. The onset of saturation is the onset of shear banding. Interestingly, above the onset, we observe a system size scaling in the number of plastic events only inside the shear band. The scaling is explained from the intervals between two consecutive hops of a particle, which decreases on an average with increasing size. We further show that there is a stronger coupling between active particles with increasing system size which helps to understand the smaller value of the intervals, so our approach captures the collective nature of plastic events. Additionally, we observe a system spanning avalanches for these sizes which exhibit shear banding, and the distribution of avalanche sizes have a different exponent from the mean field theory.

DY 40: Complex Fluids and Soft Matter 3 - organized by Uwe Thiele (Münster) (joint session DY/CPP)

Time: Wednesday 11:00–13:00 Location: DYa

DY 40.1 Wed 11:00 DYa

Thermally driven material transport in thin freestanding films — •Torsten Trittel, Kirsten Harth, Christoph Klopp, and Ralf Stannarius — Otto-von-Guericke Universität, 39106 Magdeburg, Germany

In addition to their important role in display applications, liquid crystals are attractive in the field of fundamental physics. Smectics can form thin free-standing films with aspect ratios exceeding one million to one (width/thickness). These homogeneously thin films serve as an ideal model system for the study of two-dimensional hydrodynamics. We investigate thermally driven material transport within the film plane under microgravity conditions. Temperature differences in the film lead to thermocapillary (Marangoni) flow. In materials with a normal (negative) temperature coefficient of the surface tension $d\sigma/dT < 0$, temperature inhomogeneities lead to material transport from the warm to the cold film edge. In materials with $d\sigma/dT > 0$, flow is reversed. We present a quantitative model, which predicts that the temperature difference between the hot and cold film edge is the relevant parameter, not the gradient as in conventional thermoconvection.

DY 40.2 Wed 11:20 DYa

Phase Field Crystal Model of patchy colloids in two dimensions — •Robert F. B. Weigel and Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Motivated by our recent simulation studies of quasicrystals that occur in systems of patchy colloids [1,2], we develop a Phase Field Crystal Model for such particles. We consider two-dimensional patchy colloids with symmetrically placed attractive sites on their surface, such that they interact with preferred binding angles. We construct a free energy functional that is similar to the free energy used for liquid crystals [3], but obeys the symmetry of the patchy colloids. The functional depends on both a density field and an orientation field. Free numerical minimization of the free energy yields a rich phase behavior of complex structures.

[1] Gemeinhardt et al., Eur. Phys. J. E 41, 126 (2018).
[2] Gemeinhardt et al., EPL 126, 38001 (2019).
[3] Achim et al., Phys. Rev. E 83, 061712 (2011).

DY 40.3 Wed 11:40 DYa

Orientational order parameters for arbitrary classical and quantum liquid crystals — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149, Münster, Germany

The orientational order of liquid crystals is measured using orientational order parameters such as the polarization vector and the nematic tensor. These are obtained from an angular or Cartesian multipole expansion of the one-body distribution function of the liquid crystal. In recent years, there has been an increase of interest in particles with general shapes, as well as in so-called "quantum liquid crystals" which are relevant, e.g., in superconductors. However, the standard methods for defining order parameters are not applicable to biaxial particles or quantum systems. In this talk, we discuss how the orientational expansion method can be generalized to particles with arbitrary shape [1] and to quantum soft matter [2]. This provides a unified framework for general classical and quantum liquid crystals.

[1] M. te Vrugt and R. Wittkowski, AIP Advances 10, 035106 (2020)
[2] M. te Vrugt and R. Wittkowski, Annalen der Physik 532, 2000266 (2020)
Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1

DY 40.4 Wed 12:00 DYa

Analytical classical density functionals from an equation learning network — •ShangChun Lin[1], Georg Martius[2], and Martin Oettel[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

We explore the feasibility of using machine learning methods to obtain an analytic form of the classical free energy functional for two model fluids, hard rods and Lennard Jones, in one dimension. The Equation Learning Network proposed in Ref.[1] is suitably modified to construct free energy densities which are functions of a set of weighted densities and which are built from a small number of basis functions with flexible combination rules. This setup considerably enlarges the functional space used in machine learning optimization. As a result in Ref [2], we find a good approximation for the exact hard rod functional. For the Lennard Jones fluid, we let the network learn the full excess free energy functional and the excess free energy functional related to interparticle attractions. Both functionals show a good agreement with simulated density profiles inside and outside the training region.

[1]G. Martius and C. H. Lampert, arXiv:1610.02995 (2016).
[2]S.-C. Lin, G. Martius and M. Oettel, JCP 152.2 (2020): 021102.

DY 40.5 Wed 12:20 DYa

Particle-resolved topological defects of smectic colloidal liquid crystals in extreme confinement — •René Wittmann[1], Louis Cortes[2], Hartmut Löwen[1], and Dirk Aarts[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Department of Chemistry, University of Oxford, UK

Hard particles are a standard model for colloidal systems and can be effectively studied within classical density functional theory (DFT). Fundamental mixed measure theory (FMMT) allows to predict the phase behavior of a hard-body fluid solely from the shape of individual particles. Recent experimental advances allow for the synthesis of colloids with a nearly hard interaction that can be analyzed on the single-particle level. Slices of such silica rods confined in a three-dimensional chamber under gravity can be considered a quasi-two-dimensional fluid that exhibits typical liquid-crystal behavior in confinement.

Applying FMMT to hard discorectangles in two dimensions, we study a smectic fluid in extreme complex confinement, where the optimal bulk layer spacing competes with the extrinsic geometric and topological constraints. As a result, we characterize a variety of topologically different states in an annular geometry, also observed in particle-resolved experiments with silica rods. By further comparing the free energy of the different states, naturally provided by our DFT, we map out a topological phase diagram, indicating the stable topology depending on the details of the annular geometry.

Publication: R. Wittmann et al., Nat Commun 12, 623 (2021).

DY 40.6 Wed 12:40 DYa

Full phase diagram of continuous-time self-propelled particle models with alignment interaction — •Yinong Zhao[1], Pawel Romanczuk[1], and Cristian Huepe[2,3] — [1]Institute of Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin — [2]CHuepe Labs, 2713 West Haddon Ave #1, Chicago, IL 60622, USA — [3]Northwestern Institute on Complex Systems and ESAM, Northwestern University, Evanston, IL 60208, USA

Self-propelled particle (SPP) models are widely used for exploring emergence of collective motion in nature. Despite the significant advances over the past decades in understanding self-organized active matter, many questions remain open about the general phase space of Vicsek-like alignment models and the regions of validity of corresponding analytical theories. We investigate a set of different continuous-time SPP-models with alignment interactions. We find that all these models share qualitatively the same phase diagram. Focusing on one of them, we identify three homogeneous states with long-range orientational order, that can be distinguished using statistical approaches. We tested the predictions of the Toner-Tu theory on these states and show that they do not hold

for all three of them. Furthermore, we also phenomenologically explore the role of positional repulsion on the emergent spatial structure. Our study provides a broad, over-arching perspective on continuous-time alignment-based SPP model.

DY 41: Active Matter 4 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)

Time: Wednesday 11:00–13:00 Location: DYb

DY 41.1 Wed 11:00 DYb

Wrinkling instability in 3D active nematics — Tobias Struebing, Amir Khosravanizadeh, Andrej Vilfan, Eberhard Bodenschatz, Ramin Golestanian, and •Isabella Guido — Max Planck Institute for Dynamics and Self-Organization, Goettigen, Germany

Networks of biopolymers and motor proteins are useful model systems for the understanding of emergent behaviour of active matter. An interesting class of such systems comprises active nematics, fluids constituted by self-organising elongated particles that in-vitro assemble in dynamical structures at length scales larger than those of their components by several orders of magnitude. In the last years the active nematic behaviour of biopolymer-motor networks confined on a 2D substrate was reported. Here we present an experimental and theoretical study on 3D active nematics made of microtubules, kinesin-1 motor proteins and a depleting agent. The network is subjected to the force exerted by the motors that crosslinked the filaments and let them slide against each other. In this way the system evolves toward a flattened and contracted 2D sheet that undergoes a wrinkling instability in the third dimension and subsequently transitions into an active turbulent state. We observe that the wrinkle wavelength is independent of the ATP concentration. A theoretical model describes its relation with the appearance time and a numerical simulation confirms the key role of kinesin motors in the contraction and extension of the network. Finally, we show how motor concentration and environmental cues influence the network properties

DY 41.2 Wed 11:20 DYb

A minimal model for dynamical symmetry breaking in active matter — Matthew Davison and •Patrick Pietzonka — Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

It is well known that asymmetrically shaped passive particles immersed in active matter move in a persistent direction. Recent work provides a thermodynamic framework and design principles for engines exploiting this mechanism [1]. We build on these results and reveal that symmetric passive particles in contact with active matter perform such a persistent motion as well. Its direction is determined through spontaneous symmetry breaking and remains fixed in time in the limit of a large number of active particles. We present an analytically solvable one-dimensional model for a single passive particle interacting with many active particles, which provides a physical understanding of these effects.

[1] P. Pietzonka *et al.*, Phys Rev. X **9**, 041032 (2019)

DY 41.3 Wed 11:40 DYb

Boundary-interior principle for microbial navigation in complex geometries — •Jan Cammann[1,2], Fabian Jan Schwarzendahl[2,3], Tanya Ostapenko[2], Danylo Lavrentovich[2], Oliver Bäumchen[2,4], and Marco G. Mazza[1,2] — [1]Loughborough University, UK — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]Heinrich-Heine-Universität, Düsseldorf, Germany — [4]University of Bayreuth, Germany

Microswimmers have attracted considerable interest due to the biological and ecological implications of understanding the mechanisms governing their dynamics. The motion of a motile cell appears erratic, and yet the combination of nonequilibrium forces and surfaces can produce striking examples of organization in microbial systems. While our current understanding is based on bulk systems or idealized geometries, it remains elusive how self-organization emerges in complex geometries. In this talk I will describe experiments, analytical and numerical calculations [1] to study the motion of motile cells in complex geometries, and demonstrate that a robust topology of probability flux loops organizes active motion even at the level of a single cell in an isolated habitat. Accounting for the interplay of activity and interfacial forces, we find that the boundary's curvature determines the nonequilibrium probability fluxes. We predict a universal relation between fluxes and global geometric properties that is confirmed by experiments.

[1] J. Cammann, et al. "Boundary-interior principle for microbial navigation in geometric confinement." arXiv:2011.02811 (2020).

DY 41.4 Wed 12:00 DYb

The role of inertia in active nematic turbulence — •Colin-Marius Koch and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Suspensions of active agents with nematic interactions can exhibit complex spatio-temporal dynamics such as mesoscale turbulence. Continuum descriptions for such systems are inspired by the hydrodynamic theory of liquid crystals and introduce additional effects of active stresses. The resulting equations feature an advective nonlinearity which represents inertial effects. The typically low Reynolds number of such active flows raises the question of the importance of the inertial effects. To address this question, we investigate mesoscale turbulence in a two-dimensional dense suspension of active nematic liquid crystals. We compare numerical simulations with and without nonlinear advection of the flow field. We find that for sufficiently high activity, the simulations including nonlinear advection exhibit large-scale motion which is not observed when excluding advection. Performing a spectral analysis of the energy budget, we identify an inverse energy transfer to the largest scales highlighting the importance of inertial effects in this model. We additionally show that surface friction, mimicked by a linear friction term, dissipates the transported energy and suppresses the large-scale motion.

DY 41.5 Wed 12:20 DYb

Rheotaxis of active droplets in confinements — •Ranabir Dey[1,2], Carola M. Buness[1,3], Babak Vajdi Hokmabad[1], Chenyu Jin[1,4], and Corinna C. Maass[1,3,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Germany — [2]Indian Institute of Technology Hyderabad, India — [3]Georg August Universitat Goettingen — [4]University of Bayreuth, Germany — [5]University of Twente, the Netherlands

Biological microswimmers commonly navigate confined spaces having liquid flows, e.g. locomotions of spermatozoa through the reproductive tract and bacteria in the gut. The directed motion of the microorganisms in response to the external velocity gradients is classically referred to as 'rheotaxis'. Over the last few years, rigorous efforts have been made to understand the rheotaxis of microorganims, specifically bacteria. In contrast, there is very little quantitative understanding of rheotaxis of artificial microswimmers. It must be noted that artificial microswimmers, e.g. those designed for cargo delivery, are often required to navigate confinements having external flows. Here, we elucidate the swimming dynamics of a common type of artificial microswimmer, i.e. active droplets, in micro-confinements having Poiseuille flow. We experimentally quantify the the swimming characteristics of these droplet microswimmers in response to velocity gradients of varying strength. We also try to understand the observed rheotaxis in confinements by considering the long range hydrodynamic interactions with the confining walls.

