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Fachverband Chemische Physik und Polymerphysik (CPP)

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Overview of Invited Talks and Sessions

(Lecture halls ZEU 222, ZEU 260, ZEU 255, and ZEU 114; Poster P1A, P1C, P2-EG, and P3)

Invited Talks

CPP 2.1	Mon	9:30–10:00	ZEU 222	**The Bright Future for Research with Neutrons in Europe** — •Thomas Brückel
CPP 2.7	Mon	11:30–12:00	ZEU 222	**Connecting dynamics and phase behavior of proteins: The neutron perspective** — •Frank Schreiber
CPP 2.9	Mon	12:15–12:45	ZEU 222	**Antimicrobial peptides, their mechanisms of action and self-assembly revealed by scattering techniques** — Josefine Eilsø Nielsen, Nico König, •Reidar Lund
CPP 4.1	Mon	9:30–10:00	ZEU 255	**Shear-stress fluctuations and relaxation in glassy liquids** — Liudmyla Klochko, Ivan Kriuchevskyi, Joachim Wittmer, Alexander Semenov, Hendrik Meyer, •Jörg Baschnagel
CPP 36.1	Tue	10:00–10:30	ZEU 222	**Anisotropic packing in vapor-deposited glasses** — •Mark Ediger
CPP 36.5	Tue	11:30–12:00	ZEU 222	**Influence of stability and molecular orientation on the properties of stable glasses** — •Javier Rodríguez-Viejo
CPP 37.1	Tue	9:30–10:00	ZEU 260	**Phospholipid membranes as model systems for fundamental soft matter research** — •Sebastian Jaksch
CPP 56.1	Wed	9:30–10:00	ZEU 222	**Structural and photophysical properties of blends of weakly interacting organic semiconductors** — •Katharina Broch, Clemens Zeiser, Giulio Cerullo, Roel Tempelaar, Christopher Bardeen
CPP 58.1	Wed	9:30–10:00	ZEU 255	**Structure and dynamics of semiflexible polymers in bulk and confinement** — •Arash Nikoubashman
CPP 60.3	Wed	12:00–12:30	ZEU 222	**Operando Analysis of the Lithium/Sulfur Battery by Small-Angle Neutron and X-Ray Scattering** — •Matthias Ballauff, Sebastian Risse, Eneli Härk, Günter Goerigk, Chanbum Park, Joachim Dzubiella
CPP 69.1	Wed	15:00–15:30	ZEU 222	**Modelling and Simulation of Organic Ionic Liquids** — •Pietro Ballone
CPP 69.7	Wed	17:00–17:30	ZEU 222	**Charging Dynamics and Structure of Ionic Liquids in Nanoporous Supercapacitors** — •Christian Holm, Konrad Breitsprecher, Svyatoslav Kondrat
CPP 72.1	Wed	15:00–15:30	ZEU 114	**Physics of Fiberboids** — •Igor Kulic
CPP 85.1	Thu	9:30–10:00	ZEU 222	**Molecular view on polymers adsorbed on nanoparticle surfaces** — Mozhdeh Abbasi, Sol Mi Oh, So Youn Kim, •Kay Saalwächter
CPP 85.6	Thu	11:30–12:00	ZEU 222	**Nonequilibrium Properties of Polymers in Confinement** — •Roland G. Winkler
CPP 95.4	Thu	15:45–16:15	ZEU 222	**Active Polymeric Liquid Crystals Under Confinement** — •Juan de Pablo
CPP 97.1	Thu	15:00–15:30	ZEU 255	**Grain coarsening dynamics in cylinder-forming block copolymer thin films** — •Michele Perego
CPP 100.1	Thu	17:15–17:45	ZEU 222	**Real-time Investigation of Crystallization Pathways of Organo-Metal-Halide Perovskites Solar** — •Michael F Toney

CPP 105.1	Fri	9:30–10:00	ZEU 222	**Time-resolved X-ray scattering to understand perovskite materials** — Oliver Filonik, Christopher Greve, Meike Kuhn, Michael Buchhorn, Adrian Ebert, Richard Kellnberger, •Eva M. Herzig
CPP 105.5	Fri	10:45–11:15	ZEU 222	**Structural dynamics of halide perovskites via in-situ electron microscopy** — •Chen Li
CPP 106.1	Fri	9:30–10:00	ZEU 260	**Slide electrification: charging of surfaces by moving water drops** — •Hans-Jürgen Butt

Invited talks of the joint symposium SYSD

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYBD

See SYBD for the full program of the symposium.

SYBD 1.1	Tue	9:30–10:00	HSZ 02	**Materials innovation driven by data and knowledge systems** — •Surya Kalidindi
SYBD 1.2	Tue	10:00–10:30	HSZ 02	**Network Theory Meets Materials Science** — •Chris Wolverton, Murat Aykol, Vinay Hegde
SYBD 1.3	Tue	10:30–11:00	HSZ 02	**Verification and error estimates for ab initio data** — •Claudia Draxl
SYBD 1.4	Tue	11:15–11:45	HSZ 02	**Identifying Domains of Applicability of Machine Learning Models for Materials Science** — •Mario Boley, Christopher Sutton, Luca M. Ghiringhelli, Matthias Rupp, Jilles Vreeken, Matthias Scheffler
SYBD 1.5	Tue	11:45–12:15	HSZ 02	**Deep learning of low-dimensional latent space molecular simulators** — •Andrew Ferguson

Invited talks of the joint symposium SYED

See SYED for the full program of the symposium.

SYED 1.1	Thu	9:30–10:00	HSZ 01	**Ultrafast electron dynamics at laser-irradiated surfaces** — •Baerbel Rethfeld
SYED 1.2	Thu	10:00–10:30	HSZ 01	**Unraveling Momentum-Dependent Electron-Phonon Coupling and its Role in the Origin of Charge Density Wave Phases** — •Bradley Siwick, Martin Otto, Jan-Hendrik Pohls, Laurent Rene de Cotret, Mark Sutton
SYED 1.3	Thu	10:30–11:00	HSZ 01	**Light MATTERs!!!** — •Hrvoje Petek, Andi Li, Zehua Wang, Marcel Reutzel
SYED 1.4	Thu	11:15–11:45	HSZ 01	**Quantum localization and delocalization of charge carriers in molecular organic crystals** — •Jochen Blumberger
SYED 1.5	Thu	11:45–12:15	HSZ 01	**Single-Atom Catalysis (SAC): How Structure Influences Reactivity** — •Gareth Parkinson

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — David Oriola, Benjamin Dalton, Franziska Decker, Frank Julicher, •Jan Brugues
SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch
SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch
SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Invited talks of the joint symposium SYDW

See SYDW for the full program of the symposium.

SYDW 1.1	Thu	15:00–15:30	HSZ 02	**Statics and Dynamics of Soft Wetting** — •Bruno Andreotti
SYDW 1.2	Thu	15:30–16:00	HSZ 02	**Modelling imbibition, dynamic wetting and evaporation on structured surfaces and porous coatings** — •Tatiana Gambaryan-Roisman, Noemi Ghillani
SYDW 1.3	Thu	16:00–16:30	HSZ 02	**Droplets on shaped liquid and electrically switchable surfaces** — •Glen McHale
SYDW 1.4	Thu	16:45–17:15	HSZ 02	**Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates** — •Ralf Seemann, Stefan Bommer, Roghayeh Shiri, Sebastian Jachalski, Dirk Peschka, Barbara Wagner
SYDW 1.5	Thu	17:15–17:45	HSZ 02	**Droplet durotaxis and engulfment on yielding viscoelastic gels** — •Anne Juel

Sessions

CPP 1.1–1.3	Sun	16:00–18:15	HSZ 304	**Tutorial: Nanofabrication and 3D Printing with Submicron Resolution (joint session CPP/TUT)**
CPP 2.1–2.10	Mon	9:30–13:00	ZEU 222	**Focus: Soft Matter and Nanocomposites - New opportunities with advanced neutron sources I**
CPP 3.1–3.12	Mon	9:30–12:45	ZEU 260	**Molecular Electronics and Excited State Properties I**
CPP 4.1–4.6	Mon	9:30–11:15	ZEU 255	**Glasses and Glass Transition (joint session CPP/DY)**
CPP 5.1–5.7	Mon	9:30–11:15	ZEU 114	**Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)**
CPP 6.1–6.3	Mon	11:30–12:15	ZEU 255	**2D Materials (joint session CPP/O)**
CPP 7.1–7.2	Mon	12:30–13:00	ZEU 255	**Hydrogels and Microgels**
CPP 8.1–8.11	Mon	9:30–13:00	HÜL 386	**Active Matter I (joint session BP/DY/CPP)**
CPP 9.1–9.10	Mon	9:30–12:30	POT 112	**Organic semiconductors I (joint session HL/CPP)**
CPP 10.1–10.6	Mon	9:30–12:00	POT 251	**Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar I (joint session HL/CPP)**
CPP 11.1–11.10	Mon	9:30–12:45	SCH A251	**Focus: Phase Separation in Biological Systems I (joint session BP/CPP)**
CPP 12.1–12.8	Mon	9:30–12:50	TOE 317	**Focus: High-resolution Lithography and 3D Patterning (Part I) (joint session KFM/HL/CPP)**
CPP 13.1–13.11	Mon	9:30–13:00	ZEU 250	**Membranes and Vesicles (joint session BP/CPP)**

CPP 14.1–14.4	Mon	10:15–11:30	BAR 205	**Topical Session: Data Driven Materials Science - Materials Design I (joint session MM/CPP)**
CPP 15.1–15.8	Mon	10:30–12:45	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions I (joint session O/HL/CPP/DS)**
CPP 16.1–16.13	Mon	10:30–13:45	WIL A317	**Plasmonics and Nanooptics I: Local Probes and Raman (joint session O/CPP)**
CPP 17.1–17.12	Mon	10:30–13:45	WIL C107	**2D Materials I: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)**
CPP 18.1–18.5	Mon	11:45–13:00	BAR 205	**Topical Session: Data Driven Materials Science - Materials Design II (joint session MM/CPP)**
CPP 19.1–19.8	Mon	15:00–17:00	ZEU 222	**Focus: Soft Matter and Nanocomposites - New opportunities with advanced neutron sources II**
CPP 20.1–20.5	Mon	15:00–16:15	ZEU 260	**Molecular Electronics and Excited State Properties II**
CPP 21.1–21.8	Mon	15:00–17:00	ZEU 255	**Crystallization, Nucleation and Self-Assembly**
CPP 22.1–22.5	Mon	15:00–16:15	ZEU 114	**Electrical, Dielectrical and Optical Properties of Thin Films**
CPP 23.1–23.3	Mon	16:30–17:15	ZEU 260	**Interfaces and Thin Films I (joint session CPP/O/DY)**
CPP 24.1–24.51	Mon	17:30–19:30	P3	**Poster Session I**
CPP 25.1–25.8	Mon	15:00–17:00	HSZ 101	**Bio- and Molecular Magnetism (joint session MA/CPP)**
CPP 26.1–26.10	Mon	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)**
CPP 27.1–27.6	Mon	15:00–17:00	POT 251	**Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar II (joint session HL/CPP)**
CPP 28.1–28.7	Mon	15:00–17:40	TOE 317	**Microscopy and Spectroscopy with X-rays, Ions and Positrons (joint session KFM/CPP)**
CPP 29.1–29.11	Mon	15:00–18:00	WIL A317	**Plasmonics and Nanooptics III: Ultrafast and Nonlinear Phenomena (joint session O/CPP)**
CPP 30.1–30.12	Mon	15:00–18:15	WIL C107	**2D Materials II: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)**
CPP 31.1–31.8	Mon	15:00–17:30	ZEU 250	**Biomaterials and Biopolymers (joint session BP/CPP)**
CPP 32.1–32.10	Mon	15:30–18:15	HÜL 186	**Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)**
CPP 33.1–33.10	Mon	15:00–18:00	ZEU 118	**Glasses and Glass Transition (joint session DY/CPP)**
CPP 34.1–34.9	Mon	15:00–17:45	ZEU 160	**Microswimmers (joint session DY/CPP)**
CPP 35.1–35.1	Mon	17:00–17:30	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning for Production (joint session MM/CPP)**
CPP 36.1–36.7	Tue	10:00–12:30	ZEU 222	**Focus: Exploitation of Anisotropy in Organic Semiconductors I (joint session CPP/HL)**
CPP 37.1–37.12	Tue	9:30–13:00	ZEU 260	**Interfaces and Thin Films II (joint session CPP/O/DY)**
CPP 38.1–38.5	Tue	9:30–10:45	ZEU 255	**Organic Electronics and Photovoltaics I**
CPP 39.1–39.10	Tue	9:30–12:15	ZEU 114	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids**
CPP 40.1–40.7	Tue	10:45–12:45	ZEU 255	**Polymer and Molecular Dynamics, Friction and Rheology**
CPP 41.1–41.6	Tue	9:30–11:00	CHE 91	**Organic Thin Films, Organic-Inorganic Interfaces I (joint session DS/CPP)**
CPP 42.1–42.11	Tue	9:30–13:15	GÖR 226	**Data analytics for dynamical systems I (joint session SOE/DY/CPP/BP)**
CPP 43.1–43.11	Tue	9:30–13:00	HÜL 386	**Active Matter II (joint session BP/DY/CPP)**
CPP 44.1–44.7	Tue	9:30–12:00	POT 151	**Functional semiconductors for renewable energy solutions I (joint session HL/CPP)**
CPP 45.1–45.10	Tue	9:30–12:30	POT 251	**Perovskite and photovoltaics I (joint session HL/CPP)**
CPP 46.1–46.13	Tue	9:30–13:00	ZEU 160	**Complex Fluids and Soft Matter (joint session DY/CPP)**
CPP 47.1–47.10	Tue	9:30–12:45	ZEU 250	**Focus: Phase Separation in Biological Systems II (joint session BP/CPP)**
CPP 48.1–48.6	Tue	11:15–12:45	CHE 91	**Organic Thin Films, Organic-Inorganic Interfaces II (joint session DS/CPP)**
CPP 49.1–49.53	Tue	14:00–16:00	P1A	**Poster Session II**
CPP 50.1–50.52	Tue	14:00–16:00	P1C	**Poster Session III**

CPP 51.1–51.14	Tue	14:00–16:00	P2/EG	**Poster Session III-2**
CPP 52.1–52.6	Tue	14:00–15:30	POT 151	**Functional semiconductors for renewable energy solutions II (joint session HL/CPP)**
CPP 53.1–53.8	Tue	14:00–16:00	POT 251	**Perovskite and photovoltaics II (joint session HL/CPP)**
CPP 54.1–54.8	Tue	14:00–16:00	ZEU 160	**Active Matter III (joint session DY/BP/CPP)**
CPP 55.1–55.6	Tue	14:15–15:45	IFW D	**Materials for Energy Storage and Conversion - Battery and Fuel Cell Materials (joint session MM/CPP)**
CPP 56.1–56.6	Wed	9:30–11:15	ZEU 222	**Focus: Exploitation of Anisotropy in Organic Semiconductors II (joint session CPP/HL)**
CPP 57.1–57.12	Wed	9:30–12:45	ZEU 260	**Hybrid Perovskite and Photovoltaics I (joint session CPP/HL)**
CPP 58.1–58.12	Wed	9:30–13:00	ZEU 255	**Modelling and Simulation of Soft Matter I (joint session CPP/DY)**
CPP 59.1–59.11	Wed	9:30–12:30	ZEU 114	**Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)**
CPP 60.1–60.5	Wed	11:30–13:00	ZEU 222	**Focus: Fundamentals of molecular liquids, ionic liquids and mixtures I**
CPP 61.1–61.10	Wed	9:30–12:30	POT 251	**Perovskite and photovoltaics III (joint session HL/CPP)**
CPP 62.1–62.11	Wed	9:30–13:00	SCH A251	**Single Molecule Biophysics (joint session BP/CPP)**
CPP 63.1–63.9	Wed	10:00–12:30	ZEU 160	**Active Matter IV (joint session DY/CPP/BP)**
CPP 64.1–64.4	Wed	10:15–11:30	BAR 205	**Topical Session: Data Driven Materials Science - Materials Data Management (joint session MM/CPP)**
CPP 65.1–65.11	Wed	10:30–13:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)**
CPP 66.1–66.9	Wed	10:30–13:15	REC C 213	**Focus Session: Big Data in Aquisition in ARPES (joint session O/CPP)**
CPP 67.1–67.13	Wed	10:30–13:45	WIL B321	**2D Materials IV: Interfacial Interactions (joint session O/HL/CPP)**
CPP 68.1–68.6	Wed	11:45–13:15	BAR 205	**Topical Session: Data Driven Materials Science - Descriptors (joint session MM/CPP)**
CPP 69.1–69.12	Wed	15:00–18:45	ZEU 222	**Focus: Fundamentals of molecular liquids, ionic liquids and mixtures II**
CPP 70.1–70.5	Wed	15:00–16:15	ZEU 260	**Hybrid Perovskite and Photovoltaics II (joint session CPP/HL)**
CPP 71.1–71.7	Wed	15:00–16:45	ZEU 255	**Modelling and Simulation of Soft Matter II (joint session CPP/DY)**
CPP 72.1–72.8	Wed	15:00–17:30	ZEU 114	**Polymer Networks and Elastomers**
CPP 73.1–73.8	Wed	16:15–18:30	ZEU 260	**Organic Electronics and Photovoltaics II**
CPP 74.1–74.4	Wed	15:00–16:00	GER 37	**Tribology: Surfaces and Nanostructures (joint session O/CPP)**
CPP 75.1–75.9	Wed	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)**
CPP 76.1–76.7	Wed	15:00–17:30	POT 112	**Organic semiconductors II (joint session HL/CPP)**
CPP 77.1–77.8	Wed	15:00–17:30	POT 251	**Perovskite and photovoltaics IV (joint session HL/CPP)**
CPP 78.1–78.10	Wed	15:00–17:30	TRE Ma	**Scanning Probe Techniques I: Method development (joint session O/CPP)**
CPP 79.1–79.10	Wed	15:00–17:30	WIL B321	**Nanostructured Surfaces and Thin Films I: 1D and 2D Networks (joint session O/CPP)**
CPP 80.1–80.7	Wed	15:00–16:45	ZEU 147	**Droplets and Wetting (joint session DY/CPP)**
CPP 81.1–81.11	Wed	15:30–18:15	WIL A317	**Plasmonics and Nanooptics V: Tunable Structures and Nanoparticles (joint session O/CPP)**
CPP 82.1–82.5	Wed	15:45–17:00	IFW B	**Computational Materials Modelling - Solids and Molecules (joint session MM/CPP)**
CPP 83.1–83.6	Wed	17:00–18:30	ZEU 147	**Microfluidics (joint session DY/CPP)**
CPP 84.1–84.4	Wed	18:00–19:00	HSZ 304	**Molecular Electronics and Photonics (joint session TT/CPP)**
CPP 85.1–85.9	Thu	9:30–12:45	ZEU 222	**Focus: Polymers under confinement I**
CPP 86.1–86.12	Thu	9:30–12:45	ZEU 260	**Organic Electronics and Photovoltaics III**

CPP 87.1–87.13	Thu	9:30–13:00	ZEU 255	**Wetting and Liquids at Interfaces and Surfaces I (joint session CPP/O/DY)**
CPP 88.1–88.8	Thu	9:30–11:30	ZEU 114	**Responsive and Adaptive Systems**
CPP 89.1–89.6	Thu	9:30–11:50	HSZ 301	**Materials for Energy Storage (joint session KFM/CPP)**
CPP 90.1–90.8	Thu	9:30–12:00	POT 251	**Perovskite and photovoltaics V (joint session HL/CPP)**
CPP 91.1–91.11	Thu	9:30–13:00	SCH A251	**Computational Biophysics (joint session BP/CPP)**
CPP 92.1–92.7	Thu	9:30–12:20	TOE 317	**Focus: High-resolution Lithography and 3D Patterning II (joint session KFM/HL/CPP)**
CPP 93.1–93.9	Thu	10:30–12:45	WIL C107	**Scanning Probe Techniques II: Method development (joint session O/CPP)**
CPP 94.1–94.6	Thu	14:10–16:20	HSZ 301	**TEM-based Nanoanalysis and Microstructure of thin films (joint session KFM/CPP)**
CPP 95.1–95.4	Thu	15:00–16:15	ZEU 222	**Focus: Polymers under confinement II**
CPP 96.1–96.11	Thu	15:00–18:00	ZEU 260	**Organic Electronics and Photovoltaics IV**
CPP 97.1–97.7	Thu	15:00–17:00	ZEU 255	**Nanostructures, Nanostructuring and Nanosized Soft Matter**
CPP 98.1–98.8	Thu	15:00–17:00	ZEU 114	**Composites and Functional Polymer Hybrids**
CPP 99.1–99.9	Thu	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)**
CPP 100.1–100.4	Thu	17:15–18:30	ZEU 222	**Focus: In-situ probes toward better understanding of hybrid halide perovskites (PhD symposium) I (joint session CPP/AKjDPG)**
CPP 101	Thu	18:45–19:45	ZEU 260	**Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)**
CPP 102.1–102.9	Thu	15:00–17:15	WIL B321	**Nanostructured Surfaces and Thin Films II: 1D and 2D Networks (joint session O/CPP)**
CPP 103.1–103.5	Thu	15:45–17:15	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning for Materials Characterization (joint session MM/CPP)**
CPP 104.1–104.6	Thu	17:30–19:00	BAR 205	**Topical Session: Data Driven Materials Science - Machine Learning Applications (joint session MM/CPP)**
CPP 105.1–105.8	Fri	9:30–12:15	ZEU 222	**Focus: In-situ probes toward better understanding of hybrid halide perovskites (PhD symposium) II (joint session CPP/AKjDPG)**
CPP 106.1–106.9	Fri	9:30–12:15	ZEU 260	**Wetting and Liquids at Interfaces and Surfaces II (joint session CPP/DY/O)**
CPP 107.1–107.9	Fri	9:45–12:15	ZEU 255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods**
CPP 108.1–108.1	Fri	12:30–13:15	HSZ 02	**Closing Talk: Frank Jülicher (joint session BP/DY/CPP)**
CPP 109.1–109.1	Fri	14:00–14:45	HSZ 02	**Closing Talk: Roland Wiesendanger (joint session O/CPP/DS)**
CPP 110.1–110.3	Fri	9:30–10:30	HSZ 03	**Nano- and Optomechanics (joint session TT/HL/CPP)**
CPP 111.1–111.2	Fri	9:30–10:00	GÖR 226	**Data analytics for dynamical systems II (joint session SOE/CPP/DY)**
CPP 112.1–112.6	Fri	10:00–11:30	ZEU 160	**Active Matter V (joint session DY/BP/CPP)**
CPP 113.1–113.10	Fri	10:30–13:00	WIL B321	**Nanostructured Surfaces and Thin Films III: Dots, Particles, Clusters (joint session O/CPP)**

Annual General Meeting of the Chemical and Polymer Physics Division

Thursday 18:45-19:45 ZEU 260

- Report of the current speaker team
- Miscellaneous

CPP 1: Tutorial: Nanofabrication and 3D Printing with Submicron Resolution (joint session CPP/TUT)

3D printing or additive manufacturing witnessed one of the most revolutionizing progresses in the last decade. Traditionally used for macro-scale prototyping, 3D printing currently finds applications in large-scale industrial manufacturing, medical technology, education and scientific research. More astonishingly, the resolution of lithography-free 3D printing technologies has reached to microns, pushing the borders of nanoscale and pioneering the miniaturisation of diverse tools to smallest-ever dimensions. This tutorial will present an overview on submicron 3D printing technologies and nanofabrication tools, their novel applications, and recent scientific progress in the area. Organised by: Regine v. Klitzing (TU Darmstadt) and Cagri Üzüm (Grace GmbH, Worms).

Time: Sunday 16:00–18:15 Location: HSZ 304

Tutorial CPP 1.1 Sun 16:00 HSZ 304
3D laser nanoprinting — •Martin Wegener — Institute of Applied Physics and Institute of Nanotechnology, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

This tutorial follows a recently published review and perspectives article on 3D laser nanoprinting (V. Hahn et al., Opt. Photon. News 30(10), 28-35 (2019)).

I will review the underlying physical principles, describe the state-of-the art in the context of many other alternative 3D additive manufacturing approaches, and emphasize two challenges: (i) Substantially faster and scalable 3D printing with sub-micrometer voxel sizes, and (ii) multi-material 3D nanoprinting.

(i) I will present (unpublished) results on rapid multi-focus 3D laser nanoprinting leading to printing rates around 10^7 voxels/s at sub-micrometer voxels sizes. For example, this has led to 3D mechanical metamaterials with more than 100 thousand unit cells and more than 300 billion voxels total. Furthermore, I will sketch our ideas to go well beyond this by introducing light-sheet 3D laser nanoprinting.

(ii) I will discuss three different approaches towards multi-material architectures: (a) integrated microfluidic chamber, (b) stimuli-assisted 3D laser nanoprinting, and (c) meta-inks.

This work has been supported by the Excellence Cluster "3D Matter Made to Order".

Tutorial CPP 1.2 Sun 16:45 HSZ 304
3D printed microoptics: State of the art and future challenges — •Harald Giessen — 4. Physikalisches Institut, Universität Stuttgart

3D printing using femtosecond lasers gives submicron resolution when polymerizing plastics by two-photon absorption. The small voxel size well below the diffraction limit and the combination with high-speed scanners and high-precision piezo stages allows for the creation of millimeter-sized 3D optics with unprecedented design freedom. We will demonstrate that such complex optics with aspherical and freeform surfaces without rotational symmetry can lead to novel miniature optics with wavefront aberrations as small as lambda/10. Multiple materials can be combined with different refractive indices and dispersions, thus allowing for Fraunhofer-type achromats. Diffractive optics can be 3D printed as well, and stacking several Fresnel-type surfaces leads to aplanatic imaging systems. Hybrids that combine diffractive and refractive surfaces as well as transparent and opaque materials enhance the imaging capabilities even further. When combined with imaging fibers or CMOS imaging sensors, an entire new class of miniature optical devices can be created which will revolutionize augmented and virtual reality as well as self-driving cars. Fiber-based optical trapping, side-looking OCT endoscopes, the smallest imaging endoscope in the world, as well as applications in quantum technology pave the way towards future functionalities and applications [1-2].

[1] T. Gissibl et al., Nature Communications 7, 11763 (2016). [2] T. Gissibl et al., Nature Photonics 10, 554 (2016).

Tutorial CPP 1.3 Sun 17:30 HSZ 304
Nanofabrication and 3D printing with submicron resolution — •Michael Huth — Goethe University, Frankfurt am Main, Germany

Focused electron beam induced deposition (FEBID) is a direct-write method for the fabrication of nanostructures whose lateral resolution rivals that of advanced electron beam lithography but is in addition capable of creating complex three-dimensional (3D) nano-architectures. Over the last decade several new developments in FEBID and focused electron beam induced processing (FEBIP) in general have led to a growing number of scientific contributions in solid state physics and materials science based on FEBID-specific materials and particular shapes and arrangements of the employed nanostructures. In this tutorial talk I will give an introduction to the most relevant aspects of FEBID with a particular focus on the creation of 3D functional structures. I will discuss simulation-assisted approaches to FEBID based on effective models for the reliable growth of complex 3D shapes and will briefly allude to microscopic modeling attempts that aim to go beyond growth rate and shape prediction. During the talk I will show different examples of 3D FEBID materials used in nano-magnetism, superconductivity, single-electronics and scanning probe microscopy.

CPP 2: Focus: Soft Matter and Nanocomposites - New opportunities with advanced neutron sources I

Neutrons are an essential tool in science and research for probing the structure and dynamics of matter from the mesoscale to the nanoscale and from seconds to nanoseconds. To characterize soft matter nanocomposites, nanoparticles and nanomaterials structure and dynamics of such materials can be studied to probe aspects of safety on health and environment of such new materials. Deuterated molecules allow to highlight polymer interactions or interaction of drugs and peptides. Time resolved measurements can follow the self-assembly of colloids to clusters and nano-sized structures or conformational changes in complex biological macromolecules. Neutron scattering methods are versatile to study such aspects in particular with the advent of the new European Spallation Source and future compact accelerator based neutron sources. The supposed focus session will review the possibilities for experiments with neutrons in soft matter and nanocomposites at current and the status of Research and Development on ESS and compact accelerator driven neutron sources. It will discuss the scientific and technical challenges by this new development in neutron access in the German and European scientific landscape. Organized by: Stephan Förster (FZ Jülich), Thomas Gutberlet (FZ Jülich), Peter Müller-Buschbaum (TU München) and Walter Richtering (RWTH Aachen).

Time: Monday 9:30–13:00 Location: ZEU 222

Invited Talk CPP 2.1 Mon 9:30 ZEU 222

The Bright Future for Research with Neutrons in Europe — •Thomas Brückel — Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science, Jülich, Germany

Neutron scattering has proven to be one of the most powerful methods for studying structure and dynamics of condensed matter on atomic lengths and time scales. It is essential to understand processes, phenomena and functionalities in a wide range of materials. In Europe we look forward to the start-up of the most powerful MW spallation neutron source worldwide, the European Spallation Source (ESS). Instruments at ESS will be several orders of magnitude more performant that any existing instruments and will allow entirely new type of experiments. Compact accelerator driven neutron sources (CANS) with high brilliance neutron provision are an attractive option to underpin this future flagship facility. They can provide regional access for science and industry, allow for specialized experiments and provide means for method development and training. The High-Brilliance Neutron Source (HBS) project of the Juelich Centre for Neutron Science (JCNS) will allow construction of a scalable neutron source ranging from a local neutron laboratory to a full-fledged highly competitive user facility with open access and service. A vision for the future use of neutrons in Europe will be presented emphasizing the scientific potential of these novel facilities.

CPP 2.2 Mon 10:00 ZEU 222

Reducing the recording time of neutron spectroscopy measurements to investigate kinetic processes — •Christian Beck[1,2], Marco Grimaldo[1], Felix Roosen-Runge[3], Olga Matsarskaia[1], Frank Schreiber[2], and Tilo Seydel[1] — [1]Institut Laue Langevin, Grenoble, France — [2]University of Tübingen, Germany — [3]Malmö University, Malmö, Sweden

Recent developments at the neutron backscattering spectrometer IN16b (ILL, Grenoble) allow to collect high energy resolution ($\delta E \approx 0.9\mu$eV) measurements at constant non-zero energy transfers, also called fixed window scans (FWS). Full quasi-elastic neutron scattering (QENS) spectra need to be measured for several hours while FWS only need measurement times of several minutes. Different models are established for the analysis of elastic FWS. The approaches for inelastic FWS are limited. The shorter measurement time allows to follow the short-time self-diffusive processes of kinetically changing samples. Here, slowly crystallizing protein solutions were used as a model system. We present different frameworks to analyze these data, extracting generalized mean-squared displacements [1] and global diffusion coefficients and to separate the different hierarchical contributions. The results are compared with analyzed floating average full QENS spectra with a time resolution of 15 min [2]. In addition, time-dependent neutron spin echo measurements, collected on the same systems, offer access to the short-time collective dynamics of the sample. [1] F. Roosen-Runge *et al.*; EPJ Web of Conf. 83, 02015 (2015) [2] C. Beck *et al.*; Cryst. Growth Des.; DOI:10.1021/acs.cgd.9b00858

CPP 2.3 Mon 10:15 ZEU 222

Low Background Instrumentation for Small-Angle Neutron Scattering — •Sebastian Jaksch — Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science, Garching, Germany

Current and future neutron scattering experiments in soft-matter are strongly limited by their signal-to-noise ratio, as this determines the sensitivity for weak scatterers, low contrast conditions as well as spatial resolution at very low Q. Both current and future instruments need to take this into account. Using the example of small-angle neutron scattering (SANS), also under grazing incidence conditions (GISANS), this contribution will give an overview of current developments and challenges in that area. These considerations will be mostly focused on the Small-K Advanced DIffractometer (SKADI)[1] as a future SANS instruments at the ESS, technical considerations on a compact SANS instrument at the High-Brilliance Source[2] as well as measurements at the KWS-1[3] SANS instrument at MLZ, Garching, Germany.

[1]Jaksch, S., Frielinghaus, H., Jestin, J., et al., (2014). Concept for a time-of-flight Small Angle Neutron Scattering instrument at the European Spallation Source. Nucl. Instrum. Methods Phys. Res. A, 762, 22-30.

[2]T. Gutberlet et al., (2019). The Jülich high brilliance neutron source project - Improving access to neutrons. Physica B: Condensed Matter, 570, 345-348.

[3]Feoktystov, A. V., Frielinghaus, H., Jaksch, S. et al. (2015). KWS-1 high-resolution small-angle neutron scattering instrument at JCNS: current state. J. Appl. Crystallogr., 48(1), 61-70.

CPP 2.4 Mon 10:30 ZEU 222

Evanescent wave simulations: challenges and opportunities for the interpretation of grazing incidence scattering experiments — •Tetyana Kyrey[1], Marina Ganeva[1], Judith Witte[2], Regine von Klitzing[3], Stefan Wellert[2], and Olaf Holderer[1] — [1]Forschungszentrum Jülich GmbH, JCNS am MLZ, Germany — [2]TU Berlin, Germany — [3]TU Darmstadt, Germany

Grazing incidence small angle neutron scattering (GISANS) and grazing incidence neutron spin-echo spectrometry (GINSES) are a powerful experimental method for the investigation of the structure and dynamics of adsorbed polymer systems. Neutron scattering provides access to the internal dynamics. Combination of neutron spin-echo spectrometry with grazing incidence geometry opens the possibility to probe dynamics of the polymer system in vicinity to the solid substrate in the time range up to 100 ns. In turn, the usage of the GINSES technique has some peculiarity and, due to the novelty of the method and complexity of the scattering geometry, difficulties in further data analysis appear. In the current work we present how simulations within the Distorted Wave Born Approximation (DWBA) with the BornAgain software can be used for GINSES data treatment and for the preparation to the GINSES experiment. Simultaneously we report on the possible challenges and reefs appearing in choosing the best model and the "wrong" understanding of the roughness parameter. With two showcase examples (a PNIPAM-brush and a PEG-microgel adsorbed on Si-surface), the simulation process as well as the application of the simulations to the GINSES data analysis are presented.

CPP 2.5 Mon 10:45 ZEU 222

ESS Testbeamline V20 - Pilot Experiments for Future Neutron Source — •Oliver Löhmann[1,2], Peter M. Kadletz[2], Regine von Klitzing[1], and Robin Woracek[2] — [1]Technische Universität Darmstadt, Germany — [2]European Spallation Source Lund, Sweden

Neutron scattering studies are important to gain insight into structure and dynamics of soft matter. The European Spallation Source (ESS), the future leading neutron source in Europe located in Lund (Sweden), will provide unprecedented neutron flux and a long pulsed time structure. The technical challenges associated with this together with being a 'green-field-site', triggered the motivation to design and install a dedicated testbeamline (V20) at the Helmholtz-Zentrum Berlin. [1,2]

Between 2015 and 2020, V20 was a dedicated instrument for tests of components and methods, particularly to exploit the unique time structure, and served as an integration platform for ESS technologies. Here, we will present highlights of the work done in the last year including reflectometry and SANS experiments, which are highly important for the soft matter community. Additionally, the data handling and reduction processes will be shown. The investigated concepts and methods will be able to handle both the high flux and variable wavelength resolution.

References:

[1] Woracek et al., Nucl Instrum Meth A, 839 (2016), 102-116

[2] Strobl et al., Nucl Instrum Meth A, 705 (2013), 74-84

CPP 2.6 Mon 11:00 ZEU 222

UppCANs: Bringing neutrons to the users — •Maximilian Wolff — Department for Physics and Astronomy, Uppsala University

Neutrons provide unique and essential tools for research across many disciplines ranging from basic sciences to engineering and studies of heritage artefacts. The present neutron facilities are currently decreasing in number. This overall shortage will not be compensated by ESS offering the best available brilliance but a limited total number of beam days.

Ultra-compact accelerator driven neutron sources (UCANS) can provide small facilities and enable easy accessibility by bringing neutron instruments close to the users. These use modest energy protons (~18 MeV) that impact on a light target. This allows an extremely compact design of the moderators. The small size and optimised source design provide good brilliance at reasonable cost. Dedicated instrumentation can compete in performance with current small to medium size facilities.

I will present a project for UppCANs in Uppsala. When built, this would provide neutrons for 5 to 7 beam ports and offer a broad range of modern capabilities in materials research allowing the community at modest cost to both complete straightforward measurements and prepare to exploit world leading instruments elsewhere.

15 min. break

Invited Talk CPP 2.7 Mon 11:30 ZEU 222

Connecting dynamics and phase behavior of proteins: The neutron perspective — •Frank Schreiber — University of Tuebingen, Germany

We discuss the combination of various neutron scattering techniques to shed light on the dynamics of proteins in aqueous solution. This includes several processes, such as backbone and side-chain fluctuations, interdomain motions, as well as global rotational and translational (i.e. center of mass) diffusion. Since protein dynamics is related to protein function and essential transport processes, a detailed mechanistic understanding and monitoring of protein dynamics in solution is highly desirable. In particular, we connect it to the overall phase behavior in terms of clustering, crowding, crystallization, and phase separation [1], employing a combination of elastic, quasi-elastic, and inelastic scattering [2] as well as complementary techniques. Finally, we comment on future perspectives for experiments at advanced neutron sources. Invaluable contributions by numerous collaborators are gratefully acknowledged.

[1] M. Grimaldo et al., JPCL, 10, 1709 (2019) [2] M. Grimaldo et al., Q. Rev. Biophys., 52, e7, 63 (2019)

CPP 2.8 Mon 12:00 ZEU 222

Protein Denaturing Studied by Neutron Scattering: Static and Dynamic Behaviour — •Olga Matsarskaia[1], Lena Bühl[1,2], Christian Beck[1,2], Felix Roosen-Runge[3], Marco Grimaldo[1], Ralf Schweins[1], Fajun Zhang[2], Tilo Seydel[1], and Frank Schreiber[2] — [1]Institut Laue-Langevin, Grenoble, France — [2]University of Tübingen, Germany — [3]Malmö University, Malmö, Sweden

Studying thermal protein denaturing provides valuable information on structural and dynamic aspects related to protein function. Here, we present a combined study of small-angle and quasielastic neutron scattering (SANS and QENS) to shed light on the denaturing of bovine serum albumin (BSA). To obtain insights into the influence of different parameters on protein denaturing, temperature, crowding and charge screening by NaCl are used as control parameters. SANS allows us to obtain global structural and kinetic information on the systems investigated. In addition, QENS data yield mean-squared displacement (MSD) values [1], describing the diffusive behaviour of BSA throughout denaturing. We observe that, while the pathway towards the denatured state is unchanged in the presence of salt, the dynamics of the denatured state itself changes upon the addition of NaCl. Our results offer a framework for a comprehensive, multi-method characterisation of thermal protein denaturing [2].

[1] Hennig *et al.*, Soft Matter **(8)**, 2012, 1628-1633.
[2] Matsarskaia *et al.*, *in preparation.*

Invited Talk CPP 2.9 Mon 12:15 ZEU 222

Antimicrobial peptides, their mechanisms of action and self-assembly revealed by scattering techniques — Josefine Eilsø Nielsen, Nico König, and •Reidar Lund — Department of Chemistry, University of Oslo, Norway

Antimicrobial peptides are remarkably effective towards a broad spec trum of bacteria and seem to be able to evade much of the resistance mechanisms making their interesting as therapeutics. Their main mode-of action is believed to be through selective interactions with the cytoplasmic membrane, although the microscopic mechanisms is not yet fully understood. Unfortunately, these compounds cannot easily be translated into medical applications due to degradation and hemolysis. However, self-assembly might be a promising strategy to improve the stability. First, we will consider natural antimicrobial peptides and their interactions with model lipid membranes mimicking mammalian and bacterial cells. Using Small-angle X-ray (SAXS) and neutron reflectometry, we extract the location of the peptide and the structure of the lipid bilayer. The lipid dynamics, i.e. flip-flop and molecular exchange, can be deducted using time-resolved SANS . Comparing the structure and the dynamics, we obtain unique microscopic insight into the mode-of-action. In the last part, we present results of a series of de novo designed antimicrobial peptide that assemble into nanosheet-like structures with enhanced in vivo stability. Using results various neutron scattering techniques, we will discuss the 2D/3D assembly, interfacial interactions and dynamic stability of these compounds.

CPP 2.10 Mon 12:45 ZEU 222

Quantifying Nerve fibers in the Brain Section by Small Angle Scattering — •Santanu Maiti[1,2], Henrich Frielinghaus[3], Martin Dulle[1], Markus Axer[2], and Stephan Förster[1] — [1]Jülich Centre of Neutron Science (JCNS-1/ICS-1), Forschungszentrum Jülich GmbH (FZJ), Jülich, Germany — [2]Institute of Neuroscience and Medicine (INM-1), FZJ, Jülich, Germany — [3]Jülich Centre for Neutron Science at MLZ (JCNS-MLZ), FZJ, Garching, Germany

The structure and function of a brain is intricately linked to the structural connectome, i.e. the neurons and their connections [1]. The complete structural map of its nerve fibers and the exact quantification of their constituents is essential to understand the brain function, dys-function and neurodegenerative disease. Here, we map the whole brain section by small angle neutron/x-ray scattering (SANS/SAXS) to investigate the microstructural insights of the neurons [2-4]. We quantify the spatial distribution of the nerve cells and their degree of orientation from the anisotropic scattering signals. We determine also the orientation of myelinated axon and their orientational order over the section from the myelin peak. Finally, we compare them with 3D polarized light imaging (PLI) results to have a complete map of the connectome [5]. In future, the scanning neutron/X-ray imaging can serve as an alternating technique for neuroimaging. [1] C. S. von Bartheld et al, J. Comparative Neurology, 524, 3865 (2016). [2] H. Inouye et al., PLOS One. 9, e100592, (2014). [3] M. Georgiadis et al, NeuroImage, 204, 116214 (2020). [4] S. Foerster et al, Langmuir 31, 11678, (2015). [5] M. Axer et al Front. Neuroinform., 5, 34 (2011).

CPP 3: Molecular Electronics and Excited State Properties I

Time: Monday 9:30–12:45 Location: ZEU 260

CPP 3.1 Mon 9:30 ZEU 260

A first principles study of the influence of the protein environment on electronic excitations in a bacterial reaction center — •Sabrina Kroll, Stephan Kümmel, and Linn Leppert — Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany

The reaction center (RC) lies at the heart of the photosynthetic process of energy transfer, and is strongly conserved across plants, algae and bacteria. The pigment-protein complexes of most RCs are heterodimeric and charge transfer and separation occur along only one of two similar cofactor branches. The mechanism of primary charge transfer in the RC of purple bacteria has been studied in quite some detail. However, many open questions remain, regarding the relationship between the RC's structure and functionality.

Here, we use the purple bacterium *Rh. sphaeroides* as a model system for elucidating the effect of the protein environment on electronic excitations in the RC. We explicitly include four Bacteriochlorophylls (BCL), i.e. the special pair dimer and the accessory BCLs in both branches, as well as all amino acids in their vicinity in our first principles time-dependent density functional theory calculations that use an optimally tuned range-separated hybrid. We discuss the effect of systematically including larger parts of the environment on electronic structure and excitations as a first step towards entirely non-empirical calculations of charge transfer in these systems.

CPP 3.2 Mon 9:45 ZEU 260

Electronic excitations of bacteriochlorophyll with ab initio Green's function-based many-body perturbation theory — •Zohreh Hashemi and Linn Leppert — Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany

Bacteriochlorophyll (BCL) molecules are one of the main pigments responsible for excitation energy transfer and charge separation in bacterial photosynthesis. Accurate calculation of their electronic structure and excited states from first principles, is a necessary prerequisite for simulating these processes without employing empirical parameters.

Here we present a comprehensive study of charged and neutral excitations in free-standing BCLa, as found in the Light Harvesting 2 complex of the purple bacterium Rhodobacter sphaeroides. We evaluate the accuracy of Green's function-based many-body perturbation theory within the GW+Bethe-Salpeter equation (BSE) approach and time-dependent density functional theory (TDDFT), and benchmark to theoretical values and experimental data. Furthermore, we discuss the importance of numerical convergence and partial self-consistency in the GW approach, and the role of the exchange-correlation functional used in our TDDFT calculations and as starting point for constructing zeroth order approximations to the one-particle Green's function G and the screened Coulomb interaction W.

CPP 3.3 Mon 10:00 ZEU 260

Untersuchung der Anregungsmechanismen organischer Materialien durch ultrakurz gepulste mid-IR Laserstrahlung — •Theo Pflug[1,2], Markus Olbrich[1], Philipp Lungwitz[1] und Alexander Horn[1] — [1]Laserinstitut Hochschule Mittweida, 09648 Mittweida — [2]Technische Universität Chemnitz, 09126 Chemnitz

Diese Arbeit liefert erste Erkenntnisse zur Anregung von Vibrationsmoden und nachfolgende Bearbeitung organischer Materialien mittels mid-IR Laserstrahlung. Bei der Verwendung von ultrakurz gepulster Laserstrahlung kann jedoch neben der resonanten Anregung der Moleküle auch eine nichtlineare Anregung des Elektronensystems erfolgen. Ziel der Untersuchungen ist daher ein Vergleich der resultierenden Abtragsstrukturen nach nichtlinearer elektronischer Anregung und nach der Anregung der Molekülschwingungen von PMMA mittels ultrakurz gepulster mid-IR Laserstrahlung mit Pulsdauern im Femto- bis Pikosekundenbereich, sowie die Untersuchung der Dynamik der Anregung mittels Pump-Probe-Ellipsometrie. Bei Pulsdauern im Femtosekundenbereich werden Elektronen durch Tunnelionisation angeregt, wodurch ein Anstieg des Extinktionskoeffizienten *k* und ein Abtrag unabhängig von der Wellenlänge hervorgerufen wird. Durch Erhöhung der Pulsdauer bis zu einigen Pikosekunden verringert sich die Anzahl der durch nichtlineare elektronische Anregung erzeugten quasifreien Ladungsträger, sodass lediglich bei der Resonanzfrequenz der C-H Schwingung bei $\lambda_{\text{pump}} = 3{,}4\ \mu$m Materialabtrag stattfindet und keine Änderung des Extinktionskoeffizienten für alle Wellenlängen detektierbar ist.

CPP 3.4 Mon 10:15 ZEU 260

Quantitative Predictions of Photoelectron Spectra in Amorphous Molecular Solids from Multiscale Quasiparticle Embedding — •Gianluca Tirimbò[1,4], Xander de Vries[2], Christ Weijtens[2], Peter Bobbert[2,4], Tobias Neumann[3], Reinder Coehoorn[2,4], and Björn Baumeier[1,4] — [1]Deptartment of Mathematics and Computer Science, TU Eindhoven (NL) — [2]Deptartment of Applied Physics, TU Eindhoven (NL) — [3]Nanomatch GmbH, Eggenstein-Leopoldshafen (DE) — [4]Institute for Complex Molecular Systems, TU Eindhoven (NL)

We present a first-principles-based multiscale simulation framework for quantitative predictions of the high-energy part of the Ultraviolet Photoelectron Spectroscopy (UPS) spectra of amorphous molecular solids. The approach combines a deposition simulation, many-body Green's Function Theory, polarizable film-embedding, and multimode electron-vibrational coupling and provides a molecular-level view on the interactions and processes giving rise to spectral features. This insight helps bridging the current gap between experimental UPS and theoretical models as accurate analyses are hampered by the energetic disorder, surface-sensitivity of the measurement and the complexity of excitation processes. We demonstrate the capabilities of the simulation approach studying the spectrum of two isomers of archetypal materials showing a clearly separated HOMO peak in experiment. The excellent agreement suggests that our approach provides a route for determining the HOMO energy with an accuracy better than 0.1 eV.

CPP 3.5 Mon 10:30 ZEU 260

Accuracy of optimally-tuned range-separated hybrid functionals for the calculation of excited-state molecular geometries — •Bernhard Kretz and David Alexander Egger — Department of Physics, Technical University of Munich, Germany

An accurate description of excited-state structural dynamics of molecules is essential for the computational modeling of photochemical processes (e.g., for photocatalysis). Often, geometries optimized for the lowest-lying excited state serve as the starting point of such investigations. These geometries can be obtained either by time-dependent density functional theory (TD-DFT) or by high-level wave-function methods. Even though TD-DFT based calculations are computationally very efficient, in many cases they are less accurate compared to computationally more expensive wave-function methods[1]. However, efforts made to reduce the gap in accuracy between TD-DFT and wave-function methods recently lead to the development of the very promising class of optimally-tuned range-separated hybrid (OT-RSH) functionals[2].

In this computational study, we evaluate the precision of excited-state structures obtained with TD-DFT and OT-RSH for a selection of organic molecules. Focusing on structural parameters (e.g., bond lengths, bond angles, etc.) of the lowest-excited singlet states, we benchmark our results by comparison to high accuracy wave-function data from literature.

[1] C. Azarias, J. Phys. Chem. A, 121, 32, 6122 (2017)

[2] L. Kronik et al., J. Chem. Theory Comput., 8, 5, 1515 (2012)

CPP 3.6 Mon 10:45 ZEU 260

Photophysics of tetracene-pentacene blends — •Clemens Zeiser[1], Luca Moretti[2], Margherita Maiuri[2], Giulio Cerullo[2], and Katharina Broch[1] — [1]Insititute for Applied Physics, University of Tübingen, Germany — [2]Department of Physics, Polytecnic Unitversity of Milan, Italy

Pentacene (PEN) and tetracene (TET) are prototypical compounds for the investigation of singlet fission (SF), a process that has been extensively studied in the last decade due to its potential application in solar cells. [1] Most studies on SF examine thin films, nanoparticles, single crystals or solutions of *neat* compounds, and only few studies on doped single crystals and mixed thin films have been reported [2,3]. In this study we investigate the photophysics of mixed films of PEN and TET using transient absorption spectroscopy. We find the lowest excited singlet and triplet states in PEN:TET blends to be delocalized over both compounds and will discuss the implications for the singlet fission dynamics in these blends.

[1] M. Smith et al., Chem. Rev. 110, 6891 (2010)

[2] N. Geacintov et al., Chem. Phys. Lett. 11, 504 (1971)

[3] V. O. Kim et al., J. Chem. Phys., 151, 164706 (2019)

CPP 3.7 Mon 11:00 ZEU 260

Electronic and optical properties of BCF-doped oligothiophenes from ab initio many-body theory — •Richard Schier, Ana Valencia, and Caterina Cocchi — Humboldt-Universität zu Berlin und IRIS Adlershof

Doping in organic semiconductors is an attractive research area for molecular electronics although the fundamental mechanisms ruling it are not yet fully understood. Recently, Lewis-acids such as tris(pentafluorophenyl)borane (BCF)[1] have been regarded with particular interest as a new class of dopants for organic semiconductors[2]. To gain insight into the microscopic properties of these materials, we investigate the electronic structure and optical properties of donor/acceptor interfaces formed by a single quarterthiophene (4T) molecule doped by a BCF species. For comparison, we consider also other adducts with 4T doped by hexafluorobenzene (C_6F_6) and the trihalide BF_3. We carry out our study from first principles, in the framework of hybrid density-functional theory and many-body perturbation theory. For all systems, we find that the frontier orbitals are poorly hybridized and rather segregated on the donor or the acceptor depending on the specific level alignment of the system. As a consequence, the optical spectra of the systems appear almost as a superposition of those of the respective constituents. A careful analysis reveals interaction signatures in the form of dark excitations and peak shifts[3].

[1] Körte et al., Angew. Chem. 56, 8578 (2017) [2] Yurash et al., Nat. Mater. 18, 1327 (2019) [3] Schier et al., to be submitted (2020)

15 min. break

CPP 3.8 Mon 11:30 ZEU 260

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 3.9 Mon 11:45 ZEU 260

Excited State Dynamics of Tetracene-Acceptor Blends — •Christoph Theurer[1], Julian Hausch[1], Clemens Zeiser[1], Vipilan Sivanesan[2], Petra Tegeder[2], and Katharina Broch[1] — [1]Eberhard Karls Universität Tübingen, Institut für Angewandte Physik, Tübingen — [2]Ruprecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut, Heidelberg

Charge transfer between electron donating and accepting organic semiconductors (OSCs) is pivotal for exploiting the full potential of OSCs in devices [1].

Tetracene is a prototypical OSC and exhibits interesting optical properties and effects like singlet fission, making it a promising material for solar energy conversion [2]. The competition between charge transfer to organic acceptors and singlet fission has, however, received little attention in tetracene so far [3][4]. In this work, blends of tetracene and two common, strong acceptors, F6-TCNNQ and F4-TCNQ, have been grown and investigated. Based on thorough structural and morphological investigations we studied and compared the photophysics of blends with different mixing ratios. The dynamics of these fundamentally interesting systems were examined by transient absorption spectroscopy.

[1] Forrest, S. R., Nature 428 (2004) [2] Smith, M. B., and Michl, J., Chemical Reviews 110 (2010) [3] Hu, P., et al., CrystEngComm 19 (2017) [4] Yost, S., et al., Nature Chem 6 (2014)

CPP 3.10 Mon 12:00 ZEU 260

Morphological Tuning of the Dual Luminescence in Zinc-Phthalocyanine OLEDs — Sebastian Hammer[1], •Thomas Ferschke[1], Gabriel von Eyb[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

In the field of telecommunications, a rising demand for opto-electronic devices operating in the near infrared can be identified. Moreover, in order to enhance the transmission capabilities of such future photonic devices, versatile, multi-emissive materials are required.

For this purpose, we investigate the first order α-to-β phase transition and its influence on the optical properties of crystalline Zinc-Phthalocyanine (ZnPc) thin films. Under optical excitation two distinct intensity maxima are observed at 780 nm and 930 nm. The emission component around 930 nm can be assigned to excimer emission of the ZnPc α-phase [1], whereas luminescence at 780 nm originates from bulk Frenkel excitons of the corresponding β-phase. Comprehensive temperature and time dependent studies on the phase transition show the feasibility of a controllable luminescence shift of the layers. The phase transfer kinetics can be modelled by a Johnson-Mehl-Kolmogorov-Avrami model based on growth of polyhedral grains [2]. Utilizing these findings, we demonstrate the implementation of dual luminescent OLED devices based on a single ZnPc emissive layer with balanced near infrared emission.

[1]V. Kolb and J. Pflaum, *Opt. Express* **25**, 6678 (2017)

[2]M. Avrami, *J. Chem. Phys.* **8**, 212 (1940)

CPP 3.11 Mon 12:15 ZEU 260

Substituent approach in molecular design of phosphorous compounds for OLED emitters — •Jonas Köhling, Gerd-Volker Röschenthaler, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic light emitting diodes (OLEDs) are one of the leading technologies used for display fabrication. Currently, the main challenge in OLED technology is to synthesize and design efficient and stable emitters. To achieve this goal, it is of great interest to evaluate and optimize molecular design of a large number of possible organic molecules prior to their synthesis. In this study, we have used a substituent approach to design and analyze a large number of derivatives of phosphorous compound. The core molecule is chosen so that it meets requirements of the third generation of the OLED emitters and allows for the thermally activated delayed florescence. The core molecule is systematically varied by introduction of substituents from strong electron withdrawing groups (EWG) towards strong electron donating groups (EDG). By using density functional theory (B3LYP/6-31+G(d,p)) calculations, we show that EDG substituents are able to tune the bandgap of the potential OLED emitters. On the other hand, EWG substituent groups can be used to tune the band alignment of the core molecule.

CPP 3.12 Mon 12:30 ZEU 260

Characterization and control of aggregation in doped poly(3-hexylthiophene-2,5-diyl) solutions — •Ahmed E. Mansour[1,2], Dominique Lungwitz[1], Thorsten Schultz[1,2], Malavika Arvind[3], Ana M. Valencia[1], Caterina Cocchi[1], Andreas Opitz[1], Dieter Neher[3], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt Universität zu Berlin, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany — [3]Institut für Physik und Astronomie, Universität Potsdam, Germany

Chemical doping of poly(3-hexylthiophene-2,5-diyl) (P3HT) is commonly achieved by mixing solutions of the dopant molecules and the polymer in predetermined volumes based on the desired dopant ratio. Aggregation in doped P3HT is typically observed as a result of the solution-mixing process, due to decreased solubility of the mixture. In this work, we provide means for characterizing the presence of doped aggregates and their relative amounts with respect to doped isolated polymer chains in tris(pentafluorophenyl)borane (BCF) doped P3HT solutions. This is achieved by the distinction of signatures in the optical absorption spectrum due to polarons in doped aggregates on the one hand, and doped isolated chains on the other hand. We further rely on these signatures to investigate the influence of dopant ratio and absolute concentration of the solution mixture on the relative amount and the size of the aggregates. Finally, we quantify the degree of doping as a function of the structural form, showing a larger degree of doping in the aggregates as compared to the isolated chains.

CPP 4: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 9:30–11:15 Location: ZEU 255

Invited Talk CPP 4.1 Mon 9:30 ZEU 255

Shear-stress fluctuations and relaxation in glassy liquids — Liudmyla Klochko, Ivan Kriuchevskyi, Joachim Wittmer, Alexander Semenov, Hendrik Meyer, and •Jörg Baschnagel — Institut Charles Sadron, University of Strasbourg & CNRS, 23 rue du Loess, 67034 Strasbourg Cedex, France

By means of molecular dynamics simulations we study the shear modulus μ and shear stress relaxation function $G(t)$ of a short-chain glass-forming liquid. We determine μ via the shear-stress fluctuation formalism as a function of temperature T and sampling time Δt. When cooling the system below the glass transition temperature T_g the shear modulus has a finite, T-dependent, value which depends on Δt. We show that this sampling time dependence can be traced back to the relaxation of $G(t)$, thereby establishing a relation between two often employed means—i.e. shear stress fluctuation formalism and $G(t)$—to characterize the shear response of glassy systems. We repeat the analysis for 100 independent configurations (samples) and find that the glass transition is accompanied by strong sample-to-sample fluctuations, implying that the standard deviation $\delta\mu$ of the (ensemble-averaged) modulus displays a peak near T_g and is of the same order of magnitude as μ itself. We propose a theory which explains this behavior.

CPP 4.2 Mon 10:00 ZEU 255

Molecular dynamics study of 1,4-polybutadiene supported film — •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.

CPP 4.3 Mon 10:15 ZEU 255

Dynamics of an arrested phase transition in a protein system — •Anita Girelli[1], Hendrik Rahmann[2], Nafisa Begam[1], Anastasia Ragulskaya[1], Fabian Westermeier[3], Fajun Zhang[1], Christian Gutt[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]DESY, Germany

The interest in phase transitions in biological systems has attracted much effort because of their numerous applications and its role as a mechanism underlying intracellular organization [1]. In this study the development of the spinodal decomposition near the gel/glass transition in a globular protein system was studied using X-Ray Photon Correlation Spectroscopy (XPCS) in the ultra small angle X-Ray scattering (USAXS) regime. The dynamics was probed at different quench depth, exhibiting two regimes: the first regime shows a single exponential decay of the correlation function, and the corresponding decorrelation time increases exponentially with waiting time t_w. In the second regime, a second relaxation channel appears and the associated nonergodicity parameter increases with t_w until it becomes the dominating decay. The corresponding decorrelation time increases as a power law in t_w. The dynamics was compared to simulations, which were performed by solving numerically the Cahn-Hilliard equation coupled with a gel transition. The effect of nanoscale arrested dynamics can be seen on the microscopic dynamics. Aging with quench depth dependence is visible and can be connected to real space parameters such as final concentration and mobility.

[1] Berry et al., *Rep. Prog. Phys.*, **81**, 046601, 2018

CPP 4.4 Mon 10:30 ZEU 255

molecular dynamics of glassy polynorbornenes bearing flexible side substituents: nanophase separation and glass transition — •Mohamed Aejaz Kolmangadi[1], Paulina Szymoniak[1], Glen Jacob Smales[1], Brian Pauw[1], Maxim Bermeshev[2], Martin Böhning[1], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]A.V. Topchiev Institute of Petrochemical Synthesis of Russian Academy of Science, Leninskii prospect, 29, 119991 Moscow, Russia

Polynorbornenes are latest among the high-performance polymers in the field of membrane gas separation. Not much has been studied regarding their molecular dynamics till now. In the present work, we report dielectric and calorimetric investigations of series of polynorbornenes with rigid main backbone and flexible (AlkO)3Si side groups with different length (Al = Propyl, Butyl, Octyl, Decyl). Two dielectrically active α and β relaxations observed are assigned to localized fluctuations and segmental relaxation of the flexible side groups of the polymer. A nanophase separation between the main and side chain parts is concluded from the presence of two dynamic glass transitions of the polymer, is confirmed by means of small and wide-angle X-ray scattering. Furthermore, for the first time, the glass transition temperatures of these polymers which are beyond or near to their degradation temperature are determined using Fast Scanning calorimetry employing high heating and cooling rates. The glass transition temperatures of the polymers decrease with increasing length of the alkyl side chain.

CPP 4.5 Mon 10:45 ZEU 255

Controlled crystallisation of luminescent borate-based glasses — •Marc Bürger[1], A. Charlotte Rimbach[1], and Stefan Schweizer[1,2] — [1]Faculty of Electrical Engineering, South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest

Luminescent borate glasses and glass ceramics offer a broad spectrum of optical applications. Here, the optical properties of the glass as well as the glass ceramic strongly depend on their composition and the production process. In this work, two different glass systems and their crystallization processes therein are analysed: (i) Lithium borate glass comprised of Li_2O-Al_2O_3-B_2O_3 and (ii) barium borate glass with BaO-B_2O_3. For optical activation, the lanthanide ion Dy^{3+} is added in the form of Dy_2O_3 to enable for a bright green-yellowish luminescence. To initiate the crystallization process in the glass, the samples are thermally-processed at a temperature above the glass transition temperature. The number and size as well as the phase of the grown crystallites depend significantly on annealing temperature and time as well as the heating rate. The crystallite growth is investigated and analysed in detail by differential scanning calorimetry and *in situ* x-ray diffractometry. In addition, the samples are optically characterized for transmittance, reflectance and scattering.

CPP 4.6 Mon 11:00 ZEU 255

X-ray computed tomography of glass foams with controlled bi-modal pore size distribution — •Cristine S. de Oliveira[1], Richard Kohns[2], Felix Meyerhoefer[2], Matthias Neumann[3], Dirk Enke[2], Volker Schmidt[3], Ralf B. Wehrspohn[1], and Juliana Martins de S. e Silva[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Institut für Technische Chemie, Universität Leipzig, Germany — [3]Institut für Stochastik, Universität Ulm, 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 followed by a phase-separation procedure and acid leaching. We used a powdered mixture of silica-based glasses, MnO_2 and C which we submitted to a foaming process at 815 °C. Afterwards, the material was left to cool inside the oven to temperatures around 500 °C and maintained at a constant temperature for phase separation. We then acid leached, washed and dried the samples. Based on the results obtained using X-ray CT at the micro and nanometer scales we observed that slight changes in the preparation procedure resulted in foams with different porosity, pore sizes, pore volumes and sphericity.

CPP 5: Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)

Time: Monday 9:30–11:15 Location: ZEU 114

CPP 5.1 Mon 9:30 ZEU 114

Dichroic FTIR spectrocopy on recombinant spider silk films at texturised silicon substrates — Mirjam Hofmaier[1,2], Birgit Urban[1], Sarah Lentz[3], Thomas Scheibel[3], Andreas Fery[1,2], and •Martin Müller[1,4] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry and Polymer Physics, D-01069 Dresden — [2]Technische Universität Dresden, Chair of Physical Chemistry of Polymeric Materials, D-01062 Dresden — [3]Universität

Bayreuth, Chair of Biomaterials, D-95447 Bayreuth, Germany — [4]Technische Universität Dresden, Chair of Macromolecular Chemistry, D-01062 Dresden

Films of recombinant spider silk protein eADF4 were deposited onto unidirectionally scratched silicon substrates (Si-sc) and analysed by dichroic transmission (T-) and ATR-FTIR spectroscopy addressing conformation and orientation. eADF4 films (d=0-200 nm) were casted from hexafluoroisopropanol solutions onto Si-sc. Both FTIR methods revealed low b-sheet (<10%) and high random coil content (>80%) based on Amide I band analysis. Dichroic ratios R of all Amide I components close to those of isotropic samples were found by T- and ATR-FTIR indicating no eADF4 orientation. Whereas, eADF4 films after swelling in MeOH vapor revealed higher b-sheet (>30%) and lower random coil content (<60%). By ATR-FTIR high R values for the Amide I component at 1696 cm-1 assigned to antiparallel b-sheet structure were found indicating out-of-plane orientation of b-sheets, which increased with decreasing thickness. Whereas, by T-FTIR isotropic R values indicating no in-plane orientation of b-sheets were found.

CPP 5.2 Mon 9:45 ZEU 114

Keratin films from human nail and hair as artificial nail plate model — •Kim Thomann, Andreas Späth, and Rainer H. Fink — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, 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, films from keratin extracted from human hair and nails were produced [1]. With the fingernail serving as reference, the KFs were characterized with a number of methods, including AFM, contact angle (CA) measurements, XPS, ATR-FTIR and Raman spectroscopy. In terms of composition, KFs show a good resemblance. The topography however differs as the films are much smoother than the micro-structured nail. CA measurements revealed that the surface free energy was in the same range, but the polar component was much stronger for the KFs compared to the fingernail. KFs matching the nail's microstructure represents one approach to achieve a more satisfying model, potentially realized by micro-contact printing.

[1] Lusiana, et al., Eur. J. Pharm. Biopharm. 2011, 78, 432

CPP 5.3 Mon 10:00 ZEU 114

Tracing the film formation of biotemplated titania nanostructures during spray coating with in situ GIXS techniques — •Julian E. Heger[1], Wei Chen[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

An interesting approach in soft matter science is to substitute synthetic polymers with biopolymers, such as proteins. Being water soluble and non-toxic, they open a way to greener processing. We are interested in the structure directing properties of the bovine whey protein ß-lactoglobulin (ß-lg) for thin titania films. For this, denatured ß-lg is mixed with established titania precursors to form a sol-gel, which can be eventually deposited. Spray deposition is chosen as a fast technique of low material wastage and hence of industrial relevance. In situ grazing incidence X-ray scattering measurements are performed simultaneously in small- and wide-angle regime (GISAXS/GIWAXS) to reveal the morphological changes and timescales of lateral growth upon film formation. After calcination of the as-deposited samples, the remaining titania scaffolds can be backfilled with organic semiconductors in order to build e.g. hybrid photoactive layers.

CPP 5.4 Mon 10:15 ZEU 114

Structural and physical properties of Cellulose/Silver nanoparticle multi-layer film by layer-by-layer deposition — Qing Chen[1], •Andrei Chumakov[1], Calvin Brett[1,2], Anton Plech[3], Peng Zhang[4], and Stephan Roth[1,2] — [1]Deutsche Synchrotron (DESY), 22607, Hamburg, Germany — [2]KTH Royal Institute of Technology, 10044, Stockholm, Sweden — [3]Karlsruhe Institut of Technology (KIT), 76021, Karlsruhe, Germany — [4]Sun Yat-sen University, 510275, Guangzhou, China

Silver nanoparticles and assembled structures thereof have attracted growing interest due to peculiar optical, electrical, catalytic and stimuli-responsive properties of these nanostructures during the past decade. We report a new strategy to fabricate multilayered cellulose/AgNP-based thin-film by layer-by-layer (LBL) coating method, and the kinetics during each layer coating cycle was monitored by using grazing incidence small-angle X-ray scattering (GISAXS). Multilayered films were prepared by spray-coating technique. Spray conditions and solvent treatment of cellulose and AgNP layer were optimized according to structural and morphological characterization for the formation of an AgNP layer and each cellulose interface. Atomic force microscopy (AFM) was performed to visualize the morphological characteristics of the film surface. Moreover, our strategy provides a platform for easy and scalable production of large-area AgNP LBL films.

CPP 5.5 Mon 10:30 ZEU 114

Self-assembly of aligned cellulose nanofibrils during gel drying — •Ariane Suzzoni[1], Calvin Jay Brett[1,2,3], Susumu Yada[1], Korneliya Gordeyeva[1], Stephan Volkher Roth[1,2], and Daniel Söderberg[1,3] — [1]KTH Royal Institute of Technology, SE-11428 Stockholm, Sweden — [2]Deutsches Elektronen-Synchrotron (DESY), D-22607 Hamburg, Germany — [3]Wallenberg Wood Science Centre, SE- 11428 Stockholm, Sweden

Cellulose nano fibrils (CNF) are largely studied in order to replace synthetic materials with natural ones. These materials based on natural fibers are an alternative to materials made from fossil energies, a big challenge in today's world. High mechanical performance can be related to the nanostructure of fibrils which composed the filaments. However, the mechanism involved is still unknown. A possible hypothesis is the mesoscale structure self-assembling occurs during consolidation and drying phase. Small Angle X-Ray scattering (SAXS) is a powerful technique to investigate the system arrangement at nanoscale. A flow-focusing system has been developed in a previous project to assemble CNF fibers with a highly ordered arrangement. The suspension formed using this microfluidic device is a gel containing a low concentration of CNF. SAXS experiments have been carried out directly on the gel filament lifted up in the air. The nanostructural changes were observed by SAXS during gel drying. We will present results obtained about the structure of cellulose nanofibrils as a function of drying time. This knowledge about CNF nanostructure formation will be a key to develop new eco-friendly materials.

CPP 5.6 Mon 10:45 ZEU 114

Wrinkling instability in 3D active nematics — Tobias Struebing[1], Amir Khosravanizadeh[2], Andrej Vilfan[1], Eberhard Bodenschatz[1], Ramin Golestanian[1], and •Isabella Guido[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettigen, Germany — [2]Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran

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 and subsequently loses order and transitions into a 3D active turbulent state. We observe that the wrinkle wavelength is independent of the ATP concentration and our theoretical model describes its relation with the appearance time. The experimental results are compared with a numerical simulation that confirms the key role of kinesin motors in the contraction and extension of the network.

CPP 5.7 Mon 11:00 ZEU 114

Viscoelastic AFM characterization of the S2 layer of wood pulp fibers — •Caterina Czibula[1,3], Christian Ganser[1,3], Tristan Seidlhofer[2,3], Ulrich Hirn[2,3], and Christian Teichert[1,3] — [1]Institute of Physics, Montanuniversitaet Leoben, Austria — [2]Institute of Paper, Pulp and Fibre Technology, TU Graz, Austria

— [3]CD Laboratory for Fiber Swelling and Paper Performance, TU Graz

Wood fibers consist of several cell wall layers which differ in thickness, chemical composition, and alignment of cellulose microfibrils. The S2 layer is the thickest layer, and dominates the mechanical behavior of the fibers. Several investigations with depth-sensing methods have so far focused on the characterization of the mechanical properties of the S2 layer. However, studies on the influence of relative humidity (RH) and the viscoelastic behavior of this layer are still missing. This work focusses on the viscoelastic behavior of the S2 layer at different RH by implementing an atomic force microscopy (AFM) based method. Here, wood pulp fibers have been prepared by microtome cutting, and a possible penetration of the embedding material in the cell wall layers has been ruled out by Raman spectroscopy. The evaluation of the experimental AFM data combines contact mechanics and viscoelastic models. It will be demonstrated that the Generalized Maxwell model yields reasonable results for the S2 layer measured at different RH. With increasing RH, the S2 layer shows a decrease in elastic and viscous parameters. The effect of different load rates will be discussed, and the viscoelastic results will be compared to AFM based nanoindentation data.

CPP 6: 2D Materials (joint session CPP/O)

Time: Monday 11:30–12:15 Location: ZEU 255

CPP 6.1 Mon 11:30 ZEU 255

Voltage-dependent quantitative analysis of electron-dose-limited resolution for imaging two-dimensional covalent organic framework — •Baokun Liang[1], Haoyuan Qi[1,2], Hafees Sahabudeen[2], Xinliang Feng[2], and Ute Kaiser[1] — [1]Central facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, University of Ulm, 89081 Ulm, Germany — [2]Department of Chemistry and Food Chemistry & Center of Advancing Electronics Dresden, Dresden University of Technology, 01062 Dresden, Germany

Two-dimensional covalent organic framework (2D COF) are promising candidates for organic electronics and next-generation energy storage. However, due to electron irradiation damage, high resolution (HR) TEM imaging of 2D COFs remains challenging, posing a substantial limitation on the structural elucidation of these organic 2D materials. Therefore, it is necessary to unravel the correlation between total electron dose and achievable specimen resolution for specific specimens. To investigate the relationship between total electron dose and achievable specimen resolution, we performed a dose-series analysis with 2D COF in electron diffraction mode under different acceleration voltages (300, 200, 120, 80 kV). With accumulating electron dose, the higher-order reflections gradually vanish, representing the degradation of specimen resolution. For quantitative analysis, the intensity of reflections within a specific resolution band was analyzed. Our method offers a quick and straightforward determination of dose-related specimen resolution under different voltages. These results lay the foundation for the HRTEM imaging of beam sensitive 2D COFs.