DY 41.6 Wed 12:40 DYb

Collective search strategies — •Adam Wysocki and Heiko Rieger — Department of Theoretical Physics and Center for Biophysics, Universität des Saarlandes, Saarbrücken, Germany

How long does it take to find N targets by M searchers? This question arises, for example, if animals search for food or immune cells chase for pathogens (our main motivation). The usual goal is to minimize the time needed to catch all targets. One obvious possibility would be to increase the number of ideal searchers another to search collectively by utilizing communication between the searchers. It is known, that cells of the immune system talk to and influence one another by secreting small proteins that bind to and activate each other. For instance, T cells (a type of lymphocyte) are chemotactic, i.e. they move in response to a chemical stimulus, however, it is unknown if chemotaxis is important in the coordination of the search for pathogens. We use a simulation model of chemotactic active particles together with a self-generated chemorepellent in order to test the possibility and the benefit of collective search strategies in microbiological systems.

DY 42: Glasses and Glass Transition 2 - organized by Andreas Heuer (Münster) (joint session DY/CPP)

Time: Wednesday 11:00–13:00 Location: DYc

DY 42.1 Wed 11:00 DYc

Residual stress distributions and mechanical noise in athermally deformed amorphous solids — •Céline Ruscher[1,2], Daniel Korchinski[2], and Joerg Rottler[2] — [1]Institut Charles Sadron, Strasbourg, France — [2]Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, Canada

Amorphous solids are yield stress materials whose flow consists of periods of elastic loading interrupted by rapid stress drops, or avalanches, coming from microscopic rearrangements known as shear transformations (STs). From the microscopic point of view, the density of STs, or density of local residual stresses, $P(x)$, governs the statistical properties of global collective failure events at the yielding transition.

Using atomistic simulations, we reveal the evolution of $P(x)$ upon deformation. A pseudogap form $P(x) \sim x^{\theta}$ is observed in the freshly quenched state and in the early stages of deformation. After a few percent strain, however, $P(x)$ starts to develop a system size dependent plateau in the small x limit. To explain the origin of the plateau we consider a mesoscopic elastoplastic approach. Our results show how the spatial extent of avalanches in the stationary regime has a profound effect on the distribution of local residual stresses x. While the entrance into the plateau is set by the lower cutoff of the mechanical noise produced by individual STs, the departure from the usually assumed power-law pseudogap form comes from stress fluctuations induced by collective avalanches.

DY 42.2 Wed 11:20 DYc

Evaluation of Local Atomic Structural Changes in $Cu_{50}Zr_{50}$ Cluster Assembled Metallic Glasses through Molecular Dynamics Simulations — •Syamal Praneeth Chilakalapudi[1], Shyam Katnagallu[1], Wolfgang Wenzel[1], Penghui Cao[2], and Horst Hahn[1,2,3] — [1]Institute Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Dept. Mat. Sci. & Engg., University of California-Irvine, USA — [3]KIT-TUD Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt, Germany

Cluster assembled metallic glasses (CAMGs), synthesized by cluster (amorphous) ion beam deposition (CIBD), are a prominent bottom-up approach to tailor amorphous structures. Experimental control of amorphous structure and magnetic properties [1] was demonstrated with a custom-made apparatus which offers precise control on the size and the deposition energy of the clusters under ultra high vacuum [2].

To understand the underlying mechanisms of these structural changes in CAMGs, we performed atomistic molecular dynamics simulations of $Cu_{50}Zr_{50}$ cluster assembly using LAMMPS. Our simulations model the CIBD process and evaluate changes in the local short-range order in CAMGs as a function of the deposition energy of the clusters. We notice the presence of interfacial regions, formed between every adjacent cluster. The interfaces are most prominent in soft-landing cases. We also investigate the effect of quenching rate used to generate the amorphous clusters on CAMGs.

[1] C. Benel et al., Mat. Horizons, (2019) 6, 727
[2] A. Fischer et al., Rev. Sci. Instr. (2015) 86, 023304

DY 42.3 Wed 11:40 DYc

X-ray computed tomography of glass foams with tailored hierarchical pore structure — •Cristine Santos de Oliveira[1], Richard Kohns[2], Felix Meyerhoefer[2], Simon Carstens[2], Dirk Enke[2], Ralf Boris Wehrspohn[1,3], and Juliana Martins de Souza e Silva[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Institut für Technische Chemie, Universität Leipzig, Germany — [3]Fraunhofer Gesellschaft, München, Germany

Glass foams are materials consisting of a light-weight porous glass structure of special importance in the fields of civil engineering and bio-implants. Typically, their synthesis involves the thermal foaming of a powder mixture of glass with a foaming agent that decomposes at the foaming temperature, resulting in a solid glass skeleton permeated by empty pores. In our work, we synthesized a series of glass foams with a hierarchical pore structure, obtained by combining pores generated through the foaming of a powdered mixture of silica-based glass, MnO_2 and C at 815 °C, with pores obtained by phase-separation (performed at circa 500 °C) followed by acid leaching and washing. Using a combination of mercury intrusion porosimetry, N_2 sorption and X-ray CT at the micro and nanometer scales we observed that slight changes in the preparation procedure resulted in foams with different porosity, surface area, pore size and pore volume. Furthermore, by applying machine learning segmentation to the X-ray CT data it was possible to map inhomogeneities, residues and cracks inside the foam walls.

DY 42.4 Wed 12:00 DYc

Decelerated aging in metallic glasses by low temperature thermal cycling — •Fathollah Varnik — ICAMS, Ruhr-University Bochum, Germany

It has been recently proposed that deep temperature cycling of metallic glasses may lead to a rejuvenation and improve their ductility. Here, we investigate this issue via extensive molecular dynamics simulations of a generic model glass former. We disentangle the effects of aging from those of thermal treatment and show that aging is slowed down but not stopped – neither reversed – during thermal cycling. These observations are corroborated further by a survey of energy distribution, which continues narrowing, albeit with a smaller rate. Our results are in qualitative agreement with recent differential scanning calorimetry measurements on different bulk metallic glasses, which show no measurable rejuvenation upon deeply cooled (cryogenic) thermal cycling. This applies both to as-quenched and well-annealed samples.

DY 42.5 Wed 12:20 DYc

Glassy dynamics in viscous liquids - Prospects of broadband NMR relaxometry — •Manuel Becher[1,2], Michael Vogel[2], and Ernst Rössler[1] — [1]Nordbayerisches NMR-Zentrum, Universität Bayreuth, Germany — [2]Institute of Condensed Matter Physics, TU Darmstadt, Germany

As the molecular dynamics of a liquid undergoing a glass transition features a wide range of timescales over many decades, it is beneficial to study these viscous liquids with broadband spectroscopic techniques. Besides well established methods such as dielectric spectroscopy (DS) and depolarized dynamic light scattering (DDLS) covering many decades in time/frequency, also nuclear magnetic resonance (NMR) offers detailed insights in molecular motion ranging from the boiling point of a liquid to its glassy arrest. However, in most recent publications the spectral shape of the main relaxation peak between DS, DDLS and NMR was readressed and the question of universality arised, rendering the prospect of broadband NMR experiments to a new importance. As NMR experiments can provide single-particle correlation functions of the probed molecular moieties, but are usually carried out at a single Larmor-frequency, interest lies in 'broadening' their frequency range. In this talk, ways to access the relaxation spectrum are presented, focussing on field-cycling (FC) NMR. Here, recent advances allow us to evaluate the concept of frequency-time superposition in molecular glass formers. Moreover, making use of NMR's isotope sensitivity, molecular site-dependent measurements are shown to reveal the impact of molecular flexibility on structural relaxation.

DY 42.6 Wed 12:40 DYc

The dynamics of a glassforming Lennard-Jones system below the critical mode-coupling temperature — •Juergen Horbach — Heinrich Heine-Universitaet, Duesseldorf, Germany

We present molecular dynamics (MD) computer simulations of a polydisperse glassforming Lennard-Jones model. The equation of state of this model is very similar to that of the Kob-Andersen binary Lennard-Jones (KABLJ) mixture. At a comparable density, also the critical mode coupling temperature is similar as in the KABLJ mixture. Using the swap Monte Carlo technique in combination with MD, we are able to equilibrate supercooled liquids far below the critical mode coupling temperature. We analyze the properties of these deeply supercooled samples with respect to their dynamics in the beta relaxation regime and their response to external shear. In particular, we find the formation of shear bands at sufficiently low shear rates.

DY 43: Pattern Formation - organized by Azam Gholami (Göttingen)

Time: Wednesday 14:00–16:00 Location: DYa

DY 43.1 Wed 14:00 DYa

Suppression of coarsening in a Cahn-Hilliard model with nonreciprocal coupling — •Tobias Frohoff-Hülsmann[1] and Uwe Thiele[1,2] — [1]Institute of theoretical physics, WWU Münster — [2]Center of Nonlinear Science (CeNoS), WWU Münster

When coarsening occurs, an initial patterned state develops into a fully phase-separated state. This is standard for passive mixtures and is now also frequently discussed in the field of active matter. The Cahn-Hilliard equation is the paradigmatic description for a passive system characterized by a single conserved order parameter field, e.g., concentration for a mixture. Here, we study a two-field

Cahn-Hilliard system (e.g. representing a ternary mixture). The chosen couplings maintain both conservation laws and consist of passive (reciprocal) and active (nonreciprocal) contributions. Our particular focus is the suppression of coarsening that occurs when going from the passive to the active case. We distinguish three mechanisms of suppression: Linear and nonlinear complete, and nonlinear partial suppression. They differ from the suppression of coarsening due to broken mass conservation observed in other systems.

DY 43.2 Wed 14:20 DYa

Pattern selection in reaction-diffusion systems — •Srikanth Subramanian and Seán M. Murray — Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Turing's theory of pattern formation has been used to describe the formation of self-organized periodic patterns in many biological, chemical, and physical systems. However, the use of such models is hindered by our inability to predict, in general, which pattern is obtained from a given set of model parameters. While much is known near the onset of the spatial instability, the mechanisms underlying pattern selection and dynamics away from onset are much less understood. Here, we provide physical insight into the dynamics of these systems. We find that peaks in a Turing pattern behave as point sinks, the dynamics of which is determined by the diffusive fluxes into them. As a result, peaks move toward a periodic steady-state configuration that minimizes the mass of the diffusive species. We also show that the preferred number of peaks at the final steady state is such that this mass is minimized. Our work presents mass minimization as a potential general principle for understanding pattern formation in reaction diffusion systems far from onset.

DY 43.3 Wed 14:40 DYa

Periodic patterns displace active phase separation — •Frederik Thomsen and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth

In this work we identify and investigate a novel bifurcation in conserved systems on one- and two-dimensional spatial domains. This secondary bifurcation stops active phase separation in its nonlinear regime. It is then either replaced by an extended, system-filling, spatially periodic stripe pattern in one spatial dimension or by a hexagonal pattern in two dimensions. In complementary parameter regions phase separation is replaced by a novel hybrid state with spatially alternating homogeneous and periodic states. The transition from phase separation to extended spatially periodic patterns is hysteretic. We show that the resulting patterns are multistable, as they show stability beyond the bifurcation for different wavenumbers belonging to a wavenumber band. Both transition scenarios are systems-spanning phenomena in particle conserving systems. They are predicted with a generic dissipative model as described by this contribution. Candidates for specific systems in which these generic secondary transitions are likely to occur are, for example, generalized models for motility-induced phase separation in active Brownian particles, models for cell division or chemotactic systems with conserved particle dynamics.