CPP 6.2 Mon 11:45 ZEU 255

Solvent interactions with two-dimensional materials: A computational investigation of the dispersion of graphene monolayers in commonly-used solvents. — •Urvesh Patil and Nuala Caffrey — School of Physics & CRANN, Trinity College, Dublin 2

Maintaining stable dispersions of two-dimensional (2D) materials is a prerequisite for several applications. The stability of dispersion, i.e., the ability of a solvent to maintain an adequate concentration of suspended flakes over time, depends strongly on the interaction between the 2D material and the chosen solvent. In order to identify the optimal solvent for a particular 2D material it is imperative to determine this interaction on the atomic scale. Here, we use density functional theory (DFT) combined with solvent models and molecular dynamics (MD) to study the interaction of graphene and MoS2 with solvent molecules such as NMP, cyclopentanone and toluene. Using DFT, we show that isolated solvent molecules interact via a van der Waals (vdW) interaction with pristine monolayers, with negligible charge transferred between them. MD calculations show that distinct solvation shells form around the 2D layer; the first solvation shell is formed as a result of vdW interaction irrespective of the polarity of solvent. This then interacts with rest of the solvent via a combination of both electrostatic and vdW forces. We show that the formation of this solvation shell is always favourable, and determine the relationship between the free energy of interaction and the experimental concentration of graphene in solution. Finally, we suggest a simple rule for mixing solvents that can be used to improve the 2D layer concentration in solution.

CPP 6.3 Mon 12:00 ZEU 255

Relation between topology and electronic structure of 2D polymers — •Maximilian A. Springer[1,2], Tsai-Jung Liu[2], Agnieszka Kuc[1], and Thomas Heine[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Research Site Leipzig, Permoserstrasse 15, 04318 Leipzig, Germany — [2]TU Dresden, Faculty of Chemistry and Food Chemistry, Bergstrasse 66c, 01062 Dresden, Germany

New 2D materials open access to a whole new world of compounds and properties. Graphene monolayer is such a material, since it has special electron transport features due to its honeycomb topology. Apart from the honeycomb net, there are many more 2D topologies which promise a manifold of new properties, e.g. the kagomé or the Lieb lattice. As recently shown in the case of the kagomé net, 2D polymers (covalent organic frameworks) can be designed in a way that their geometric and electronic structure match the desired topology [Y. Jing, T. Heine, J. Am. Chem. Soc. 2019, 141, 2, 743-747]. We investigate electronic properties including topological signatures of different 2D nets using a tight-binding approach. Based on these findings, we want to propose new 2D polymers with the desired structures and new properties using density-functional theory.

CPP 7: Hydrogels and Microgels

Time: Monday 12:30–13:00 Location: ZEU 255

CPP 7.1 Mon 12:30 ZEU 255

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 sub-micron 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.

CPP 7.2 Mon 12:45 ZEU 255

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

Time: Monday 9:30–13:00 Location: HÜL 386

Invited Talk CPP 8.1 Mon 9:30 HÜL 386

Spontaneous and driven active matter flows — •Eric Clement — PMMH-ESPCI-Sorbonne University, Paris, France

Understanding the individual and the macroscopic transport properties of motile micro-organisms in complex environments is a timely question, relevant to many ecological, medical and technological situations. At the fundamental level, this question is also receiving a lot of attention as fluids loaded with swimming micro-organisms has become a rich domain of applications and a conceptual playground for the statistical physics of active matter. The existence of microscopic sources of energy borne by the motile character of micro-swimmers is driving self-organization processes at the origin of original emergent phases and unconventional macroscopic properties leading to revisit many standard concepts in the physics of suspensions. In this presentation, I will report on a recent exploration on the question of collective motionspontaneous formation, in relation with the rheological response of active suspensions. I will also present new experiments showing how the motility of bacteria can be controlled such as to extract work macroscopically.

CPP 8.2 Mon 10:00 HÜL 386

Light-regulated motility of microbial suspensions induces phase separation in confinement — •Alexandros Fragkopoulos[1], Jeremy Vachier[1], Johannes Frey[1], Flora-Maud Le Menn[1], Michael Wilczek[1], Marco Mazza[1,2], and Oliver Bäumchen[1] — [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

A highly concentrated suspension of self-propelled particles can form large-scale concentration patterns, separating into regions of high and low particle concentrations, due to the activity of the particles and their mutual interactions. However, such a phenomenon has so far been rarely seen in biological systems. Here, we present that a sufficiently concentrated suspension of *Chlamydomonas reinhardtii* cells, a model organism of puller-type microswimmers, forms such large-scale aggregations under confinement in specific light conditions. We find that cell-cell interactions need to be dominated by collisions for the aggregation to form, resulting to a generic coupling of the cell's motility and local cell density. In addition, the cell's motility decreases with decreasing light intensity, which regulates the cell aggregation. Through active Brownian particle simulations, we show that for our system the change of the motility is sufficient to induce the aggregation. Finally, we provide evidence that the photosynthetic activity controls the cell's motility, and consequentially, the separation of the active suspension into regions of high and low cell density.

CPP 8.3 Mon 10:15 HÜL 386

Motility induced transport in microbial environments — •Jayabrata Dhar, 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 industry due to high local concentrations. Studies in aquatic ecosystems have demonstrated nutrient mixing via bioconvection by high concentrations of motile microbes [1] potentially impacts species distributions in natural settings. However, to date, we lack a systematic framework to capture the role of microbial traits (for instance, morphology or motility) on the onset and progression of bioconvection. Here, using different bloom-forming algal species as model organisms, we study how microbial traits underpin the onset of bioconvection and modulate mass transfer due to local density changes. Combining micro-PIV analysis of dispersed particles and auto-fluorescence imaging of algal cells, we quantify the emergent transport properties in real-time, revealing a plume-driven primary convective field. Interestingly, our results further capture relatively weak, secondary eddies that create local mixing patches with short lifetimes. Thus, bioconvection may alter the chemical environment of the microbes through distinct modes, impacting the distribution of nutrients, toxins or secondary metabolites, all of which could be vital for large-scale phenomena like harmful algal blooms.

[1] T. Sommer, et al., Geophysical Research Letters 44, 9424, 2017.

CPP 8.4 Mon 10:30 HÜL 386

Reactivation of isolated axonemes by light-driven ATP regeneration system — Raheel Ahmed[1], Christin Kleinberg[2], Tanja Vidakovich-Koch[2], Kai Sundmacher[2], Eberhard Bodenschatz[1], and •Azam Gholami[1] — [1]MPI for Dynamics and Self-Organization — [2]MPI for Dynamics of Complex Technical Systems

Cilia and flagella are slender cellular appendages whose regular beating pattern pumps fluids, for example the mucus in mammalian airways, or propels unicellular organisms such as the green algae Chlamydomonas reinhardtii. Cilia and flagella have a microtubule-based structure called axoneme which performs whip-lash-like motion to provide motility. This oscillatory motion is powered by dynein molecular motors that generate active stresses for ciliary beat in the presence of ATP. In this work, we have successfully integrated light-driven energy module for continuous generation of ATP. This light-driven ATP regeneration system is built through bottom-up assembly of FOF1- ATP synthase and bacteriorhodopsin into two different types of artificial hybrid membranes based on a diblock copolymer (PBd-PEO) and a graft copolymer (PDMS- g-PEO). After illumination of the energy module with light, we mixed it with axonemes isolated from Chlamydomonas reinhardtii and observed actively beating axonemes for many hours. Interestingly, the axonemes beat even at low concentrations of ATP well below 50 μM.

CPP 8.5 Mon 10:45 HÜL 386

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 multimode 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. coffee break

CPP 8.6 Mon 11:30 HÜL 386

Synthetic minimal active cilia — •Isabella Guido — Max Planck Institute for Dynamics and Self-Organization, Goettigen, Germany

Cilia and flagella are microtubule based filamentous organelles that protrude into the extracellular environment from the surface of many cells for promoting fluid transport or propelling organisms in fluids by producing rhythmic bending waves. The main contribution to their beating is due to motor proteins that drive sliding of the microtubule doublets. However, the fundamental mechanism of the motor-microtubule interaction is still a puzzle. Here we present a synthetic minimal active cilium, a two-filaments system, in which the beat is initiated by a buckling instability in one of the filaments. The system presents continuous beating through association and dissociation cycles, similar to the sliding of a pair of doublet microtubules observed in a Chlamydomonas flagellum. The analysis of the conformational dynamics gives us a quantification of dynein force, motor density and bending energy. We develop a theoretical model to study the dynamics of active elastic filaments induced by internal force in which the attachment and detachment kinetics of motors play as important a role as their force generation. The active stroke of the synthetic cilium occurs due to a buckling instability between two clamped filaments, while the recovery stroke follows a "catastrophic failure" of the bound motors.

This work is in collaboration with Prof. Ramin Golestanian and Dr. Andrej Vilfan.

CPP 8.7 Mon 11:45 HÜL 386

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.

CPP 8.8 Mon 12:00 HÜL 386

Self-organization of active surfaces — •Alexander Mietke[1,2,3,4,7], V. Jemseena[5], K. Vijay Kumar[5], Ivo F. Sbalzarini[2,3,4,6], and Frank Jülicher[1,3,6] — [1]MPI for the Physics of Complex Systems — [2]Faculty of Computer Science, TU Dresden — [3]Center for Systems Biology Dresden — [4]MPI of Molecular Cell Biology and Genetics — [5]ICTS-TIFR — [6]Cluster of Excellence PoL, TU Dresden — [7]Department of Mathematics, MIT, Cambridge, MA

Self-organization of morphogenetic events often arises through a feedback loop in which active forces, by inducing deformations and material flows, indirectly affect their own mechano-chemical regulation. In recent years, the existence of generic mechano-chemical patterning mechanisms in simple, fixed geometries has been demonstrated theoretically and experimentally. However, the interplay of mechano-chemical processes with the surface geometry remains to be explored. In our work, we employ the theory of active gels in complex geometries to study the properties of dynamically evolving active surfaces. Within those surfaces, diffusive and advective transport processes can redistribute molecules responsible for local stress generation. This resembles the interplay between active forces, the shape changes they imply and the effects this has on their regulation. Within our framework, a contractile ring formation, as well as the peristaltic motion of active tubular structures can be understood as natural emergent phenomena. Our approach provides novel opportunities to explore different scenarios of mechano-chemical self-organization and can help to better understand the role of shape as a regulatory element in morphogenetic processes.

CPP 8.9 Mon 12:15 HÜL 386

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 states.

CPP 8.10 Mon 12:30 HÜL 386

Fast vs. gradual death in assemblies of immotile growing cells — •Yoav G. Pollack, Philip Bittihn, and Ramin Golestanian — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Göttingen, Germany

Cell life-cycle processes such as growth, division and death, often all happen on a similar timescale, as do the resultant mechanical and dynamical responses of the cell assembly (such as a colony, biofilm or tissue). An archetypal example is *E. Coli* where growth, division and the subsequent relative motion of the daughter cells all happen at roughly the same rate. However there are also examples of another type of system showing abrupt processes, including 'snapping' cell division in *Actinobacteria* and 'explosive' bacterial lysis.

Here we test whether going from the first type of system to the other by introducing a second *fast* timescale in one of the microscopic processes can affect the macroscopic mechano-dynamics, such as the homeostatic pressure. Specifically we simulate a closed 1D channel of cells that grow and divide to fill up the channel and are removed (via death or extrusion) when pressure builds up. We focus on varying the timescale of the cell removal process, keeping growth and division timescales fixed. We show a clear distinction in the macroscopic system properties between abrupt vs. gradual cell removal, such as a significant increase in the homeostatic pressure.

CPP 8.11 Mon 12:45 HÜL 386

Simulations of an active surface immersed in viscous fluids — •Lucas D. Wittwer and Sebastian Aland — Faculty of Informatics / Mathematics, University of Applied Science Dresden, Germany

Mechanochemical processes play a crucial role during morphogenesis, the formation of complex shapes and tissues out of a single cell. On the cellular level, the actomyosin cortex governs shape and shape changes. This thin layer of active material underneath the cell surface exerts an active contractile tension, the strength of which being controlled by the concentration of force-generating molecules. Advective transport of such molecules leads to a complex interplay of hydrodynamics and molecule concentration which gives rise to pattern formation and self-organized shape dynamics.

In this talk, we present a novel numerical model to simulate an active surface immersed in viscous fluids. We show the resulting patterning and cell shape dynamics for different parameter configurations as well as the flow profiles in the surrounding fluids and compare it to results from other models.

CPP 9: Organic semiconductors I (joint session HL/CPP)

Time: Monday 9:30–12:30 Location: POT 112

CPP 9.1 Mon 9:30 POT 112

Towards a plastic brain — •Matteo Cucchi, Hans Kleemann, Hsin Tseng, Alexander Lee, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, 01062 Dresden, Germany

Interconnectivity, fault tolerance and dynamic evolution of the circuitry have been long sought-after objectives of bio-inspired electronics and engineering. The massive parallelization of the neuronal circuitry grants the human brain superior efficiency and capabilities in cognitive learning and pattern recognition compared to digital, transistor-based machines. Here, we developed a technique to grow conductive networks and artificial synapses based on organic semiconductors. Their dendritic growth, stimulated by an AC signal, resembles the formation of new synapses in the nervous system (synaptogenesis). Moreover, their functions in saline solution emulate numerous brain features over multiple orders of magnitude in the time domain, such as learning, forgetting, time-dependent-spiking plasticity, and Pavlovian conditioning. We employ the artificial synapses to show a new device-concept capable of recognizing numerical patterns and explore possible pathways towards biocompatibility, neuroprosthetics and brain-inspired computing.

CPP 9.2 Mon 9:45 POT 112

Dibenzopentacene single crystals: growth, characterization and exciton dispersion — •Lukas Graf, Fupin Liu, Bipasha Debnath, and Martin Knupfer — IFW Dresden

Pentacene and its hydrocarbon relatives continue to attract researchers world-wide, as they promise applications due to their relatively high charge carrier mobilities and their intriguing photophysical behavior including singlet fission processes. We have studied a relatively unexplored member of this family, Dibenzopentacene (DBP).

Single crystals of DBP have been grown using the vapor phase transport method, which to the best of our knowledge are the first DBP single crystals reported so far. We have determined the DBP crystal structure using X-ray diffraction and complementary electron diffraction experiments. The electronic excitations of DBP have been investigated using electron energy-loss spectroscopy (EELS). We present results on the strongly anisotropic electronic excitations across the band gap, and in addition their momentum behavior, i.e. their dispersion. An analysis of this exciton dispersion using a simple model from the literature allowed to gain first information on the charge carrier hopping parameters in DBP.

This is supported by the DFG (KN393/25, KN293/26).

CPP 9.3 Mon 10:00 POT 112

Self-alignment OTFT structures — •Jörn Vahland, Hans Kleemann, and Karl Leo — TU Dresden, IAP

Organic thin film transistor (OTFT) parameters have significantly improved in regard to static transistor performance, e.g. contact resistance and mobility. The dynamic performance, though, is mainly governed by the device capacitance. A large device capacitance restricts the switching frequency and might ultimately lead to inefficient circuits. Historically, this limitation has been overcome in inorganic device architectures by employing a so-called self-aligned gate structure, which allows structuring of source- and drain-electrode with virtually no overlap to the gate, yielding low overlap capacitance.

The transfer to OTFTs is not trivial, since subtractive process steps such as etching need to be selective to various materials within a typical device stack i.e. the semiconductor and the gate dielectrics. First implementations of self-alignments for OTFTs employ process steps which are unfortunately not scalable (such as through-plane exposure or lift-off), effectively prohibiting such devices in actual circuits.

We propose a coplanar OTFT in top gate configuration where selective etching processes and additional passivation layers are used in order to form a truely self-aligned organic transistor. We discuss the scaling of the overlap capacitance and highlight the potential of such self-aligned devices for high-frequency operation. Furthermore, we discuss the influence of etching process on the channel properties, and describe how charge carrier mobility and on/off ratio of the transistor can be preserved.

CPP 9.4 Mon 10:15 POT 112

Exciton dispersion in rubrene single crystals — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster

Rubrene single crystals are proposed as components of various organic (opto-)electronic devices. Their electronic (quasiparticle) bandstructure shows an anisotropic behaviour with a relatively strong dispersion of several 100 meV along the Γ-Y direction, whereas the bands are almost flat along the Γ-X direction [1].

Corresponding to the electronic bands, excitons can also exhibit dispersion of their excitation energies as a function of their total momentum (related to their centre-of-mass motion). This dispersion and its anisotropy might be relevant for excitonic hopping transport. In this talk we use the GW/BSE approach of many-body perturbation theory (MBPT) to calculate the excitonic bandstructure of rubrene single crystals in order to investigate if the anisotropy is still present or mitigated by excitonic effects.

[1] S. Yanagisawa et al., Phys. Rev. B **88**, 115438 (2013)

CPP 9.5 Mon 10:30 POT 112

Conductivity studies at the crystal-film charge transfer interfaces — •Bipasha Debnath[1], Michael Bretschnieder[1], Shu-Jen Wang[2], Martin Knupfer[1], Yulia Krupskaya[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Material Research Dresden, Dresden, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAP), Dresden, Germany

The charge transfer occurs at the interface of two organic semiconductor materials known as donor and acceptors. The alignment of the electron affinity of one material with the ionization potential of other material leads to enhance electrical conductivity at their interface by exchanging charge carriers between them. Herein, we try to explore the underlying mechanism of charge transfer with a systematic study by preparing interfaces between Rubrene and F6-TCNNQ, as donor and acceptor semiconductor materials, respectively. By thermally evaporating F6-TCNNQ film on the surface of highly-ordered Rubrene single-crystals, the charge transfer interfaces are fabricated. The electrical characterization of these interfaces reveals enhanced conductivity. Furthermore, temperature-dependent measurements demonstrate thermally activated conductivity. The fundamental properties such as charge carrier density and mobility are investigated through additional Hall-effect measurements. This work is financially supported by DFG (KR 4364/4-1)

30 min. break.

CPP 9.6 Mon 11:15 POT 112

Investigation of biodegradable devices — •Kevin Krechan[1], Daniel Firzlaff[2], Hans Kleemann[1], Karl Leo[1], and Kathrin Harre[2] — [1]Technische Universität Dresden, Deutschland — [2]HTW Dresden, Deutschland

In an aging society there is an increasing need for innotative health care and monitoring solutions. Sensor solutions for health monitoring are vital for improved treatment quality and the reduction of costs.

In particular, there is a strong need to continuous postoperative in-vivo surveillance systems. However, such sensor systems are required to be bio-compatible and ideally biodegradable in order to undesired postoperative complications.

In this contribution we discuss sensor concepts for e.g. in-vivo pressure or ion sensing based on bio-compatible organic semiconductor materials. Most importantly, we make use of biodegradable collagen-based substrate materials and discuss their decomposition behavior as well as the associated challenges during the fabrication of the sensor system. Overall, we believe that our approaches will enable the development of fully degradable sensor tags in future.

CPP 9.7 Mon 11:30 POT 112

High-gap donor-acceptor blends exhibiting both efficient emission and charge-generating properties — •Xiangkun Jia[1], Sascha Ullbrich[1], Johannes Benduhn[1], Vasileios C. Nikolis[1], Jinhan Wu[1], Yuan Liu[1], Axel Fischer[1], Donato Spoltore[1], Sebastian Reineke[1], and Koen Vandewal[1,2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Hasselt University, Hasselt, Belgium

We demonstrate that the intermolecular charge-transfer (CT) states at the donor-acceptor interfaces are crucial for the operation of organic optoelectronics. Such D-A based OLEDs show electroluminescence external quantum yields (EQE_{EL}) of up to 16%, while in contrast, D-A systems for state-of-the-art OSCs typically only feature $EQE_{EL} \approx 0.01 - 0.0001\%$. The dominating non-radiative recombination in the latter is the main reason for their large voltage losses and low power-conversion efficiencies. Here, we adopt high-gap materials to increase the energy of CT states. This blend shows a fill factor of 70% and an internal quantum efficiency of 83% upon solar illumination, comparable to well performing OCSs. Meanwhile, its non-radiative voltage loss is reduced to $0.10V$ and EQE_{EL} reaches 1.5%. This work therefore shows that efficient photogeneration of free carriers and a high electroluminescence quantum yield do not necessarily need to be mutually exclusive in organic semiconductors.

CPP 9.8 Mon 11:45 POT 112

Quantifying the Damage Induced by Monoatomic Ion Beam Etching during X-ray Photoemission Spectroscopy Depth Profiling of Conjugated Polymers — •Yvonne Jasmin Hofstetter[1,2] and Yana Vaynzof[1,2] — [1]Integrated Center for Applied Physics and Photonics, Dresden, Germany — [2]Center for Advancing Electronics Dresden, Dresden, Germany

X-ray photoemission spectroscopy (XPS) depth profiling using monoatomic Ar+ ion etching sources is commonly used to probe the vertical compositional profiles of polymer-based organic photovoltaic devices, focusing on compositional variations across interfaces and vertical phase separation within bulk-heterojunction active layers. The damage induced by the monoatomic etching is generally considered to be very shallow and is assumed to not significantly alter the XPS signal acquired at each step of the depth profile. Herein, we quantify the damage depth for a variety of conjugated polymers for monoatomic Ar+ ion beams of variable energy from 0.5 to 4 keV. Our results indicate that even when etching with the lowest available ion beam energy for as little as 3 s, the damage inside the polymer bulk material significantly exceeds the XPS probing depth (approx. 10 nm). We find that the damaged material exhibits a distorted composition which strongly changes the resulting XPS depth profile. In contrast, we find that Ar gas cluster ion beam etching is significantly less damaging and preserves compositional information demonstrating its superior suitability for XPS depth profiling of organic materials.

CPP 9.9 Mon 12:00 POT 112

Momentum dependent investigation of electronic excitations in β-metal-phthalocyanines — •Louis Philip Doctor and Martin Knupfer — Leibniz Institut für Festkörper- und Werkstoffforschung, Helmholtz Str. 20, 01069 Dresden

This work presents an investigation of the electronic excitations of β-metal-phthalocyanines. We prepared 120 nm thick thin films by physical vapour deposition, which afterwards underwent an annealing process. Infrared spectroscopy revealed that the annealed films were in the β-phase. The films were further characterised in the visible regime. The prominent feature in this regime is the Q-band, which consists of four peaks arising from the HOMO to LUMO transition split by solid-state effects. Furthermore, the dispersion of the Q-band was measured using electron energy loss spectroscopy. We found a complex momentum dependent behaviour. Most interesting is the negative dispersion of the lowest-lying excitation, which also has a tremendous effect on the performance of optoelectronic devices. This redshift partially correlates with the intermolecular distance and the charge carrier transfer integrals. The latter were determined by a theoretical model, which describes the interaction of Frenkel and charge transfer excitons in metal-phthalocyanines. Our results clearly indicate a prominent influence of charge transfer excitons to the lowest electronic excitations.

CPP 9.10 Mon 12:15 POT 112

Comparing Charge Generation and Extraction in Y6 and LM11 Devices — •Seyed Mehrdad Hosseini[1], Yingping Zou[2], and Safa Shoaee[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, Potsdam-Golm D-14476, Germany — [2]College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, P.R. China

In the last few years, non-fullerene acceptors (NFA) have dominated organic solar cells. Whilst in thin films, exceptional fill-factor (FF) can be obtained, in thicker junctions however, FF is usually affected. Reduced FF is the manifestation of voltage-dependent charge photogeneration and/ or inefficient free charge extraction3. In this study, we compare two NFAs, named Y6 and LM11, when blended with PM6. Our results show that although PM6:LM11 device has a higher open-circuit voltage (Voc) than PM6:Y6, lower FF limits the efficiency. We employed time-delayed collection field (TDCF) measurements to reveal the reason behind the poorer FF in PM6:LM11 device by studying charge generation and recombination in both systems.

CPP 10: Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar I (joint session HL/CPP)

Hybrid halide perovskites are by now well established solar absorber and emitter materials, with power conversion efficiencies of single cell devices exceeding 20%. We have observed - with notable exceptions - a widening gap between experimental and theoretical efforts in the literature on halide perovskites. Further, a large fraction of the literature focuses on properties relevant for optoelectronic applications, while we envision a much wider scope for these materials, e.g in spintronic and electro-chemical applications. The purpose of this focus session is to provide a platform for theorists and experimentalists working in this field, to interact, present state-of-the-art methods, and exchange their ideas on future directions for this technologically relevant class of materials beyond the current focus on optoelectronics.

Organizers: Linn Leppert (Universiät Bayreuth) and Felix Deschler (TU Munich)

Time: Monday 9:30–12:00 Location: POT 251

Invited Talk CPP 10.1 Mon 9:30 POT 251

Anharmonic semiconductors - Lessons Learned from Halide perovskites — •Omer Yaffe — Weizmann Institute of Science, Rehovot, Israel

In semiconductor physics, the dielectric response, charge carrier mobility and other electronic material properties at finite temperatures, are always treated within the framework of the harmonic approximation. This approach is very successful in capturing the properties of tetrahedrally bonded semiconductors such as silicon and GaAs.

In my talk, I will show that 2D and 3D halide perovskites are fundamentally different due to their strongly anharmonic lattice dynamics. Large amplitude, local polar fluctuations induced by lattice anharmonicity localize the electronic states and enhance the screening of electric charge within the material. In other words, in some aspects, halide perovskites behave more like a liquid than a crystalline solid. I will also discuss the implications of these findings on other families of semiconductors such as organic and rock-salt semiconductors.

Invited Talk CPP 10.2 Mon 10:00 POT 251

Lattice Screening of Excitons in Lead Halide Perovskites from First Principles — •Marina R. Filip[1], Jonah B. Haber[2], and Jeffrey B. Neaton[2,3,4] — [1]Department of Physics, University of Oxford — [2]Department of Physics, UC Berkeley — [3]Molecular Foundry and Materials Science Division, Lawrence Berkeley National Laboratory — [4]Kavli Energy NanoSciences Institute at Berkeley

Dielectric screening in semiconducting and insulating crystals generally originates both from electrons and polar phonons. Since photoexcited electron-hole pairs interact within this dielectric environment, both the electronic and lattice components of the screening can have important contributions to excitonic properties; for lead-halide perovskites, this is suggested from both theoretical and experimental evidence [1,2]. However, standard ab initio GW-BSE methodology for calculating optical excitations does not capture dynamic lattice polarization effects. In this talk I will present our extension of the GW-BSE method, to include lattice contributions to the screening. I will show that in heteropolar semiconductors with weakly bound excitons, dynamic lattice polarization can significantly reduce the exciton binding energy, and I will demonstrate this effect for the CsPbX3 (X = Cl, Br, I) perovskites. Furthermore, I will discuss more generally the lattice contribution to the exciton binding energy in heteropolar semiconductors, as it emerges from a generalization of the Wannier-Mott model to include dynamical lattice polarization effects. [1] Miyata et al, Nat. Phys. 11, 582 (2015) [2] Umari et al, JPCL, 9, 3, 620 (2018). Work supported by the US DoE in the C2SEPEM center; computational resources from NERSC.

15 min. break.

Invited Talk CPP 10.3 Mon 10:45 POT 251

Structural dynamics and disorder in halide perovskites — •David Egger — Department of Physics, Technical University of Munich, 85748, Garching, Germany

Halide perovskites (HaPs) are highly promising materials for several optoelectronic applications. HaPs are also very interesting scientifically because of the peculiar structural dynamics that occur in the material. These include the appearance of massive structural disorder and anharmonic effects already at room temperature, which challenge our currnent understanding of coupling between lattice vibrations and optoelectronic properties in a semiconductor.

In this talk, I will present our recent explorations of the consequences of the unusual structural phenomena in HaPs for their optoelectronic properties. Theoretical calculations based on density functional theory, molecular dynamics, and tight-binding modeling will be used to examine the impact of structural dynamics on pertinent device-relevant observables. Consequences of the structural dynamics and anharmonicity in HaPs will be discussed for the charge-carrier mobility, Urbach energy, and defect energetics. It will be shown that the impact of the unusual structural dynamics on the optoelectronic properties of HaPs cannot be neglected when understanding these materials microscopically and designing new functional compounds.

CPP 10.4 Mon 11:15 POT 251

Optoelectronic properties of lead-free double-perovskites from first principles — •Raisa I. Biega[1], Marina R. Filip[2,3], Linn Leppert[1], and Jeffrey B. Neaton[2,3,4] — [1]Institute of Physics, University of Bayreuth, Bayreuth, Germany — [2]Department of Physics, University of California, Berkeley, USA — [3]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Kavli Energy NanoSciences Institute, Berkeley, USA

Power conversion efficiencies of single junction solar cells with lead-based halide perovskite absorbers have exceeded 25%. However, stability concerns have stimulated efforts for finding substitutes with similar optoelectronic properties, i.e., small band gaps, low effective masses and small exciton binding energies. Double perovskites containing alternating mono- and trivalent metal cations have emerged as one such alternative. Here we present first principles calculations of the electronic structure and excited states of the double perovskites Cs_2AgBX_6 (B=Bi, Sb and X=Br, Cl). We use density functional theory and *ab initio* Green's function-based many-body perturbation theory within the GW and Bethe-Salpeter equation approach to calculate band structures and absorption spectra of these materials. Our results provide insights into the nature of optical excitations and suitability for photovoltaic and other light harvesting applications.

We acknowledge computational resources provided by NERSC, a DOE Office of Science User Facility supported by the U.S. Department of Energy and financial support by the DFG Programs SFB840 and GRK1640.

CPP 10.5 Mon 11:30 POT 251

First principles calculations for blue-emitting organic-inorganic halide perovskites — •Ivor Loncaric[1], Luca Grisanti[1], Jasminka Popovic[1], and Aleksandra Djurisic[2] — [1]Rudjer Boskovic Institute, Zagreb, Croatia — [2]The University of Hong Kong

Ruddlesden-Popper halide perovskite (RPP) materials are of significant interest for light-emitting devices since their emission wavelength can be controlled by tuning the number of inorganic layers n. However, RPP films typically contain phases with different n which hinders the achievement of pure blue emission from n=2 films. Furthermore, energy funneling phenomenon, which involves energy transfer from lower n (higher energy) to higher n (lower energy) domains resulting in a brighter, but red-shifted emission, represents the further difficulty in obtaining pure blue emission from n=2 RPP emitters. By performing DFT calculations at room temperature we obtained an improved understanding of the effect of spacer cation on RPP properties. The calculations can be compared to real experimental conditions and give an insight into the feasibility of the stabilization of n=2 perovskite phase.

CPP 10.6 Mon 11:45 POT 251

Computing temperature-dependent band gap distributions of halide perovskites with a first-principles tight-binding approach — •Maximilian J. Schilcher[1], Matthew Z. Mayers[2], Liang Z. Tan[3], David R. Reichman[2], and David A. Egger[1] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Department of Chemistry, Columbia University, New York, NY 10027, USA — [3]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Due to their remarkably soft lattice and large temperature-induced nuclear fluctuations, it is challenging to understand the microscopic origin of the fascinating optoelectronic properties of halide perovskites (HaPs). In order to reveal their electronic and optical characteristics, one can apply well-established theoretical methods, such as density functional theory (DFT). However, conventional DFT calculations are limited in addressing the impact of complex structural effects in HaPs that require the simulation of large supercell sizes and nuclear dynamical phenomena.

In this work, we employ a recently developed tight-binding (TB) approach [1], which is parametrized on the basis of DFT calculations, and apply it to trajectories obtained from efficient molecular dynamics calculations at various temperatures. We compute dynamic band-gap distributions for several HaPs to estimate the influence of temperature on these distributions, in order to explain the electronic and optical characteristics of HaPs around room temperature.

[1] M. Z. Mayers, et al., Nano Lett. 18, 8041-8046 (2018).

CPP 11: Focus: Phase Separation in Biological Systems I (joint session BP/CPP)

Time: Monday 9:30–12:45 Location: SCH A251

CPP 11.1 Mon 9:30 SCH A251

ATP-arrested phase separation of an abundant nuclear protein — •Davide Michieletto — University of Bath

The formation and regulation of phase separated condensates is an important and ubiquitous process in biology. However, the biological functions of these condensates and how they are regulated, i.e. assembled and disassembled in vivo, are still poorly understood

I will present our recent work on an abundant nuclear protein called Scaffold Attachment Factor A, or SAF-A, that is involved in organizing the genome. It contains an intrinsically disordered RNA binding domain and an ATP-binding and hydrolysis domain. We discovered that the RGG domain of this protein undergoes phase separation in the nucleus upon transcriptional inhibition and that the size of the droplets can be controlled by tuning the amount arginine/lysine residues in the RGG domain and, more importantly, the coarsening of these droplets is arrested when the RGG domain is fused with the ATPase domain. To explain our findings, we propose a non-equilibrium extension of the classical Model B equations in which AAA-RGG fragments can switch between binding and non-binding states.

In summary, we provide evidence that not only does SAF-A undergo phase separation but we are able to show that this behavior can be regulated using an ATP-switch linked to its functional role in the nucleus.

CPP 11.2 Mon 9:45 SCH A251

Experimental measurement of the phase diagram of liquid-liquid phase separating proteins and peptides — •Emmanouela Filippidi[1,2], Anthony Hyman[1], and Frank Jülicher[2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Pfotenhauerstrasse 108

Peptides and proteins of a variety of organisms are known to undergo liquid-liquid phase separation to a dense and a dilute phase under certain conditions of temperature, pH, salt and macromolecular concentrations. Our goal is to create and study model peptide systems with sequences inspired by proteins in order to study the effect of amino acid sequence to phase separation. Herein, we will present parallel studies of both a protein, FUS, and simplified peptides of known, repetitive sequences.

As our first step, we will present quantitative measurements of both branches of the binodal curves of the phase diagrams obtained via quantitative phase imaging microscopy. We shall focus on how the multiplicity (multivalency) of pi-cation interactions at constant linear density affects their phase diagrams.

CPP 11.3 Mon 10:00 SCH A251

Measuring protein concentrations in biomolecular condensates via quantitative phase microscopy — •Patrick M McCall[1,2], K Kim[3], J Wang[1], AW Fritsch[1], A Poznyakovskiy[1], B Diederich[4], M Kreysing[1], R Heintzmann[4], J Guck[3], S Alberti[3], J Brugués[1,2], and AA Hyman[1] — [1]MPI-CBG, Dresden — [2]MPI-PKS, Dresden — [3]TU Dresden — [4]Leibniz IPhT, Jena

Many compartments in eukaryotic cells are protein-rich biomolecular condensates formed via phase separation from the cyto- or nucleoplasm. Although knowledge of condensate composition is essential for a full description of condensate properties and potential functions, measurements of composition pose a number of technical challenges. To address these, we use quantitative phase microscopy and optical diffraction tomography to measure the refractive index of model condensates, from which the protein concentration may be inferred. Here, model condensates are formed by phase separation of purified protein constructs derived from the primarily disordered RNA-binding domain (RBD) of TAF15. Surprisingly, we find that phase separation of TAF15(RBD) is attenuated only weakly by salt (0.05-3 M KCl) or temperature (10-50 °C), suggesting that Coulombic and entropic interactions, respectively, play only minor roles in controlling the phase equilibria. Interestingly, we also find that partition coefficients determined by fluorescence microscopy dramatically underestimate protein concentrations in condensates. A simple model including inner filter and excited-state saturation effects suggests that the discrepancy stems primarily from reduced fluorescence quantum yields in condensates.

CPP 11.4 Mon 10:15 SCH A251

Phase separation in protein solutions – a colloid physics' perspective — •Florian Platten and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Protein solutions undergoing phase separation are relevant for physiological functions (e.g., intracellular compartmentalization), disease pathology (e.g., cataract and amyloid plaque formation), biopharmaceutical formulations (e.g., their solubility and aggregation stability), the tunable design of soft solids (e.g., food gels) as well as a non-classical route to crystallization. The metastable liquid-liquid phase separation of lysozyme solutions was studied in terms of their phase coexistence temperatures and static structure factors $S(Q)$. If scaled by a property of dilute solutions, namely the second virial coefficient B_2, instead of temperature, the experimental binodals fall onto a master curve, which is similar to that of an adhesive hard-sphere fluid; i.e., the extended law of corresponding states holds for protein solutions. Accordingly, $S(Q)$ of moderately concentrated solutions can be described by B_2 using Baxter's model. The interactions between protein molecules – even in test tubes – are highly complex, i.e., patchy and directional. Nevertheless, coarse-grained colloid models provide effective descriptions. These simple models facilitate further insights into the physics of protein phase separation.