DY 43.4 Wed 15:00 DYa

Chimera solitons and soliton turbulence in oscillatory media — •Arkady Pikovsky[1], Lev Smirnov[2], Maxim Bolotov[3], Dmitry Bolotov[3], and Grigory Osipov[3] — [1]University of Potsdam, Germany — [2]Institute of Applied Physics of the Russian Academy of Sciences, Nizhny Novgorod, Russia — [3]Department of Control Theory, Nizhny Novgorod State University, Nizhny Novgorod, Russia

Chimera states are coexisting patterns of synchrony and asynchrony in oscillatory media. Here we report on stable solitary chimera states in an infinite medium: a finite region of synchrony coexists with an infinite asynchronous background. When this state becomes unstable, soliton turbulence appears, where solitons merge and reappear randomly. With a further change of parameters, this regime evolves into a spatial-temporal intermittency, where the synchronous state is absorbing. Close to the transition point, where the spatial-temporal intermittency disappears, it is dominated by traveling dark solitons: moving patches of asynchrony on a synchronous background.

DY 43.5 Wed 15:20 DYa

A hierarchy of protein patterns robustly decodes cell shape information — •Tzer Han Tan[1,4], Manon C. Wigbers[2], Fridtjof Brauns[2], Jinghui Liu[1], Zak Swartz[3], Erwin Frey[2], and Nikta Fakhri[1] — [1]MIT, Cambridge, USA — [2]LMU, Munich, Germany — [3]Whitehead Institute, Cambridge, USA — [4]MPI-CBG, Dresden, Germany

Many cellular processes rely on precise positioning of proteins on the membrane. Such protein patterns emerge from a combination of protein interactions, transport, conformational state changes, and chemical reactions at the molecular level. Recent experimental and theoretical work clearly demonstrates the role of geometry and advective cortical flow in modulating membrane protein patterns. How can regulatory proteins form a robust spatiotemporal organization on the membrane in the face of dynamic cell-shape changes during physiological processes? Here, we use the oocytes of the starfish *Patiria miniata* as a model system and elucidate a shape-adaptation mechanism that robustly controls spatiotemporal protein dynamics on the membrane despite cell-shape deformations. By combining experiments with biophysical theory, we show how cell-shape information contained in a cytosolic gradient can be decoded by a bistable regulator of Rho. In turn, this bistable front precisely controls a mechanochemical response by locally triggering excitable dynamics of Rho. We posit that such a shape-adaptation mechanism based on a hierarchy of protein patterns may constitute a general physical principle for cell-shape sensing and control.

DY 43.6 Wed 15:40 DYa

Wavelength selection by interrupted coarsening in reaction–diffusion systems — Fridtjof Brauns[1], •Henrik Weyer[1], Jacob Halatek[2], Junghoon Yoon[1], and Erwin Frey[1] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — [2]Biological Computation Group, Microsoft Research, Cambridge CB1 2FB, UK

Intracellular pattern formation may be described by (nearly) mass-conserving reaction–diffusion systems. Of these, two-component mass-conserving reaction–diffusion systems are paradigmatic models, also used to describe for example precipitation patterns or granular media systems. We will discuss that these mass-conserving models generically show uninterrupted coarsening because of positive feedback in the mass transport between neighbouring pattern domains. From this, a general coarsening criterion follows and the coarsening law may be determined.

We use this understanding to explain the arrest of coarsening due to weak source terms and predict the wavelength thereby selected. This analysis will exemplify how the phase-space structure of pattern-forming systems may be used to study wavelength selection far from equilibrium.

DY 44: Invited Talk Sujit S. Datta (Princeton)

Time: Wednesday 14:00–14:30 Location: DYb

Invited Talk DY 44.1 Wed 14:00 DYb

Life in a tight spot: How bacteria swim in complex spaces — •Sujit Datta — Princeton University, Princeton NJ, USA

Bacterial motility is central to processes in agriculture, the environment, and medicine. While motility is typically studied in bulk liquid or on flat surfaces, many bacterial habitats – e.g., soils, sediments, and biological gels/tissues – are complex porous media. Here, we use studies of E. coli in transparent 3D porous media to demonstrate how confinement in a heterogenous medium fundamentally alters motility. In particular, we show how the paradigm of run-and-tumble motility is dramatically altered by pore-scale confinement, both for cells performing undirected motion and those performing chemotaxis, directed motion in response to a chemical stimulus. Our porous media also enable precisely structured multi-cellular communities to be 3D printed. Using this capability, we show how spatial variations in the ability of cells to perform chemotaxis enable populations to autonomously stabilize large-scale perturbations in their overall morphology. Together, our work thus reveals new principles to predict and control the behavior of bacteria, and active matter in general, in complex environments.

DY 45: Brownian Motion and Anomalous Transport - organized by Ralf Metzler (Potsdam)

Time: Wednesday 14:00–16:30 Location: DYc

Invited Talk DY 45.1 Wed 14:00 DYc

Small diffusive systems warm up faster than they cool down — Alessio Lapolla and •Aljaz Godec — Mathematical bioPhysics Group, Max Planck Institute for Biophysical Chemistry, Göttingen

The celebrated laws of linear irreversible thermodynamics dictate that the relaxation of an extensive thermodynamic observable to its equilibrium value depends linearly on the departure from equilibrium, and is therefore independent of the direction of the departure. However, these linear laws rely on the assumption of "local thermodynamic equilibrium" which is expected to break down when systems become sufficiently small. It turns out that the relaxation of nano-scale systems driven out of equilibrium by a rapid change in temperature depends not only on the distance but also on the direction of the displacement from thermodynamic equilibrium. Contrary to intuition nano-scale systems in fact warm up faster than they cool down. This asymmetry is a general feature of reversible overdamped diffusive systems with smooth single-well potentials and also occurs in multi-well landscapes when quenches disturb predominantly intra-well equilibria. In the talk we will explain the physical origin of this intriguing asymmetry in relaxation to equilibrium.

[1] A. Lapolla, A. Godec, *Phys. Rev. Lett* **125**, 110602 (2020) with focus article in *Physics* **13**, 144 (2020)

DY 45.2 Wed 14:30 DYc

Cooperatively enhanced reactivity and stabilitaxis of dissociating oligomeric proteins — •Jaime Agudo-Canalejo[1], Pierre Illien[2], and Ramin Golestanian[1] — [1]Department of Living Matter Physics, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Sorbonne Universite, CNRS, Laboratoire PHENIX, UMR CNRS 8234, Paris, France

Many functional units in biology, such as enzymes or molecular motors, are composed of several subunits that can reversibly assemble and disassemble. This includes oligomeric proteins composed of several smaller monomers, as well as protein complexes assembled from a few proteins. By studying the generic spatial transport properties of such proteins, we investigate here whether their ability to reversibly associate and dissociate may confer on them a functional advantage with respect to non-dissociating proteins [1]. In uniform environments with position-independent association-dissociation, we find that enhanced diffusion in the monomeric state coupled to reassociation into the functional oligomeric form leads to enhanced reactivity with localized targets. In non-uniform environments with position-dependent association-dissociation, caused by, for example, spatial gradients of an inhibiting chemical, we find that dissociating proteins generically tend to accumulate in regions where they are most stable, a process that we term "stabilitaxis."

[1] Agudo-Canalejo, J., Illien, P., & Golestanian, R. (2020). Proceedings of the National Academy of Sciences, 117(22), 11894-11900.

DY 45.3 Wed 14:50 DYc

Hot Brownian Motion in the Ballistic Timescale — •Xiaoya Su[1], Alexander Fischer[1], Frank Cichos[1], and Klaus Kroy[2] — [1]Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany — [2]Institute of Theoretical Physics, University Leipzig, Leipzig, Germany

Brownian motion is the erratic motion of particles in a fluid due to the bombardment of the particle with solvent molecules providing thermal energy and viscous friction. It is fundamental for the dynamics of soft matter and defines the prototype of a fluctuation dissipation relation. While at long timescales the motion is purely stochastic, it is at shorter times influenced by hydrodynamic effects and even ballistic at ultrashort times. Yet, the ballistic motion is still determined by the temperature of the system. Here we explore the transition to the ballistic regime for a hot Brownian particle, i.e. a microparticle which is heated by a laser in an optical trap. In this case the particle temperature is different from the solvent temperature and so far, only theoretical predictions exist for the relevant temperature determining the particle velocity.

We report the first measurements of the thermal non-equilibrium process in a specially designed optical trap which is able to resolve particle displacements of about 20 pm with a time-resolution of 5ns. We show how the mean squared displacement of the particle from the nanoseconds to the seconds timescale changes as a function of the surface temperature of the particle and discuss the model of a frequency dependent effective temperature of hot Brownian motion.

DY 45.4 Wed 15:10 DYc

Stochastic action for tubes: Connecting path probabilities to measurement — •Julian Kappler[1], Jannes Gladrow[2], Ulrich F. Keyser[2], and Ronojoy Adhikari[1] — [1]Department of Applied Mathematics and Theoretical Physics, Cambridge University, Cambridge, United Kingdom — [2]Cavendish Laboratory, University of Cambridge

The trajectories of diffusion processes are continuous but nondifferentiable, and each occurs with vanishing probability. This introduces a gap between theory, where path probabilities are used in many contexts, and experiment, where only events with nonzero probability are measurable. We bridge this gap by considering the probability of diffusive trajectories to remain within a tube of small but finite radius around a smooth path. This probability can be measured in experiment, via the rate at which trajectories exit the tube for the first time, thereby establishing a link between path probabilities and physical observables. In my talk I will show how this link can be used to both measure ratios of path probabilities [1], and to extend the theoretical stochastic action from individual paths to tubes [2].

[1] J. Gladrow, U. F. Keyser, R. Adhikari, and J. Kappler. Direct experimental measurement of relative path probabilities and stochastic actions. arXiv:2006.16820

[2] J. Kappler and R. Adhikari. Stochastic action for tubes: Connecting path probabilities to measurement. Physical Review Research, 2(2), June 2020.

DY 45.5 Wed 15:30 DYc

Diffusion and random search in (in)homogeneous media — •Trifce Sandev[1,2] and Ralf Metzler[1] — [1]University of Potsdam — [2]Macedonian Academy of Sciences and Arts

Different approaches to diffusion in both homogeneous and heterogeneous media will be discussed. Such processes often become anomalous due to the geometric constraints, random potential effects or variations of the diffusion coefficients. Such problems of heterogeneous diffusion might be closely related to inhomogeneous advection-diffusion processes and geometric Brownian motion used to analyze stock prices in financial markets in the Black-Scholes model. The search strategies of many animals follow similar laws but they often return to their nest or resting place, after some (random) search time. We will give results on the first passage and first hitting times for different random search processes with and without external forces for which we will show that introduction of stochastic resetting in such systems leads to various interesting realizations. The investigation of resetting mechanism in aforementioned systems may also be important for description of experiments of random motion with resetting using optical trap techniques, or economic models of income dynamics.

DY 45.6 Wed 15:50 DYc

Disentangling the origins of anomalous diffusion in data: the Moses/ Noah and Joseph effects — •Erez Aghion[1], Philipp G. Meyer[1], Vidushi Adlakha[2], Holger Kantz[1], and Kevin E. Bassler[2] — [1]Max-Planck Institute for the Physics of complex systems, Dresden, Germany — [2]University of Houston, Houston Texas, USA

We study a method for detecting the precise elements that lead to anomalous diffusion, when it is observed in a experimental data, where we do not have exact knowledge about the underlying dynamics.

The reasons for anomalous diffusion are decomposed into three effects: Increment correlations are expressed by the *Joseph effect*, fat-tails of the increment probability density lead to a *Noah effect*, and non-stationarity, to the *Moses effect*. Telling these three effects apart is crucial when one tries to infer the underlying structure of the system, and build a model to describe it.

We present this decomposition method by analysing the example of a widely-applicable model for coupled Levy walk. We infer the properties of the dynamics from data using methods of time-series analysis, and compare our results with theoretical predictions.

DY 45.7 Wed 16:10 DYc

Dynamics of a point-like colloid in a confined critical fluid — •Markus Gross — MPI for Intelligent Systems, Stuttgart

We study analytically and via simulations a point-like colloidal particle (tracer) immersed in a confined critical fluid. Particle and fluid are governed by a system of coupled stochastic PDEs. In addition to a white noise, the particle experiences a random force due to the coupling to the fluctuating fluid density, which is spatially correlated and strongly non-Markovian. By adiabatically eliminating the fluid degrees of freedom, we obtain an effective Langevin equation for the particle, which entails a fluctuation-induced (Casimir) potential, a spatially dependent Markovian noise, and a spatially dependent mobility. The stochastic interpretation of the noise is found to depend on the type of coupling between particle and fluid.