CPP 11.5 Mon 10:30 SCH A251

Kinetics and dynamics of LLPS in protein solutions exhibiting a LCST phase behavior probed by XPCS — •Anastasia Ragulskaya[1], Anita Girelli[1], Nafisa Begam[1], Hendrik Rahmann[2], Fabian Westermeier[3], Fajun Zhang[1], Christian Gutt[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]DESY, Hamburg

Kinetics and dynamics of liquid-liquid phase separation (LLPS) are usually intimately intertwined. We investigated a model system of bovine serum albumin (BSA) with YCl_3 which shows a lower critical solution temperature (LCST) phase behavior [1]. The dynamics of spinodal decomposition after a temperature jump was studied by X–ray photon correlation spectroscopy (XPCS) and the kinetics was probed simultaneously by ultra-small angle X–ray scattering (USAXS). The analysis of two-time correlation functions obtained from XPCS shows a two-mode behavior of the dynamics. The slow mode has a relaxation rate behavior similar to the kinetic one and corresponds to the transition from a density fluctuation to a coarsening stage. The relaxation time of the fast mode has a transition from an exponential growth to a monotonic increase with a modulation as a function of time, corresponding to the further growth of domains. Results are supported by Cahn-Hilliard simulations [2]. The work demonstrates the successful use of XPCS in USAXS-mode approach to study evolution of the domains during LLPS .

[1] O.Matsarskaia et. al., Phys. Chem. B, 120 (2016), 5564.
[2] D. Sappelt, J. Jäckle, Physica A , 240 (1997) , 453.

CPP 11.6 Mon 10:45 SCH A251

Quantitative droplet FRAP based on physical principles — •Lars Hubatsch[1,2], Louise Jawerth[1,2], Anthony Hyman[2], and Christoph 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

Fluorescence recovery after photobleaching (FRAP) is used to characterize a range of dynamic processes, for example binding kinetics and mobility of intracellular proteins, and recently liquid-liquid phase separation (LLPS) in vitro and in vivo. To gain an understanding of the relevant molecular mechanisms, data analysis must be based on the underlying physics. Strikingly, for FRAP of phase-separated droplets, no physical model from first principles has been derived, which severely restricts data interpretation. Here, we first derive a FRAP model from the physical principles underlying LLPS. Second, we use the full spatio-temporal imaging data within the droplet for fitting. This results in the following improvements: we can (i) distinguish the time scales of exchange through the droplet interface (set by bulk diffusion and boundary kinetics) from diffusion inside the droplet, (ii) quantify the impact of the interface (iii) provide improved measurements for several biologically important proteins, and (iv) use our analysis framework to explore several multi-component scenarios. Finally, we provide experimental guidelines for highly quantitative in vitro FRAP, e.g. the necessity to perform a full bleach to allow robust analysis and routines to allow spatio-temporal fitting.

30 min. coffee break

CPP 11.7 Mon 11:30 SCH A251

Stress granule formation via ATP depletion-triggered phase separation — Jean David Wurtz and •Chiu Fan Lee — Imperial College, London, U.K.

Stress granules (SG) are droplets of proteins and RNA that form in the cell cytoplasm during stress conditions. We consider minimal models of stress granule formation based on the mechanism of phase separation regulated by ATP-driven chemical reactions. Motivated by experimental observations, we identify a minimal model of SG formation triggered by ATP depletion. Our analysis indicates that ATP is continuously hydrolysed to deter SG formation under normal conditions, and we provide specific predictions that can be tested experimentally.

Reference: JD Wurtz and CF Lee (2018) New Journal of Physics 20, 045008.

CPP 11.8 Mon 12:00 SCH A251

Sequence dependent gelation, accumulation and sedimentation — •Alexandra Kühnlein[1], Christof Mast[1], Hannes Mutschler[2], and Dieter Braun[1] — [1]Biophysics and Center for NanoScience, LMU Munich, Amalienstrasse 54, 80799 München — [2]Max Planck Institute of Biochemistry, Martinsried, Germany

The origins of biological information constitutes a major challenge for understanding the origins of life. Under Darwinian evolution, a localized, homogeneous sequence phenotype is selected. How could this state of matter emerge from random sequence mixtures?

To jumpstart Darwinian evolution, a random mixture of sequences have to show physical phenotypes, most likely in non-equilibrium settings. We show preliminary results that indicate a self-selection of sequences by cooperative binding.

Eight 80mer sequences, derived from tRNA to implement a hybridization-based replicator, revealed upon cooling a sharp transition to hydrogels with the size of millimeters. These agglomerates, if broken up by flow, sediment under gravity. If one of the eight sequences are missing, no significant gelation and no sedimentation is found.

Secondly, we subjected random sequences to steep thermal gradients where convection and thermophoresis lead to a size-dependent accumulation. By sequencing, we found that the initial random sequence pool accumulated end sequences with a higher affinity for binding. We speculate that in the long run, only a small number of cooperative binding sequences could remain in such a non-equilibrium setting.

CPP 11.9 Mon 12:15 SCH A251

Shedding light on biomolecular condensates: optical trapping of protein & RNA liquids — •Marcus Jahnel[1,2], Titus M. Franzmann[1,2], Simon Alberti[1,2], and Stephan W. Grill[1,2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]BIOTEC / TU Dresden, Dresden, Germany

Membraneless organelles formed by liquid-liquid phase separation of proteins and RNAs influence vital aspects of cellular biology. However, the transient nature and broad chemical combinatorics of the underlying weak molecular interactions makes these materials challenging to study and reason about, requiring new approaches to make progress.

Optical tweezers use changes in light's linear momentum to measure or apply tiny molecular forces and displacements accurately. This ability has revolutionized single-molecule experiments but also bears great potential to unravel the physics of mesoscopic biomolecular assemblies.

Here, we demonstrate the use of high-resolution dual-trap optical tweezers to study various aspects of biomolecular condensation phenomena, bridging the scales from the single-molecule level to microscopic collections and multi-component mixtures of intrinsically disordered proteins and RNAs. Using this approach, we highlight the rules governing the liquid-to-solid transition in prion-like protein liquids and the influence of RNA-to-protein ratios on the material properties of compositionally complex biomolecular condensates.

CPP 11.10 Mon 12:30 SCH A251

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.

CPP 12: Focus: High-resolution Lithography and 3D Patterning (Part I) (joint session KFM/HL/CPP)

Chair: Robert Kirchner (TU Dresden)

Time: Monday 9:30–12:50 Location: TOE 317

Invited Talk CPP 12.1 Mon 9:30 TOE 317

Novel device integration - combining bottom-up and top-down approaches — •Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Scaling electronic devices to smallest structure sizes well below 10nm will require novel developments for the fabrication of single components. Smallest functional devices can be assembled using chemical methods leading to, e.g., single molecules with electronic functionalities. Reliable contacting of single molecules using metallic contacts is, however, an extremely challenging task which has not been solved so far. We have therefore developed techniques which use self-assembly for the creation of conducting nanostructures in order to create small, self-assembled circuits which then can be contacted reliably using standard lithographic methods. In this talk, we demonstrate how single organic molecules can be contacted using mechanically controllable break junctions. In addition, we show how DNA Origamis can be used for the self-assembly of metallic nanowires, which are contacted using electron beam lithography and electrically characterized. Further integration of such nanostructures into standard silicon electronics may be achieved by connecting them with 1d- or 2d-semiconductors. We have therefore developed transistors based on 2d-materials and silicon nanowires using electron beam lithography and dry etching (i.e. using a classical top-down approach), which are reconfigurable. With the combination of these devices with self-assembled nanostructures, a large variety of electronic nanocircuits can be constructed in future applications.

CPP 12.2 Mon 10:00 TOE 317

Fabrication of NbC Josephson-junction arrays by focused-ion-beam-induced deposition — •Fabrizio Porrati, Felix Jungwirth, Sven Barth, and Michael Huth — Goethe-University, Institute of Physics, Frankfurt a. M.

In this work, a Ga focused-ion-beam is used in combination with the precursor Nb(NMe2)3(N-t-Bu) to fabricate 2D Josephson-junction arrays made of NbC nanodots with typical diameter of 40 nm. Square-arrays with lattice constant between 70 nm and 100 nm are characterized by transport measurements. The ratio Ej/Ec between Josephson coupling energy and the charging energy can be varied by tuning either the dot thickness or the inter-dot distance. As a consequence, a superconductor to insulator transition takes place, as shown by temperature-dependent resistivity measurements. In the Josephson regime, the arrays show magnetic frustration. The resistance as function of the magnetic field exhibits an oscillating behavior with a period of 380 mT for the square-array with lattice constant of 70 nm.

CPP 12.3 Mon 10:20 TOE 317

Avoiding amorphization during semiconductor nanostructure ion beam irradiation — •G. Hlawacek[1], X. Xu[1], W. Möller[1], H.-J. Engelmann[1], N. Klingner[1], A. Gharbi[2], K.-H. Heinig[1], S. Facsko[1], and J. von Borany[1] — [1]Ion Beam Physics and Materials Research, Helmholtz—Zentrum Dresden – Rossendorf, Dresden, Germany — [2]CEA-Leti, Grenoble, France

Ion beam induced amorphization of semiconductor nanostructures limits the applicability of ion beam processing to semiconductor nanostructures. Here, we present an approach that not only avoids this amorphization but in addition allows to tailor the lateral device dimensions of pillars and fins used in modern GAA and Fin-FET designs. Si nanopillars (diameter: 25–50 nm) have been irradiated by either 50 keV broad beam Si^+ or 25 keV focused Ne^+beam from a helium ion microscope (HIM) at various temperatures using fluences of 2×10^{16} cm^{-2} and higher. While at room temperature strong deformation of the nanopillars has been observed, the pillar shape is preserved above 325°C. This is attributed to ion beam induced amorphization of Si at low temperatures allowing plastic flow due to the ion hammering effect and surface capillary forces. Plastic deformation is suppressed for irradiation at elevated temperatures. Above 325°C, as confirmed by diffraction contrast in BF-TEM, the nanopillars remain crystalline, and are continuously thinned radially with increasing fluence down to 10 nm. This is due enhanced forward sputtering through the sidewalls of the pillar, and agrees well with 3D ballistic computer simulations.

Supported by the H-2020 under Grant Agreement No. 688072.

CPP 12.4 Mon 10:40 TOE 317

Grayscale Lithography: Creating complex 2.5D structures in thick photoresist by direct laser writing — •Dominique Collé — Heidelberg Instruments, Heidelberg, Germany

Heidelberg Instruments's lithography systems make it possible to expose any pattern directly without fabricating a mask, which results in a significantly shorter prototyping cycle. The use of a digital mask also allows some quick modification of the design when necessary. The possibility to modulate the energy of each pixel exposed brings the control over the 3rd dimension. This localized dose modulation can be represented as gray tones in a design between black (no dose / no depth in the resist) and white (highest dose / maximum depth in the resist) with up to 1024 different gray tones. Grayscale lithography opens a new world of application from texturing to micro-optic. Micro lenses array, light diffusers, Fresnel lenses, blazed gratings and diffractive optic elements are some typical micro-structures made with grayscale lithography.

20 min. break

Invited Talk CPP 12.5 Mon 11:20 TOE 317

Shapeable materials technologies for high resolution patterning of 3D microelectronic devices — •Daniil Karnauschenko — Institute for Integrative Nanosciences, Leibniz IFW, Helmholtz str. 20, 01069 Dresden, Germany

Electronic devices are continually evolving to offer improved performance, smaller sizes, lower weight, and reduced costs, often requiring state of the art manufacturing and materials to do so. An emerging class of materials and fabrication techniques, inspired by self-assembling biological systems shows promise as an alternative to the more traditional methods that are currently used in the microelectronics industry. Mimicking unique features of natural systems, namely flexibility and shapeability, the geometry of initially planar microelectronic structures can be tailored. Heavily relying on cylindrical geometry, fabrication of microwave helical antennas, coils, resonators and magnetic sensors is challenging, when conventional fabrication techniques are applied. Involving high resolution lithographic patterning and self-assembly strategies realization of these spatially non-trivial devices in a compact form and with a reduced number of fabrication steps become feasible. This spatial self-assembly process, triggered by an external stimulus, offers a possibility of an improved performance while reducing overall manufacturing complexity of devices and components by harnessing the relative ease in which it can produce microscopic 3D geometries such as a *Swiss-roll* architecture. These benefits can lead to tighter a system integration of electronic components including active electronics with reduced costs fabricated from a single wafer.

CPP 12.6 Mon 11:50 TOE 317

Coupling Single Mode Fibers to Single Quantum Emitters using Femtosecond 3D Printing Technology — •Ksenia Weber[1], Simon Thiele[2], Simon Ristok[1], Sarah Fischbach[3], Jan Hausen[3], Lucas Bremer[3], Mark Saritson[4], Simone Protalupi[4], Alois Herkommer[2], Stefan Reitzenstein[3], Peter Michler[4], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart — [2]Institute for Applied Optics and Research Center SCoPE, University of Stuttgart, Stuttgart — [3]Institute of Solid State Physics, Technische Universität Berlin — [4]Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, University of Stuttgart

We propose a method to efficiently couple single photon quantum emitters to optical single mode fibers. Due to the undirected emission of single photon sources, such as quantum dots or defect centers in crystals, coupling into optical fibers which is essential for long range quantum communication is typically associated with high losses. To overcome this limitation, femtosecond two-photon lithography can be used to directly fabricate a combination of a microlens and an optical fiber holder onto a quantum emitter. A single mode optical fiber is then integrated into the fiber holder. Due to the high precision of the femtosecond 3D printing process, the position of the fiber core can be adjusted with sub-micrometer accuracy to match the focal point of the microlens. Light from the emitter which is focused by the microlens can therefore efficiently be coupled into the fiber. We present a number of different optical layouts and discuss their pros and cons.

CPP 12.7 Mon 12:10 TOE 317

Optical properties of photoresists for femtosecond 3D printing: Refractive index, extinction, luminescence - dose dependence, aging, heat treatment and comparison between 1-photon and 2-photon exposure — •Michael Schmid, Dominik Ludescher, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Femtosecond 3D printing has emerged as an important technology for manufacturing nano- and microscopic optical devices and elements. Detailed knowledge of the dispersion in the visible and near-infrared spectral range is crucial for the design of these optical elements. Here we provide refractive index measurements for different UV-doses, aging times, heat treatment and 2-photon exposed structures for the photoresists IP-S, IP-Dip, IP-L, OrmoComp, IP-Visio, and PO4. We use a modified and automized Pulfrich refractometer setup, utilizing critical angles of total internal reflection with an accuracy of $5{\cdot}10^{-4}$ in the visible and near-infrared spectral range. We compare Cauchy and Sellmeier fits to the dispersion curves. We also give Abbe numbers and Schott Catalog numbers of the almost entirely polymerized resists. Additionally, we provide quantitative extinction and luminescence measurements for all photoresists.

CPP 12.8 Mon 12:30 TOE 317

Acoustic Impedance Matching on Ultrasonic Devices using Additive Manufacturing — •Severin Schweiger, Sandro Koch, Marcel Krenkel, and Marco Kircher — Fraunhofer Institute for Photonic Microsystems, Dresden, Germany

Acoustic impedance matching layers are attached to ultrasonic transducers to increase acoustic energy transmission into the load medium. A capacitive micromachined ultrasonic transducer (CMUT) emits sound via electrostatic deflection of a flexible electrode. Especially air-coupled CMUTs with protective or focusing layers exhibit a notable impedance mismatch. We propose a new approach to fabricate impedance matching metamaterials with low load-side specific acoustic impedance values, by employing a photolithographic additive manufacturing technology using two photon absorption. It will enable improved impedance matching, which has a beneficiary effect on acoustic bandwidth, efficiency and sensitivity of the CMUT. The center operating frequency of the CMUT can be influenced via this process as well. The technology also allows for direct fabrication of microstructures on the chip, foregoing any adhesion layers that disturb the impedance matching and enabling the protective and/or focusing aspects of the layer. This contribution will show analytic and FEM simulations of CMUTs with matching layers. Fabricated impedance matching layer samples and on chip fabrication will be presented as well. Electric impedance and acoustic measurements are in progress and will be featured accordingly.

CPP 13: Membranes and Vesicles (joint session BP/CPP)

Time: Monday 9:30–13:00 Location: ZEU 250

CPP 13.1 Mon 9:30 ZEU 250

Regulated ensembles and lipid membranes — •Martin Girard and Tristan Bereau — Max-Planck-Institut für Polymerforschung

Cellular membranes are composed of lipid bilayers, amphiphilic molecules with polar headgroups and hydrophobic tails. Their composition is highly complex, involving hundreds of different lipid types and the regulation mechanism is still the subject of intense research. A recent experiment [1] has shown that cholesterol concentration increases with temperature in zebrafishes, as well as the demixing temperature, two results which appear to be contradictory results since cholesterol promotes mixing. Here, we show that many aspects of the zebrafish experiments can be replicated if one assumes a chemical reaction network for regulation of acyl tails. Effectively, this would mean that acyl tail saturation is loosely regulated by cells and mainly directed by cholesterol fraction. This view also explains trends seen along the secretory pathway between cholesterol concentration and acyl tail saturation.[1] M. Burns, K. Wisser, J. Wu, I. Levental, S. L. Veatch, "Miscibility transition temperature scales with growth temperature in a zebrafish cell line" Biophysical Journal 113 (2017)

CPP 13.2 Mon 9:45 ZEU 250

Effect of reactive oxygen species on phospholipid monolayers — •Florian Gellert, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald

Oxidative degeneration of lipids can lead to severe damages of the biological cell membrane. The phenomenon is initiated by reactive radicals, such as certain reactive oxygen/nitrogen species (ROS/ RNS). To investigate this behaviour, we use monolayers at the air/ water interface of unsaturated lipids as model membranes and measure isotherms. ROS induce an oxidation of the double bond. The double bond turns hydrophilic, thus increases the molecular area per lipid at the same surface pressure. This is demonstrated by using phosphocholines with the same head group, but either one or two double bonds in one alkyl chain and no double bond in the other alkyl chain. In another series of experiments, both alkyl chains contained a double bond. We conclude that the ROS/ RNS attacks mostly the unsaturated alkyl chains and has little effect on the head group of the lipid.

CPP 13.3 Mon 10:00 ZEU 250

From UV to Near Infrared Optical Control of Photolipid Vesicles — •Theresa S. Kehler[1], Stefanie D. Pritzl[1], Alexander F. Richter[1], David B. Konrad[2], Dirk Trauner[2], and Theobald Lohmüller[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany — [2]Department of Chemistry, New York University, Silver Center, 100 Washington Square East, New York 10003, United States

Photoswitchable azobenzene phospholipids or "photolipids" can be employed as molecular reagents in bilayer membranes to control a variety of characteristic membrane properties such as lateral fluidity, permeability or stiffness. A general drawback of the azobenzene photoswitch, however, is that illumination with UV light is required to trigger trans-to-cis isomerization, which limits the wider applicability of photolipids in biological systems.

Here, we report on the photophysical properties of a new group of halogenated azobenzene photolipids, where the wavelengths required to control photoisomerization are shifted to the visible and near-infrared range. The isomerization dynamics of red-shifted photolipid vesicles are characterized by absorption measurements, fluorescence microscopy and membrane fluctuation analysis. Notably, we observe a wavelength dependence of the switching rates, which can be harnessed to reversibly control the membrane rigidity up to a factor of two.

CPP 13.4 Mon 10:15 ZEU 250

Structural and dynamical changes of biomimetic myelin membranes induced by myelin basic protein — •Benjamin Krugmann[1], Andreas Stadler[2], Aurel Radulescu[1], Alexandros Koutsioumpas[1], Marie-Sousai Appavou[1], Martin Dulle[2], Laura Stingaciu[3], and Stephan Förster[2] — [1]FZJ JCNS-1, 52428 Jülich, Germany — [2]FZJ JCNS-MLZ, 85748 Garching, Germany — [3]ORNL, Oak Ridge TN 37831, USA

A major component of the saltatory nerve signal conduction is the multilamellar myelin membrane around axons. In demyelinating diseases like multiple sclerosis, this membrane is damaged. In literature different values for the lipid composition of healthy myelin sheath and myelin with experimental autoimmune encephalomyelitis - the standard animal model for multiple sclerosis - have been found. In this work we try to elucidate the interaction mechanism of myelin basic protein - the structural protein responsible for the cohesion of the cytoplasmic leaflets of the myelin sheath - with membranes mimicking both compositions. As samples we use unilamellar vesicles and supported bilayer systems. With neutron and x-ray small angle scattering methods combined with cryo-TEM we can follow the rapid aggregation which leads to a slow process in which different structures are formed depending on the lipid composition. Those structural information can be associated with the bending rigidity of the respective membrane measured with Neutron Spin Echo. Neutron reflectometry gives insights on how the interaction mechanism between membrane and protein functions and reveals how modified membranes are destabilised by the protein.

Invited Talk CPP 13.5 Mon 10:30 ZEU 250

How do lipids and proteins diffuse in cell membranes, and what do the diffusion experiments actually measure? — •Ilpo Vattulainen — Dept Physics, Univ Helsinki, Finland

There are numerous techniques able to gauge diffusion in biomembranes. For instance, quasi-elastic neutron scattering measures diffusion in a non-perturbative manner over the nanosecond time scale, yet sampling in space is in these experiments done over large distances. Meanwhile, single-particle tracking allows one to measure the dynamics of individual molecules in almost nanometer resolution, but these measurements are based on the use of markers that may interfere with the diffusion process. Here we discuss nanoscale simulation studies designed to explore the underlying molecular-scale diffusion mechanisms of lipids and membrane proteins. Also, we discuss the bases of single-particle tracking experiments by considering the effects of streptavidin-functionalized Au nanoparticle probes on the lateral diffusion. The results show that lipids diffuse in a concerted fashion as clusters of lipids whose motion is highly correlated, and membrane proteins move as dynamical complexes with tens of lipids dynamically bound to the protein. Meanwhile, lipids linked to a streptavidin-nanoparticle complex also turn out to move in a concerted manner but as a complex with the linker protein and numerous non-labeled lipids, slowing down the motion of the probe by an order of magnitude. The results highlight that prior to using any technique, it is crucial to understand the physical basis of the diffusion process that one aims to measure. Otherwise, interpretation of experimental data can be a surprisingly difficult task.

30 min. coffee break

CPP 13.6 Mon 11:30 ZEU 250

Prerequisites and kinetics of lipid bilayer fusion with living cell membrane — •Justus Bednár[1,2], Anastasia Svetlova[1,2], Vanessa Maybeck[1], and Andreas Offenhäusser[1] — [1]Forschungszentrum Jülich, Institute of Complex Systems: Bioelectronic (ICS-8) — [2]Fakultät für Mathematik, Informatik und Naturwissenschaften RWTH Aachen

Fusion processes between artificial lipid vesicles and living cell membrane are studied for a variety of reasons. The delivery of anti-cancer therapeutics or the method known as lipofection are only two applications that would benefit from a detailed understanding of the prerequisites and kinetics of this fusion process.

While usually this process takes place between liposomes that have a small size relative to the cell membrane they are fusing to, an inverse approach is presented in the current work. Producing an artificial solid-supported lipid bilayer (SLB) first and letting extracts of living cell membrane fuse with it afterward allows for the application of a quartz crystal microbalance with dissipation monitoring (QCM-D). Tracking the changes in resonance frequency and energy dissipation of a quartz sensor underneath the SLB allows for real-time tracking of adhesion and fusion processes.

Using the proposed setup along with dynamic light scattering and fluorescence microscopy, the dependence of fusion efficiency and kinetics on lipid composition of the artificial lipid bilayer as well as on the concentration of cell membrane vesicles is evaluated.

CPP 13.7 Mon 11:45 ZEU 250

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. Because of the two channels, asymmetric bilayers can be formed by making the two lipid leaflets of different composition. Furthermore, proteins, such as transmembrane, peripheral, and pore-forming proteins, 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.

Small, 2019, 10.1002/smll.201900725

CPP 13.8 Mon 12:00 ZEU 250

Statistics on Red Blood Cell Flow in Microchannels — •Felix Maurer, Thomas John, and Christian Wagner — Experimentalphysik Universität des Saarlandes

Half of the human blood volume consists of erythrocytes, also refered to as red blood cells. Most of the pressure induced by the heart muscle is used for microcirculation through capillary vessels. Capillary flow is strongly characterized by the soft body physics of red blood cells often described as vesicles. We established an experimental method to record individual cells during flow through straight artificial microfluidic channels. Stationary shapes could be classified. We measured the speed as a function of position at different external pressure drops and channel geometries. The velocity distributions reveal intrinsic differences between individual erythrocytes. These have been found to be the root cause of pairing in this setup. Interaction forces have no influence on the examined flow.

CPP 13.9 Mon 12:15 ZEU 250

The mechanism of vesicle-vesicle detachment under shear flow — •Mehdi Abbasi, Alexander Farutin, and Chaouqi Misbah — Univ Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Red blood cells (RBCs) suspended in plasma tend to aggregate and form rouleaux, during the aggregation they start by forming doublets of RBCs. In the physiological conditions the aggregation is reversible, the RBCs aggregate and disaggregate by the shear rate. In contrast, under some pathological conditions the aggregation becomes irreversible and once the aggregates formed they can not be dispersed again. Recently, D, Flormann et al analysed the doublet shape in the absence of applied flow in vitro and in silico. They observe that contact surface of the doublet starts by flat then sigmoid shape with the increase of adhesion energy. We performed two dimensional simulations to study the doublet dynamics under shear flow in different conditions and the effect of the doublet dynamics on the doublet suspension rheology, we also invesitigate the mechanism of vesicle-vesicle detachment.

CPP 13.10 Mon 12:30 ZEU 250

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. We also found that these buds are responsible for regulation of tension in the membrane which can give rise to activation or deactivation of different chemical signaling pathways.

CPP 13.11 Mon 12:45 ZEU 250

Conformal wrapping of nanoparticles — •Piermarco Fonda[1,2] and Luca Giomi[1] — [1]Lorentz Instituut, Leiden University, Leiden, The Netherlands — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

It is well-known that wrapping of nanometer-sized particles by lipid membranes can happen spontaneously for sufficient adhesion energy between the particle surface and lipid molecules. In this work we show the surprising result that, even in absence of adhesion forces, there exist solutions to the shape equation that describe a stable, spontaneous wrapping of spherical particles. Mathematically, these solutions can be found analytically thanks to the scale invariant nature of the bending energy, which allows to reduce the problem to the one of finding minimal surfaces in hyperbolic and spherical spaces. From a physical standpoint, such shapes are well-behaved since, unlike for adhesive forces, they do not require any in-plane stress at the contact points, and hence they easily preserve the liquid nature of the membrane. Finally, the relevance of these solutions to experimental and biological systems will be discussed.

CPP 14: Topical Session: Data Driven Materials Science - Materials Design I (joint session MM/CPP)

Time: Monday 10:15–11:30 Location: BAR 205

Topical Talk CPP 14.1 Mon 10:15 BAR 205

Data-Mining Strategies for Understanding Strength and Failure of Materials — •Stefan Sandfeld — TU Bergakademie Freiberg, Lampadiusstr. 4, 09599 Freiberg

Experimental observations and simulation data should – in principle – help to shed light on the 'inner workings' of a physical system, say, a material or specimen. There, the 'inner workings' would be the interaction of microstructural features among themselves, with the surfaces of the specimen, with defects, or with phase boundaries, to name but a few. Both experiment and simulation, however, suffer from particular problems which in many situations makes it difficult to directly compare them or to use results from one as input or support for the other.

In this presentation, we will start by giving an overview over current attempts for integrating experiment and simulation. We will then demonstrate, on the one hand, how data science approaches might be used to access data from experiments that would be otherwise inaccessible and, on the other hand, how data science also might help to reduce the high level of abstraction inherent to most simulations. With those methods, experiment and simulation might get a little closer to each, thereby helping to understand relevant mechanisms in strength and failure from a new point of view.

CPP 14.2 Mon 10:45 BAR 205

Stabilities of novel Mg-based light metal high entropy alloys — •Wernfried Mayr-Schmölzer[1], Johannes Kirschner[2], Clemens Simson[4], Christoph Eisenmenger-Sittner[2], Johannes Bernardi[3], Stefan Müller[1], and Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]Institute of Solid State Physics, TU Vienna — [3]USTEM, TU Vienna — [4]LKR, Austrian Institute of Technology GmbH

Compositionally Complex Alloys (CCAs) consist of four or more elements alloyed in approximately equal fractions and often crystallize in a simple crystal lattice. In many cases, their mechanical properties like structural stability or ductility exceed that of common modern alloys. Usually, they contain heavy d-Orbital metals, but investigations into low density light metal CCAs have been rare up to now due to the complex binding modes of their constituents.

We use both a Cluster Expansion approach, augmented by stochastic prescreening steps, and neural network based pair potentials to scan the large configuration space of the Mg-Al-Cu-Zn system for stable phases. The training data was generated using density functional theory calculations implemented in the VASP code. In conjunction with experiments, we find that while the introduction of Al into the brittle $MgZn_2$ hexagonal Laves phase leads to phase separation and does not improve the mechanical properties of the alloy, the addition of Cu inhibits this process and leads to the formation of a highly stable cubic phase.

CPP 14.3 Mon 11:00 BAR 205

Automatic design of reversible shape changing metamaterials — Silvia Bonfanti, Francesc Font Clos, Roberto Guerra, and •Stefano Zapperi — University of Milan, Milan, Italy

We have developed a computational method to design metamaterials that perform pre-determined input/output mechanical operations. Our numerical scheme to design metamaterials combines a reinforced dynamic Monte Carlo method with finite element simulations. We performed 3D printing of selected metamaterial configurations, showing that the machine-generated solutions present effciencies far exceeding those of man-designed ones. Finally, we show that machine learning algorithms can be trained to identify efficient solutions without performing simulations. The designed metamaterial units can be exploited as the building blocks of generic metamaterial machines or other actuators with higher complexity.

This work is supported by the European Research Council through the PoC project METADESIGN. The presenting author thanks the Alexander von Humboldt foundation for the Humboldt Research Award.

CPP 14.4 Mon 11:15 BAR 205

Towards Building New Zeolites with Machine Learning — •Benjamin A. Helfrecht[1], Rocio Semino[1,2], Giovanni Pireddu[1,3], Scott M. Auerbach[4], and Michele Ceriotti[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Université de Montpellier, Montpellier, France — [3]Università degli Studi di Sassari, Sassari, Italy — [4]University of Massachusetts Amherst, Amherst, Massachusetts USA

Synthesizing new zeolites, which are useful for applications like gas separation and catalysis, with specific properties is an ongoing challenge in the zeolite community. Ideally, one would like to select a handful of compatible "building blocks" from which a new zeolite with desired properties can be synthesized. In this work, we make progress toward this goal by constructing an "atlas" of local atomic environments comprising several thousand all-silica zeolites from the Deem SLC PCOD database [1] using machine learning techniques. We evaluate the utility of this atlas by examining correlations between the locations of the atomic environments in the atlas and their energy and volume contributions to their parent frameworks.

[1] R. Pophale, P. A. Cheeseman, M. W. Deem, A database of new zeolite-like materials, Phys. Chem. Chem. Phys 13(27):12407-12412, 2011.

CPP 15: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions I (joint session O/HL/CPP/DS)

Electronic-structure calculations from first principles have become an indispensable and ubiquitous tool in materials modeling, design, and discovery. One of the outstanding challenges in this area is to study materials at finite temperature, in order to achieve a more realistic description of materials properties and to enable direct comparison with experimental data. To address this challenge it will be necessary to move beyond the static-ions approximation, and to devise systematic approaches for incorporating the effects of electron-phonon coupling, phonon-phonon interactions, and phonon-assisted quantum processes in state-of-the-art electronic-structure methods. The invited lectures will cover recent progress in the broad area of electron-phonon physics from the point of view of first-principles calculations. More generally, the symposium will also cover other areas of first-principles computational materials science (basic methods and applications).

Claudia Draxl (Humboldt-Universität zu Berlin, Germany), Feliciano Giustino (University of Texas at Austin, USA), Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)

Time: Monday 10:30–12:45 Location: GER 38

Invited Talk CPP 15.1 Mon 10:30 GER 38

Predominance of non-adiabatic effects in zero-point renormalization of electronic energies. — •Xavier Gonze[1,2], Anna Miglio[1], Véronique Brousseau-Couture[3], Gabriel Antonius[4,5], Yang-Hao Chan[4], Steven Louie[4], Giantomassi Matteo[1], and Michel Côté[3] — [1]UCLouvain, Belgium. — [2]Skoltech, Moscow, Russia. — [3]Dept. Physique, U. Montréal, Canada. — [4]Dept. Physics, U. California Berkeley & Materials Sci. Div. NBNL Berkeley, CA, USA. — [5]Dept. Chim., Bio. & Physique, U. Québec Trois-Rivières, Canada.

Electron-phonon interaction induces variation of bandgaps with temperature, and zero-point motion renormalization (ZPR) even at 0K. Ignored in most calculations, ZPR has been evaluated recently for several materials, often relying on the adiabatic approximation, reasonably valid for materials without infrared (IR) activity, but eagerly applied to other materials. We present the first large-scale (29 materials) first-principles evaluation of ZPR beyond the adiabatic approximation [1]. For materials with light elements the ZPR is often larger than 0.3 and up to 1.1 eV: it is useless to go beyond G0W0 without including ZPR in such materials. For IR-active materials, global agreement with experimental data is obtained only with nonadiabatic effects. They even dominate ZPR for many materials. A generalized Fröhlich model that represents accurately nonadiabatic effects accounts for more than half the ZPR for a large set of materials.

[1] A. Miglio, V. Brousseau-Couture, G. Antonius, Y.-H. Chan, S.G. Louie, M. Giantomassi, M. Côté, and X. Gonze. Submitted.

CPP 15.2 Mon 11:00 GER 38

A generalized first-principles formalism for the electron-phonon renormalization of electronic energy eigenvalues — •Jae-Mo Lihm[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

The interaction between electrons and phonons induce a temperature-dependent renormalization of electronic energy eigenvalues [1]. The perturbative theory of Allen, Heine, and Cardona (AHC) [2] enables an efficient first-principles calculation of the renormalized electronic eigenenergies. The temperature dependence of the electronic bandgap, optical responses, and topological properties of real materials have been investigated within the AHC formalism. In this study, we generalize the AHC formalism [3] so that it could be applied to a broader class of materials. We demonstrate our formalism by calculating the temperature-dependent electronic energy eigenvalues of representative materials.

[1] F. Giustino, Rev. Mod. Phys. 89, 015003 (2017)

[2] P. B. Allen and V. Heine, J. Phys. C 9, 2305 (1976); P. B. Allen and M. Cardona, Phys. Rev. B 24, 7479 (1981); 27, 4760 (1983).

[3] J.-M. Lihm and C.-H. Park, unpublished.

CPP 15.3 Mon 11:15 GER 38

Electron-phonon interactions beyond the Born-Oppenheimer approximation in Kohn Sham theory — •Nikitas Gidopoulos — Department of Physics, Durham University, South Road, Durham, DH1 3LE, U.K.

I shall present our work on non-adiabatic corrections to the electron-phonon matrix elements, in density functional theory beyond the Born Oppenheimer approximation, where the Kohn-Sham single-particle potential contains a non-adiabatic correction term [1]. This term depends self-consistently on the nuclear vibrational wave function. The standard expansion of the non-adiabatic KS potential around the nuclear equilibrium positions yields electron-phonon matrix elements beyond the BO approximation.

[1] NI Gidopoulos, EKU Gross, Phil. Trans. R. Soc. A 372, 20130059 (2014). http://dx.doi.org/10.1098/rsta.2013.0059

CPP 15.4 Mon 11:30 GER 38

Renormalized second-order perturbation theory for the band gap and single-particle excitations of solids — •Maria Dragoumi[1], Sergey V. Levchenko[2,1], Igor Ying Zhang[3,1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Skolkovo Institute of Science and Technology, Moscow, RU — [3]Fudan University, Shanghai, CN

We report an efficient implementation of renormalized second-order single-particle energies for periodic systems in an all-electron numeric atomic orbital framework. Starting from second-order perturbation theory, which is single-electron self-interaction free as a virtue of the first-order and second-order exchange diagrams, we use the Dyson equation to sum up infinite number of diagrams [1,2]. In our implementation we use Ewald summation for the long-range part of the Coulomb interaction. This results in an integrable singularity in k-space, which has to be carefully evaluated in order to ensure proper convergence with k-point mesh density. For this purpose we develop an approach based on a generalization of the Gygi-Baldereschi method. The dependence on the starting point of the perturbation theory is examined. The new approach shows a competitive or even superior performance for the description of band-energies compared to the current state-of-the-art methods such as hybrid functionals and G^0W^0 approximation. Thus, with a good starting point this method becomes a powerful tool for the prediction of band energies for a variety of materials.
[1] J. Sun and R. J. Bartlett, J. Chem. Phys. 104, 8553 (1996).
[2] A. Grüneis *et al.*, J. Chem. Phys. 133, 074107 (2010).

CPP 15.5 Mon 11:45 GER 38

Band structure of semiconductors and insulators from Koopmans-compliant functionals — •Riccardo De Gennaro[1], Nicola Colonna[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institute, 5232 Villigen, Switzerland

Koopmans-compliant functionals provide a novel orbital-density-dependent framework for an accurate evaluation of spectral properties, obtained imposing a generalized piecewise-linearity condition on the total energy of the system with respect to the occupation of each orbital. In crystalline materials, due to the orbital-density-dependent nature of the functionals, minimization of the total energy leads to a ground-state set of variational orbitals that are localized and break the periodicity of the underlying lattice. Despite that, thanks to the Wannier-like character of the variational orbitals, we show that the Bloch symmetry is still preserved and it is possible to describe the electronic energies through a band structure picture. In this talk I will present results for some benchmark semiconductors and insulators, obtained by unfolding the electronic bands obtained with Gamma-point-only calculations.

CPP 15.6 Mon 12:00 GER 38

Dynamical vertex corrections beyond GW from time-dependent density-functional theory — •Georg S. Michelitsch[1,2], Lucia Reining[1,2], and Matteo Gatti[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

Strong many-body effects in solid state materials are the reason for features such as satellites in electronic excitation spectra. Many-body perturbation theory approaches based on the Green's function formalism are the state-of-the-art in their understanding, commonly applied in terms of the GW approximation to the self-energy, which neglects the so-called vertex correction in Hedin's equations. Although successful for some observables such as band gaps, this approximation cannot sufficiently well describe satellite peaks observed in experiment. Vertex corrections beyond GW can be taken into account thanks to time-dependent density-functional theory[1]. However, only adiabatic approximations have been considered so far. Here we make use of a non-adiabatic approximation[2] to investigate dynamical vertex corrections within a model self-energy. We compare our results to calculations where a static vertex is included and report first successes in terms of a correction to the satellites in the spectral function of sodium.
[1] R. Del Sole et al. *Phys. Rev. B*, 49, 8024 (1994)
[2] M. Panholzer et al. *Phys. Rev. Lett.*, 120, 166402 (2018)

CPP 15.7 Mon 12:15 GER 38

Large-scale benchmark of exchange-correlation functionals for the determination of electronic band gaps of solids — •Pedro Borlido[1], Thorsten Aull[2], Ahmad Huran[2], Fabien Tran[3], Miguel Marques[2], and Silvana Botti[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

We compile a large dataset designed for the efficient benchmarking of exchange-correlation functionals for the calculation of electronic band gaps.The dataset comprises information on the experimental structures and band gaps of 472 non-magnetic materials, and includes a diverse group of covalent-, ionic-, and van der Waals-bonded solids.

We used it to benchmark a set of 30 functionals sampling the entirety of Jacob's Ladder. This includes well established functionals such as PBE, mBJ and HSE06, as well as several other less known functionals.

The comparison of experimental and theoretical band gaps shows that mBJ is at the moment the best available density functional, closely followed by HSE06. Other functionals such as HLE16, HLE17, AK13 and TASK also show overall good performance.

CPP 15.8 Mon 12:30 GER 38

Assessment of Approximate Methods for Anharmonic Free Energies — •Venkat Kapil[1], Edgar Engel[2], Mariana Rossi[3], and Michele Ceriotti[1] — [1]Swiss Federal Institute of Technology, Switzerland — [2]Department of Physics, University of Cambridge, UK — [3]MPI for Structure and Dynamics of Matter, Hamburg, Germany

Quantitative estimations of thermodynamic stabilities, measured by free energies, must take into account thermal and quantum zero-point nuclear motion. While these effects are easily estimated within a harmonic approximation, corrections arising from the anharmonic nature of the interatomic potential are often crucial and their accurate computations require expensive path integral simulations. Consequently, different approximate methods for computing affordable estimates of anharmonic free energies have been developed. Understanding which of the approximations involved are justified for a given system is complicated by the lack of comparative benchmarks. We here assess the accuracy of some of the commonly used approximate methods: vibrational self-consistent field and self-consistent phonons by comparing anharmonic corrections to Helmholtz free energies against reference path integral calculations. We study a diverse set of systems, ranging from simple weakly anharmonic solids to flexible molecular crystals with freely-rotating units and conclude that efforts towards obtaining computationally-feasible anharmonic free-energies of molecular systems must focus at reducing the expense of path integral methods.
Kapil, Venkat, et al. Assessment of Approximate Methods for Anharmonic Free Energies. JCTC, 2019, doi:10.1021/acs.jctc.9b00596.

CPP 16: Plasmonics and Nanooptics I: Local Probes and Raman (joint session O/CPP)

Time: Monday 10:30–13:45 Location: WIL A317

CPP 16.1 Mon 10:30 WIL A317

Light emission from charged Hydrogen-Phthalocyanine molecules on NaCl layers — •Vibhuti Rai[1], Lukas Gerhard[1], Sun Qing[1], and Wulf Wulfhekel[1,2] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany — [2]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Recently, light emission studies from single molecules on insulating layers studied by scanning tunneling microscopy (STM) has had made considerable progress. However, many fundamental aspects of light emission remain unclear. In this report, we used a home build STM[1] with high light collection efficiency to investigate the light emission from single Hydrogen-Phthalocyanine (H_2Pc) molecules thermally evaporated onto bi- and trilayers of NaCl on Au(111) surface. For the first time we have observed light emission from both charged and neutral H_2Pc molecules and mapped the spatial dependence of light emission. We find that the photon yield of the charged species is significantly higher than the neutral one and that the tautomerization of the charged H_2Pc molecule is reflected in the energy and spatial distribution of the emitted light. For further understanding of the fundamental processes of light emission we performed detailed current and voltage dependence of light emission spectra from charged H_2Pc molecule.

1. Edelmann et al., Review of Scientific Instruments 89, 123107 (2018).

CPP 16.2 Mon 10:45 WIL A317

Anti-Stokes Light Scattering in an Electrically Biased Plasmonic Nanojunction — •Shuyi Liu[1], Martin Wolf[1], and Takashi Kumagai[1,2] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany. — [2]JST-PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.

Photon scattering and emission from plasmonic nanostructures have attracted increasing attention but the underlying mechanisms have been debated. [1,2] We report on light scattering from an electrically-biased plasmonic nanocavity, which composed of a Ag tip and Ag(111) surface, using a low-temperature scanning tunneling microscope (STM). It is found that anti-Stokes shifted scattered light is observed occurs when a bias voltage (< 2V) is applied to the junction. By observing the scattering spectra in dependence on the spectral shape of the localized surface plasmon resonance (LSPR) in the STM junction, we revealed that either electronic Raman scattering (ERS) or photoluminescence (PL) dominates the process depending on spectral matching of the LSPR with excitation wavelength. We discuss the possibility that ERS occurs by the interaction of the LSPR with a "gap exciton" in the STM junction. Reference: [1] Mertens et al, Nano Lett. 17, 2568-2574 (2017).[2] Cai et al, Anti-Stokes Emission from Hot Carriers in Gold Nanorods. Nano Lett. 19, 1067-1073 (2019).

CPP 16.3 Mon 11:00 WIL A317

Broadband measurement of local density of optical states by plasmonic nanofocusing spectral interferometry — •Abbas Chimeh[1], Martin Esmann[2], Anke Korte[1], Jinhui Zhong[1], Nahid Talebi[3], and Christoph Lienau[1] — [1]Universität Oldenburg, Oldenburg, Germany — [2]Centre de Nanosciences et de Nanotechnologies, Paris, — [3]Universität Kiel, Kiel, Germany

The local density of optical states (LDOS) is one of the most fundamental quantities in nanophotonics [1]. Experimental mapping of the LDOS enables to understand how a quantum emitter is coupled to its nanostructred photonic environment. Here, we demonstrate a novel experimental approach to directly measure the LDOS with <10 nm spatial resolution in a broad spectral range. Surface plasmon polaritons (SPPs) propagating along a conical gold taper are adiabatically converted to a local dipole mode at the very apex [2], which can locally excite and detect the optical states around single gold nanoparticles. Integration of an inline interferometer in this plasmonic nanofocusing taper allows us to extract amplitude a phase of local light scattering spectra of gold nanoparticles and quantify line broadenings and spectral shifts induced by tip-sample coupling [3]. We show that, in the limit of weak tip-sample coupling, this measurements directly probe the projected local density of optical states of the plasmonic system.

[1] R. Carminati et al., Surf. Sci. Rep. 70, 1 (2015) [2] M. Esmann et al., Nature Nanotechnol. 6, 6040 (2019) [3] M. Esmann et al., Nanophotonics, in press (2020)

CPP 16.4 Mon 11:15 WIL A317

Spatial and spectral mode mapping of a Sb_2S_3 nanodot by broadband interferometric homodyne scanning near-field spectroscopy — Jinxin Zhan[1], Wei Wang[2], Jens Brauer[1], Lukas Schmidt-Mende[2], Christoph Lienau[1], and •Petra Gross[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]University of Konstanz, Konstanz, Germany

We present and demonstrate a novel approach towards broad-bandwidth scattering-type near-field scanning optical spectroscopy based on homodyne mixing and on rapid acquisition of spectra facilitating tip-modulated spectroscopy. We aim at a fast and spectrally resolved near-field measurement of plasmonic and dielectric nanostructures. The weak, broad-bandwidth near field is amplified above the background by homodyne mixing using a Michelson interferometer, and spectral interferograms over a >150 nm bandwidth are recorded. For rapid acquisition of complete spectra, we use a monochromator and a line camera with 210-kHz readout rate. The near-field spectra obtained after demodulation show supreme background suppression.

We apply this new method to the characterization of Sb_2S_3 semiconductor nanodots fabricated by electron beam lithography. Sb_2S_3 recently became attractive as photovoltaic material, and patterning the surface of a thin film with nanodots of the same material is a strategy to achieve light trapping. Here, we present spatially and spectrally resolved measurements of waveguide-like modes that are excited by below-bandgap illumination. These constitute a practical mechanism for improved below-bandgap absorption in Sb_2S_3 thin film solar cells.

CPP 16.5 Mon 11:30 WIL A317

Polarization-sensitive near-field optical nanoscopy for investigating optical phonon anisotropies at mid-infrared to THz wavelengths — •Lukas Wehmeier[1], Tobias Nörenberg[1], Thales V. A. G. de Oliveira[1,2], J. Michael Klopf[2], Susanne C. Kehr[1], and Lukas M. Eng[1,3] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany — [3]ct.qmat, Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Polarization-sensitive techniques, such as ellipsometry, are of essential value when investigating optically anisotropic (low-dimensional) materials. Yet, polarization is often neglected in scattering scanning near-field optical microscopy (s-SNOM) and spectroscopy. In a first attempt towards quantitative nano-ellipsometry, we demonstrate here the phonon-enhanced resonant near-field excitation when using both p- and s-polarized incident photons. Notably, we find their near-field responses to be on the same order of magnitude [1]. We apply this s-SNOM mimic for inspecting a broad set of crystalline perovskite materials, i.e. $BiFeO_3$, $PbZrTiO_3$, $SrTiO_3$, and $LiNbO_3$. Their phonon resonances are easily excited by our setup, making use here of the broad tunability range of the free-electron laser FELBE at Dresden-Rossendorf, Germany [1,2]. Hence, we are able to resonantly excite specific phonons, i.e. a single type of vibronic bonding within the crystal in our s-SNOM setup [2].

[1] L. Wehmeier et al., Phys. Rev. B 100, 035444 (2019).

[2] L. Wehmeier et al., Appl. Phys. Lett., submitted (2019).

CPP 16.6 Mon 11:45 WIL A317

Single-molecule vibrational signature and redox-states probed with STM-Induced Fluorescence Microscopy — •Benjamin Doppagne, Michael C. Chong, Etienne Lorchat, Stephane Berciaud, Michelangelo Romeo, Hervé Bulou, Alex Boeglin, Fabrice Scheurer, and Guillaume Schull — Institut de Physique et Chimie des Matérieux de Strasbourg, 67034 Strasbourg, France

Infrared, Raman and fluorescence spectroscopies are powerful methods to obtain precise information regarding the chemical structure or environment of an organic system. In this presentation, I report the use of a STM to obtain the fluorescence spectrum of a single Zinc-Phthalocyanine molecule, to go beyond the limitations commonly observed in conventional optical techniques. We have shown that in such configuration, it is possible to obtain optically an accurate vibrational signature of the probed molecule with a sub-molecular resolution, without light excitation. This technique has allowed us to obtain, for the first time, the fluorescence spectrum of a charged single molecule. Comparison between fluorescence spectra of the neutral and the charged species shows that these latters exhibit different vibrational signatures. Thanks to this identification, we performed a complete optical monitoring of the redox state of a single molecule with STM-Induced Fluorescence Microscopy.

CPP 16.7 Mon 12:00 WIL A317

Optical tracking of a tautomerization process with STM-Induced Fluorescence Microscopy — •Benjamin Doppagne[1], Tomas Neuman[2], Ruben Soria Martinez[1], Luis E. Parra Lopez[1], Hervé Bulou[1], Michelangelo Romeo[1], Stephane Berciaud[1], Fabrice Scheurer[1], Javier Aizpurua[2], and Guillaume Schull[1] — [1]Institut de Physique et Chimie des Matérieux de Strasbourg, 67034 Strasbourg, France — [2]Center for Materials Physics, San Sebastian 20018, Spain

Optical spectroscopies are powerful techniques to obtain precise information regarding the chemical structure or the environment of organic molecules. Therefore, gathering the optical signal from a single molecule represents the ultimate limit in terms of chemical analysis and provide a way to probe its local environment. In this presentation, I report recent results, where we used a STM to induce fluorescence emission from a single H2Pc molecule. Two different emission lines, which are relative to each tautomer of the molecule are observed in the STM-Induced fluorescence spectrum. Spatial mapping of these fluorescence lines coupled with a theoretical model using the concept of plasmonic picocavity, where the light is confined by the last atoms of the tip within volumes of the order of 1 nm3, allowed us to obtain optical images of the two tautomers. Thanks to this identification, real-time optical tracking of the tautomerization process is carried out, providing the tautomers lifetimes. This result shows that STM-Induced single-molecule fluorescence experiments constitute a complete optical microscopy technique at the atomic scale.

CPP 16.8 Mon 12:15 WIL A317

Compensating for electrostatically-induced artifacts in scanning near-field optical microscopy — •Tobias Nörenberg[1], Susanne C. Kehr[1], and Lukas M. Eng[1,2] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Nanotechnology and modern material sciences demand reliable local probing techniques with nanometer resolution. In particular, scattering-type scanning near-field optical microscopy (s-SNOM) is a well-established method that is sensitive to the local optical response of a sample, yielding a wavelength-independent lateral resolution on the order of $\sim$10 nm. Nevertheless, local variations of the electric potential at the sample surface may dramatically affect the tip-sample interaction, thereby introducing artifacts in both optical near-field signal and topography.

Here, we present a comprehensive experimental study investigating the mentioned artifacts for different sample systems, i.e. metals (Au), semiconductors (Si), and insulators (SiO_2). By combining s-SNOM with Kelvin-probe force microscopy (KPFM) we firstly fully compensate for these errors, while secondly also being able to measure such local potentials. Optical, topographic, and electronic information hence become well separated and quantified.

CPP 16.9 Mon 12:30 WIL A317

Tip-Enhanced Raman Scattering of CdSe-CdS Nanoplatelets on Plasmonic Substrates — •Ilya Milekhin[1], Mahfujur Rahaman[1], Tatyana Duda[2,3], Ekaterina Rodyakina[2,3], Kirill Anikin[2,3], Roman Vasiliev[4], Volodymyr Dzhagan[5], Alexander Milekhin[2,3], Alexander Latyshev[2,3], and Dietrich RT Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]A.V. Rzhanov Institute of Semiconductor Physics RAS, Novosibirsk, Russia — [3]Novosibirsk State University, Novosibirsk, Russia — [4]Department of Material Science, Moscow State University, Moscow, Russia — [5]V.E. Lashkaryov Institute of Semiconductor Physics, Kiev, Ukraine

We present the results on a gap-plasmon tip-enhanced Raman scattering (TERS) study of core-shell CdSe-CdS nanoplatelets (NPs) deposited on periodic arrays of Au nanodisks which serve as plasmonic substrates. The fabrication of Au nanodisks with a diameter of 110 nm and a height of 50 nm on Si substrates covered with a 77 nm of SiO2 was performed by electron beam lithography. NPs with a characteristic size of 100x30x3 nm were deposited onto the plasmonic substrate using the Langmuir-Blodgett technique. We observe a remarkable Raman enhancement of the phonon modes of CdSe and CdS from NPs located in the plasmonic gap between Au nanodisks and TERS tip. Gap-mode TERS imaging was performed at 638 and 785 nm excitation and allowed us to visualize the near field distribution of the gap-plasmon with relative TERS contrast of 30. A phonon response of the single NP was achieved with a spatial resolution of 2 nm.

CPP 16.10 Mon 12:45 WIL A317

The influence of size and shape of tip and substrate in gap-mode tip-enhanced Raman spectroscopy — •lu he, mahfujur rahaman, teresa i. madeira, and d.r.t. zahn — Semiconductor physics, University of technology Chemnitz, Germany

Tip-enhanced Raman Spectroscopy (TERS) utilizes the confined electric field in the vicinity of a metal tip. The typical spatial resolution is around 2 nm[1] and even sub-nanometer can be achieved[2,3]. Many factors play a role in the TERS technique[4]. Our simulation focuses on the comparison of the two configurations. The first one consists of various tip radii with thin film while the second one consists of a constant tip radius with various radii of spherical substrates in a metal-metallic gap-mode TERS system using the finite element method (FEM). An unusual shift in the first case is observed. An improved expression of the above approximation is obtained for the second case.

CPP 16.11 Mon 13:00 WIL A317

Probing the Local Generation and Diffusion of Active Oxygen Species on a Pd/Au Bimetallic Surface by Tip-Enhanced Raman Spectroscopy — Hai-Sheng Su[1], •Jin-Hui Zhong[2,1], and Bin Ren[1] — [1]State Key Laboratory of Physical Chemistry of Solid Surfaces, iChEM, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China. — [2]Institute of Physics, Carl von Ossietzky University, Oldenburg 26129, Germany

In this contribution, we discuss the application of tip-enhanced Raman spectroscopy (TERS) to image local atomic site-specific electronic and catalytic properties of bimetallic Pd monolayer/Au(111) [1] and Pt nanoisland/Au(111) surface [2]. The high spatial resolution (<3 nm) of TERS allows us to reveal distinct properties of surface atoms that correlate to the catalytic properties. We further probe the local generation and diffusion of OH radicals on a Pd monolayer/Au(111) bimetallic catalyst surface [3]. The reactive OH radicals can be catalytically generated from hydrogen peroxide (H2O2) at the active Pd step edge site and could diffuse to both the Au and Pd surface sites to induce oxidative reactions, with a diffusion length estimated to be about 5.4 nm. The results suggest the capability of TERS, as a plasmon-enhanced nanoscopy, to in-situ study catalysis with unprecedent spatial resolution and rich molecular identity. [1] J.-H. Zhong, B. Ren*, et al., Nat. Nanotech., 2017, 12, 132. [2] H.-S. Su, J.-H. Zhong*, B. Ren*, et al., Angew. Chem. Int. Ed. 2018, 57, 13177. [3] H.-S. Su, J.-H. Zhong*, B. Ren*, et al., submitted.

CPP 16.12 Mon 13:15 WIL A317

Strong surface plasmon localization in gold nanosponges probed by plasmonic nanofocusing spectroscopy — •Anke Korte[1], Abbas Chimeh[1], Jinhui Zhong[1], Dong Wang[2], Peter Schaaf[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität Oldenburg, Germany — [2]Technische Universität Ilmenau, Germany

Porous gold nanosponges, percolated with a three-dimensional network of 10 nm sized ligaments, recently emerged as promising substrates for plasmon-enhanced spectroscopy. Experimental and theoretical studies suggest surface plasmon localization in small hot-spots. To probe the existence of such hot-spots, we have first used scattering-type scanning near-field optical microscopy with homodyne detection of the scattered signal from individual nanosponges to reveal such strong spatially and spectrally confined modes. By recording local near-field scattering spectra, high quality factors of 40 for individual hot-spots are demonstrated. More recently, we combined this method with plasmonic nanofocusing, where surface plasmon polaritons propagate along the shaft of a conical gold taper and form an isolated nano light source. This removes unwanted background since hot-spot modes are locally excited just by the nano-localized tip dipole field, resulting in a highly improved signal-to-noise-ratio and a simplified image interpretation. This advanced technique is used to investigate the coupling behaviour between such hot-spot modes and small quantum emitters, which were deposited inside the pores of a nanosponge.

CPP 16.13 Mon 13:30 WIL A317

Resonant, plasmonic enhancement of alpha-6T molecules encapsulated in CNTs — •Sören Wasserroth[1], Sebastian Heeg[1,2], Niclas Mueller[1], Patryk Kusch[1], Uwe Hübner[3], Etienne Gaufrès[4], Nathalie Tang[4], Richard Martell[4], Aravind Vijayaraghavan[2], and Stephanie Reich[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]The University of Manchester, Manchester, UK — [3]Leibniz IPHT, Jena, Germany — [4]Université de Montréal, Montréal, Canada

Surface-enhanced and resonant Raman scattering are widely used techniques to enhance the Raman intensity by several orders of magnitude. SERS uses plasmonic near-fields to enhance the Raman scattering process, whereas electronic transitions are the origin of the enhancement in resonant Raman scattering. Typical Raman reporters in SERS are molecules; in SERS experiments, the intrinsic resonance of the molecules is often ignored. We present a wavelength dependent Raman study of sexithiophenes encapsulated in carbon nanotubes. To distinguish between the intrinsic resonance and plasmonic enhancement we investigate different tube bundles with and without plasmonic near field. The filled nanotubes are placed precisely in a gold dimer gap by dielectrophoretic deposition. Polarization dependent Raman measurements confirmed the alignment of the molecules within the nanotubes and the influence of the plasmonic near-field. By tuning the excitation wavelength, we were able to determine the intrinsic molecular resonance and observed a strong redshift towards the plasmon resonance of maximum Raman intensity under plasmonic enhancement.

CPP 17: 2D Materials I: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)

Time: Monday 10:30–13:45 Location: WIL C107

Invited Talk CPP 17.1 Mon 10:30 WIL C107

A microscopic view of graphene quantum Hall edge states with STM and AFM measurements — •Joseph A. Stroscio — NIST, Gaithersburg, MD 20899, USA

2D heterostructed devices with electrostatic pn junction boundaries provide a convenient geometry for the examination of Quantum Hall edge states with microscopic probes. In this talk I will review our work in circular and rectangular geometries to examine the quantum Hall edge states which form in high magnetic field using scanning tunneling microscopy (STM) and atomic force microscopy (AFM) measurements. In circular graphene pn junctions a concentric series of compressible and incompressible rings form due to electron interactions, and show single electron charging when probed by scanning tunneling spectroscopy. In a rectangular Hall bar geometry defined by pn junction boundaries, the compressible strips form the topological protected edge states in the quantum Hall effect. For the graphene Hall bar device, we utilize simultaneous AFM, STM, and quantum transport measurements at mK temperatures. The Kelvin probe force microscopy (KPFM) mode of AFM detects the chemical potential transitions when Landau levels are being filled or emptied as a function of back gate potential. In particular, symmetry breaking states can be resolved at filling factors $\nu = *1$ inside the N=0 Landau level manifold, showing the lifting of the graphene four-fold degeneracy due to spin and valley. With KPFM we can map the dispersion of the Landau levels across the quantum Hall edge boundary as a function of density and spatial position, including resolving the $\nu = *1$ edge modes.

CPP 17.2 Mon 11:00 WIL C107

Energy dissipation on suspended graphene quantum dots — •Alexina Ollier[1,2], Marcin Kisiel[1], Urs Gysin[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel,Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Swiss Nanoscience Institute, Klingelbergstrasse 82, 4056 Basel

Here we report on a low temperature (T=5K) measurement of striking singlets or multiplets of dissipation peaks above graphene nanodrums surface. The stress present in the structure leads to formation of few nanometer sized graphene quantum dots ribbons (GQDRS) and the observed dissipation peaks are attributed to tip-induced charge state transitions in quantum-dot- like entities. The dissipation peaks strongly depend on the external magnetic field (B=0T-2T), the behavior we attributed to crossover from quantum dot carrier confinement to the confinement by magnetic field.

CPP 17.3 Mon 11:15 WIL C107

The edge morphology and electronic properties of ballistic sidewall zig-zag graphene nanoribbons on SiC (0001) — •T.T.Nhung Nguyen[1], H. Karakachian[2], J. Aprojanz[1], U. Starke[2], A. Zakharov[3], C. Polley[3], and C. Tegenkamp[1] — [1]TU Chemnitz, Germany — [2]Max Planck Institute, Germany — [3]MAX IV Lab, Sweden

Epitaxial graphene nanoribbons grown on SiC(0001) mesa structures were shown to reveal ballistic transport at room temperature. The subsequent improvement of preparation parameters allows us to fabricate large scale zig-zag type ribbons with 40nm in widths with a pitch size down to 200 nm. We analyzed the electronic structure of the ribbons and their edges by ARPES and STM/STS. Indeed, ARPES reveals clearly the Dirac cone from the ribbon. The Fermi energy coincides with the Dirac point. This finding is corroborated by STS, revealing an elastic tunneling gap of around 130meV. STM shows that the zigzag edge merges into the SiC substrate. Exactly at the position of this edge, a metallic state is seen at 0V. The gradual decrease of its intensity within 3nm comes along with a peak splitting. Moreover, the valence and conduction band states reveal close to the edge a larger gap of around 300 meV. We assign these findings to a hybridization of the zig-zag GNR edge with SiC. Furthermore, we propose that the ballistic transport is rather mediated by a 1D interface state rather than by a GNR edge state. The interface state mimics massive particles, which is consistent with the energy positions of electron transmission peaks found in GNR nanoconstrictions of various lengths.

CPP 17.4 Mon 11:30 WIL C107

Attosecond-fast current control at graphene-based interfaces — •Tobias Boolakee, Christian Heide, Heiko B. Weber, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Epitaxially grown monolayer graphene on bulk n-doped silicon carbide (SiC) forms a Schottky contact with remarkable electronic and optical properties. We show that charge transfer across the graphene-SiC solid-state interface takes place within (300 ± 200) attoseconds (1 as = 10^{-18} s), which is the fastest charge transfer observed across a solid-state interface [1]. To reveal the attosecond dynamics, we apply femtosecond laser pulses and use saturable absorption in graphene as an intrinsic clock to determine how long an excited state stays excited before charge transfer and thermalization depopulate this state. Recent experimental results and a simple theoretical modelling based on rate equations and on a quantum mechanical model will be presented [2,3].

[1] Heide, C. et al. accepted in Nat. Photon.
[2] Higuchi, T. et al. Nature **550**, 224–228 (2017).
[3] Heide, C. et al. New J. Phys. **21** (2019).

CPP 17.5 Mon 11:45 WIL C107

Sideband generation & pseudospin-flip excitations in graphene using tr-momentum microscopy — •Marius Keunecke[1], David Schmitt[1], Christina Möller[1], Davood Momeni Pakdehi[2], Hendrik Nolte[1], Wiebke Bennecke[1], Marie Gutberlet[1], Matthijs Jansen[1], Marcel Reutzel[1], Klaus Pierz[2], Daniel Steil[1], Hans Werner Schumacher[2], Sabine Steil[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen. I. Physikalisches Institut, 37077 Göttingen, Germany — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The coherent control of quantum states is a promising route towards new emerging phases in solids. One of these phases are the so called Floquet-Bloch states, created by a periodic driving laser. Other light-matter coupled states (Volkov states) arise close to the surface of a solid and are understood as a final state dressing by the laser light. In graphene, the driving by circularly polarized light is predicted to open up a bandgap at the dirac point and thus creating a Floquet topological insulator [1]. In our experiment, the electronic bandstructure of ML graphene on SiC (0001) is mapped during photo-excitation using a momentum microscope in combination with a 1 Mhz femtosecond

HHG lightsource (26.6 eV). Different pump wavelengths and polarizations are used to disentangle the excited states dynamics and the sideband generation at high momenta. We will discuss the nature of the generated sidebands and the photoinduced anisotropic hot carrier distributions. [1] M. A. Sentef et al., Nat. Commun. 6, 7047 (2015)

CPP 17.6 Mon 12:00 WIL C107

Melting the low temperature gap in monolayer VSe_2, in time resolved ARPES — •Deepnarayan Biswas[1,2], Alfred Jones[1], Paulina Majchrzak[1,3], Klara Volckaert[1], Charlotte Sanders[1,3], Igor Marković[2], Federico Andreatta[1], Akhil Rajan[2], Yu Zhang[3], Gabriel Karras[3], Tsung-Han Lee[4], Chang-Jong Kang[4], Byoung Ki Choi[5], Richard Chapman[3], Adam Waytt[3], Emma Springate[3], Jill Miwa[1], Philip Hofmann[1], Phil D. C. King[2], Young Jun Chang[5], Nikola Lanata[1], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]University of St Andrews, UK — [3]Central Laser Facility, UK — [4]Rutgers University, USA — [5]University of Seoul, Republic of Korea

The group V transition metal dichalcogenide VSe_2 shows a charge density wave (CDW) transition at 110 K with $(4 \times 4 \times 3)$ charge ordering in its bulk form. In contrast, recent experiments on monolayer (ML) VSe_2 have shown an enhanced transition at ~ 140 K with very different charge ordering. Moreover, this transition is accompanied by a full gapping of the Fermi surface. Here, we have used time and angle resolved photoelectron spectroscopy (TR-ARPES) to understand the electron dynamics in ML VSe_2 above and below the transition temperature. We have also modelled the ARPES intensity using a modified BCS self energy and density functional theory calculated bare bands. We find the gapped phase vanishes upon pumping and takes unusually long time to recover (more than 10 ps). This behaviour points toward a hot electron relaxation bottleneck coupled with an electronic phase transition in this sample.

CPP 17.7 Mon 12:15 WIL C107

Time-dependent momentum distributions of bright and dark excitons in bulk WSe2 — •Shuo Dong[1], Samuel Beaulieu[1], Dominik Christiansen[2], Maciej Dendzik[1], Tommaso Pincelli[1], Rui Patrick Xian[1], Julian Maklar[1], Malte Selig[2], Andreas Knorr[2], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Transition metal dichalcogenide semiconductors feature exceptional optoelectronic properties. The investigation of excited states in k-space provides access to optically-bright and dark states on equal footing. Here, we perform the momentum-resolved excited-state mapping in the entire first Brillouin zone of bulk WSe2 using time-resolved momentum microscopy. Upon resonant excitation of band gap, the bright excitons with trARPES signal in the K valleys rapidly scatter to finite-momentum dark excitons in the Σ valleys. We analyze the shape and size of momentum distribution of the excited state. Under the plane wave final state approximation, the Fourier transform of photoemission signal yields real-space image of excitonic wave function. Combined with a microscopic theoretical description of exciton dynamics, the momentum-resolved valley carrier distribution provides information of fundamental exciton properties, like size, binding energy and exciton-phonon coupling.

CPP 17.8 Mon 12:30 WIL C107

Sub-picosecond photo-induced displacive phase transition in two-dimensional $MoTe_2$ — •Bo Peng[1,2], Hao Zhang[2], Heyuan Zhu[2], Bartomeu Monserrat[1], and Desheng Fu[3] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Optical Science and Engineering, Fudan University, China — [3]Department of Optoelectronics and Nanostructure Science, Shizuoka University, Japan

Photo-induced phase transitions (PIPTs) provide an ultrafast, energy-efficient way for precisely manipulating the topological properties of transition-metal ditellurides, and can be used to stabilize a topological phase in an otherwise semiconducting material. By first-principles calculations, we demonstrate that the PIPT in monolayer $MoTe_2$ from the semiconducting 2H phase to the topological 1T' phase can be driven purely by electronic excitations. The photo-induced electronic excitation changes the electron density, and softens the lattice vibrational modes. These pronounced softenings lead to structural symmetry breaking within sub-picosecond timescales, which is far shorter than the timescale of a thermally driven phase transition. The transition is predicted to be triggered by photons with energies over 1.96 eV, corresponding to an excited carrier density of 3.4×10^{14} cm^{-2}, which enables a controllable phase transformation by varying the laser wavelength. Our results provide insight into the underlying physics of the phase transition in 2D transition-metal ditellurides, and show an ultrafast phase transition mechanism for manipulation of the topological properties of 2D systems.

CPP 17.9 Mon 12:45 WIL C107

Understanding electron beam damage in 2D materials from first-principles calculations: Effects of chemical etching and electronic excitation — •Silvan Kretschmer[1] and Arkady V. Krasheninnikov[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

Two-dimensional (2D) materials are routinely characterized nowadays in the transmission electron microscope (TEM). The high-energy electron beam in TEM can create defects in the target, and as the influence of defects on materials properties is expected to be stronger in systems with reduced dimensionality, understanding defect production in 2D materials is of particular importance. Irradiation-induced defects can appear through three mechanisms, namely ballistic or knock-on damage (1), ionization and electronic excitations (2) and beam-induced chemical etching (3). Only the first channel is well understood, while observations of defects formation in 2D transition metal dichalcogenides below the knock-on threshold point out that other mechanism should be important. Here we investigate the role of beam-induced chemical etching and electronic excitations in defect production by using ab-initio molecular dynamic simulations and advanced first-principles simulation techniques based on the Ehrenfest dynamics combined with time-dependent density-functional theory. We demonstrate that the adsorption of small beam-induced radicals and electronic excitations dramatically lower the displacement threshold.

CPP 17.10 Mon 13:00 WIL C107

Interaction of highly charged ions with single, bi- and trilayer graphene — •Anna Niggas[1], Janine Schwestka[1], Sascha Creutzburg[2], Benjamin Wöckinger[1], Tushar Gupta[3], Bernhard C. Bayer-Skoff[3], Friedrich Aumayr[1], and Richard A. Wilhelm[1,2] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [3]TU Wien, Institute of Materials Chemistry, Vienna, Austria

The interaction of highly charged ions (HCIs) with surfaces has been in the focus of many groups over the last decades. Recently, the rise of 2D materials has provided access to study the neutralisation dynamics of HCIs as they have not reached their equilibrium charge state inside atomically thin materials yet.

In our experiment, we use Xe ions (Xe^{1+} to Xe^{44+}) with energies in the range of 1-400 keV as projectiles and we then record the exit charge states of the ions after transmission through 2D materials. Additionally, we are able to determine the energy loss during the interaction through time of flight measurements, the yield and energy of emitted secondary electrons and forward sputtered target atoms in coincidence.

We now focus especially on the dependence of the neutralisation process on the thickness of the target. Thus, we employ single, bi- and trilayer graphene to mimic graphite with adjustable thickness. In order to ensure that this target structure is not affected by contaminations, it is crucial to implement cleaning procedures. Possible *in-situ* techniques and their effects will also be discussed in this context.

CPP 17.11 Mon 13:15 WIL C107

Neutralization of ions transmitted through graphene and MoS_2 monolayers — •Sascha Creutzburg[1,7], Janine Schwestka[2], Anna Niggas[2], Heena Inani[3], Anthony George[4], Lukas Madauss[5], Stefan Facsko[1], Jani Kotakoski[3], Marika Schleberger[5], Andrey Turchanin[4], Pedro L. Grande[6], Friedrich Aumayr[2], and Richard A. Wilhelm[1,2] — [1]HZDR, Ion Beam Center, Dresden, Germany — [2]TU Wien, Institute of Applied Physics, Vienna, Austria — [3]University Vienna, Faculty of Physics, Vienna, Austria — [4]Friedrich Schiller University Jena, Institute of Physical Chemistry, Germany — [5]University Duisburg-Essen, Faculty of Physics and CENIDE, Germany — [6]Federal University of Rio Grande do Sul, Porto Alegre, Brazil — [7]TU Dresden, Germany

Ion irradiation is a widely used technique for material modification. The use of ion irradiation for defect engineering in 2D materials requires a high sensitivity of energy deposition in the surface during the ion's impact. Ions of high charge states (e.g. Xe^{30+}) deposit their potential energy of up to tens of keV in shallow surface depths triggering nanostructure formation. In fact, nanostructure formation in 2D materials, like carbon nanomembranes or MoS_2, due to the impact of Xe ions of charge states larger than 28 was observed. In contrast, no nanostructures on graphene were found, even after irradiation with Xe^{40+} ions. Here, we investigated the ion's neutralization during the transmission through freestanding graphene and MoS_2 monolayers. We deduce the lost energy of the ions (kinetic and potential) in experiment and put our results into context of nanostructuring.