Reference: M. Gross, arXiv:2101.02072

DY 46: Active Matter 5 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP)

Time: Wednesday 14:30–15:50 Location: DYb

DY 46.1 Wed 14:30 DYb

Barrier-mediated predator-prey dynamics — •Fabian Jan Schwarzendahl and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

The survival chance of a prey chased by a predator depends not only on their relative speeds but importantly also on the local environment they have to face. For example, a wolf chasing a deer might no be able to cross a river which can be crossed by the deer. Here, we propose a simple predator-prey model for a situation in which both the escaping prey and the chasing predator have to surmount an energetic barrier. Different barrier-assisted states of catching or final escaping are classified and suitable scaling laws separating these two states are derived. We discuss the effects of diffusion on the catching times and determine states in which catching or escaping is more likely. Including hydrodynamic and chemotactic interactions, we further identify trapping or escaping states which are determined by hydrodynamics and chemotaxis. Our results are of importance for both microbes and self-propelled unanimous microparticles following each other by non-reciprocal interactions in inhomogeneous landscapes.

DY 46.2 Wed 14:50 DYb

Irreversibility of active particles: Fluctuation Theorem and Mutual Information — Lennart Dabelow[1], •Stefano Bo[2], and Ralf Eichhorn[3] — [1]Fakultät für Physik, Universität Bielefeld — [2]Max Planck Institute for the Physics of Complex Systems — [3]Nordita, Royal Institute of Technology and Stockholm University

The defining feature of active particles is that they locally consume energy, which enables them to self-propel and prevents them from equilibrating with their thermal environment. Within the framework of active Ornstein-Uhlenbeck particles we derive the path probability of a particle subject to both, thermal and active noise. By comparing the path probabilities for observing a particle trajectory forward in time versus observing its time-reserved twin trajectory we obtain a generalized "entropy production" for active Brownian motion, which fulfills an integral fluctuation theorem. We show that those parts of this "entropy production", which are different from the usual dissipation of heat in the thermal environment, can be associated with the mutual information between the particle trajectory and the history of the non-equilibrium environment. We then investigate the time-reversal properties of steady-state trajectories of a trapped active particle. We find that steady-state trajectories in a harmonic potential fulfill path-wise time-reversal symmetry exactly despite their active nature, while this symmetry is typically broken in anharmonic potentials.

DY 46.3 Wed 15:10 DYb

Shape-anisotropic Microswimmers: Influence of Hydrodynamics — •Arne W. Zantop and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Constituents of active matter, e.g. bacteria or active filaments, are often elongated in shape. The shape and the stiffness of the active components clearly influence their individual dynamics and collective pattern formation. On length scales much larger than the size of the constituents, active materials exhibit many fascinating phenomena such as the formation of vortices or turbulent structures [1,2]. To identify how steric and hydrodynamic interactions as well as thermal fluctuations influence collective behavior is subject of current research.

In this context, we model shape-anisotropic microswimmers with rod shape by composing them of overlapping spherical squirmers. We simulate their hydrodynamic flow fields using the method of multi-particle collision dynamics. With increasing aspect ratio of the rods, we find that a force quadrupole moment dominates the hydrodynamic flow field, whereas in quasi-2D confinement between two parallel plates (Hele-Shaw geometry) the far field is determined by a two-dimensional source dipole moment [3]. Investigating the collective dynamics of the squirmer rods, we identify with increasing density and aspect ratio of the rods a disordered, a swarming, and a jamming state.

[1] Dunkel *et al.*, Phys. Rev. Lett. **110**, 228102 (2013)
[2] Wensink *et al.*, Proc. Natl. Acad. Sci. **109**, 14308-14313 (2012)
[3] A. W. Zantop and H. Stark, Soft Matter **16**, 6400-6412 (2020)

DY 46.4 Wed 15:30 DYb

Feedback Control of Multiple Active Microswimmers — •Alexander Fischer[1], Giovanni Volpe[2], and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Universität Leipzig — [2]Physics Department, Gothenburg University

Sensing and reacting to signals is a fundamental component of life. The exchange of information is used to organize ensembles of active objects into collective states that appear as flocks, swarms or even tissue. Here we explore the emergent collective behavior as a result of an information exchange between synthetic microswimmers by computer-controlled feedback processes. We have created a setup where multiple active microswimmers can respond to local signals in space or their distance to other microswimmers [1]. Our system consists of symmetric self-thermophoretic swimmers that are propelled by light-to-heat conversion allowing us to implement almost arbitrary control of propulsion speed and direction. Using this system, we study in particular the delayed response of the swimmers to environmental signals, where the swimmers remember previous information on a signaling landscape or infers future signals from experience. We find that this type of delayed response is modifying the collective behavior enhancing local swimmer densities depending on delay time, extrapolation or memory and the rotational diffusion time. Our data suggest the existence of optimal delays for the given landscapes.

[1] U. Khadka, V. Holubec, H. Yang, F. Cichos, Nat. Commun. 9, 3864 (2018)

Physics of Socio-economic Systems Division
Fachverband Physik sozio-ökonomischer Systeme (SOE)

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Overview of Invited Talks and Sessions

Invited Talks

SOE 1.1	Mon	9:00– 9:40	SOEa	**Mathematical modelling of COVID-19: dynamics and containment** — •Yuliya Kyrychko
SOE 1.5	Mon	11:00–11:40	SOEa	**data-driven modeling of COVID-19 pandemic** — •Yamir Moreno

Sessions

SOE 1.1–1.9	Mon	9:00–13:00	SOEa	**COVID-19 pandemics through the lens of physics (org.: Fakhteh Ghanbarnejad and Philipp Hövel)**
SOE 2.1–2.6	Mon	14:00–16:00	SOEa	**Networks and Social Dynamics**
SOE 3.1–3.8	Mon	17:30–19:30	SOEp	**Poster**
SOE 4.1–4.5	Tue	11:00–12:40	SOEa	**Data Analytics for Complex Dynamical Systems (joint SOE/DY Focus Session) (joint session SOE/DY)**
SOE 5.1–5.3	Tue	14:00–15:00	SOEa	**Financial and Economic Systems and Evolutionary Game Theory**
SOE 6	Tue	17:45–18:30	BPb	**Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)**
SOE 7	Tue	19:00–19:40	SOEa	**Member's Assembly of SOE**
SOE 8.1–8.3	Wed	9:00–10:00	SOEa	**Partial Synchronization in Networks (Focus Session joint with DY and BP) (joint session SOE/DY)**
SOE 9.1–9.4	Wed	11:00–12:20	SOEa	**Opinion Formation**
SOE 10.1–10.8	Wed	13:00–15:40	SOEa	**Transport, Regional and Urban Dynamics**

Annual General Meeting of the Physics of Socio-economic Systems Division

Tue 19:00–19:40 SOEa

Sessions

– Invited Talks, Contributed Talks, and Posters –

SOE 1: COVID-19 pandemics through the lens of physics (org.: Fakhteh Ghanbarnejad and Philipp Hövel)

Time: Monday 9:00–13:00 Location: SOEa

Invited Talk SOE 1.1 Mon 9:00 SOEa

Mathematical modelling of COVID-19: dynamics and containment — •Yuliya Kyrychko — Department of Mathematics, University of Sussex, Falmer, Brighton, United Kingdom

COVID-19 disease caused by the novel SARS-CoV-2 coronavirus has already brought unprecedented challenges for public health and resulted in huge numbers of cases and deaths worldwide. In this talk I will discuss mathematical models developed to analyse the dynamics of COVID-19 spread in some regions of the UK and Ukraine. A particular emphasis will be made on the non-exponential distribution of infection and recovery times as well as age- and location-specific contact matrices used to represented mixing patterns. I will show how the model can be used to provide an accurate short-term forecast for the numbers and age distribution of cases and deaths, as well as the effects of different lockdown scenarios [1,2].

[1] Y.N. Kyrychko, K.B. Blyuss, I. Brovchenko (2020). Mathematical modelling of the dynamics and containment of COVID-19 in Ukraine . Nature Sci. Rep., 2020;10:1-11.DOI: 10.1038/s41598-020-76710-1

[2] K.B. Blyuss, Y.N. Kyrychko, Effects of latency and age structure on the dynamics and containment of COVID-19, J.Theor.Biol. 2021; 513: 110587:DOI:10.1016/j.jtbi.2021.110587.

SOE 1.2 Mon 9:40 SOEa

An all-Ireland SIRX Network Model for the Spreading of SARS-CoV-2 — •Rory Humphries[1], Mary Spillane[1], Kiernan Mulchrone[1], Sebastian Wieczorek[1], Michael O'Riordain[1,2], and Philipp Hövel[1] — [1]School of Mathematical Sciences, University College Cork, Western Road, Cork T12 XF64, Ireland — [2]Department of Surgery, Mercy University Hospital, Grenville Place, Cork, T12 WE28, Ireland

The Republic of Ireland and Northern Ireland have been severely impacted by the recent history of the spreading of the Severe Acute Respiratory Syndrome Corona Virus 2 (SARS-CoV-2). Our work contributes to the goal of an island with zero community transmissions and careful monitoring of routes of importation in the absence of effective pharmaceutical interventions.

In the model, nodes correspond to locations or communities that are connected by links indicating travel and commuting between different locations. The network comprises 4330 nodes, which corresponds to local administrative units below the NUTS 3 regions. The local dynamics within each node follows a phenomenological SIRXD compartmental model including classes of Susceptibles, Infected, Recovered, Quarantined (X) and Deaths. We consider various scenarios including the 5-phase roadmap for Ireland, where the parameters are chosen to match the current number of reported deaths. In addition, we investigate the effect of dynamic interventions that aim to keep the number of infected below a given threshold.

SOE 1.3 Mon 10:00 SOEa

Scenario projections of the Covid-19 pandemic using a data-driven macroscopic model — •Martin Treiber — TU Dresden, Germany

Modelling the pandemic dynamics is a prime example of an interdisciplinary topic combining biology, the dynamics of social systems, and econometric data analysis. The proposed model is of the delayed SEIR type including delays caused by the infection period and the delayed effect of vaccinations. Moreover, it also includes a complete measurement model including the delay between infection and test, the number of tests, test strategies, the percentage of reported infections, and the test sensitivity and specificity.

The time varying model parameters base reproduction number R_0 and infection fatality rate are calibrated, for different countries, to the reported cases and fatalities of RKI and OWID data. Relating the R_0 values to social behavior (mask usage, distance, different stages of a "lockdown") I estimate the effect of different measures, of the season, and possibly of different virus strains, in terms of changes of R_0.

Using the interactive online tool `traffic-simulation.de`, I present projections for several timelines of social behaviour, vaccination process, and interactions with neighboring countries. As of Jan 28, the projection of the weekly incidence for the time of the Spring Meeting is, ceteris paribus, about 30 confirmed cases/week/100000 persons.

SOE 1.4 Mon 10:20 SOEa

Analyzing protests against COVID-19 mitigation strategies on the German internet — •Andrzej Jarynowski[1], Alexander Semenov[2], and Vitaly Belik[3] — [1]Interdisciplinary Research Institute, Wroclaw, Poland — [2]Herbert Wertheim College of Engineering, University of Florida, Gainesville, USA — [3]System Modeling Group, Institute of Veterinary Epidemiology and Biostatistics, Freie Universität Berlin, Berlin, Germany

In this study we quantitatively assess perception of protests agains COVID-19 mitigation strategies in Germany from the late July till the end of August 2020 in the Internet media. To this end we investigate Google searches, Twitter and Telegram posts, as well as selection of news articles collected via EventRegistry. We focus on demonstrations on August 1st and August 29th, 2020 in Berlin [1]. Although the dominant actors of the protest are on the far-right political spectrum, based on network analysis, we demonstrate that left-wing activists could both sympathize with and oppose the protest. We observe a constant interest in the protest movements in traditional media, in contrast, their popularity on social media was growing. The revealed insights shed light on social dynamics in the context of such major disruptive events as COVID-19 pandemic and could serve as a basis for optimization of risk awareness campaigns by the government.

[1] Jarynowski A., Semenov A., Belik V. (2020) In: Chellappan S., Choo KK.R., Phan N. (eds) Computational Data and Social Networks. CSoNet 2020. Springer Lecture Notes in Computer Science, vol 12575, 524 (2021) https://doi.org/10.1007/978-3-030-66046-8_43

20 min. break

Invited Talk SOE 1.5 Mon 11:00 SOEa

data-driven modeling of COVID-19 pandemic — •Yamir Moreno — Institute BIFI, University of Zaragoza, Zaragoza 50018

The new Coronavirus disease 2019 (COVID-19) has forced an unprecedented response from health authorities worldwide and the World Health Organization. Despite the adoption of drastic measures, the pandemic is still ongoing worldwide, and surges of infections are being observed in more than 188 countries. Even with vaccination campaigns starting to roll out, specific pharmaceutical interventions need to be adopted nowadays to reduce the pressure over health-care systems. Here we show results that correspond to different stages of the pandemic using data-driven modeling. Specifically, we present simulations using data-driven models tailored to mobility data from China, Spain, and the U.S. The models are used to estimate the effectiveness of customary public interventions on the spread of COVID-19 in these locations as well as to calculate heard immunity thresholds of realistic populations and vaccine coverage needed to protect them. Our main findings highlight that having a coordinated response system could be key for the containment of the spread of COVID19 and its possible eradication at the lowest possible cost.

SOE 1.6 Mon 11:40 SOEa

How to estimate the macroscopic epidemic dynamics with a random testing strategy — Yasaman Asgari[1], Sepideh Abdollahi[2], Aryana Haghjoo[2], Farnoush Farahpour[3], and •Fakhteh Ghanbarnejad[1,4] — [1]Department of Mathematics, Sharif University of Technology, Tehran, Iran — [2]Department of Physics, Sharif University of Technology, Tehran, Iran — [3]Bioinformatics and Computational Biophysics, University of Duisburg-Essen, Germany — [4]Institute for Theoretical Physics, Technical University of Dresden, Dresden, Germany

The world has suffered from epidemics and pandemics especially the most recent one: COVID-19 in many ways. Having a more precise estimation of how an epidemic evolves, can help us to make better interventions policies. Molecular and Antibody tests, not only can help the physicians for a more accurate individual diagnosis (microscopic level) but also can help to have a macroscopic picture of the spreading dynamics. However, due to some limitations, different testing strategies have to be made. In this work, we want to show how to estimate the real epidemic dynamics with random sampling at a macroscopic level. So we developed a mathematical model based on SIR dynamics and introduced a quantitative method on how to extract information from the empirical data, i.e. daily test results. Moreover, we show the impact of daily test capacity on the estimation. Finally, we studied two empirical data, namely the daily positive PCR cases at Paris and Massachusetts, and compared our estimations with their COVID-19 wastewater analysis. Our estimations present reliable error bars.

SOE 1.7 Mon 12:00 SOEa

Discontinuous epidemic transition due to limited testing — Davide Scarselli[1], •Nazmi Burak Budanur[1], Marc Timme[2], and Björn Hof[1] — [1]Institute of Science and Technology Austria, Klosterneuburg, Austria — [2]Chair for Network Dynamics, Center for Advancing Electronics Dresden (cfaed), Institute for Theoretical Physics and Center of Excellence Physics of Life, Technical University of Dresden, Dresden, Germany

High impact epidemics constitute one of the largest threats humanity is facing in the 21st century. In the absence of pharmaceutical interventions, physical distancing together with testing, contact tracing and quarantining constitute crucial measures in slowing down epidemic dynamics. Yet, here we show that if testing capacities are limited, containment may fail dramatically because such combined countermeasures drastically change the rules of the epidemic transition: Instead of continuous, the response to countermeasures becomes discontinuous [1]. Rather than following the conventional exponential growth, the outbreak that is initially strongly suppressed eventually accelerates and scales faster than exponential during an explosive growth period. As a consequence, containment measures either suffice to stop the outbreak at low total case numbers or fail catastrophically if marginally too weak, thus implying large uncertainties in reliably estimating overall epidemic dynamics, both during initial phases and during second wave scenarios. [1] D. Scarselli, N. B. Budanur, M. Timme, B. Hof. Discontinuous epidemic transition due to limited testing. Under review (2021).

SOE 1.8 Mon 12:20 SOEa

A control theory approach to optimal pandemic mitigation — Prakhar Godara[1], Stephan Herminghaus[1,2], and •Knut Heidemann[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany

The recent outbreak of the illness COVID-19, has resulted in a pandemic with unprecedented impact on societies all over the globe. A major focus of governments is on designing containment strategies which are as mild as possible, but substantial enough to limit the severity of the outbreak in order not to overwhelm the health service system (HSS). In the framework of homogeneous susceptible-infected-recovered (SIR) models, we use a control theory approach to identify optimal pandemic mitigation strategies [1]. We derive rather general conditions for reaching herd immunity while minimizing the costs incurred by the introduction of societal control measures (such as closing schools, social distancing, lockdowns, etc.), under the constraint that the infected fraction of the population does never exceed a certain maximum corresponding to public health system capacity. Optimality is derived and verified by variational and numerical methods for a number of model cost functions. The effects of immune response decay after recovery are taken into account and discussed in terms of the feasibility of strategies based on herd immunity.

[1] Prakhar Godara, Stephan Herminghaus and Knut M. Heidemann. "A control theory approach to optimal pandemic mitigation." arXiv preprint arXiv:2009.02513 (2020).

SOE 1.9 Mon 12:40 SOEa

Statistsiche Untersuchungen der Covid-Inzidenzzahlen des RKI — •Rainer Gottwald[1], Stefan Scheingraber[2] und Uli Spreitzer[3] — [1]Dr. Rainer Gottwald, 86899 Landsberg am Lech — [2]PD. Dr. Stefan Scheingraber, 93413 Cham — [3]Löw & Spreitzer GmbH, 92277 Hohenburg

Inzidenzzahlen für Corona-positive des RKI sind umstritten wegen der Änderungen der Teststrategie, methodische Grenzen des PCR-Testverfahrens, Meldedatenverzug u.a. Die Daten des RKI zur Inzidenz der "Coronafälle" für 2020 wurden mit mathematischen Verfahren untersucht. Zeitreihenanalyse ergaben abweichende Werte für wichtige Punkte wie Trendumkehr. Der Einfluß des weißen Rauschen wurde aufgezeigt. Korrelationsrechnungen zeigten den Einfluß geänderter Testbedingungen auf die Werte. Medizinische Analysen der Inzidenzahlen ergänzen und plausibilisieren die statistischen Erkenntnisse.

SOE 2: Networks and Social Dynamics

Time: Monday 14:00–16:00 Location: SOEa

SOE 2.1 Mon 14:00 SOEa

Degree irregularity and rank probability bias in network-meta analysis — •Annabel L Davies[1] and Tobias Galla[1,2] — [1]The University of Manchester, Manchester, United Kingdom — [2]Instituto de Fisica Interdisciplinar y Sistemas Complejos, IFISC (CSIC-UIB), Palma de Mallorca, Spain

Network meta-analysis (NMA) is a statistical technique for the comparison of treatment options. The nodes of the network graph are the competing treatments and the edges represent comparisons made between the treatments in the trials. Outcomes of Bayesian NMA include estimates of treatment effects, and the probabilities that each treatment is ranked best, second best and so on. How exactly network topology affects the accuracy and precision of these outcomes is not fully understood. We conduct a simulation study and find that disparity in the number of trials involving different treatments leads to a systematic bias in estimated rank probabilities. This bias is associated with an increased variation in the precision of treatment effect estimates. Using ideas from network theory, we define a measure of 'degree irregularity' to quantify asymmetry in the number of studies involving each treatment. Our simulations indicate that more regular networks have more precise treatment effect estimates and smaller bias of rank probabilities. We also find that degree regularity is a better indicator for the accuracy and precision of parameter estimates in NMA than both the total number of studies in a network and the disparity in the number of trials per comparison. Reference: A. L. Davies, T. Galla, Research Synthesis Methods 2020, 1-17, https://doi.org/10.1002/jrsm.1454

SOE 2.2 Mon 14:20 SOEa

Revealing network size from the dynamics of a single node? — •Georg Börner, Hauke Haehne, Jose Casadiego, and Marc Timme — Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden

Networks are ubiquitous in the natural and human-made world and their dynamics fundamentally underlie the function of a variety of systems, from gene regulation in the cell and the activity of neuronal circuits to the distribution of electric power and the transport of people and goods.

Recent work [1] introduced a method to infer the size of a network, its number of dynamical variables, from measuring times series of a fraction of the its units only. Here we demonstrate that size inference is possible even from the observed time series of a single unit. We state mathematical conditions required for such inference in principle and show that, in practice, the success depends strongly on numerical constraints as well as on experimental decisions. We illustrate successful size inference for systems of $N = 20$ variables and point to ways for improving the reliability and power of the reconstruction. We briefly comment on how the success of the approach depends on the quality and quantity of collected data and formulate some general rules of thumb on how to approach the measurement of a given system.

[1] H. Haehne et al., Detecting Hidden Units and Network Size from Perceptible Dynamics Phys. Rev. Lett. 122:158301 (2019).

SOE 2.3 Mon 14:40 SOEa

Blind identification of stochastic block models from dynamical observations — •Michael Schaub — RWTH Aachen University, Aachen, Germany

In many applications we are confronted with the following system identification problem: we observe a dynamical process that describes the state of a system at particular times. Based on these observations we want to infer the (dynamical) interactions between the entities we observe. In the context of a distributed system, this typically corresponds to a "network identification" task: find the edges of the graph of interconnections.

However, often the number of samples we can obtain from such a process are far too few to identify the edges of the network exactly. Can we still reliably infer some aspects of the underlying system?

Motivated by this question we consider the following identification problem: instead of trying to infer the exact network, we aim to recover a (low-dimensional) statistical model of the network based on the observed signals on the nodes. More concretely, here we focus on observations that consist of snapshots of a diffusive process that evolves over the unknown network. We model the (unobserved) network as generated from an independent draw from a latent stochastic blockmodel (SBM), and our goal is to infer both the partition of the nodes into blocks, as well as the parameters of this SBM. We present simple spectral algorithms that provably solve the partition and parameter inference problems with high-accuracy. We further discuss some possible variations and extensions of this problem setup.

SOE 2.4 Mon 15:00 SOEa

Detection and Analysis of Fake News on Twitter — Zahra Ghadiri, Sima Hashemi, Milad Ranjbar, •Fakhteh Ghanbarnejad, and Sadegh Raeisi — Sharif University of Technology, Tehran, Iran

Fake news on social media has become a major problem that impacts many aspects of our lives. In this work, we try to combine ideas from complex systems and networks with techniques from natural language processing (NLP) to develop intelligent agents that can distinguish real and fake news. Our approach is based on the intuition that one of the more effective ways to detect fake news is to cross-check with reliable sources such as well-established news agencies. To this end, first we collect tweets from the Twitter accounts of official news agencies

which are posted around the posting time of the target tweets. We use clustering algorithms to cluster tweets based on the topic and content. Next we identify the cluster that best matches the target tweet. Then we extract features from our tweets and train a classifier that based on the comparison with the corresponding cluster would identify fake tweets. This provides a NLP tool that enables us to check a posted tweet with news from news agencies or any other reliable source of information based on the content. We also build and investigate the evolution/dynamic trees of retweets. We analyze the topological features of the trees as well as the dynamical properties. We should note that there are challenges associated with the reconstruction of the network and dynamics of a tweet on Twitter that could potentially influence our results and conclusion.

SOE 2.5 Mon 15:20 SOEa

A physics of governance networks: critical transitions in contagion dynamics on multilayer adaptive networks with application to the sustainable use of renewable resources — •Jonathan Donges[1,2], Fabian Geier[1], Wolfram Barfuss[1,3], and Marc Wiedermann[1] — [1]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]Stockholm Resilience Centre, Stockholm University, Stockholm, Sweden — [3]School of Mathematics, University of Leeds, Leeds, United Kingdom

Adaptive network models are promising tools to analyze complex interactions in coupled human-economy-nature systems in the context of climate change mitigation and sustainability transformations. Here, we focus on a three-layer adaptive network model, where a polycentric governance network interacts with a social network of resource users which in turn interacts with an ecological network of renewable resources. We uncover that sustainability is favored for slow interaction timescales, large homophilic network adaptation rate (as long it is below the fragmentation threshold) and high taxation rates. We also observe a trade-off between an eco-dictatorship and the polycentric governance network of multiple actors. In the latter setup, sustainability is enhanced for low but hindered for high tax rates compared to the eco-dictatorship case. These results highlight mechanisms generating emergent critical transitions in contagion dynamics on multilayer adaptive networks and show how these can be understood and approximated analytically, relevant for understanding complex adaptive systems from various disciplines ranging from physics to epidemiology.