CPP 17.12 Mon 13:30 WIL C107

Ab-initio Exciton-polaritons: Cavity control of two-dimensional Materials — •Simone Latini[1], Enrico Ronca[1], Hannes Hübener[1], Umberto De Giovannini[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free Electron Laser Science, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth avenue, New York NY 10010

We put forward a novel way of controlling the optical features of two-dimensional materials by embedding them in a cavity. The cavity light-matter interaction leads to the formation of exciton-polaritons, mixed states of matter and light. We demonstrate a reordering and mixing of bright and dark excitons leading to the direct optical observation of the latter. In type II van-der-Waals heterostructure, we show that the cavity provides control on the stabilization of inter- over intralayer excitons. Our theoretical predictions are based on a newly developed non-perturbative many-body framework that involves the ab-initio solution of the coupled quantized electron-photon Schrödinger equation in a quantum-electrodynamics plus Bethe-Salpeter approach. Within this framework we are able to investigate exciton-polariton states and predict their dispersion and response in a strong cavity light-matter coupling regime. Our method lends itself to the investigation of more complex polaritonic, so called phonoriton, a mixture of excitons, phonons and photons. In particular we were able to identify elusive phonoritonic spectral features observed in a state-of-the-art pump and probe experiment.

CPP 18: Topical Session: Data Driven Materials Science - Materials Design II (joint session MM/CPP)

Time: Monday 11:45–13:00 Location: BAR 205

CPP 18.1 Mon 11:45 BAR 205

Versatile Bayesian deep-learning framework for crystal-structure recognition in single- and polycrystalline materials — •Andreas Leitherer, Angelo Ziletti, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Physical properties of a given material are directly related to its structure. In particular, in polycrystalline materials the location and nature of grain boundaries are crucial features determining their properties. For instance, mechanical characteristics of steels are strongly influenced by grain boundaries. In this work, we propose *strided pattern matching* which is a framework using single-crystal classification to investigate polycrystals. Accessible crystal-structure identification methods are either very robust – but can treat only few classes – or include a large number of classes – but are not very robust. We use a Bayesian neural network in combination with the smooth-overlap-of-atomic-positions (SOAP) descriptor, allowing us to classify, robustly and without any predefined threshold, more than 100 prototypes including not only bulk but also two- and one-dimensional materials (e.g., fullerenes). Furthermore, we are able to quantify the uncertainty in the model predictions. As an example for polycrystal investigation, we apply our model to recognize an ordered $L1_2$ phase in a disordered fcc matrix. This serves as a model system for precipitate detection in Ni-based superalloys, which are materials used in aircraft engines.

CPP 18.2 Mon 12:00 BAR 205

Parametrically Constrained Geometry Relaxations for High-Throughput Materials Science — •Maja-Olivia Lenz[1], Thomas A. R. Purcell[1], David Hicks[2], Stefano Curtarolo[1,2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Department of Materials Science and Mechanical Engineering, Duke University, Durham, USA

Exploiting crystal symmetries is a common technique to accelerate and improve electronic-structure calculations. However, this method usually fails when the global symmetry is broken, e.g., in materials with defects. We present a relaxation scheme that uses parametric geometry constraints to allow symmetry conservation at all levels [1]. We demonstrate how it can be used to relax metastable structures that are otherwise poorly addressable. Using the example of polarons in MgO [2], we showcase the ability to relax structures with local symmetry breaking with known distortion patterns. The flexibility of our constraints is particularly useful to accelerate high-throughput searches for novel materials. A performance study on several hundreds of different materials throughout the structural space has been done using the AFLOW Library of Crystallographic Prototypes [3]. The assignment of prototypes is helpful not only to enable user-friendly searches in materials databases like NOMAD Archive but also to describe and refine terms and concepts in a prospective materials ontology.

[1] M.-O. Lenz, *et al.*, accepted in Npj Comput. Mater. (2019).
[2] S. Kokott, *et al.*, New J. Phys. **20** (3):33023 (2018).
[3] M. J. Mehl, *et al.*, Comp. Mater. Sci. **136**, S1 (2017).

CPP 18.3 Mon 12:15 BAR 205

Combining ab-initio and data-guided approaches for refractory multi-principal element alloys design — •Yury Lysogorskiy[1], Alberto Ferrari[2], and Ralf Drautz[1] — [1]AMS, ICAMS, Ruhr University Bochum, Bochum, Germany — [2]Delft University of Technology, Delft, Netherlands

Refractory multiple principal element alloys (MPEA) nominally consist of several elements of the groups IV-VI at near-equal compositions in a single crystalline bcc phase that is characterized by exceptional high-temperature mechanical properties and a very high melting point. In this work we introduce a computationally tractable and accurate method, based on first-principles calculations and alloy modelling, to predict phase stability in MPEAs at arbitrary compositions. We reconstruct the complete phase diagram of the prototypical refractory MPEAs Mo-Nb-Ta-W and detect the regions where the formation of a solid solution is favorable at a given transition temperature. We then extend the modeling of temperature dependent properties with supervised machine learning (ML) and combine these results to a ML model for Vickers hardness, trained on experimental data from literature, to identify out-of-equiatomic composition regions of lower solid-solution formation temperature and higher hardness.

CPP 18.4 Mon 12:30 BAR 205

Data-Efficient Machine Learning for Crystal Structure Prediction — •Simon Wengert[1], Gábor Csányi[2], Karsten Reuter[1], and Johannes T. Margraf[1] — [1]Chair of Theoretical Chemistry, TU Munich, Germany — [2]Department of Engineering, University of Cambridge, UK

The combination of modern machine learning (ML) approaches with high-quality data from quantum mechanical (QM) calculations can yield models with an unrivalled accuracy/cost ratio. However, such methods are ultimately limited by the computational effort required to produce the reference data. In particular, reference calculations for periodic systems with many atoms can become prohibitively expensive. This trade-off is critical for crystal structure prediction. Here, a data-efficient ML approach would be highly desirable, since screening a huge space of polymorphs with small stability differences requires the assessment of a large number of trial structures with high accuracy.

In this contribution, we present tailored hybrid-ML models that allow screening a wide range of crystal candidates while adequately describing the subtle interplay between intermolecular interactions such as H-bonding and many-body dispersion effects. This is achieved by enhancing a physics-based description of long-range interactions —for which an efficient implementation is available— with a short-range ML model trained on high-quality first-principles reference data. The presented workflow is broadly applicable to different molecular systems, without the need for a single periodic calculation on the reference level of theory.

CPP 18.5 Mon 12:45 BAR 205

Uncovering Anharmonicity in Material Space — •Thomas Purcell, Florian Knoop, Chuanqi Xu, Matthias Scheffler, Luca Ghiringhelli, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Identifying materials with ultra-low thermal conductivities κ is the pivotal challenge in the development of more efficient thermoelectric devices. One strategy to achieve this goal is to find materials with a high level of anharmonicity, and therefore reduced phonon lifetime and κ. To help discover such materials, we calculate the anharmonicity of materials ranging from simple binary compounds to complex perovskites using the high-throughput framework *FHI-vibes* [1]. The framework automatically generates an accurate harmonic model for a material's vibrational properties, from which we determine its anharmonicity by statistically comparing the harmonic and *ab initio* forces of thermally displaced structures. Our screening not only demonstrates that anharmonicity is more prevalent in material space than previously thought, but also shows that the developed metric strongly correlates with various thermal properties. Using classes of simple binaries as an example, we show that the anharmonicity of a material can be related to its atomic, bulk, and harmonic properties via the sure independence screening and sparsifying operator (SISSO) approach [2], thus facilitating an even more efficient screening.

[1] https://vibes.fhi-berlin.mpg.de

[2] R. Ouyang, *et al. Phys. Rev. Mat.* **2**, 083802 (2018)

CPP 19: Focus: Soft Matter and Nanocomposites - New opportunities with advanced neutron sources II

Time: Monday 15:00–17:00 Location: ZEU 222

CPP 19.1 Mon 15:00 ZEU 222

TOF-NR investigation of cononsolvency in PNIPAM-based block copolymer thin films — •Christina Geiger[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 Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Institut Laue-Langevin, 38042 Grenoble, France — [3]Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam, Germany — [4]TU München, Physik-Department, Physik weicher Materie, 85748 Garching, Germany

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 also be induced upon addition of organic cosolvents due to the competitive attachment and detachment of water and cosolvent to the PNIPAM chains. We demonstrate that the cononsolvency effect is transferrable from solutions to thin polymer films. The film swelling and collapse kinetics due to the uptake of water and cosolvent from a saturated vapor atmosphere 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 cosolvent within the polymer films.

CPP 19.2 Mon 15:15 ZEU 222

On the structure and inner dynamics of zwitterionic polysulfobetaine brushes — •Judith Witte[1], Olaf Holderer[2], Jörg Lahann[3,4], and Stefan Wellert[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Heinz Maier-Leibnitz Zentrum, Garching, Germany — [3]University of Michigan, Ann Arbor, MI, USA — [4]Karlsruhe Institute of Technology, Karlsruhe, Germany

PMEDSAH brushes are zwitterionic polysulfobetaine brushes, which are investigated as a microenvironment for the attachment and lift-off of cells and proteins. Structure and dynamics of polymer brushes influence the motion of macromolecules, nanoparticles or proteins at and along the interface and their potential adsorption at or penetration into the brushes. So far, a rather simple approach is used to discuss the complex self-association behavior. Still, a more detailed understanding of the structure and dynamics within PMEDSAH brushes, especially of the self-association behavior, is lacking. We conduct a series of complementary laboratory and neutron scattering experiments to improve the basic understanding of the influence of the grafting density on the brush structure and inner dynamics. Beside X-ray-reflectometry and ellipsometry measurements on dry polysulfobetaine brushes with different grafting densities also multi contrast neutron reflectometry measurements on the wet brushes were performed to investigate the brush structure in dependence on the grafting density. Additionally, neutron spin echo spectroscopy under grazing incidence is applied to study the influence of the self-association on the segmental dynamics in the polysulfobetaine brushes.

CPP 19.3 Mon 15:30 ZEU 222

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 19.4 Mon 15:45 ZEU 222

Polyelectrolyte Multilayer Films from Mixtures of Polyanions: Different Composition in Film and Preparation Solution — •Annekatrin Sill, Antonia Weltmeyer, Peter Nestler, Malte Passvogel, Sven Neuber, and Christiane A. Helm — University Greifswald, Institute of Physics, Germany

Polyelectrolyte multilayer films were prepared from polyanion PSS and polycation PDADMA in 0.1 M NaCl by sequential adsorption of oppositely charged polyelectrolytes. PSS consisted of binary mixtures of long deuterated PSSd (Mw(PSSd) = 80.8 kDa) and short protonated PSS (Mw(PSS) = 10.6 kDa). With neutron reflectivity, it was found that the mole fraction of long PSSd in the film exceeded the one in the deposition solution. Indeed, the film consisted of only PSSd if the mole fraction of PSSd in the deposition solution exceeded 5%. This observation can be explained by the adsorption kinetics which were studied with in-situ ellipsometry. Two mechanisms determined the film composition: (i) during PSS deposition, adsorption of short PSS was reversible while adsorption of long PSSd was irreversible; thus, the PSSd fraction increased with adsorption time; (ii) if short PSS was present, each polycation adsorption step was followed by slow desorption of polyelectrolyte complexes consisting of PDADMA and short PSS molecules. Short PSS is bound with fewer electrostatic monomer/monomer bonds to the film and can easier desorb, or form complexes with PDADMA. These studies show how to measure and control film composition when polydisperse polyelectrolyte solutions are used for film preparation.

CPP 19.5 Mon 16:00 ZEU 222

Functional Nanocomposites: Neutron Scattering Study — •Margarita Kruteva[1], Lisa Fruhner[1,2], Artur Feld[3], Rieke

Koll[3], Hauke Heller[3], Jürgen Allgaier[1], Wim Pyckhaut-Hintzen[1], Artem Feoktystov[4], Olaf Holderer[4], Michaela Zamponi[4], Horst Weller[3], and Stephan Förster[1] — [1]Jülich Centre for Neutron Science (JCNS-1) and Institute for Complex Systems (ICS-1), Forschungszentrum Jülich GmbH, Germany — [2]Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany — [3]Institut für Physikalische Chemie, Universität Hamburg, Germany — [4]Jülich Centre for Neutron Science JCNS at MLZ, Garching, Germany

Nowadays adaptive synthetic polymer materials which are able to change their properties on demand play important role in nanotechnology. In contrary to conventional polymer nanocomposites, the nanoparticles functionalized with a polymeric shell, which takes the role of a matrix, allow to control the distance between the nanoparticles and homogeneously dispersed per definition. Determining factors are size of the core, grafting density, length of the grafting chain and temperature. Supramolecular functionalization (H-bonds) of the grafting chains leads to additional steps in adaptiveness. Moreover, using magnetic nanoparticle as a core extends the application area to e.g. magnetorheological nanocomposites. In this talk I will focus (1) on the structure of magneto-elastomeric nanocomposites with supramolecular activity and (2) polymer chain dynamics in one component nanocomposites (OCNC) studied by neutron scattering.

CPP 19.6 Mon 16:15 ZEU 222

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 polythiophene. 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 19.7 Mon 16:30 ZEU 222

Ionic liquid cation dynamics in carbon nanoconfinement: A pore size and temperature-dependent neutron spectroscopy study — •Mark Busch[1], Tommy Hofmann[2], Bernhard Frick[3], Jan P. Embs[4], Boris Dyatkin[5], and Patrick Huber[1] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, Switzerland — [5]Dept. of Materials Science and Engineering, Drexel University, Philadelphia, U.S.A.

The temperature-dependent cation dynamics of the room-temperature ionic liquid [BuPy][Tf_2N] within the nanoconfinement of carbide-derived carbons with various pore sizes are investigated by quasi-elastic neutron spectroscopy. An overview of the dynamic landscape over a wide temperature range is obtained by employing fixed window scans, where one sample parameter is scanned, while only one specific energy transfer value is observed. These data that provide already a quite comprehensive understanding of the confinement-induced alteration of the molecular mobility in comparison to the bulk are complemented by a more detailed analysis of full energy transfer spectra. Two diffusive processes on different time scales are found. Both are considerably slower than in the bulk and the corresponding self-diffusion coefficients decrease with decreasing nanopore size. In spite of this dynamic slow down, the temperature range of the liquid state upon nanoconfinement is found to be notably extended to much lower temperatures.

CPP 19.8 Mon 16:45 ZEU 222

The impact of water on functional nanocellulose thin films — •Calvin J. Brett[1,2], Lucas P. Kreuzer[3], Tobias Widmann[3], Elisabetta Nocerino[1], Ola K. Forslund[1], Lionel Porcar[4], Peter Müller-Buschbaum[3,5], Martin Månsson[1], Daniel L. Söderberg[1], and Stephan V. Roth[1,2] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Deutsches Elektronen-Synchrotron, Hamburg, German — [3]Technische Universität München, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [4]Institut Laue-Langevin, Grenoble, France — [5]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

Sustainable devices experience a massive increase of attention over the last decade. Our whole economy is starting to minimize the use of fossil resources. Nevertheless, it is yet not fully understood how sustainable devices perform and degrade under environmental influences and how we could improve possible drawbacks. Cellulose, as one of the most earth abundant nature materials, consists of so-called cellulose nanofibrils. These nanoscale building blocks have high potential in applications due to their low density, high material strength and sustainability. Within this project, we show how to manufacture materials with desired physical properties such as electrical conductance, optical transmittance, and the tunability of wetting behavior. For real-life applications, we tested the water impact on these functional thin films by applying humidity and studying the films by means of grazing incidence small-angle neutron/X-ray scattering (GISAXS/GISANS) at P03 / PETRA III (Hamburg) and D22 / ILL (Grenoble).

CPP 20: Molecular Electronics and Excited State Properties II

Time: Monday 15:00–16:15 Location: ZEU 260

CPP 20.1 Mon 15:00 ZEU 260

Modeling the Complex Band Structure of Conjugated Polymers via Kronig-Penney-like Models — •Florian Günther[1], Kevin Preis[2], and Sibylle Gemming[2,3] — [1]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [2]Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany — [3]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

In molecular electronics, it is crucial to understand and control the electronic properties of the involved materials. Due to the small length scale, which is in the range of nanometers and below, the coherent electron tunneling plays an important role in the conduction behavior of the used compounds. Its exponential decay with the length can be studied by considering the complex band structure in the region of the Fermi energy.

In our work, we calculate the real and the complex bands of various conjugated polymers using the density functional based tight binding approach. The results are fitted with the analytical solutions arising from the two-band tight binding and the Kronig-Penney models. While the former exhibits less free parameters, the latter is able to reproduce the non-symmetric shape of the complex bands with respect to the Fermi energy. We found that the product of the barrier height and width of the Kronig-Penney model correlates with the tunneling inverse decay length. Our results suggest that the coherent electron tunneling through conjugated polymers can be estimated by fitting the Kronig-Penney model to the real band structure.

CPP 20.2 Mon 15:15 ZEU 260

Understanding Ultrafast Proton transfer reaction in Molecular Crystals — •Hyein Hwang[1,2], Vandana Tiwari[1,2], Simon Bittmann[1], Hong-Guang Duan[1], Friedjof Tellkamp[1], Ajay Jha[1], and R. J. Dwayne Miller[1,3] — [1]MPSD, Hamburg, Germany — [2]Department of Chemistry, University of Hamburg, Germany — [3]Departments of Chemistry and Physics, University of Tornoto, Canada

Ultrafast proton transfer reactions is a topic of great interest particularly due to their association with the understanding of primary elementary reaction pathways in functional electrochemical and biological systems. Although these reactions have been extensively investigated in solution for the role of interaction between the solute and the solvent-bath, but the reaction dynamics in bulk single molecular crystals remains elusive. Here, we study ultrafast intramolecular proton transfer reaction in hydroxyanthraquinones in crystalline form, where molecular system forms the 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.

CPP 20.3 Mon 15:30 ZEU 260

Exciton dynamics in optically active surface-mounted metal-organic frameworks: A time-resolved second harmonic generation study — •Vipilan Sivanesan[1], Ritesh Haldar[2], Christof Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Germany

For the optimization of organic optoelectronic devices it is important to understand the ultrafast electronically excited state dynamics in organic semiconductors after optical excitation. For instance, different molecular packing and relative orientations of the optically active chromophores can affect the excitonic coupling strength. This can be studied in crystalline molecular assemblies by integrating these chromophores into surface-mounted metal-organic frameworks (SURMOFs) as organic linkers. Varying the side-groups of the molecules enables to engineer the crystal structure to tune the excitonic coupling. To analyse the influence of this crystal engineering on the ultrafast dynamics we investigated thin films of chromophore functionalized Zn-SURMOF by means of femtosecond time-resolved second harmonic generation.

Literature: [1] R. Haldar et al., Chem. Eur. J, 23, 14316 (2017) [2] R. Haldar et al., Nature Commun. 10:2048 (2019)

CPP 20.4 Mon 15:45 ZEU 260

Optical absorption of azobenzene-derivatives in solution and in metal-organic frameworks via embedded orbital-tuned Bethe-Salpeter calculations — •Aseem Rajan Kshirsagar and Roberta Poloni — Univ. Grenoble-Alpes, CNRS, Grenoble-INP, SIMaP, Grenoble 38000, France

The use of UV-Vis light has been proposed as an energy-efficient strategy for capture and release of CO_2 in azobenzene-functionalized metal-organic frameworks (MOFs). We recently demonstrated that the mechanism behind the observed reversible change in gas adsorption is metal-node blocking by the *cis* isomer upon UV-Vis excitation [1]. Large photo-isomerization yields are needed in order to achieve large changes in CO_2 uptake, underlining the importance of a highly selective optical absorption by each isomer. For this, the Bethe-Salpeter formalism with a non-equilibrium embedding scheme has been employed to accurately compute the paradigmatic case of S_1 band separation between *cis* and *trans* in azobenzene derivatives in solution. Besides embedding, we show that the choice of the DFT functional is critical, despite the iterative convergence of *GW* quasiparticle energies. In light of this result, we employ an environment-consistent orbital-tuning method to study 20 azobenzene derivatives in solution and then extend this approach to study the nature of the lowest energy excitons of MOF and the implications of using periodic versus non-periodic models of MOFs. [1] Yang, Kshirsagar, Eddin, Lin, Poloni, *Chem. Eur. J.* **24**, 15167 (2018); [2] Kshirsagar, D'Avino, Blase, Li, Poloni, *ChemRxiv* (2019), url: https://chemrxiv.org/s/a7791c5ab68368b15dce.

CPP 20.5 Mon 16:00 ZEU 260

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 $\leq$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 21: Crystallization, Nucleation and Self-Assembly

Time: Monday 15:00–17:00 Location: ZEU 255

CPP 21.1 Mon 15:00 ZEU 255

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

The formation of tetragonal lysozyme crystals from supersaturated solutions has been monitored by isothermal microcalorimetry. The weak dependence of the crystallization enthalphy ΔH on salt concentration and pH value can be explained by a linearized Poisson-Boltzmann theory. The calorimetric signal is related to the concentration change during nucleation and growth, from which the induction time t_{ind} and, using a finite difference model, the growth rate G are determined. The dependences of t_{ind} and G on the chemical potential are in line with previous findings and can be modelled by classical nucleation theory and the growth of 2D clusters, respectively.

CPP 21.2 Mon 15:15 ZEU 255

Specific ion selection of protein crystal structures and growth — •Ralph Maier[1], Christian Simo[1], Aafiya Idrees[1], Georg Zocher[1], Fajun Zhang[1], Thilo Stehle[1,2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Vanderbilt University School of Medicine, Nashville, USA

We study protein crystallization in aqueous solutions of β-lactoglobulin (BLG) with $ZnCl_2$ by microscopy and small angle X-ray scattering (SAXS). This system is compared to a previously investigated system of BLG with another divalent salt ($CdCl_2$). Both systems exhibit a reentrant condensation phase behavior with phase transitions at the salt concentration (c_s) c^* and *pseudo*-c^{**} and a morphology change of the resulting crystals by increasing c_s [1]. Importantly, in contrast to BLG with Cd where all crystals share the same structure [2], the morphology change with Zn is accompanied by a change of the crystal structure as verified by SAXS measurements. While the needle-like crystals nucleate in a $P3_221$ structure, the structure of the more compact crystals, which is similar as for Cd, could not yet been resolved due to twin crystals for Cd. Interestingly, for BLG-Cd, a two-step crystallization mechanism has been proposed and an intermediate phase between the initial solution and the final crystal was identified by a specific SAXS correlation peak, which, however, has not yet been observed for Zn [2] despite forming the similar structure. This provides a model system to investigate different crystallization pathways leading to different structures. [1] Sauter *et al.*, *J. Am. Chem. Soc.*, 2015, 137, 1485-1491. [2] Sauter *et al.*, *Cryst. Growth Des.*, 2014, 14, 6357-6366.

CPP 21.3 Mon 15:30 ZEU 255

Crystal structure prediction for benzene using basin-hopping global optimisation — •Atreyee Banerjee[1] and David Wales[2] — [1]MPIP — [2]Cambridge University

Organic molecules can be stable in distinct crystalline forms known as polymorphs, which are important for industrial application. Here we use basin-hopping global optimization [1] to predict different low energy structures for crystalline benzene. An anisotropic pair potential is employed using rigid benzene molecules and periodic boundary conditions [2]. We find that basin-hopping can rapidly locate most of the stable crystal structures even for a small cell, validating the methodology as well as the accuracy of the potential. We adopted a recently developed methodology where the supercell is adjusted dynamically to contain the cutoff radius for the real space interaction. During the basin-hopping run, we find a number of unphysical structures that are eliminated by choosing a larger system size. A critical size of the cell is proposed in order to eliminate the system-size effects. Our results suggest that the basin-hopping framework is effective for structure prediction of crystalline systems, in addition to clusters and biomolecules, without additional information from experimental data or symmetry constraints.

References:

[1] D.J. Wales and J. P. K Doye, J. Phys. Chem. A, 101, 5111, 1997.

[2] T. S. Totton, A. J. Misquitta, and M. Kraft, J. Chem. Theory Comput., 6, 683, 2010.

CPP 21.4 Mon 15:45 ZEU 255

Ordering of small polymer systems through the prism of partition function zeros. — •Timur Shakirov and Wolfgang Paul — Institute of Physics, University of Halle, Halle, Germany

Typical low temperature conformations of small alkane systems (single chains and few chain aggregates) differ frequently from the melt ones: even relatively short chains are folded in non-trivial structures at low temperatures [1]. The ordering of a system is related to change of thermodynamic and conformational characteristics of chains. In the case of big systems, the changes occur at one the same transition temperature, whereas for small systems the typical temperatures of the changes can be shifted relative to each other. The sensitivity of thermodynamic functions to the shift differs and can be hidden because of a widening of the transition region of the small system. We present here the results of an analysis of the partition function zeros, which helps to identify a two stage conformational reorganization of small alkane systems. Our calculations are based on Wang-Landau-type Monte Carlo simulations [2,3] of a chemically realistic united atom model [4].

[1] T. Shakirov, and W. Paul, J. Chem. Phys. 2019, 150, 084903.

[2] F. Liang, C. Liu, R. J Carroll, J. Am. Stat. Assoc. 2007, 102, 305-320.

[3] T. Shakirov, Comp. Phys. Commun. 228 (2018), 38-43.

[4] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. 103 (1995) 1702-1709.

CPP 21.5 Mon 16:00 ZEU 255

Independent Variation of Transition Temperature and Order Parameter at Prefreezing Transition — •Muhammad Tariq, Oleksandr Dolynchuk, Ann-Kristin Flieger, and Thomas Thurn-Albrecht — Institute of Physics, Martin Luther University Halle-Wittenberg, Germany

A solid substrate can induce crystallization of a liquid by either heterogeneous nucleation or prefreezing. Prefreezing refers to the formation of a crystalline layer of thickness l_{min} at the melt-solid interface at a temperature T_{max} above the melting point T_m, and is an equilibrium phenomenon. Recently developed phenomenological theory of first-order prefreezing predicts that the transition temperature T_{max} depends mainly on the difference of interfacial free energies $\gamma_{sm} - (\gamma_{sc} + \gamma_{cm})$, whereas the order parameter l_{min} depends on the ratio $\frac{\gamma_{sc}+\gamma_{cm}}{\gamma_{sm}}$. To test these predictions, we performed series of in situ AFM experiments on different polymer-substrate systems. Experiments on polyethylene PE films on a molybdenum disulfide MoS_2 substrate evidence a significantly higher T_{max} than on highly oriented pyrolytic graphite HOPG. In case of poly(ϵ-caprolactone) PCL, where direct experimental measurements of the prefrozen layer thickness are possible, T_{max} of the prefrozen PCL on MoS_2 remains nearly same as on HOPG, whereas l_{min} decreases to a smaller value and, thereby, indicates that T_{max} and l_{min} are independent. As such, these experimental findings are consistent with the above-mentioned predictions of the phenomenological theory.

CPP 21.6 Mon 16:15 ZEU 255

Intramolecular inhomogeneities during glassy densification as studied for polyalcohols by FTIR-spectroscopy — •Friedrich Kremer, Wilhelm Kossack, and Jan Gabriel — Peter Debye Institute for Soft Matter Physics, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

The intra-molecular potentials of a series of short polyalcohols (glycerol, threitol, xylitol, sorbitol) are studied by Fourier-Transform InfraRed (FTIR) Spectroscopy far above and below the calorimetric glass transition temperature. Analyzing the temperature dependencies of specific IR absorption bands reflecting dedicated molecular moieties, enables one to unravel on an intra-molecular scale the process of glass formation. For the v(O)-H) stretching vibration with increasing temperature a pronounced red shift is observed which enables one to deduce quantitatively the change in the extension of the inter-molecular N-H*O bonds. The intra-molecular vibrations being not involved in H-bonding show in contrast an albeit weak blue shift. The relative variation oft the width oft their respective potentials can be extracted from fits based on the Morse-function. By that the characteristic signature oft he intra-molecular inhomogenieties in the glassy systems far above and below the calorimetric glass transition temperature is obtained.

CPP 21.7 Mon 16:30 ZEU 255

Simultaneous SAXS-SANS to study direct influence of surfactant on anisotropic gold nanorod growth — •Tobias Zech[1], Ezzeldin Metwalli[1], Klaus Götz[1], Lionel Porcar[2], Anne Martel[2], and Tobias Unruh[1] — [1]Friedrich-Alexander-University Erlangen-Nuremberg, Institute for Crystallography and Structural Physics, Erlangen, Germany — [2]Institut Laue-Langevin, Grenoble, France

Despite many years of research on understanding the anisotropic growth of gold nanorods (AuNR), some questions remain. One is the influence of the ligand CTAB on shape, size and purity of synthesized gold nanorod solutions. However, in-situ studies, typically done with UV-Vis spectroscopy or SAXS, are only sensitive to the scattering volume of the inorganic gold nanoparticle. The influence of the organic parts, which make up most of the non-aqueous constituents in the solution are often treated as constant during the synthesis. We performed in-situ experiments to observe both inorganic and organic parts during AuNR synthesis via the unique SAXS/SANS instrument developed at our institute. This device is readily positioned at the D22 beamline at ILL. We not only observed, that the micelle structure is changing over time during the synthesis of AuNR but could also link those changes to the stages of growth of the nanoparticles. Furthermore, the influence of modified micelle structures via addition of n-alcohols can be directly correlated to differences in shape and size of the synthesized AuNR. This study shows a new perspective on how ligands can control anisotropic growth of noble metals on a nanoscale.

CPP 21.8 Mon 16:45 ZEU 255

Vertically aligned silica in the hard X-ray spotlight: an in situ GISAXS study of EASA — •Gilles E. Moehl[1], Li Shao[1], Samuel S. Fitch[1], Chris Nicklin[2], Jonathan Rawle[2], Philip N. Bartlett[1], and Andrew L. Hector[1] — [1]Chemistry, University of Southampton, Southampton, SO17 1BJ, UK — [2]Diamond Light Source, Didcot, OX11 0DE, UK

Under the Advanced Devices by Electroplating EPSRC programme grant (EP/N035437/1) we are working on the integration of nanowire semiconductor structures into electronics, by electrodepositing high quality chalcogenide semiconductors into aligned mesoporous templates. Mesoporous silica films are typically produced by evaporation-induced self assembly (EISA), but vertical alignment of the pores to the substrate is very difficult to achieve. Hexagonal arrays of vertically aligned mesopores can be achieved by electrochemically assisted surfactant assembly (EASA). The application of a negative potential to an electronically conductive substrate results in the self-assembly of a cationic surfactant (typically cetyltrimethylammonium bromide) close to the substrate surface, but also the formation of spheroidal surface aggregates, limiting the obtainable film thickness to a few hundreds of nm. The resulting pore spacing and diameter of only a few nanometres make the characterisation of such structures very challenging and time consuming. In this work, we show the results obtained from in situ GISAXS experiments done during the EASA of silica, following the evolution of the structure formation in real time with sub-second time resolution.

CPP 22: Electrical, Dielectrical and Optical Properties of Thin Films

Time: Monday 15:00–16:15 Location: ZEU 114

CPP 22.1 Mon 15:00 ZEU 114

Ionic liquid post-treatment of PEDOT:PSS thin films to increase their thermoelectric properties — •Anna Lena Oechsle[1], Julian Heger[1], Nian Li[1], Shanshan Yin[1], Hartmut Stadler[2], Sigrid Bernstorff[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Bruker, AXS Advanced X-ray Solutions GmbH, 76187 Karlsruhe, Germany — [3]ELETTRA Sincrotrone Trieste S. C. p. A., AREA Science Park Basovizza, 34149 Trieste, Italy

In times of constantly increasing energy demand, climate change and scarcity of fossil resources thermoelectric materials are of great interest as they enable waste heat recovery and the use of solar thermal energy. In particular thermoelectric polymers are attractive, as in contrast to so far used inorganic materials, they own some advantages like low cost, high mechanical flexibility, low or no toxicity, light weight and intrinsically low thermal conductivity. Thermoelectric properties of materials can generally be evaluated by the so called power factor. This parameter depends on the Seebeck coefficient S and the electrical conductivity σ, which again are affected by the electronic and morphological features of the polymer. In terms of improving both S and σ simultaneously we post-treat fabricated PEDOT:PSS thin films with ionic liquids (ILs). By performing measurements of the Seebeck coefficient, the electrical conductivity, UV-Vis, layer thickness changes and determination of the structure we attempt to find the influence of ILs on the morphology-function relation of the PEDOT:PSS thin films.

CPP 22.2 Mon 15:15 ZEU 114

Printed colloidal PbS quantum dots solids for optoelectronics — •Wei Chen[1], Haodong Tang[2], Nian Li[1], Manuel Andree Scheel[1], Yue Xie[2], Volker Körstgens[1], Matthias Schwartzkopf[3], Stephan Roth[3], Kai Wang[2], Xiao Wei Sun[2], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, 85748 Garching, Germany — [2]SUSTech, 518055 Shenzhen, China — [3]DESY, 22607 Hamburg, Germany

Colloidal PbS quantum dots (QDs) are attractive in photovoltaics applications due to not only the larger spectral range for the photon-electron response but also the compatibilities with various thin-film deposition methods, including spray and printing depositions. In this work, we use a slot-die coating method for particle deposition integrated with a layer-by-layer method for ligand exchange treatment to fabricate QDs planar structured solar cells with larger effective areas and less waste of QDs than commonly applied deposition methods. The particle kinetics of QDs during the printing deposition for pristine QD films is studied by time-resolved grazing-incidence small-angle X-ray scattering (GISAXS). Further, the surface morphologies and the inner structures of ligand exchanged QDs solid are studied by scanning electron microscope, atomic force microscope, and GIWAXS. Moreover, the time-resolved photoluminescence spectroscopy with spectral mapping is used to compare and discuss the charge carrier dynamics of ligand exchanged QD solids made by printing and regularly spin-coating deposition methods respectively.

CPP 22.3 Mon 15:30 ZEU 114

Ultrathin electrically conductive films created from different polycations and oxidized carbon nanotubes for bioelectrical applications — •Sven Neuber, Peter Nestler, Annekatrin Sill, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald, 17489 Greifswald, Germany

Surface functionalization by ultrathin films is becoming increasingly important for technological and biological applications such as the electrically active implants. nm-thick films were made by sequential adsorption of different polycations (strong polycation PDADMA; weak polycations PAH and branched PEI) and oxidized carbon nanotubes (CNT). The degree of oxidation of CNTs was determined by XPS and UV-vis absorption spectroscopy. Quartz crystal microbalance and ellipsometry have shown that film structure depends on the used polycation. Films from strong polycation PDADMA/CNT (9 layer CNTs) are more compact, thinner (d = 33.88 nm), less rough (Rq = 13.87 nm) and more electrical conductive (σ = 60.6 mΩ-1m-1) compared to films from weak polycations like PEI/CNT (9 layer CNTs, d = 42.5nm, Rq = 20.25 nm, σ = 16.4 mΩ-1m-1). AFM images show that the films have a network structure with random nanopores, making them ideal structures for biomedical applications.

CPP 22.4 Mon 15:45 ZEU 114

Investigation on Light-Matter Interactions in Tunable Colloidal Nanocavities — •Fabian R. Gossler[1] and Tobias A.F. König[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden — [2]TU Dresden, 01069 Dresden

For large-scale fabrication of optical circuits, tailored subwavelength structures are required to modulate the refractive index. Here, we introduce a colloid-to-film-coupled nanocavity whose refractive index can be tailored by various materials, shapes, and cavity volumes.[1,2] With this colloidal nanocavity setup, the refractive index can be adjusted over a wide visible wavelength range. For many nanophotonic applications, specific values for the extinction coefficient are crucial to achieve optical loss and gain. We employed bottom-up self-assembly techniques to sandwich optically active ternary metalchalcogenides between a metallic mirror and plasmonic colloids. The spectral overlap between the cavity resonance and the broadband emitter makes it possible to study the tunable radiative properties statistically. For flat cavity geometries of silver nanocubes with sub-10 nm metallic gap, we found a fluorescence enhancement factor beyond 1000 for 100 cavities and a 112 meV Rabi splitting. In addition, we used gold spheres to extend the refractive index range. By this easily scalable colloidal nanocavity setup, gain and loss building blocks are now available, thereby leading to new generation of optical devices. [1] F. Goßler et al., The Journal of Physical Chemistry C 2019 123 (11), 6745-6752 [2] M. Mayer et al., Advanced Optical Materials 2019, 7, 1800564.

CPP 22.5 Mon 16:00 ZEU 114

Optical band structures of self-assembled colloidal metasurfaces — •Olha Aftenieva[1] and Tobias A.F. König[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Institute of Physical Chemistry and Polymer Physics, Dresden, Germany — [2]Technical University of Dresden, Physical Chemistry, 01062 Dresden, Germany

In order to obtain mixed plasmon states from the periodic arrangement we follow the concept of colloidal metasurface [König, Fery et al. Adv. Optical Mater. 2018, 1800564]. We avail of the rational design of such structures through numerical simulation, colloidal self-assembly manufacturing, and spectroscopic evaluation to obtain the optical band structures. This contribution will focus on the quantitative characterization of the interaction between Bragg diffraction and plasmonic modes by angle-resolved spectroscopy. The energy-momentum measurements are supported by the finite-difference time-domain (FDTD) simulations. Such a unique assembly of colloidal nanoparticles at a flat interface allows accessing subwavelength polaritonic states that go beyond conventional optics.