SOE 2.6 Mon 15:40 SOEa

Public goods games on networks: endogeneous reference groups — •Adrian Fessel[1], Martin Kocher[2], and Hans-Günther Döbereiner[1] — [1]Institute for Biophysics, University of Bremen, Bremen, Germany — [2]Department of Economics, University of Vienna, Vienna, Austria

Public goods games are a paradigm for understanding cooperative behavior within some reference group, whereas the field of complex networks provides powerful frameworks for modeling the dynamics and structure of interactions between individual agents. Combining these approaches, we study the formation and evolution of endogeneous reference groups in a network model. Between iterations of public goods games played within each connected component, the model evolves by edge addition or removal based on expected utility. In simulations, we observe fragmented or percolated states depending on the set of parameters, as well as dynamical solutions characterized by oscillations of the network structure.

SOE 3: Poster

Time: Monday 17:30–19:30 Location: SOEp

SOE 3.1 Mon 17:30 SOEp

Effective curvature of street networks — •David Bantje, Stephan Herminghaus, and Knut M. Heidemann — Max-Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

Demand responsive ride pooling (DRRP) could contribute significantly to the transition towards sustainable mobility. In mean-field theories of DRRP [1], such systems are currently modelled in the Euclidean plane. We investigate if by assigning an effective Gaussian curvature, the metric properties of the street network can be incorporated into the existing theoretical framework. This poster illustrates the calculation scheme of effective curvature and presents results for model and real street networks.

[1] S. Herminghaus (2019). Mean field theory of demand responsive ride pooling systems. Transportation Research Part A: Policy and Practice, 119. https://doi.org/10.1016/j.tra.2018.10.028

SOE 3.2 Mon 17:30 SOEp

Persistence length of ride-sharing bus trajectories — •Steffen Mühle and Helge Heuer — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

On-demand ride-sharing services have the potential to drastically decrease urban traffic, mobility costs, carbon emissions and the need for owning a private car. While the benefits of a well-coordinated bus fleet capable of serving live incoming transport requests are compelling, predicting the spatio-temporal dynamics even of single buses is far from trivial. Typically, a bus' trajectory does not originate in isolation but emerges from its interplay with incoming requests, the street network, other buses and fleet-wide policies.

Given the latter, namely the maximally allowed detour an accepted request may entail, $\delta_{\max}$, we treat bus trajectories as random walks and inspect them from the perspective of polymer theory. To this end, we generate random walks purely geometrically, and also run full-scale ride-sharing simulations using MatSim. In both cases, we observe that for long times a bus' trajectory becomes diffusive, which allows us to assign a persistence length to them.

This creates a quantitative link between the (tunable) parameter $\delta_{\max}$ and the (observed) typical length scale on which a bus changes its direction, enabling us to predict e.g. how much time a bus spends in a certain district or how far it travels over the course of one day.

SOE 3.3 Mon 17:30 SOEp

Evaluation of demand responsive ride pooling on real life taxi data — •Michael Sternbach[1,2,3], Felix Jung[1], Puneet Sharma[1,2], Stepahn Herminghaus[1,2], and Knut Heidemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institut for Dynamics and Complex Systems, University of Göttingen, Germany — [3]Campus Institute for Dynamics of Biological Networks, Göttingen, Germany

Climate change caused by human greenhouse gas (GHG) emissions is one of the vital challenges of humankind. Passenger cars contribute significantly to human GHG emissions. To reduce this effect, more eco-friendly transport modes are needed. Demand responsive ride pooling (DRRP) offers door-to-door service similar to taxi or personal car while pooling customers with similar routes on the same vehicle, thereby reducing emissions and the number of cars needed. In this study, we measure the performance of a DRRP system on real life taxi request data and evaluate under which conditions e. g. request rate, number of vehicles, allowed detour or waiting time DRRP can operate more efficiently than taxi service at a reasonable service quality. We compare our results to a mean field description of DRRP [1] to analyze the effect of road network structure and spatial request distribution. Our results provide significant insight on the prerequisites for ecological and economic feasibility of DRRP.

[1] Herminghaus, S. (2019). Mean field theory of demand responsive ride pooling systems. Transportation Research Part A: Policy and Practice, 119, 15-28.

SOE 3.4 Mon 17:30 SOEp

Bi-modal demand responsive ride pooling — •Puneet Sharma, Helge Heuer, Stephan Herminghaus, and Knut Heidemann — Max Planck Institute for Dynamics and Self-Organization, Goettingen

Commuting is an indispensable part of modern human lives. While modern cities offer various modes of transportation, considered separately, none of them is both efficient, i.e., sustainable, and convenient. A taxi service is convenient, in a sense, due to door-to-door service, but is inefficient since it usually serves one customer only. Demand responsive ride pooling (DRRP) with minibuses is more efficient, but leads to undue competition with line services (LS), which provide even better pooling (average number of passengers per vehicle) but are less convenient due to fixed routes and stops. A combination of both modes, DRRP and LS, may provide an ideal solution but is challenging to organize. Here we derive conditions for efficient and convenient transportation for a bi-modal service based on a simple square-grid geometry. We relate the optimal mesh size, i.e., distance between stations, to external parameters like passenger density and traveling behavior. We also compare the carbon footprint of the bi-modal service with private cars so as to measure it*s efficiency.

SOE 3.5 Mon 17:30 SOEp

Numerical study of phase transition in the bipartite z-matching — •Till Kahlke[1], Martin Fränzle[2], and Alexander K. Hartmann[1] — [1]Institut of Physics, University of Oldenburg, Germany — [2]Institut of Computer Science, University of Oldenburg, Germany

We study numerically [1] the many-to-one bipartite *z-matching*, a generalisation of the matching problem. It can be used, e.g., to model a wireless communication network of users and servers, where z denotes the maximum number of users a server can treat at one time. Within a bipartite graph representation, there are links from each user to all servers which are feasible, e.g., close enough. The maximum matching capacity of this graph is the largest total number of users all servers can serve. After mapping to standard maximum matching, we use a nu-

merically *exact algorithm* (Edmonds blossom shrinking) to solve the z-matching problem. First, we compare it with previous analytic results [2]. Next, we look at the saturation probability as order parameter and *observe phase transitions* when varying the average number of neighbors. We describe these transitions by their critical points and an universal critical exponent. When comparing the matchings of the exact algorithm with a commonly used matching *heuristic*, we observe that the heuristic starts to differ from the optimal solution right at the critical point.

[1] A.K. Hartmann, *Big Practical Guide to Computer Simulations* (World Scientific, 2015).
[2] E. Kreačić and G. Bianconi, Europhys. Lett. **126**, 28001 (2019).

SOE 3.6 Mon 17:30 SOEp

Burstiness and accuracy of collective decision-making — •Mariko Ito — Rikkyo University, Tokyo, Japan

In the decision-making of an individual, others' opinions can significantly affect when and what he/she states. Kurvers et al. [1] empirically showed that informative individuals tend to answer earlier than the others when each individual in a group is allowed to answer any time for a binary choice problem. They also exhibited that the group performance is high in the collective decision-making with such self-organised orders compared to that in the case where individuals make decisions independently. Here my interest is whether the distribution of the interval between statements has any information about the quality of their collective decision-making as well as the order of the statements.

I analysed the data in Kurvers et al. and derived the burstiness parameter B, the strength of burstiness [2]. Burst is the phenomenon where events, i.e., statements in our case, frequently occur in short periods while that rarely occur in long periods. I found that the greater is B, the higher is the group performance. The value of B was positively correlated with the group performance even when individuals made decisions independently. These results suggest that individuals with stronger confidence can cause a more bursty sequence of their statements.

[1] Kurvers et al., R. Soc. Open Sci., 2015. [2] Goh and Barabási, EPL, 2008.

SOE 3.7 Mon 17:30 SOEp

Cascade dynamics in Reddit communities — •Joao Pinheiro Neto and Knut Heidemann — Max Planck Institute for Dynamics and Self-Organization

Social media has a large role in modern society, making studying its dynamics fundamental to understand social and political events. Reddit is one of the biggest social media platforms in the world, and individual subcommunities (called "subreddits") have been involved in some of the biggest events in recent times. Discussions in Reddit happen in threads that follow a tree structure, with each comment spawning a new branch. This has been modeled with directed percolation-like models such as the Hawkes process, and it has been shown that the probability distributions of both thread size and total score follow power-laws [1,2]. Here we explore how these distributions and other observables vary across different subreddits. In particular, we show that i) subreddits can display both power-laws and non-power-law distributions, and ii) that the measured power-law exponents can vary considerably. We relate that to subreddit features such as the type of content and size of the userbase.

References

1. Medvedev, A. N., Delvenne, J. C., Lambiotte, R., & Cherifi, H. (2018). Journal of Complex Networks, 7(1), 67-82

2. Medvedev, A. N., Lambiotte, R., & Delvenne, J.-C. (2019) In Springer Proceedings in Complexity (pp. 183-204).

SOE 3.8 Mon 17:30 SOEp

Dirac Algebra Generalized Matrix Inverses — •Martin Erik Horn — IUBH - Internationale Hochschule, Campus Berlin

More and more introductory business mathematics textbooks present generalized matrix inverses as elementary part of the foundations of mathematical economics. Therefore Moore-Penrose generalized matrix inverses as the scalar part of Pauli Algebra generalized matrix inverses had been discussed at the DPG spring meeting 2018 of the Physics of Socio-economic Systems Division in Berlin in a geometric way.

As this geometry is based on the Euclidean structure of space, it is quite reasonable to ask, what happens if generalized matrix inverses are constructed in pseudo-Euclidean, hyperbolic spacetimes. This will be discussed in this poster presentation: Spacetime generalized matrix inverses are constructed as the scalar part of Dirac Algebra generalized matrix inverses. And again the algebraic reasoning of textbooks will be completed by analyzing the geometry it is based on.

SOE 4: Data Analytics for Complex Dynamical Systems (joint SOE/DY Focus Session) (joint session SOE/DY)

Time: Tuesday 11:00–12:40 Location: SOEa

SOE 4.1 Tue 11:00 SOEa

Network inference from event sequences: Disentangling synchrony from serial dependency — •Reik Donner[1,2], Adrian Odenweller[2], Frederik Wolf[2], and Forough Hassanibesheli[2] — [1]Magdeburg-Stendal University of Applied Sciences, Magdeburg, Germany — [2]Potsdam Institute for Climate Impact Research (PIK) - Member of the Leibniz Association, Potsdam, Germany

Inferring coupling among interacting units or quantifying their synchronization based on the timing of discrete events has vast applications in neuroscience, climate, or economics. Here, we focus on two prominent concepts that have been widely used in the past: event synchronization (ES) and event coincidence analysis (ECA). Numerical performance studies for two different types of spreading processes on paradigmatic network architectures reveal that both methods are generally suitable for correctly identifying the unknown links. By further applying both concepts to spatiotemporal climate datasets, we demonstrate that unlike ECA, ES systematically underestimates linkages in the presence of temporal event clustering, which needs to be accounted for in network reconstruction from data. In turn, for spike train data from multi-channel EEG recordings (with relatively narrow inter-event time distributions), the obtained results are practically indistinguishable. Our findings allow deriving practical recommendations for suitable data preprocessing in the context of network inference and synchronization assessment from event data.

SOE 4.2 Tue 11:20 SOEa

Identification of Stochastic Differential Equations from Data — •Tobias Wand[1] and Oliver Kamps[2] — [1]Westfälische Wilhelms-Universität Münster — [2]Center for Nonlinear Science Münster

In recent years, methods to identify dynamical systems from experimental or numerical data have been developed [1, 2]. In this context, the construction of sparse models of dynamical systems has been in the focus of interest and has been applied to different problems. These data analysis methods work with hyper-parameters that have to be adjusted to improve the results of the identification procedure. Non-deterministic systems require a refined identification algorithm. In this talk, we will introduce an approach to optimally select hyper-parameters for the identification of sparse differential equations from non-deterministic data.

[1] Brunton et al. Proceedings of the National Academy of Sciences, 2016, 113, 3932-3937
[2] Mangan et al. Proceedings of the Royal Society A, 2017, 473, 20170009

SOE 4.3 Tue 11:40 SOEa

Data-driven analysis of the power grid frequency — •Benjamin Schäfer[1], Christian Beck[1], Leonardo Rydin Gorjão[2,3], Johannes Kruse[2,3], and Dirk Witthaut[2,3] — [1]School of Mathematical Sciences, Queen Mary University of London, London E1 4NS, United Kingdom — [2]Forschungszentrum Jülich, Institute for Energy and Climate Research-Systems Analysis and Technology Evaluation (IEK-STE), Jülich, Germany — [3]Institute for Theoretical Physics, University of Cologne, Köln, Germany

The Paris conference 2015 set a path to limit climate change to "well below 2°C". To reach this goal greenhouse gas emissions have to be reduced and renewable generators, electrical mobility or smart grids are integrated into the existing power system.

The introduction of these new technologies raises several questions about control, stability and operation and therefore requires a solid understanding of existing and future systems and new conceptional approaches.

Here, we use data-driven approaches to work towards a quantitative understanding of the power grid with a particular focus on the power grid frequency. We analyse time series from various synchronous areas such as Continental Europe, Great Britain but also two US areas and several European islands.

We highlight significant deviations from Gaussianity in several regions, scaling laws and spatio-temporal dynamics. Finally, we discuss how past information may be used to forecast the frequency.

SOE 4.4 Tue 12:00 SOEa

Tipping and transition paths in high-dimensional agent-based models — •Luzie Helfmann[1,2,3], Peter Koltai[1], Jobst Heitzig[3], and Christof Schütte[2,1] — [1]Freie Universität Berlin — [2]Zuse Institute Berlin — [3]Potsdam Institute for Climate Impact Research

Agent-based models are a popular choice for modeling complex social systems. Here, we are concerned with studying noise-induced tipping between relevant subsets of the agent state space, e.g., in order to understand drastic opinion

changes in a population of agents. Due to the large number of interacting individuals, agent-based models are usually very high-dimensional. We therefore apply Diffusion Maps, a non-linear dimension reduction, to reveal the intrinsic low-dimensional structure of the model dynamics. We will characterize the tipping behavior by means of Transition Path Theory, a theory for gaining statistical understanding of the tipping paths (e.g., their density, flux, rate). We will illustrate our approach on two examples, both exhibiting a multitude of tipping pathways.

SOE 4.5 Tue 12:20 SOEa

Quasi-stationary states in temporal correlations for traffic systems: Cologne orbital motorway as an example — •Shanshan Wang, Sebastian Gartzke, Michael Schreckenberg, and Thomas Guhr — Fakultät für Physik, Universität Duisburg–Essen, Lotharstraße 1, 47048 Duisburg, Germany

Traffic systems are complex systems that exhibit non-stationary characteristics. Therefore, the identification of temporary traffic states is significant. In contrast to the usual correlations of time series, here we study those of position series, revealing structures in time, i.e. the rich non-Markovian features of traffic. Considering the traffic system of the Cologne orbital motorway as a whole, we identify five quasi-stationary states by clustering reduced-rank correlation matrices of flows using the k-means method. The five quasi-stationary states with non-trivial features include one holiday state, three workday states and one mixed state of holidays and workdays. In particular, the workday states and the mixed state exhibit strongly correlated time groups shown as diagonal blocks in the correlation matrices. We map the five states onto reduced-rank correlation matrices of velocities and onto traffic states where free or congested states are revealed in both space and time. Our study opens a new perspective for studying traffic systems. This contribution is meant to provide a proof of concept and a basis for further study.

SOE 5: Financial and Economic Systems and Evolutionary Game Theory

Time: Tuesday 14:00–15:00 Location: SOEa

SOE 5.1 Tue 14:00 SOEa

Uncovering the Dynamics of Correlation Structures Relative to the Collective Market Motion — •Anton J. Heckens, Sebastian M. Krause, and Thomas Guhr — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Complex systems are characterized by a variety of interactions and often produce a strong correlated behavior of their system components. Stock markets are particularly well-suited as examples of such complex systems due to their abundance of data for the analysis of correlated phenomena. Münnix et al. [1] used correlation matrices over short time horizons, in order to analyze their dynamics with respect to their non-stationarity. Using a cluster procedure, it became apparent that there are quasi-stationary periods, so-called market states. They emerge, disappear or reemerge, but they are dominated by the collective motion of all stocks. To extract more refined information, we present a new approach by clustering correlation matrices which are free from the collective market motion [2]. The resulting dynamics is remarkably different, and the corresponding market states are quasi-stationary over a long period of time.

[1] M. C. Münnix, T. Shimada, R. Schäfer, F. Leyvraz, T. H. Seligman, T. Guhr and H. E. Stanley, Identifying States of a Financial Market, Scientific Reports 2, 644 (2012), arXiv:1202.1623

[2] A. J. Heckens, S. M. Krause, T. Guhr, Uncovering the Dynamics of Correlation Structures Relative to the Collective Market Motion J. Stat. Mech. 2020, 103402 (2020), arXiv:2004.12336

SOE 5.2 Tue 14:20 SOEa

Explosive amortization times in the dynamics of photovoltaic implementation? — •Raoul Schmidt, Malte Schröder, and Marc Timme — Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden

To combat climate change, renewable energy supply such as through photovoltaics (PV) becomes increasingly important. The amortization time of a single PV unit relates the energy (and CO2) expended for production, transport and installation of a unit to its electric power generation (and thus potential savings in CO2 emissions). Here, we analyze the CO2 budgeting dynamics of many PV units continuously added by new installations [1,2]. Intriguingly, the resulting systemic amortization time necessarily is substantially larger than that of a single unit. We demonstrate analytically that already at constant installation rate, it already is twice the amortization time of a single unit, whereas at an exponentially increasing rate, it may be arbitrarily much larger, with resulting relevant time scales in between 10 and more than 30 years - potentially beyond the life time of a PV unit. Intriguingly, evaluating installation data of the past two decades indicates an exponential installation rate on the global scale that may cause such explosive increase of CO2 budget amortization times.

[1] N. von der Heydt, DPG Spring Meeting Berlin (2018). [2] R. Schmidt et al., in prep. (2021).

SOE 5.3 Tue 14:40 SOEa

Should the government reward cooperation? Insights from an agent-based model of wealth redistribution — Frank Schweitzer, Luca Verginer, and •Giacomo Vaccario — ETH, Zurich, Switzerlan

In our multi-agent model agents generate wealth from repeated interactions for which a prisoner's dilemma payoff matrix is assumed. Their gains are taxed by a government at a rate α. The resulting budget is spent to cover administrative costs and to pay a bonus to cooperative agents, which can be identified correctly only with a probability p. Agents decide at each time step to choose either cooperation or defection based on different information. In the local scenario, they compare their potential gains from both strategies. In the global scenario, they compare the gains of the cooperative and defective sub-populations. We derive analytical expressions for the critical bonus needed to make cooperation as attractive as defection. We show that for the local scenario the government can establish only a medium level of cooperation, because the critical bonus increases with the level of cooperation. In the global scenario instead full cooperation can be achieved once the cold-start problem is solved, because the critical bonus decreases with the level of cooperation. This allows to lower the tax rate, while maintaining high cooperation.

SOE 6: Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)

Time: Tuesday 17:45–18:30 Location: BPb

Details will be published in a programme update.

SOE 7: Member's Assembly of SOE

Time: Tuesday 19:00–19:40 Location: SOEa

Online Member's Assembly. The ordinary Annual Member's Assembly will be held in September.

SOE 8: Partial Synchronization in Networks (Focus Session joint with DY and BP) (joint session SOE/DY)

Time: Wednesday 9:00–10:00 Location: SOEa

SOE 8.1 Wed 9:00 SOEa

Partial synchronization as a model for uni-hemispheric sleep — •Jakub Sawicki[1], Lukas Ramlow[1,2], and Eckehard Schöll[1,3] — [1]Institute of Theoretical Physics, Technische Universität Berlin, Germany — [2]Humboldt University of Berlin, Berlin, Germany — [3]Potsdam Institute for Climate Impact Research, Potsdam, Germany

Uni-hemispheric slow-wave sleep is a dynamical state of the brain where one hemisphere is asleep while the other remains awake. This state can also be characterized by simultaneous but spatially separated occurrence of high and low degree of synchronization in the sleeping and the awake hemisphere, respectively. Therefore, this real world phenomenon can be described in terms of partial synchronization characterizing patterns of coexistence of synchronized and desynchronized parts of a network. Here we investigate the occurrence of partial synchronization patterns in empirical structural connectivities of the human brain. The connectivities consist of ninety regions of interest using the Automated Anatomical Labeling (AAL) Atlas, and were derived by magnetic resonance imaging (MRI) based probabilistic diffusion tractography. The local dynamics is modeled by FitzHugh-Nagumo oscillators. We demonstrate under which conditions partial synchronization patterns with respect to the brain hemispheres can be found.

SOE 8.2 Wed 9:20 SOEa

Effect of Topology upon Relay Synchronization in Triplex Neuronal Networks — •Fenja Drauschke, Iryna Omelchenko, Rico Berner, Jakub Sawicki, and Eckehard Schöll — Institute of Theoretical Physics, Technische Universität Berlin

Complex networks consisting of several interacting layers allow for remote synchronization of distant layers via an intermediate relay layer. We investigate relay synchronization in a three-layer neuronal network and study the effect of the topology of the layers upon the synchronization scenarios. Introducing random topologies either in the outer layers or in the middle (relay) layer leads to an increase of the range of inter-layer coupling strength for which the relay-synchronized state is preserved, compared with regular nonlocal coupling topologies.

SOE 8.3 Wed 9:40 SOEa

Complexified Kuramoto model – synchrony in the weak coupling regime — •Moritz Thümler, Sheshagobal Srinivas, Malte Schroeder, and Marc Timme — TU Dresden, Dresden, Germany

Networks of Kuramoto oscillators constitute paradigmatic models for the emergence of temporal patterns – foremost synchrony – across oscillatory systems. Here we extend the Kuramoto model to complex dynamical variables. We uncover a transition from traditional synchrony emerging for sufficiently large coupling strengths to a second type of synchrony that exists in the weak coupling regime, i.e. below the coupling required for the real-variable model to synchronize. The new type of synchrony state is known from systems that are not dissipative but conservative, compare [1,2] for relations of the two system types. We introduce a novel, two dimensional order parameter for networks of N oscillators that enables us to consistently quantify synchrony.

[1] D. Witthaut and M Timme, Phys. Rev. E 90:032917 (2014)
[2] D. Witthaut et al., Nature Comm. 8:14829 (2017)

SOE 9: Opinion Formation

Time: Wednesday 11:00–12:20 Location: SOEa

SOE 9.1 Wed 11:00 SOEa

Social nucleation: From physics to group formation and opinion polarization — •Georges Andres and Frank Schweitzer — Chair of Systems Design, ETH Zurich, Weinbergstrasse 58, 8092 Zurich, Switzerland

Individuals form groups, which subsequently develop larger domains via competition and coalescence. How much have these social processes in common with established mechanisms of phase transitions in physics? Are nucleation in metastable systems or spinodal decomposition of thermodynamic phases or percolation in porous media suitable paradigms for modeling the emergence of large social groups? We answer this challenging question by providing an agent-based model that combines group formation and opinion dynamics in a novel manner. Opinion formation is a fast process and determines the formation of groups. On a slower time scale, groups can form larger clusters of various numbers, density and stability. These clusters can merge, split or rearrange, to develop either compact phases, networks of high modularity, or quasistable cluster distributions. Dependent on the choice of parameters for opinion dynamics and social influence, our model can reproduce social phenomena such as consensus, weak or strong polarization, social networks of various densities or stable minorities.