CPP 23: Interfaces and Thin Films I (joint session CPP/O/DY)

Time: Monday 16:30–17:15 Location: ZEU 260

CPP 23.1 Mon 16:30 ZEU 260

In Situ Monitoring Mesoscopic Deformation of Nanostructured Porous Titania Films Caused by Water Ingression — Lin Song[1,2], Monika Rawolle[1], Nuri Hohn[1], Jochen S. Gutmann[3], Henrich Frielinghaus[4], and •Peter Müller-Buschbaum[1,5] — [1]Lehrstuhl für funktionelle Materialien, Physik Department, TU München, 85748 Garching, Germany — [2]Xian Institute of Flexible Electronics, Northwestern Polytechnical University, Xian 710072, Shaanxi, China — [3]Fakultät für Chemie, Universität Duisburg-Essen, 45141, Essen, Germany — [4]JCNS at MLZ, Forschungszentrum Jülich GmbH, 85748 Garching, Germany — [5]MLZ, TU München, 85748 Garching, Germany

Nanostructured porous titania films are used in many energy related applications. We investigate the temporal evolution of the mesoscopic deformation of mesoporous titania films synthesized via block copolymer assisted sol-gel chemistry with in situ grazing incidence small-angle neutron scattering (GISANS) during exposure to water vapor. Two types of mesoporous titania films are compared, which have a different degree of structural stability, depending on the applied annealing temperature in nitrogen atmosphere. Water ingression causes a gradual structure deformation in terms of decreasing center-to-center distances and broadening of the size distribution of the titania nanostructures. Based on the evolution of the mesopore size obtained from in situ GISANS measurements, the results show which type of titania structure is more stable against water infiltration.

CPP 23.2 Mon 16:45 ZEU 260

In situ GISAXS Investigations of Multi-responsive Block Copolymer Thin Films during Solvent Vapor Annealing — •Florian A. Jung[1], Panayiota A. Panteli[2], Detlef-M. Smilgies[3], Dorthe Posselt[4], Constantinos Tsitsilianis[5], Costas S. Patrickios[2], and Christine M. Papadakis[1] — [1]Physics Department, Soft Matter Group, Technical University of Munich, Garching, Germany — [2]Department of Chemistry, University of Cyprus, Nicosia, Cyprus — [3]Wilson Laboratory, Cornell University, Ithaca, USA — [4]Department of Science and Environment, Roskilde University, Denmark — [5]Department of Chemical Engineering, University of Patras, Greece

Responsive block copolymer thin films are of interest for many applications, e.g. as fast sensors or switchable membranes. In the present work, we investigate a pH and temperature responsive pentablock quaterpolymer in thin films during solvent vapor annealing (SVA). The end blocks are temperature-responsive and hydrophobic while the midblock is pH-responsive and hydrophilic. Structural information was obtained by employing in situ grazing-incidence small-angle X-ray scattering (GISAXS) and by model fitting the obtained 2D patterns. We find that, varying the pH value of the solution for spin-coating as well as the nature of the solvent used for SVA gives the opportunity to tune the structures in a wide range.

CPP 23.3 Mon 17:00 ZEU 260

Self-assembly of large magnetic nanoparticles in ultrahigh molecular weight linear diblock copolymer films — •Wei Cao[1], Senlin Xia[1], Xinyu Jiang[1], Markus Gallei[2], Matthias Opel[3], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]DESY, Notkestrasse 85, 22603 Hamburg — [5]KTH Royal Institute of Technology, FPT, SE-100 44 Stockholm, Sweden

The fabrication of diblock copolymer nanocomposite films that consist of magnetic nanoparticles (NPs) with diameters (D) of more than 20 nm is a challenging task. Herein, ultrahigh molecular weight (UHMW) linear polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) diblock copolymer is spin-coated as a template for the self-assembly of large iron oxide NPs ($D = 27$ nm), and the morphology of hybrid nanocomposites is governed by the concentration of the iron oxide NPs. The NPs are functionalized with carboxylic acid groups showing an affinity to the PMMA blocks. Due to the rearrangement of the polymer chains for accommodating the NPs, well-ordered spherical nanostructures are readily generated at a NP concentration of 0.5 wt%. Most interestingly, a chain-like network appears inside the hybrid films at a high NP loading. All hybrid films show ferromagnetism at room temperature, proven with a superconducting quantum interference device magnetometer.

CPP 24: Poster Session I

Topics: Biopolymers, Biomaterials and Bioinspired Functional Materials (24.1-24.9); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (24.10-24.14); Crystallization, Nucleation and Self-Assembly (24.15-24.27); Electrical, Dielectrical and Optical Properties of Thin Films (24.28-24.33); Interfaces and Thin Films (24.34-24.37); Polymer Networks and Elastomers (24.38-24.42), Soft Matter and Nanocomposites - New opportunities with advanced neutron Sources (24.43-24.51).

Time: Monday 17:30–19:30 Location: P3

CPP 24.1 Mon 17:30 P3

Multivalent Cation-Induced Actuation of DNA-Mediated Colloidal Superlattices — Devleena Samanta[1,3], •Aysenur Iscen[2], Christine R. Laramy[2,3], Sasha B. Ebrahimi[2,3], Katherine E. Bujold[1,3], George C. Schatz[1,3], and Chad A. Mirkin[1,2,3] — [1]Department of Chemistry — [2]Department of Chemical and Biological Engineering — [3]International Institute for Nanotechnology, Northwestern University, Evanston IL USA

Nanoparticles functionalized with DNA can assemble into ordered superlattices with defined crystal habits through programmable DNA “bonds”. Here, we examine the interactions of multivalent cations with these DNA bonds as a chemical approach for actuating colloidal superlattices. Multivalent cations alter DNA structure on the molecular scale, enabling the DNA “bond length” to be reversibly altered between 17 and 3 nm, ultimately leading to changes in the overall dimensions of the micron-sized superlattice. The identity, charge, and concentration of the cations each control the extent of actuation, with Ni^{2+} capable of inducing a remarkable >65% reversible change in crystal volume. Molecular dynamics simulations provide insight into the conformational changes in DNA structure as the bond length approaches 3 nm and show that cations that screen the negative charge on the DNA backbone more effectively cause greater crystal contraction. Taken together, the use of multivalent cations represents a powerful strategy to alter superlattice structure and stability, which can impact diverse applications through dynamic control of material properties, including the optical, magnetic, and mechanical properties.

CPP 24.2 Mon 17:30 P3

Cross-scale characterization of the interaction of polymers on cellulose interfaces: Construction of a model surface of cellulose — •Cassia Lux, Thomas Tilger, Olaf Soltwedel, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

As a functional material, cellulose based paper has a high importance in a variety of sectors, such as packaging, print media and speciality papers. This is especially crucial with regard to reducing plastic use and waste and replacing it with renewable and biodegradable resources.

The interactions of cellulose fibers with functional additives, such as the wet-strength increasing polymer PDADMAC, have been investigated in the past with respect to the mechanical properties of the resulting paper. Yet, a systematic understanding of the effects of the chemistry and structure of the polymer on the properties of the fibers is still missing and would lead to an exhaustive knowledge of the functionalization of paper.

For a detailed examination, model surfaces are prepared by dip and spin coating from both soluble carboxymethyl cellulose (CMC) and suspended microcrystalline cellulose (MCC) under the variation of extrinsic conditions such as concentration and pH value of the polyelectrolyte solutions and deposition time. Ellipsometry and AFM measurements allow for a comprehensive investigation of the influence of these conditions on features like thickness and roughness of the synthesized films.

CPP 24.3 Mon 17:30 P3

Development of a new paper-based test system using electrochemical reactions — Marc Riedel[1], •Oliver Nagel[2], Werner Wirges[2], Robert Niedl[2], Fred Lisdat[1], and Carsten Beta[3] — [1]Technische Hochschule Wildau — [2]Universität Potsdam — [3]Diamond

Inventics

Paper-based sensors have reached a wide popularity in research and industry. Such systems are low cost in production and simple to fabricate. Furthermore, the benefit in analysis speed and availability made them attractive and easy to use as analytical tools. Paper is available in a wide range of thicknesses, it is biodegradable, and environmentally friendly. The hydrophilicity and porosity of the paper provide a natural substrate for the fabrication of microfluidic channels and can be operated without an external power source for fluid control. It is possible to easily print, coat, and link chemical reagents or (bio)molecules to the paper surface. This work will show a new paper-based test system consisting of a carbon and a silver electrode printed on the paper to detect electrochemical reactions on the chip. To test the μPAD (microfluidic paperbased analytical device), a peroxidase/ferrocene redox system was used for amperometric measurements.

CPP 24.4 Mon 17:30 P3

Folding kinetics within recombinant spider silk coatings — •Mirjam Hofmaier[1,2], Birgit Urban[1], Sarah Lentz[3], Thomas Scheibel[3], Andreas Fery[1,2], and Martin Müller[4] — [1]Leibniz Institute of Polymer Research Dresden, Institute of Physical Chemistry and Polymer Physics, Hohe Straße 6, D-01069 Dresden — [2]Technical University Dresden, Chair of Physical Chemistry of Polymeric Materials, 01069 Dresden — [3]University of Bayreuth, Chair of Biomaterials, Rüdiger-Bormann Str. 1, D-95447 Bayreuth — [4]Technical University Dresden, Chair of Macromolecular Chemistry, 01062 Dresden

The folding kinetics of the recombinant spider silk protein eADF4(C16) in thin films was analysed by in-situ ATR-FTIR spectroscopy. eADF4(C16) was cast from hexafluoroisopropanol solutions (1-50 mg/ml) to respective thin and thick films onto unidirectionally scratched silicon substrates (Si-sc). To quantify secondary structure portions, the Amide-I band was examined using line shape analysis (LSA). Five relevant components in the range between 1585 and 1730 cm-1 were identified and assigned to typical secondary structures. Significant decrease of random coil and increase of beta-sheet content was recorded by ATR-FTIR measurements over 24 hours while treating the initial eADF4(C16) films with methanol vapour (MeOH-v) or liquid methanol (MeOH-l). The protein folding appears to be a two-state kinetic process. Received rate constants indicate folding kinetics of first order by MeOH-v treatment and both zero and first order by MeOH-l treatment. No dependence of folding kinetics on the layer thickness could be found.

CPP 24.5 Mon 17:30 P3

Structural properties and chain connectivity in squid-based biopolymer networks analysed by 1H time-domain NMR experiments — •Lucas Löser[1], Huihun Jung[2], Melik Demirel[2], and Kay Saalwächter[1] — [1]Inst. f. Physik - NMR, Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Dep. of eng. science and mechanics, Pennsylvania State University, Pennsylvania

A variety of structural and topological factors is known to strongly influence the mechanical properties of a polymer network. Here, we focus on a molecular-engineered biopolymer network consisting of random coils and nano-sized β-sheet crystals (acting as physical crosslinks) that was obtained by modifying and expressing repetitive elements in the genetic code of squid-ring teeth proteins. Usage of different solvents and different chain lengths of the expressed biopolymer yields the possibility of variations in crystallinity and the amount of topological defects. Using 1H time-domain NMR experiments, namely free induction decay (FID) analysis and a double-quantum (DQ) experiment, we investigate the crystalline and mobile fraction, as well as the different chain connectivities being present in the network. Additionally, we investigate the segmental mobility along the elastic chain and show that a mobility gradient exists, which is possibly induced by confinement of the elastic chains due to the β-sheet crystals. We show that we can correlate β-sheet content and the crystallinity measured by FID analysis, and additionally we discuss a previously published entropic-elasticity model [1] in the context of our DQ-NMR results.[1] A. Pena-Francesch et. al., ACS Biomater. Sci. Eng. 2018, 4, 3, 884-891

CPP 24.6 Mon 17:30 P3

Ramanspectroscopic investigation of eco-friendly binder systems for carbon-bonded filters — •Simon Brehm[1], Cameliu Himcinschi[1], Benjamin Bock[2], Christos Aneziris[2], and Jens Kortus[1] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, Germany — [2]Institute of Ceramic, Glass and Construction Materials, TU Bergakademie Freiberg, Germany

Environmentally friendly binder systems for carbon-bonded filters based on lactose/tannin were investigated by Raman spectroscopy. In earlier samples, the carcinogenic material CarboresP was used as a binder [1], which is replaced by a lactose/tannin mixture in this work.

With Raman spectroscopy, the size of the sp^2 carbon clusters using the intensity ratio of the D- and G-bands [2] and the -OH content can be qualitatively compared between different samples.

Temperature-dependent in-situ Raman measurements of the pure materials lactose and the tannin derivatives (tannic acid, gallic acid, ellagic acid) were performed.

Also two test series of the binder system were examined, one series was annealed to 1000°C and one was untreated. Both series consist of six samples, whereby the initial CarboresP portion of 20% is gradually replaced by a lactose/tannin mixture.

[1] C. Himcinschi et al., J. Eur. Ceram. Soc. 38, 5580 (2018),
[2] C. Röder et al., J. Raman Spectrosc. 45, 128 (2013)

CPP 24.7 Mon 17:30 P3

Supermolecular ordering in monolayers of lipids with extended polymer head groups - DSPE-PEG — •Heiko Ahrens, Olaf Soltwedel, Jens-Uwe Günther, and Christiane A. Helm — Institut für Physik, Uni-Greifswald, 17489 Greifswald

Depending on area per molecule, lipid monolayers - like Distearoylphosphatidyl-ethanolamine (DSPE) - at the air-water interface exhibit a phase transition form a liquid expanded to a condensed phase with tilted alkyl tails. On further compression the tilt angle decreases. Larger head groups increase the tilt angle and disturb the crystalline order.

DSPE with chemically attached short PEG (poly ethylene glycol) to the head group was investigated with GID and x-ray reflection. DSPE with longer PEG chains show a transition from fluid molecules to heterogeneous monolayer consisting of domains with condensed tilted lipid chains immersed in PEG chains adsorbed into the hydrophobic moiety of the lipid monolayer. These domains are then arranged in a hexagonal super structure with lattice constants up to 16 nm.

With a short PEG chain (8 monomers) an incompressible condensed phase with coherence length in the 10 nm range is found. The alkyl tails are strongly tilted - 39°- in a strongly distorted oblique lattice. Perpendicular to the tail axis they are arranged in the dense herring bone structure. Additional diffraction peaks due to an extended unit cell consisting of four alky tails were observed.

CPP 24.8 Mon 17:30 P3

Studying the nanomechanical properties of functional organic and biologic macromolecules — •Ilka M. Hermes[1], Mina Hong[2], Gerald Pascual[2], Byong Kim[2], and Keibock Lee[2] — [1]Park Systems Europe, Mannheim, Germany — [2]Park Systems, Inc., Santa Clara, USA

As the functionality of organic and biologic macromolecules is often determined by their nanomechanical properties, visualizing the distribution of mechanical properties on the nanoscale provides crucial insights for soft matter research. Here, we present a study on structural and nanomechanical properties of functional organic and biologic macromolecules depending on the respective environment as well as external stimuli, such as temperature, ion concentration and pH. Force-distance measurements with atomic force microscopy (AFM) resolve adhesion and elasticity by pressing a nanometer-sized tip on the end of a cantilever onto the surface. However, the correlation of mechanical data from force-distance measurements to the local sample morphology additionally requires topographic sample information. PinPoint nanomechanical imaging simultaneously acquires topographic and force-distance data within short amounts of time and is therefore ideally suited to investigate organic and biologic macromolecules.

CPP 24.9 Mon 17:30 P3

Correlation between secondary structures and viscous properties of xanthan polymers — •Jenny Fjodorova[1], Gerd Hublik[3], Vera Ortseifen[2], Karsten Niehaus[2], Volker Walhorn[1], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, Bielefeld University, Germany — [2]Proteome and Metabolome Research, Bielefeld University, Germany — [3]Jungbunzlauer Austria AG, Pernhofen 1, 2064 Wulzeshofen, Austria

Xanthan is an extracellular polysaccharide secreted by the bacterium *Xanthomonas campestris*. Due to its unique viscosifying properties over a wide range of salt concentrations, xanthan has numerous industrial applications e.g. in food, cosmetic or oil industry. Therefore, the optimisation of xanthan production and its rheological properties is of particular interest. Targeted genetic modification of the Xanthomonas metabolism and subsequent change of salt concentrations can be a powerful tool to optimise the shear-thickening potency of the polysaccharide.

Using atomic force microscopy (AFM) imaging and rheological measurements, we analysed the structure of single xanthan polymers in different environments. We identified structures ranging from single-stranded coiled networks to branched double-strands. Viscosity measurements show a link between the microscopic structural features and the macroscopic viscosity. Thus, we will discuss a model, which describes a correlation between the secondary structure of the polymer with its shear-thickening properties.

CPP 24.10 Mon 17:30 P3

Lithium Ion Transport in Block–Copolymer Electrolytes – A Molecular Dynamics Study — •Len Kimms, Diddo Diddens, and Andreas Heuer — Institut für physikalische Chemie, Westfälische Wilhelms–Universität Münster, Corrensstraße 28/30, 48149 Münster, {len.kimms, d.diddens, andheuer}@uni-muenster.de

On this poster we will present insights into the ion transport in block–copolymer electrolytes with lamellar microstructure. Traditional solid polymer electrolytes (SPE) consist of salt accommodated in an amorphous poly(ethylene oxide) (PEO) melt. Subsequently other polymers have been tried in order to improve conductivity and safety. From a safety point of view rigid polymers are favored since they can suppress dendrite growth and provide mechanical stability. Unfortunately, those types of polymers exhibit decreased segmental dynamics which hinders the ion mobility. Block–copolymers provide the ability to tune the mechanical and ion–transport properties of the blocks independent from each other. Here we report results about the ion transport in block–copolymer electrolytes with lamellar microstructure which experimentally have displayed very high conductivities. In those observations the ionically conducting PEO domain consists of short PEO chains that can accommodate high salt concentrations. From the preparation of the lamellae there remains non–volatile Tetrahydrofuran (THF). We employ Molecular Dynamics (MD) simulations to understand the ion transport mechanism and compare our findings to earlier MD simulations of classical PEO-based SPEs. First conjectures on the role of the remaining THF are presented.

CPP 24.11 Mon 17:30 P3

Fundamental principles of polyelectrolyte hydrogel pressure sensors and diodes from molecular simulations — •Joerg Rottler[1], Vasilii Triandafilidi[2], and Savvas Hatzikiriakos[2] — [1]Dept. of Physics and Astronomy and Quantum Matter Institute, University of British Columbia, Vancouver BC Canada V6T 1Z1 — [2]Dept. of Chemical Engineering, University of British Columbia, Vancouver BC Canada V6T 1Z4

The function of many novel soft electronic materials arises from electrostatic effects at interfaces between polyelectrolyte networks. This talk uses coarse-grained molecular simulations to elucidate the molecular principles of two distinct effects: the emergence of a pressure gradient between two differently ionized gels that results in the buildup of a Nernst-Donnan potential, and the ability of a junction of two oppositely charged crosslinked networks to rectify an electric current. In both cases, the simulations are used to probe the regime of strong electrostatic coupling where counterion condensation becomes important. The Nernst-Donnan potential at the interface is found to scale linearly with temperature with the coefficient of proportionality given by the fraction of uncondensed counterions. Similarly, a Poisson-Boltzmann continuum electrostatic description of the gel diode interface is only applicable at weak electrostatic coupling, and modifications are developed to describe more strongly ionized gels.

CPP 24.12 Mon 17:30 P3

Structure of Micelles Formed by Multi-responsive Triblock Terpolymers — •Yanan Li[1], Athanasios Skandalis[2], Varvara Chrysostomou[2], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]Physik-Department, Technische Universität München, Garching, Germany — [2]Theroretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Positively charged core-shell micelles are of interest for gene-transfer applications. Such systems may be formed by PDMAEMA-b-PLMA-b-POEGMA terpolymers. PDMAEMA is responsive to pH, ionic strength and temperature, whereas PLMA is strongly hydrophobic and POEGMA is permanently water-soluble and ensures biocompatibility. As a reference system, we investigate the simpler diblock copolymer PDMAEMA-b-PLMA as well. Detailed structural information is obtained from small-angle X-ray scattering.

CPP 24.13 Mon 17:30 P3

Adsorption of Dodecyl Sulfonate Surfactants and Alkali Ions at Extended and Nanoscopic Oil/Water Interfaces — •Dana Glikman, Eric Weissenborn, and Björn Braunschweig — Institute of Physical Chemistry and Center for Soft Nanoscience, Corrensstr. 28/30, 48149 Münster, Germany

Emulsions find many applications in different everyday life and industrial applications. However, a complete molecular-level understanding of the soft oil/water interface inside emulsions is still missing, but is prerequisite for targeted manipulation of emulsions. In this contribution, we report on the influence of anionic dodecyl sulfate (DS^-) surfactants and their counter ions (Li^+, Na^+, Cs^+) at the extended- and nanoscopic hexadecane/water interface. In order to study the oil/water interface as a function of surfactant concentration and ionic strength on different length scales, we have applied a thin-film pressure balance and the captive bubble method for extended surface, but also recorded the zeta-potential and second-harmonic light scattering (SHS) profiles from nanoscopic oil drops. Due to the higher affinity of DS^- to oil, the surface pressure is higher at the oil/water interface than at the air/water interface. Nevertheless, we find similar trends for the alkali cations at the oil/water interface as for the air/water interface: in dependence on the counter ion, the maximal surface excess of DS^- decreases with decreasing ion size ($Cs^+ > Na^+ > Li^+$). In addition, the zeta-potential of nanoemulsions is for NaDS more negative than for CsDS, which is corroborated by SHS experiments that can address the double-layer potential directly.

CPP 24.14 Mon 17:30 P3

Influence of added salt on the foam film properties of NaPSS/C_{14}TAB-mixtures — •Kevin Gräff, Larissa Braun, and Regine von Klitzing — Technische Universität Darmstadt, Soft Matter at Interfaces, Darmstadt, Germany

The properties of foams are of interest in many applications such as in personal care products and in food technology.

To understand the properties of macroscopic foam, it is essential to investigate foam films - the framework of foams.

Due to the formation of highly surface-active complexes, mixtures of oppositely charged polyelectrolytes and surfactants are widely used in many industrial applications. There exist many studies that focus on a big variety of surfactant-polyelectrolyte mixtures. However, the influence of the ionic strength - especially on the foam films - is still unclear.

In this work, a thin film pressure balance (TFPB) is used to study foam films of NaPSS/C_{14}TAB-mixtures in terms of disjoining pressure, surface potential and foam film stability. We add NaBr (the combination of the two counterions) to get insights on the influence of the ionic strength on the foam film properties. Our current investigation shows an unexpected increase in foam film stability with added NaBr which might be explained by a change of the conformation of NaPSS at the air/water interface. To study the effects of the presence of NaBr in detail, the NaBr concentration is further varied.

CPP 24.15 Mon 17:30 P3

Hierarchical assembly of non-spherical colloids by critical Casimir forces — •Timo Knippenberg, Jakob Steindl, Tian Li, and Clemens Bechinger — FB Physik, Universität Konstanz

Recent experiments demonstrated the use of critical Casimir forces in the context of spherical colloidal aggregation processes. Such forces arise due to the geometrical confinement of a critical mixture. Critical Casimir induced particle assembly essentially takes advantage of the fact, that the strength of such forces strongly depends on the temperature of the fluid and the adsorption preference of the colloidal particles. Here, we experimentally study the aggregation of semi-disk like particles under the influence of critical Casimir forces. We observe a preferential attraction between the flat facets of the particles which leads to their assembly into disk-shaped aggregates. At larger particle densities, the assembled disks form a hexagonal lattice. This hierarchical assembly process is explained by the strong curvature dependence of critical Casimir forces which leads to a strong alignment of non-spherical particles. This alignment strongly depends on the particle thickness which has been systematically varied in our experiments.

CPP 24.16 Mon 17:30 P3

Packing polydisperse colloids into crystals: when charge-dispersity matters — •Lucas Goehring[1], Guillaume Bareigts[2], Pree-Cha Kiatkirakajorn[3], Joaquim Li[4], Robert Botet[5], Michael Sztucki[6], Bernard Cabane[4], and Christophe Labbez[2] — [1]Nottingham Trent University — [2]University Bourgogne — [3]Max Planck Institute for Dynamics and Self-Organisation — [4]ESPCI ParisTech — [5]University Paris-Sud — [6]ESRF-The European Synchrotron

Here we show that even modest amounts of polydispersity can dramatically change how colloidal crystallization occurs. Monte-Carlo simulations, fully constrained by experimental parameters, are found to agree well with a measured phase diagram of aqueous dispersions of nanoparticles with a moderate size polydispersity over a broad range of salt concentrations, c_s, and volume fractions, ϕ. Upon increasing ϕ, the colloids freeze first into coexisting compact solids then into a body centered cubic phase (bcc) before they melt into a glass forming liquid. The surprising stability of the bcc solid at high ϕ and c_s is explained by the interaction (charge) polydispersity and vibrational entropy.

CPP 24.17 Mon 17:30 P3

Crystallization kinetics in colloidal hard spheres by confocal microscopy — •Sahana Kale and Hans-Joachim Schoepe — University of Tuebingen, Germany

We study the homogeneous crystallization of meta-stable colloidal hard sphere fluids using laser scanning confocal microscopy. Direct imaging in three dimensions offers the unique possibility to observe crystal nucleation and growth on the particle level.

We present nucleation rate densities for various volume fraction in comparison with previous data from light scattering and simulation. In addition, we analyse the temporal evolution of the local structure of the crystallizing clusters.

CPP 24.18 Mon 17:30 P3

Modeling epitaxial film growth of C_{60} — •William Janke and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland

Epitaxial films evolve on time and length scales that are inaccessible to atomistic computer simulation methods like molecular dynamics (MD). To numerically predict properties for such systems, a common strategy is to employ kinetic Monte Carlo (KMC) simulations, for which one needs to know the transition rates of the involved elementary steps. The main challenge is thus to formulate a consistent model for the set of transition rates and to determine its parameters. We revisit a well-studied model system, the epitaxial film growth of the fullerene C_{60} on an ordered C_{60} substrate(111). We implement a systematic multiscale approach in which we determine transition rates through MD simulations of specifically designed initial configurations. These rates follow Arrhenius' law, from which we extract energy barriers and attempt rates. We discuss the issue of detailed balance for the resulting rates. Finally, we study the morphology of submonolayer and multilayer film growth and compare simulation results to experiments.

CPP 24.19 Mon 17:30 P3

Machine learning for DNA self-assembly: a numerical case study — •Jörn Appeldorn, Arash Nikoubashman, and Thomas Speck — Inst. für Physik, Universität Mainz, Germany

We study the spontaneous self-assembly of single-stranded DNA fragments using the coarse-grained oxDNA2 implementation [1]. A successful assembly is a rare event that requires to cross a free energy barrier. To employ advanced numerical algorithms like forward-flux sampling or Markov state modeling one needs to identify one or more collective variables (order parameters) that faithfully describe the transition towards the assembled state. Formulating appropriate order parameters typically relies on physical insight, which is then verified, e.g., through a committor analysis. Here we explore the use of machine learning to automize this process and to find suitable collective variables based on structural information. For this step one still needs to map configurations onto structural descriptors, which is a non-trivial task. Specifically, we investigate the latent space of EncoderMap [2] and how it changes with the amount of information contained in the descriptor.

[1] - Snodin et al., J. Chem. Phys.(2015), 142, 234901 [2] - T. Lemke and and C. Peter,J.Chem.TheoryComput.(2019), 15, 1209*1215

CPP 24.20 Mon 17:30 P3

Characterisation of the Free Energy Landscape of Syndiotatic Polysterene — •Atreyee Banerjee, Tristan Bereau, and Joseph F. Rudzinski — MPIP

Syndiotatic polysterene (sPS) is known to crystallise in distinct forms, commonly known as polymorphs [1]. Traditional molecular dynamics simulations are powerful tools for characterizing the molecular mechanism of transition between polymorphs, but require extreme computational resources due to the strong metastability of the polymorph states. Enhanced sampling methods have the potential to largely remedy this problem, but require prior knowledge of collective variables (CVs) that can resolve the relevant transition pathways, typically identified through physical or chemical expertise. CVs are also often used for constructing a kinetic model to better characterise the transition pathways of the characteristic long timescale processes of the system. A huge interest has grown to apply neural networks to automate the discovery of a low-dimensional representation [2]. Autoencoders are potentially powerful tools to identify good CVs, since the technique forces an information compression in the bottleneck region. A specialised autoencoder architecture, the Gaussian mixture variational autoencoder (GMVAE), performs dimensionality reduction and clustering within a single unified framework, and can identify the inherent dimensionality of the system by enforcing physical constraints in the latent space. In contrast to manually constructed CVs, we apply the GMVAE approach to accurately characterise the pathways of transition between polymorphs in sPS.

CPP 24.21 Mon 17:30 P3

Self-Assembly of Polymers in Presence of Solvent Evaporation — •Gregor Ibbeken and Marcus Müller — Georg-August Universität, Göttingen, Deutschland

Integral asymmetric polymer membranes are promising functional macromolecular systems which have numerous applications, like water purification and protein separation. Since their synthesis requires high control over kinetic pathways, a description in terms of statistical physics and exploiting computer simulations will help improve understanding and production. Here we tackle a process combining self-assembly of asymmetric diblock copolymers and non-solvent induced phase separation using continuum descriptions of self-assembling polymer systems. First, model B for the Ohta-Kawasaki free energy functional, which successfully describes dynamics of diblock copolymers, is phenomenologically altered to feature space and time dependent parameters. This mimics the impact of solvents. In a second step the impact of solvents is explicitly investigated using the Uneyama-Doi functional, a model capable of describing arbitrary polymer mixtures. Appropriate parameter regions and thus corresponding kinetic pathways in which the copolymers form ideal standing cylinders, later functioning as pores, are identified. Finally, bridging the gap between simulation and experiment, the parameters are mapped to experimental ones, such as mobilities and Flory-Huggins parameters.

CPP 24.22 Mon 17:30 P3

Unraveling kinetically driven self-assembly of nanoplatelets — •Nanning Petersen, Rebecca Momper, Martin Girard, Andreas Riedinger, and Omar Valsson — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz

CdSe can form thin rectangular semiconductor nanoparticles. These nanoplatelets are remarkably uniform in thickness and size [1]. To make use of their extraordinary properties the colloidal particles have to be collectively orientated in solid state films. Previous experiments in our group have demonstrated that effective control over the collective orientation can be gained by exploiting kinetic effects in the self-assembly process. This yields well defined monolayer films with controlled nanoplatelet orientation. Through variation of the solvent, the temperature or the partial pressure the evaporation rate can be tuned, yielding monolayers with nanoplatelets either orientated "face-down" or "edge-up". However, the mechanism behind the kinetically driven self-assembly is not well understood.

Recently there have been major efforts to understand self-assembly processes in different nanoparticle systems. Molecular simulations have been proven to be a promising strategy to get a microscopic understanding of these processes. For nanoplatelets we have taken the first steps in this direction by employing coarse-grained molecular dynamics simulations using the MARTINI force field. Here we present our initial results on model nanoplatelet systems.

[1] A. Riedinger *et al.*, Nat. Mater. 16, 743-748 (2017)

CPP 24.23 Mon 17:30 P3

In-situ investigation of sputter deposition of electrodes for non-fullerene organic photovoltaics application — •Xinyu Jiang[1], Simon J. Schaper[1], Matthias Schwartzkopf[2], Stephan V Roth[3], Jonas Drewes[4], Oleksandr Polonskyi[4], Thomas Strunskus[4], and Peter Müller-Buschbaum[1] — [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

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. Electrodes of aluminum are widely used in organic photovoltaic devices. For understanding the mechanism of Al 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 sputter 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 24.24 Mon 17:30 P3

Versatile approach to well-defined conjugated oligomers and polymers with narrow molecular weight distribution for fundamental studies on structure-property relationships — •Frank-Julian Kahle[1], Julia Wollmann[2], Irene Bauer[2], Anna Köhler[1], and Peter Strohriegl[2] — [1]Soft Matter Optoelectronics, University of Bayreuth, Germany — [2]Macromolecular Chemistry I, University of Bayreuth, Germany

In this work, we present a versatile approach to achieve well-defined conjugated polymers and oligomers from a single standard synthesis route via preparative Size Exclusion Chromatography. Using a special recycle mode and well-defined end-cappers, we are able to prepare pure oligomers with three to eight repeat units and high molecular weight polymers with dispersity D as low as 1.06 in just one preparation step with reasonable yield. To demonstrate the capabilities of our method, we conducted a fundamental spectroscopic study on the influence of chain length and molecular weight distribution on electronic properties and aggregation behavior of a series of fluorene based oligo- and polymers. Due to the well-defined nature of the investigated compounds we consistently find a first-order phase transition and an increase of the critical transition temperature from amorphous to β-phase as function of the number of repeat units in accordance with the Sanchez model on coil-globule transitions.

CPP 24.25 Mon 17:30 P3

Thermophoretic Trapping of Single Amyloid Fibrils — Martin Fränzl[1], •Tobias Thalheim[1], Juliane Adler[1], Daniel Huster[1], Juliane Posseckardt[2], Michael Mertig[2,3], and Frank Cichos[1] — [1]Leipzig University, Germany — [2]Kurt-Schwabe-Institut für Mess- und Sensortechnik e.V. Meinsberg, Germany — [3]TU Dresden, Germany

The formation of aggregates of peptides is responsible for a number of neurodegenerative diseases. The individual steps of this aggregation from single soluble monomers or oligomers to highly ordered, insoluble amyloid fibrils, however, are commonly hidden in the ensemble average of common measurement techniques. The heterogeneity of the ensemble at all stages of the aggregation process hides the growth details such as secondary nucleation processes or fibril fragmentation. I will present on my poster a method that is able to trap single amyloid fibrils freely diffusing in solution relying on thermophoresis. This thermophoretic trap allows us to extract a lot of properties of the individual fibrils, like their Soret coefficients as well as the translational and rotational diffusion coefficients over time periods of at least several 10 minutes up to even hours. Repeating the measurement for several single fibrils permits us to measure a length dependence of the translational and rotational diffusion coefficients. Due to the high sensitivity of the rotational diffusion coefficient on length changes, we are furthermore able to study the growth of single fibrils down to a few 10 nm in the presence of monomers or monitor secondary nucleation events and fragmentation which have not been seen directly before.

CPP 24.26 Mon 17:30 P3

Effect of entanglements on the morphology and crystallinity of semi-crystalline polymer — •Zefan Wang, Mareen Schäfer, Albrecht Petzold, Thomas Thurn-Albrecht, and Kay Saalwächter — Institute for Physics, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

Recent simulation work indicates that the thickness of crystalline lamellae in the semi-crystalline polymer might be controlled by the entanglement density of the crystallizing melt. However, experimental evidence of how the morphology and the crystallinity of the semi-crystalline polymer is influenced by the topological restriction of entanglement density is scarce. By diluting high molecular weight polycaprolactone (PCL) with its own oligomer, a series of PCL samples with different entanglement density in equilibrium were prepared. The reduced entanglement density in the melt state was confirmed by rheological measurements. In addition, after crystallization, the semicrystalline morphology was characterized by SAXS and solid state NMR. At low crystallization temperatures the long chain polymer and the oligomer cocrystallize. SAXS data indicate that the lamellar thickness remains constant while the thickness of the amorphous regions decreases with decreasing entanglement density in the melt state. NMR measurements confirmed the corresponding increase of the crystallinity. These observations suggest that the thickness of the amorphous regions and therefore also the of semicrystalline polymers is controlled by the entanglement density in the melt state.

CPP 24.27 Mon 17:30 P3

Strain induced polymer crystallization — •Rajdeep Singh Payal[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute for Polymer Research, Hohe Str. 06, Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

Crystallization behavior of polymers is known to be influenced by the processing conditions. Lamellar thickness and crystallinity can be enhanced by the application of strain. Here, we have utilized molecular dynamics simulations and primitive path analysis to establish a direct correspondace between the themo-mechnical history of the molten state and crystallization behavior. Within linear extension regime, crystalline behavior is governed by the mixture of thermodynamic and topological effects. Partial disentanglement of the polymer chains due to applied force results in higher lamellar thickness and crystallinity. Furthermore, predicted behavior cannot be accounted using the kinectic theory of polymer crystallization.