SOE 9.2 Wed 11:20 SOEa

Ideological differences in engagement in public debate on Twitter — •Felix Gaisbauer, Armin Pournaki, Sven Banisch, and Eckehard Olbrich — Max Planck Institute for Mathematics in the Sciences, Inselstrasse 22, 04103 Leipzig

We analyse public debate on Twitter via network representations of retweets and replies. We show that through the interplay of the two networks, it is possible to identify ideological differences in activity patterns between different opinion groups on the platform. The method is employed to observe public debate about two events: The Saxon state elections and violent riots in the city of Leipzig in 2019. We show that in both cases, (i) opinion groups differ in their propensities to get involved in debate, and therefore have unequal impact on public opinion. Users retweeting far-right parties and politicians are significantly more active, hence their positions are disproportionately visible. (ii) Said users act significantly more confrontational, as becomes visible in the local assortativity distribution of the reply network, while other opinion groups tend to debate largely amongst themselves.

SOE 9.3 Wed 11:40 SOEa

Modeling Opinion Formations in Europe: A new Perspective — •Martin Gestefeld, Jan Lorenz, Nils Henschel, and Klaus Boehnke — Jacobs University Bremen, Bremen, Deutschland

In recent years, politics and especially election results appear to be more polarized than in the years before. Empirical evidence for opinion polarization has been found regarding specific topics but there is still a lack of evidence for a general trend in society. The presented work compares the characteristics of various polarization measurements and determines similarities between them in empirical data. In an exploratory data analysis of the European Social Survey, individual responses are analyzed on the left-right political self-placements and similar attitudes. By applying a new model, we demonstrate that people who placed their opinions on a 0 to 10 scale can be split up into five distinct groups. In addition to this model, we are able to decompose a formal measurement and provide detailed information on the degree of polarization in each of our distinct groups. Over the complete data set, cross-topic, cross-country, and time-trends are analyzed and compared to establish an overview and new perspective on polarization in Europe.

SOE 9.4 Wed 12:00 SOEa

Opinion Formation in distributed topologies: the voter model on hierarchical networks — •Kateryna Isirova[1,2], Oleksandr Potii[2], and Jens Christian Claussen[1] — [1]Department of Mathematics, Aston University, Birmingham, UK — [2]V. N. Karazin Kharkiv National University, Ukraine

The voter model is a paradigmatic stochastic model that has been widely employed especially for modeling of emergent social phenomena as opinion formation. Consensus formation protocols however also occur in the dynamics of computer networks, where the verification of nodes may become time-critical in large networks, and depend on the network topology. In society, consensus is formed (or not) via messages to neighbours in the network and likewise depends on the network structure. Here, we investigate the average time to consensus in a variety of different hierarchical and other network topologies, namely, small-world networks, various tree structures and hierarchical networks. For hierarchical networks, we consider the straightforward generalization where influencing a node occurs with different probability depending on the direction of hierarchy. Systemeatic Monte-Carlo simulations show that the average time to consensus in hierarchical networks is considerably larger than in regular graphs and small-world networks.

SOE 10: Transport, Regional and Urban Dynamics

Time: Wednesday 13:00–15:40 Location: SOEa

SOE 10.1 Wed 13:00 SOEa

Adaptive Stop-Pooling for Sustainable Shared Mobility? — •Charlotte Lotze, Malte Schröder, and Marc Timme — Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden

Ride-sharing – the bundling of simultaneous trips of several people in one vehicle – may help us to reduce the carbon footprint of human mobility [1,2]. Ride-sharing trades reduced total route traveled by vehicles for increased passenger travel times. Yet standard door-to-door ride sharing services come with the burden of many stops and detours to pick up individual passengers. Requiring some passengers to walk to nearby shared stops may reduce detours yet may become inefficient if spatio-temporal demand patterns do not well fit the stop locations. Here, we present a simple model of adaptive, on-demand stop pooling and analyze its influence on the performance of ride-sharing services. We find counteracting effects of stop pooling on the number of and distance between stops, inducing a roughly constant route length despite stop pooling benefits. Intriguingly, however, stop pooling also reduces the average travel time although passengers walk parts of their trip. Stop pooling may thus break the trade-off between route lengths and travel times. We conclude, that dynamic stop pooling could enable higher sustainability and service quality simultaneously, potentially also in real world ride sharing systems. References: [1] Molkenthin et al., Scaling Laws of Collective Ride-Sharing Dynamics, Phys. Rev. Lett. 125:248302 (2020); [2] Storch et al., Incentive-driven discontinuous transition to high ride-sharing adoption, arXiv:2008.11079 (2020).

SOE 10.2 Wed 13:20 SOEa

The future of traffic jams: Forward propagating congestion in electric vehicle charging infrastructure — •Philip Marszal[1], Malte Schröder[1], and Marc Timme[1,2] — [1]Chair for Network Dynamics, Center for Advancing Electronics and Institute for Theoretical Physics, Technical University of Dresden, Dresden, Germany — [2]Lakeside Labs, Klagenfurt, Austria

Individual motorized mobility is becoming increasingly electrified. The unique properties of electric vehicles promise to give rise to new collective traffic flow dynamics, which are largely unexplored as of now. Here we demonstrate a new type of congestion in the utilization of charging infrastructure, emerging solely from correlations in driver's charging dynamics due to queue-avoidance behavior on long range trips. We explain the formation of forward-propagating congestion waves as phase separation of the traffic flow into free and congested phases, occurring already before the system reaches its theoretical capacity limit. While current numbers of electric vehicles compared to available charging stations are far below the onset of congestion, these results reveal collective dynamics that may influence how future infrastructure supporting sustainable modes of mobility will be built.

SOE 10.3 Wed 13:40 SOEa

Towards Optimal Bikeability of Urban Mobility Networks — •Christoph Steinacker, David-Maximilian Storch, Marc Timme, and Malte Schröder — Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden

Individual transport in cities is most commonly enabled by private cars, an unsustainable status quo both ecologically and socially. On typical urban distance scales, bicycling constitutes a more sustainable alternative that is broadly accessible. Yet, insufficient and poorly designed bike path networks often hinder more prevalent bike use. Here, we propose an optimisation scheme for bike path networks that enables smooth and safe bicycle travel in cities. Evaluating bike-sharing data on millions of city trips, we estimate bike travel demand and find greatly bike-friendly network topologies. Interestingly, a reverse percolation process that starts from a complete bike path network covering all streets and systematically lowers the number of bike paths by eliminating least used bicycle paths yields topologies much more suitable than a forward process with optimised iterative addition of paths. Even just a small number of bike paths, if chosen wisely, may result in a bike-friendly network. These results may support the planning of sustainable mobility networks, strongly improving urban bikeability.

SOE 10.4 Wed 14:00 SOEa

Purely fluctuation-induced congestion in street traffic — •Verena Krall[1], Max Burg[2,3], Malte Schröder[1], and Marc Timme[1] — [1]Chair for Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, Technical University Dresden, Germany — [2]Institute for Theoretical Physics and Centre for Integrative Neuroscience, University of Tübingen, Germany — [3]Bernstein Center for Computational Neuroscience, Tübingen, Germany

Traffic congestions may emerge spontaneously - out of nowhere. Statistical physics studies provide both qualitative and quantitative insights, yet so far they focused on the consequences of external factors such as street bottlenecks or human behavioral imperfections. Here we present a simple model of traffic flow on a street segment in which congestion spontaneously emerges purely due to fluctuations in the number of incoming vehicles [1]. Agent-based simulations and analytical estimates indicate that this instability exists even in regimes where mean field theory predicts stable traffic flow. Our results thus underline the limitations of mean field analysis for predicting the collective nonlinear dynamics of mobility systems.

[1] V. Krall et al., Number Fluctuations Induce Persistent Congestion, Transport Findings, December 2020. https://doi.org/10.32866/001c.18154.

SOE 10.5 Wed 14:20 SOEa

On the relation between transversal and longitudinal scaling in cities — •Fabiano L. Ribeiro — Universidade Federal de Lavras, Lavras, Brazil

Empirical evidence has been shown that some urban variables scale non-linearly with the city population size. More specifically, some socio-economic variables, such as the number of patents, wages and GDP, show a super-linear behaviour with the population of the city. On the other hand, infrastructure variables, such as the number of gas stations and length of streets, scale sub-linearly with the city population, generating a scale economy. However, does this scaling properties observed in a system of cities (transversal scaling) also work for individual cities in different stages of their growth process (longitudinal scaling)? The answer to this question has important policy implications, but the lack of suitable data has so far hindered rigorous empirical tests. The work that will be presented was developed looking at the evolution of two urban variables, GDP and water network length, for over 5500 cities in Brazil. It will be shown that longitudinal scaling exponents are city-specific, however they are distributed around an average value that approaches the transversal scaling exponent provided that the data is decomposed to eliminate external factors, and only for cities with a sufficiently high growth rate. This result adds complexity to the idea that the longitudinal dynamics is a micro-scaling version of the transversal dynamics of the entire urban system.

SOE 10.6 Wed 14:40 SOEa

Bimodal Transport: Combining Demand Responsive and Public Transport — •Helge Heuer, Puneet Sharma, Stephan Herminghaus, and Knut M. Heidemann — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Bimodal Transport describes the combination of traditional Public Transport (PT), also called Fixed Route Transport (FRT), and Demand Responsive Transport (DRT). In many of the existing DRT services there is the option to share the rides with other customers to reduce the price and increase the ecological efficiency of the individual rides. Bimodal Transport aims to combine the flexibility of DRT services with the efficiency of classical line services. An advantage of shared mobility in general is the comparably low carbon footprint and less general pollution, resulting from the reduction of active vehicles in comparison to unshared transportation.

Here we study bimodal transport via simulations on a square lattice. We analyze the performance of the system under various parameter settings and identify under which conditions the overall ecological footprint can be minimized while maintaining satisfactory customer service. Simulations are compared to an effective analytical theory.

SOE 10.7 Wed 15:00 SOEa

Policy and Innovation Spreading on the Global City Network — •Niklas Kitzmann[1], Jonathan Donges[1], Xuemei Bai[2], Pawel Romanczuk[3], and Ricarda Winkelmann[1] — [1]Potsdam Institute for Climate Impact Research, Germany — [2]Fenner School of Environment & Society, Australian National University, Australia — [3]Institute for Theoretical Biology, Humboldt University of Berlin, Germany

In the much-needed global sustainability transformation, cities may play an important role. Being among the prime drivers of GHG emissions, as well as of sustainable policy innovation and adoption, cities are known to learn from each other to reduce, prepare for and react to the coming environmental changes. In this way, they can be conceptualized as nodes in a globe-spanning learning network, potentially yielding insights into the social tipping dynamics that are so urgently needed to control the human impacts on the Earth System.

Here, we aim to identify whether network-based contagion effects are dominant in sustainability policy adoption by cities. An attempt is made to approximate the inter-city innovation spreading network using empirical data of the global air traffic network and other city-to-city connections. We analyze the spreading of several municipal policies and innovations related to sustainability, such as the implementation of Bus Rapid Transit public transport systems, as contagion processes on these inter-city networks. Surrogate data methods and a dose-response-contagion approach are used to identify network-spreading-

correlations. We then investigate the nature of the spreading process by attempting to reproduce it using generative models.

SOE 10.8 Wed 15:20 SOEa

Indication of correlations between urban scaling and Zipf's exponent — Haroldo V. Ribeiro[1], Milena Oehlers[2], Ana I. Moreno-Monroy[3], Jürgen P. Kropp[2,4], and •Diego Rybski[2,5] — [1]Departamento de Fisica, Universidade Estadual de Maringa, PR 87020-900, Brazil — [2]Potsdam Institute for Climate Impact Research - PIK, Member of Leibniz Association, P.O. Box 601203, 14412 Potsdam, Germany — [3]OECD Centre for Entrepreneurship, SMEs, Regions and Cities, Honorary Associate, Geography and Planning Department, University of Liverpool, 2 rue Andre-Pascal, 75016 Paris, France — [4]Institute for Environmental Science and Geography, University of Potsdam, 14476 Potsdam, Germany — [5]Department of Environmental Science Policy and Management, University of California Berkeley, 130 Mulford Hall #3114, Berkeley, CA 94720, USA

Zipf's law and urban scaling are two fundamental paradigms researched in urban science. They have mostly been investigated independently and are perceived as disassociated matters. Here we present a large scale investigation about the connection between these two laws using population and GDP data from 96 countries. We empirically demonstrate that both laws are tied to each other and derive an expression relating the exponents, capturing the main tendency of the empirical relation. Simulations yield very similar results to the real data after accounting for fluctuations. Our research puts forward the idea that urban scaling of GDP does not solely emerge from intra-city processes.

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