CPP 24.28 Mon 17:30 P3

Controllable Au Nanoparticle Plasmonic Effects via Sputter Deposition on TiO2 Templates — •Suzhe Liang[1], Wei Chen[1], Shanshan Yin[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany

Due to the localized surface plasmon resonances (LSPR) effect, plasmonic metal nanostructures exhibit unique optical properties and have been applied in various fields, such as plasmon-enhanced sensing and chemistry, biotechnologies, and lighting harvesting for solar energy. Generally, plasmonic mantel nanostructures can be fabricated by colloid chemical methods, electron-beam lithography, and laser ablation. The wavelength of LSPR can be tuned form the ultraviolet to the infrared regions by changing the structure size and shape. In this work, we have introduced a facile and scalable method to obtain plasmonic nanoparticle array, with uniformed size and inter-distance distribution, by sputtering gold on TiO2 template. The sputtering measurement is realized by a unipolar reactive pulsed DC magnetron sputtering device. The uniform distribution of gold nanoparticles can be controlled by sputtering time and the customized TiO2 templates with designable morphologies. The growth dynamics of gold nanoparticles are studied by GISAXS. Combined with SEM and UV-vis spectroscopy measurements, the relationship between gold nanoparticles distribution and LSPR effects is established and explained.

CPP 24.29 Mon 17:30 P3

Hybrid Energy Harvester based on Solar Cell and Triboelectric Nanogenerator — •Tianxiao Xiao[1], Wei Cao[1], Wei Chen[1], Sven-Jannik Wöhnert[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Deutsches Elektronen-

Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany

Developing clean energy plays a central role in the sustainable development of human society. Solar energy is one of the most promising energy sources in replacement of conventional used fossil fuels. However, the daily and seasonal fluctuations in weather limit solar cell's applications. Integrating the solar cell with other kinds of energy harvesters in one device is a possible solution. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvesters. Due to its advantages of light-weight, low-cost, and easily fabricated, TENG attracts worldwide attention in the past years. In the present work, a flexible hybrid energy harvester is designed and fabricated based on quantum dots (QDs). This device consists of a PbS-QD solar cell part and a polydimethylsiloxane (PDMS) based TENG part, which can harness both, solar and mechanical energy from ambient environment to generate electricity. GISAXS measurements are used to characterize the bending stability and morphology changes of the mesoscale structure.

CPP 24.30 Mon 17:30 P3

A surface treatment recipe for significantly enhancing thermoelectric PEDOT: PSS films — •Suo Tu and Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Organic semiconductors have attracted intense attention because of their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially, 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 devices. The energy conversion efficiency of a TE material is evaluated by a dimensionless figure of merit ZT. However, it is generally considered that it is difficult to obtain a high ZT value of TE materials, due to the fact that the parameters are interdependence as a function of carrier concentration and hard to be optimized simultaneously. Mostly methods employing film treatment or both film treatment and additives in the solution show better conductivity than the mere additives in the PEDOT:PSS aqueous solution. Herein, a facile multi-step surface treatment was applied to enhance TE properties of pristine PEDOT:PSS thin films. Subsequently, the surface morphology and the inner morphology were probed using atomic force microscopy and grazing-incidence wide/small-angle X-ray scattering, respectively. Additionally, UV-Vis spectroscopy, Raman spectroscopy and X-ray photoelectron spectroscopy were employed to investigate the mechanism behind for TE performance improvement.

CPP 24.31 Mon 17:30 P3

DC and AC conductivity of ultra-thin carbon nanotube/polycation multilayers in air and different aqueous solutions — •Sven Neuber, Peter Nestler, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald, 17489 Greifswald, Germany

To prepare implants covered by an electrically conductive film it is necessary to control the device surface and properties. Electrically conductive multilayers were built by the layer-by-layer technique, sequential adsorption of oppositely charged chemically modified carbon nanotubes and polycations. Quartz crystal microbalance, atomic force microscopy and ellipsometry measurements were used to determine surface coverage, thickness and roughness on nm-scale. Also, frequency-dependent conductivity (kHz range, DC and AC) measurements at ambient conditions (20°C), at different humidities (r.h. between 0 * 100%) and in physiological solutions were investigated to get an overview of the multilayer capability for cell stimulation. It was found that the electrical conductivity depends on the environment. For PDADMA/CNT films (7 layer pairs) in air a current of 22.4 mA was obtained, in 100 mM NaCl solution 20.8 mA and in deionized water 10.5 mA. Also no phase change occurred during the frequency shift up to 100 kHz, indicating an ohmic behavior. The results are discussed in terms of film swelling, electron conductivity through the film and ionic conductivity through the solution.

CPP 24.32 Mon 17:30 P3

Dispersion Relations of Metal/Organic Hybrid Structures caused by Strong Coupling between Plasmons and Excitons — •Maximilian Rudloff[1], Maximilian Rödel[1], Thomas Stark[2], Jochen Manara[2], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Light-matter interaction in the vicinity of a metal surface is an intensely researched topic motivated by the possibility of tuning the optical properties of thin film devices on sub-wavelength scales [1]. By extending this concept to organic semiconductors on top of a metal surface, new hybrid states appear, labelled plexcitons. In our contribution we analyze the dispersion relations of plexcitons emerging by the coupling of localized excitons in ZnPc molecular layers and the collective electronic excitations at gold surfaces by means of a surface plasmon resonance setup. The resulting coupling strength is in the order of $\approx 100\,\text{meV}$ and is interpreted by the characteristics inherent to the individual systems. In addition we discuss the influence of the morphology on the plexcitonic dispersion branches, which provides an additional degree of freedom upon implementing this concept in future opto-electronic devices.

[1] V. Kolb, Opt. Express 25 (2017) 6678

CPP 24.33 Mon 17:30 P3

The Gradient Contribution to Light Scattering in an Interface Layer — •Reinhard Sigel — 88677 Markdorf

The effect of the refractive index gradient in an interface layer on the diffuse interface scattering is investigated theoretically. An extension of the transfer matrix method for a layered interface profile by small fluctuations in the layers provides predictions for diffuse interface light scattering. While the s-polarization follows the conventional wave equation, there is an extra term with a first order derivative in the wave equation for p-polarization. Within the transfer matrix method there are step-like gradients located at the layer boundaries. The gradient term in p-polarization produces an extra scattering contribution at the layer boundaries. It becomes significant for an evanescent wave illumination with an angle of incidence close to the critical angle and can be used for a new approach to depth resolution in interface scattering experiments. A comparison to the Distorted Wave Born Approximation (DWBA) which is highly celebrated within the X-ray community is discussed.

CPP 24.34 Mon 17:30 P3

Protein adsorption at the solid-liquid interface tuned by the choice of trivalent cations — •Nina Conzelmann, Madeleine Fries, Fajun Zhang, and Frank Schreiber — University of Tübingen, Germany

In biological processes, such as cell adhesion, protein adsorption at solid-liquid interfaces plays a crucial role since it is often observed as one of the first steps. Our study focuses on the effect of trivalent cations (La^{+3}, Y^{+3}) on globular proteins such as bovine serum albumin (BSA) which exhibits a rich phase behavior including reentrant condensation between two critical salt concentrations (c*, c**) and liquid-liquid phase separation [1]. Ellipsometry and quartz crystal microbalance were used to investigate the effect of increasing amounts of salt on the protein-interface system. The interaction of BSA with net-negatively charged surfaces like SiO$_2$ is dominated by electrostatic repulsion and minimum protein adsorption. First, an increasing amount of absorbed protein on the surface was observed while increasing salt concentration. Then, in the regime II, the thickness of absorbed protein reaches a maximum. At high salt concentrations, the adsorbed layer first decreases and then approaches a constant value. This behavior can be explained by using the ion-activated patchy interactions model [2]. Both salts used show the same overall adsorption trend, yet the absolute adsorbed amount in regime II (c*<c<c**) differs. The difference in regime II for LaCl$_3$ and YCl$_3$ is caused by LaCl$_3$ having weaker effective attractive protein-protein interactions.

[1] Matsarskaia et al, PCCP (2018); [2] Fries et al, PRL (2017)

CPP 24.35 Mon 17:30 P3

Real-time observations of alkali metal doped 6-Phenacene films — •Matthias Zwadlo, Martin Hodas, Alexander Gerlach, Nadine Russegger, Berthold Reisz, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

The characterization of growth and structure formation in molecular und hybrid systems is an important topic in fundamental organic semiconductor research. In order to study and influence this process different real-time methods have to be used [1]. A promising strategy for tuning the properties of these materials is alkali metal doping, which for example, can lead to superconductivity under specific circumstances [2]. In this work, the growth and structure formation of 6-Phenacene doped with potassium has been investigated. Thin films of pure 6-Phenacene have been grown in ultra-high vacuum (UHV) and investigated with x-ray, AFM and optical methods. Furthermore, grazing incidence wide angle scattering (GIWAXS) measurements of thin films of 6-Phenacene with potassium doping were performed insitu during growth at PETRA 3 (beamline P03) in Hamburg. First results show small distortions in crystal structure after potassium doping. The results allow us to get a better understanding on the structural behavior and growth process in theory and experiment.

[1] Hosokai, T., Gerlach, A., Hinderhofer, A., Frank, C., Ligorio, G., Heinemeyer, U., * Schreiber, F. Appl. Phy. Lett. , 97(6), 9 (2010) doi:10.1063/1.3478450

[2] Mitsuhashi, R., Suzuki, Y., Yamanari, Y. et al. Nature 464, 76 (2010) doi:10.1038/nature08859

CPP 24.36 Mon 17:30 P3

Gold Sputter Deposition on Polystyrene Thin Films: Influence of Template Thicknes and Molecular Weight — •Vivian Waclawek[1,2], Matthias Schwartzkopf[2], Marc Gensch[2,5], Pallavi Pandit[2], Michael Rübhausen[1,3], and Stephan V. Roth[2,4] — [1]Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg — [2]DESY, Notkestr. 85, D-22607 Hamburg — [3]Center for Free Electron Laser Science (CFEL), Luruper Chaussee 149, D-22761, Hamburg — [4]KTH, Teknikringen 56-58,SE-10044 Stockholm — [5]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str.1, D-85748 Garching

Nanostructured noble metal films on polymer layers promise various potentials applications in solar cells, biosensors, reflective or antireflective coatings. Moreover, such material combinations have recently gained importance for stabilizing thin polymer films during annealing above glass temperature. In order to study the effect of polymer film thickness d_{PS} and molecular weight M_W we combine sputter deposition with grazing incidence X-ray scattering (GISAXS) to investigate in-situ the growth kinetics of Au on polystyrene thin films with different thin (3-80nm) thicknesses and two different M_Ws (4 and 270kDa). We analyze quantitatively the metal nanoparticle layer growth and compare our results within the different polymer thicknesses. It is mandatory to understand the influence of the growth kinetics on the metal film morphology during sputter deposition for understanding the influence of M_W and d_{PS} on Au cluster growth. For future studies the results could be compared with different homopolymers.

CPP 24.37 Mon 17:30 P3

Influence of Wavy-Interface on the Dynamics of Drop-Interface Coalescence — •Kuntal Patel — Indian Institute of Technology, Bombay, India

In drop-interface type coalescence, when a droplet is placed gently on a liquid pool, it will try to merge with the liquid pool (by draining the liquid within the droplet into the pool), which may result in either partial or complete coalescence. It primarily depends on the relative competition among the surface tension, viscous resistance, and gravity [1]. In present work, we perform numerical simulations using the ghost-fluid method based sharp-interface level-set method [2] to study the coalescence dynamics of an ethanol droplet (of diameter 1.07 mm) with a wavy pool of ethanol (surrounded by air).

Numerical experiments show that the dual coalescence-cascade pattern observed with a planar ethanol pool gets altered in the case of a wavy pool. This deviation in the coalescence dynamics is attributed to the complex interaction between two different capillary waves, one originated due to the coalescence, and other from the waviness of the ethanol pool. We demonstrate the transition from dual coalescence-cascade to single and zero coalescence-cascade (i.e., complete coalescence) for different waviness (defined here using amplitude and frequency) of ethanol pool.

[1] B. Ray, et al., Journal of Fluid Mechanics 655, 72-104 (2010).

[2] J. Shaikh, et al., Chemical Engineering Science 176, 77-95 (2018).

CPP 24.38 Mon 17:30 P3

The Aging Mechanism of Silicone Molds for Vacuum Casting — •Natalie Frese[1], Martin Wortmann[2], Alexander Heide[2], Johannes Brikmann[2], Elmar Moritzer[3], Bruno Hüsgen[2], and Armin Gölzhäuser[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Bielefeld University of Applied Sciences, Bielefeld, Germany — [3]Paderborn University, Paderborn, Germany

The use of silicone casting molds in the vacuum casting process for the production of prototypes made of polyurethane is state of the art. Although the process is widely used for prototype replication, it is rarely considered for an extensive use in small batch production. With this, the gap in plastic processing between very small (rapid prototyping) and very large quantities (injection molding) might one day be closed. We present an in-depth investigation of the aging effects in silicone casting molds for vacuum casting processes. Their lifetime is limited to a few production cycles due to contamination with the diisocyanate component of the polyurethane casting resin. By using a wide variety of characterization methods, the chemical and physical mechanisms of the aging process have been identified. It has been shown that an anomalous diffusion process of diisocyanate into the silicone surface leads to the formation of interpenetrating polymer networks of polyurea derivatives in the poly(dimethylsiloxane) matrix. This has been proven by extracting and analyzing polyurea of low molecular weights from the silicone.

CPP 24.39 Mon 17:30 P3

Measuring Diffusion Coefficients of Methylene Diphenyl Diisocyanate in Polymeric Coatings on Poly(dimethylsiloxane) — •Martin Wortmann[1], Richard Petkau[1], Waldemar Keil[2], Natalie Frese[3], Elmar Moritzer[2], Armin Gölzhäuser[3], Andrea Ehrmann[1], Claudia Schmidt[2], and Bruno Hüsgen[1] — [1]Bielefeld University of Applied Sciences, Bielefeld, Germany — [2]Paderborn University, Paderborn, Germany — [3]Bielefeld University, Bielefeld, Germany

Methylene diphenyl diisocyanate (MDI), as a common constituent of polyurethane, is the most frequently produced isocyanate and therefore of vital industrial importance. The diffusivity of MDI in polymeric materials is relevant i.a. due to its health hazardous properties but also due to its use in technical processes. In this work, the diffusion coefficients of MDI in eight different amorphous polymers were determined by means of a newly proposed test methodology. For this purpose, the polymers were dissolved in various volatile solvents and coated by solvent casting on individually pretreated poly(dimethylsiloxane) (PDMS) samples. By measuring the mass transfer rate and the MDI concentrations on both sides of the coating, the diffusivity could be calculated with the stationary Fickian diffusion equation. To determine the MDI concentrations, nuclear magnetic resonance spectroscopy (NMR) was used. DOSY NMR was used to determine the concentration of MDI in the liquid state and a combination of 1H MAS solid-sate NMR and thermogravimetric analysis was used to determine the MDI concentration in the PDMS substrate.

CPP 24.40 Mon 17:30 P3

Development of a process to characterize an elastomer-metal contact with the aim of leakage prediction — •Felix Senf[1], Marius Pätzold[1], Robin Fonk[2], Sean Schneeweiss[2] und Othmar Marti[1] — [1]Institut für Experimentelle Physik, Ulm — [2]Ulmer Zentrum für wissenschaftliches Rechnen, Ulm

The following investigation describes the connection between surface structures, elastomers and tightness of critical leakage systems. In technical applications the sealing of hardware components is described with leakage rates based on different boundary conditions of the system. In general, physical rules state that an absolutely sealed system is not possible. Different parameters like materials, surface structures, roughness parameters, closing forces and not least the design of the sealing system influence the function of the sealing joint. The research program investigates the alignment between elastomers and metal surface structures and the resulting open volumes. The theory of contact problems, FEA simulation tasks and compression experiments help us to describe this alignment. An experimental set-up for leakage measurements and the combination with CFD simulations are the main tool to understand the leakage nature more in detail. Out of this toolbox we create a new process to describe leakage cases in a time efficient manner. Filter methods like morphological filters and Voronoi diagrams help us to work out the process.

CPP 24.41 Mon 17:30 P3

Analysis of liquid distribution in micro-channel systems using the electro-hydraulic analogy — •Marius Pätzold[1], Felix Senf[1], Carl Krill[2] und Othmar Marti[1] — [1]Institut für Experimentelle Physik, Ulm — [2]Institut für funktionelle Nanosysteme, Ulm

The research program investigates the calculation of leakages in hydraulic systems by modelling the systems using electric resistor networks as an alternative to simulations using computational fluid dynamics. Based on a rigid geometry, describing a network of channels with rectangular cross sections of constant height, the hydraulic properties of the network are examined. The system is then modelled using an electric resistor network using these hydraulic properties. For a given pressure drop between the in- and outlets the model can be solved and the leakages can be calculated using the modified nodal analysis. The results show that modelling the geometry this way can be an alternative to simulations using computational fluid dynamics within the requirements set by the electric-hydraulic analogy. Modelling hydraulic networks that are not within these requirements, like those with very short channels or highly complex channel networks, results in errors spreading through the network resulting in significant differences between the modelling and simulation approach.

CPP 24.42 Mon 17:30 P3

Studies on the Effect of Stoichiometric Changes on Thermomechanical Properties of Anhydride-cured Epoxy Resin — •Farnaz Emamverdi — BAM, Berlin, Germany

Introducing boehmite nanoparticles (BNPs) to anhydride-cured epoxy networks can improve the mechanical properties of the polymer. Understanding of the interaction between BNPs and the epoxy system is crucial since previous studies reveal that the interaction between the BNPs and the epoxy induces changes in the curing reaction locally. AFM-based studies revealed that the anhydride molecule has a preferential interaction with the BNP. It is hypothesized that such preferential absorption disturbs the curing reaction and causes a stoichiometric imbalance at the interphase in the epoxy matrix. To explain this behavior, we prepared off-stoichiometric samples where ratio between epoxy and anhydride were systematically altered. Previous studies have failed to focus on stoichiometric changes of epoxy-anhydride system. The effect of stoichiometric imbalance on the thermomechanical properties like the shear modulus and Tg is the focus of this study. The characterization for rich-hardener, poor-hardener and standard samples were done by FT-IR, TGA, DMA and DSC. Brown discoloration occurred is poor hardener sample. TGA results showed that all samples are thermally stable up to 200°C where the poor-hardener sample is the most stable one. DMA measurements show a post-curing effect for all samples, which is most pronounced in rich-hardener sample where G* dropped by 28%. Poor-hardener sample shows the highest Tg and crosslinking density.

CPP 24.43 Mon 17:30 P3

From flower-like micelles to bridged networks: Thermo-responsive block-polymers in solution studied by small-angle neutron scattering. — •Albert Prause[1], Michelle Hechenbichler[2], Benjamin von Lospichl[1], André Laschewsky[2,3], and Michael Gradzielski[1] — [1]Technische Universität Berlin, Department of Chemistry, Berlin, Germany — [2]Universität Potsdam, Department of Chemistry, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [3]Fraunhofer Institute for Applied Polymer Research IAP, Geiselbergstr. 69, 14476 Potsdam, Germany

Mediation between hydrophilic and hydrophobic phases is necessary for almost every application or process, e.g. cleaning, solubilization and stabilization. Best known for this purpose are amphiphilic molecules like surfactants. Usually, it is important to be able to control and adjust rheologic properties like the viscosity of a solution, wherefore polymers were commonly used to obtain the desired rheologic behavior. With this, inducing the possibility of a distinct temperature response to a rheologic property can become highly favorable for applications where temperature can be used to manipulate the rheology. To combine these properties, in this work hydrophobically modified thermo-responsive block-polymers are characterized between 20°C and 60°C in D_2O. The block-polymers are built of a permantently hydrophilic and a hydrophilic/hydrophobic temperature switchable block with a lower critical solution temperature (LCST). Used monomers are *N*-dimethylacrylamide (DMA) and monomers with LCST like *N*-isopropylacrylamide (NiPAm), respectively.

CPP 24.44 Mon 17:30 P3

Phase transition kinetics in a doubly thermo-responsive poly(sulfobetaine)-based block copolymer thin film — •Lucas P. Kreuzer[1], Tobias Widmann[1], Lorenz Biessmann[1], Raphael Märkl[1], Jean-Francois Moulin[2], Viet Hildebrand[3], André Laschewky[3], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]HZG at MLZ, 85747 Garching — [3]Universität Potsdam, Institut für Chemie, 14476 Potsdam Golm

Thermo-responsive polymers show a strong change in volume towards slight changes of their surrounding temperature. While this behavior is well understood for polymers in solution, less is known about the underlying mechanisms in thin film geometry. In our work, we investigate the phase transition kinetics upon increasing temperature in a thermo-responsive block copolymer thin film, that shows both, upper and lower critical solution temperature (UCST and LCST) behavior. Time-of-flight neutron reflectometry (ToF-NR) is used to follow the phase transition kinetics with high time resolution. At temperatures, below the UCST, the polymer film is first swollen in D2O atmosphere to increase the mobility of the polymer chains. Subsequent, temperature is increased to an intermediate regime (between UCST and LCST) and high regime (above LCST). In addition ToF grazing incidence small angle neutron scattering (GISANS) measurements are performed at the beginnnig and in between the kinetic processes to gain detailed information about the thin film morphology at different temperatures.

CPP 24.45 Mon 17:30 P3

Kinetics of shell collapse and aggregation in thermoresponsive PMMA-*b*-PNIPAM micelles revealed by time-resolved small-angle neutron scattering and fast pressure jumps — •Geethu P. Meledam[1], Chia-Hsin Ko[1], Shu-Hsien Huang[1], Bart-Jan Niebuur[1], Leonardo Chiappisi[2], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]University of Central Florida, Orlando, U.S.A.

The amphiphilic diblock copolymer, poly(methyl methacrylate)-*b*-poly(N-isopropylacrylamide) (PMMA-*b*-PNIPAM) self-assembles into core-shell micelles in aqueous solution, and the thermoresponsive PNIPAM shell collapses upon heating through its cloud point. Here, we explore the kinetics of structural modifications and intermicellar interactions in PMMA-*b*-PNIPAM micelles during its phase transition by performing time-resolved small-angle neutron scattering (SANS) in combination with millisecond pressure jumps. Because of the fast equilibration in a pressure jump, we are able to observe different stages of micellar shell collapse and aggregation while undergoing phase transition. At high pressures, the micellar shell stays rather hydrated and the growth proceeds via diffusion-limited aggregation. On the contrary, at low pressures, a hydrophobic-driven micellar aggregation occurs due to the strong dehydration of the PNIPAM shell. In general, the strategy of combining time-resolved SANS with rapid pressure jump experiments provides an exclusive possibility to probe the initial stages of phase transitions in macromolecules.

CPP 24.46 Mon 17:30 P3

Dehydration process of thermoresponsive molecular brushes with copolymer side chains — •Jia-Jhen Kang[1], Junpeng Zhao[2], Lester C. Barnsley[3], Fabian Kohler[1], Hendrik Dietz[1], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Athens, Greece — [3]FZ Jülich, JCNS at MLZ, Garching, Germany

Molecular brushes are densely grafted polymers composed of a backbone and side chains attached to virtually every monomer of the backbone. In the present study, we investigate molecular brushes with PEO-*ran*-PPO or PEO-*block*-PPO copolymer side chains in aqueous solution. Both PEO, poly(ethylene oxide), and PPO, poly(propylene oxide), exhibit lower critical solution temperature (LCST) behavior with very different cloud points. Their structural evolution upon heating from ambient temperature to temperatures above the corresponding cloud points is resolved using dynamic light scattering (DLS) and small-angle neutron scattering (SANS). The results reveal that the vastly different dehydration process strongly affects the side chain conformation, and thus the overall brush conformation as well as the collapse and the aggregation behavior.

CPP 24.47 Mon 17:30 P3

Increase of the diffusion constant of polyanion PSS in polyelectrolyte multilayers on approach to the glass transition temperature in dependence of salt concentration and pH — •Annekatrin Sill, Sven Neuber, and Christiane A. Helm — University Greifswald, Institute of Physics, Germany

Using neutron reflectivity, the vertical diffusion of polyanion PSS within polyelectrolyte multilayers is probed. We used a slab architecture with selective polyanion deuteration. The temperature-, salt- and pH-dependent change of the diffusion constant was determined. The films were measured as prepared and after annealing for different times (i) in 1 M NaCl solution at different temperatures approaching the glass transition at 55°C, (ii) at 40°C and different NaCl concentrations of the annealing solution and (iii) in 100 mM NaCl solution with different pH values. As the temperature of the annealing solution increases, the diffusion constant increases by five orders of magnitude. If the salt concentration in the annealing solution is reduced, the diffusion constant becomes smaller by two orders of magnitude. Preliminary measurements show that the diffusion constant decreases as the pH of the annealing solution increases. We conclude that for a large diffusion constant not only electrostatic monomer/monomer bonds need to be replaced by monovalent/ion bonds, but the most important effect is the increased mobility of the water molecules on approach to the glass transition temperature.

CPP 24.48 Mon 17:30 P3

Polyelectrolyte Microemulsion Complexes (PEMECs) Studied by Scattering Methods — •Michael Gradzielski[1], Miriam Simon[1], Laurence Noirez[2], Emmanuel Schneck[3], and Hoffmann Ingo[4] — [1]Stranski Laboratorium für Physikalische Chemie, Technische Universität Berlin, Germany — [2]Laboratoire Leon Brillouin (LLB) Saclay, France — [3]MPI für Kolloide und Grenzflächen, Golm/Potsdam, Germany — [4]Institut Laue-Langevin (ILL), 38000 Grenoble, France

Charged oil-in-water microemulsion droplets one can form polyelectrolyte/microemulsion complexes (PEMECs), where colloidal stability and structure are controlled by the properties of the individual components. In our experiments we varied systematically Mw and type of the polyelectrolyte as well as size and charge density of the microemulsion droplets and determined the phase behaviour and mesoscopic structure by means of static and dynamic light scattering, and small-angle neutron scattering (SANS). The formed structures are typically elongated but elongation and total size depend strongly on the mixing ratio, the Mw of the PE and its persistence length - and show and interesting pH response. Further dynamic experiments with PFG-NMR and neutron spin-echo (NSE) showed a remarkably high internal dynamics of these systems. In summary, PEMECs are an interesting and so far only little explored colloidal system that is a well-defined model system suitable for fundamental investigations but also highly relevant for formulations in cosmetics and pharmacy, due to their high loading with hydrophobic components.

CPP 24.49 Mon 17:30 P3

New insights of the gold nanoparticle growth: Simultaneous SAXS/SANS study — •Ezzeldin Metwalli[1], Klaus Götz[1], Tobias Zech[1], Christian Bär[1], Anne Martel[2], Lionel Porcar[2], and Tobias Unruh[1] — [1]ICSP, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Institut Laue-Langevin, 71, Avenue des Martyrs, Grenoble, 38042, France

Exploiting small angle X-ray and neutron scattering SAXS/SANS methods on the same sample volume at the same time offers a unique possibility to obtain complementary nanoscale structural information at two different contrast situations. A custom-made portable SAXS system has been designed, constructed and installed at D22-ILL for simultaneous SAXS/SANS experiments. For the first time, the temporal structural cross-correlation between organic stabilizing agent (cetyltrimethylammonium bromide; CTAB micelles) and gold seeds, which cooperate in the formation of different size/shape of large stabilized gold nanoparticles [1], has reliably been determined on the same sample. Compared with an independent experimental approach, the current experimental approach ensures the exactness of the probed samples, especially for time-resolved studies. This novel nanoanalytical method at ILL will answer yet unresolved scientific questions allowing real time investigations of a wide range of innovative materials such as smart self-assembling nanomaterials and multifunctional materials as well as enabling comprehensive in situ studies on biological systems. [1] T. Schmutzler, et al., ACS Applied Nano Materials 2, 3206 (2019).

CPP 24.50 Mon 17:30 P3

Grazing incidence scattering for the study of buried interfaces — •Max Wolff — Department for Physics and Astronomy, Uppsala University

Neutrons can penetrate deeply into matter and are sensitive to light elements. If applied under grazing incidence beam geometry they offer surface sensitivity and the opportunity to address highly relevant scientific challenges on solid-liquid boundaries, like e.g. the hydrodynamic boundary condition. From specular reflectivity the density profile, along the normal of the interfaces, of a liquid close to a solid substrate can be extracted.

Lateral correlations, parallel to an interface, are accessible by off-specular (μm) or grazing incidence scattering (nm length scale). Moreover, by using time of flight (TOF) methods a range of Q (momentum transfers) vectors and related penetration depth can be addressed. In turn the measurements are flux hungry and demanding with respect to brilliance of the source. This in combination with the low absorption of the neutrons in the liquid limits the achievable depth resolution. A combined approach of further improved instrumentation and sample design may allow to overcome this limitations by careful control of the wave amplitude using reference layers and resonators.

CPP 24.51 Mon 17:30 P3

RheoNSE for the study of topological interactions in polymers — •Max Wolff — Department for Physics and Astronomy, Uppsala University

Entangled polymers show unique flow behaviors, since the relaxation processes occur on time scales relevant for our daily lives, ranging from milliseconds to hours or even days. Yet, due to experimental limitations, the nonlinear rheological behavior of complex fluids is only modestly understood. We investigate the microscopic structure and dynamics of highly entangled polymers under shear with small angle neutron scattering (SANS) and neutron spin echo (NSE), respectively.

The viscoelastic properties of materials are typically investigated by rheology. If such measurements are done in shear rate controlled mode, the formation of a stress plateau can be observed above a critical shear rate. It is known that for these systems the measured stress shows a plateau when investigated under controlled shear rate. At these shear rates the polymer might disentangle resulting in a change in the topological interactions between the chains. This transition can only be observed in the dynamics of the chains studied with NSE.

CPP 25: Bio- and Molecular Magnetism (joint session MA/CPP)

Time: Monday 15:00–17:00 Location: HSZ 101

CPP 25.1 Mon 15:00 HSZ 101

HF-EPR investigations on Co(II)- and Fe(IV)-coordination complexes — •Lena Spillecke[1], Changhyun Koo[1], Shalini Tripathi[2], Maheswaran Shanmugam[2], Saskia Krieg[3], Peter Comba[3], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Department of Chemistry, Indian Institute of Technology, Mumbai, India — [3]Institute of Inorganic Chemistry, Universität Heidelberg, Heidelberg, Germany

We present high-frequency/high-field electron paramagnetic resonance (HF-EPR) studies on Co(II) and Fe(IV) coordination complexes. For Co(II) systems, we show that ligand exchange in the 2nd coordination sphere on $[Co(L_1)_4]X_2$, with L_1 = thiourea (NH_2CSNH_2) and X = I (**1**),Br (**2**), SiF6 (**3**)) has significant effects on the crystal field and hence on magnetic anisotropy of the Co-ion. While the substitution of I by Br only has small impact on the axial anisotropy ($D =$ -153(2)/-168(5) GHz, respectively), we observed strong enhancement of anisotropy in the SiF_6 containing sample ($|D| > 800$ GHz). Furthermore, our data enables precise determination of weak intermolecular coupling in the range of several hundred mK which sign changes by ligand substitution. In additon, we present HF-EPR data on an octahedrally coordinated Fe(IV)-complex which was prepared under liquid N_2 conditions. Our results confirm the intermediate-spin state and detect axial anisotropy of $D = 107(3)$ GHz.

CPP 25.2 Mon 15:15 HSZ 101

Magnetic field tuning of low energy spin dynamics in the single-atomic magnet $Li_2(Li_{1-x}Fe_x)N$ with $x \ll 1$ — •Sascha Albert Bräuninger[1], Sirko Kamusella[1], Felix Seewald[1], Rajib Sarkar[1], Manuel Fix[2], Stephan Jantz[2], Anton Jesche[2], Andre Zvyagin[3], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany —

[2]Institute of Physics, University Augsburg, D-86135 Augsburg, Germany — [3]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str., 38, D-01187 Dresden, Germany

We present a systematic ^{57}Fe-Mössbauer study on highly diluted Fe centers in $\mathrm{Li_2(Li_{1-x}Fe_x)N}$ single-crystals as a function of temperature and magnetic field applied transverse and longitudinal with respect to the single-ion anisotropy axis. Below 30 K the Fe centers exhibit a giant magnetic hyperfine field of $\bar{B}_A = 70.25(2)\,\mathrm{T}$ parallel to the axis of strongest electric field gradient $\bar{V}_{zz} = -154.0(1)\,\mathrm{V/Å^2}$. Fluctuations of the magnetic hyperfine field are observed between 50 K and 300 K and described by the Blume two-level relaxation model. An Arrhenius analysis yields a single thermal activation barrier of $\bar{E}_A = 570(6)\,\mathrm{K}$. Mössbauer spectroscopy studies with applied transverse magnetic fields up to 5 T reveal a large increase of the fluctuation rate by more than one order of magnitude. The experimental observations are qualitatively reproduced by a single-ion effective spin Hamiltonian analysis assuming a Fe^{1+} d^7 charge state with unquenched orbital moment and a $J = 7/2$ ground state.

CPP 25.3 Mon 15:30 HSZ 101

Intramolecular crossover from 2D diamagnetism to 3D paramagnetism — •Carolin Schmitz-Antoniak[1], Alevtina Smekhova[2], Detlef Schmitz[2], Natalya V. Izarova[1], S. Fatemeh Shams[1], Maria Stuckart[3], Frank M. F. de Groot[4], and Paul Kögerler[1,5] — [1]Forschungszentrum Jülich (PGI-6), 52425 Jülich — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin — [3]Inst. f. Chem. Reaktionstechnik, FAU Erlangen-Nürnberg, 91058 Erlangen — [4]Inorganic Chemistry and Catalysis Group, Debye Inst. for Nanomaterials Science, Utrecht University, Utrecht 3584 CG — [5]Inst. f. Anorgan. Chemie, RWTH Aachen University, 52074 Aachen

In a 2D square-planar coordination with four surrounding oxygen anions, Pd(II) ions in polyoxopalladates are diamagnetic with a large orbital contribution to the magnetic response as revealed by XANES and XMCD. Supported by atomic multiplet calculations the dependence of electronic and magnetic properties on 4d spin-orbit coupling, bond lengths, and delocalization of 4d electrons was investigated. We found that (i) four additional out-of-plane oxygen anions around Pd(II) lead to an effective 3D symmetry causing a paramagnetic response in external magnetic fields and (ii) in the crossover region between common diamagnetism and paramagnetism, the large spin-orbit coupling of Pd facilitates an unusual diamagnetic state modified by significant mixing. Furthermore, by measuring and analysing characteristic fine structures of the diamagnetic states in the XMCD spectrum, we overcome the common limitation of XMCD to ferro/ferrimagnetic and paramagnetic materials in external magnetic fields.

CPP 25.4 Mon 15:45 HSZ 101

Chemical Doping of Individual Polynuclear Molecular Magnets on Surfaces — •Fabian Paschke[1], Vivien Enenkel[1], Tobias Birk[1], Jan Dreiser[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universitaet Konstanz, 78457 Konstanz, Germany — [2]Swiss Light Source, 5232 Villigen PSI, Switzerland

The controlled deposition, characterization and manipulation of single molecule magnets (SMMs) on surfaces is one of the crucial topics to investigate with regard to their possible implementation as units in future electronic and spintronic devices. $\mathrm{Fe_4}$ derivatives are among the most investigated SMMs showing a giant spin and a variety of quantum mechanical phenomena. We showed that a flat derivative of this SMM is suitable for defined adsorption on decoupling monatomic layers of h-BN and graphene [1,2]. We proved the robust molecular magnetism to be retained on a global and single molecule scale, even on metallic substrates [2-4]. In order to manipulate electronic and magnetic properties of individual SMMs chemical doping with alkali atoms has shown to be a feasible technique [5]. Unfortunately, large polynuclear compounds like $\mathrm{Fe_4}$ can host numerous adsorption sites for dopants. Here we present successful chemical doping with a defined adsorption configuration for the prototypical $\mathrm{Fe_4}$ SMM and study the effect on its electronic and magnetic properties.

[1] P. Erler et al., Nano Lett. 15, 4546 (2015). [2] L. Gragnaniello et al., Nano Lett. 17, 7177 (2017). [3] F. Paschke et al., ACS Nano 13, 780 (2019). [4] F. Paschke et al., *submitted* (2019). [5] C. Krull et al., Nat. Mat. 12, 337 (2013).

CPP 25.5 Mon 16:00 HSZ 101

Numerical Challenges in Studying Families of $3d$-$4f$ Heterometallic Single-Molecule Magnets — •Julius Mutschler[1], Hetti M. Jayawardena[1], Christopher E. Anson[2], Annie K. Powell[2], and Oliver Waldmann[1] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institut für anorganische Chemie, Universität Karlsruhe, KIT, Germany

The discovery of slow relaxation and quantum tunneling of the magnetization in single molecule magnets (SMMs) has inspired both physicists and chemists alike. This class of molecules has been expanded to heterometallic clusters incorporating transition metal and rare earth ions. The $4f$ ions are of interest because of their large angular momentum and magnetic anisotropy, but present unexpected challenges in the numerical analysis of experimental powder susceptibility and magnetization curves. For example in the case of the $3d$-$4f$ SMM $\mathrm{Mn_2Ho_2}$-square, the dimension of the Hilbert space is 7225, and the computation time for a full exact diagonalization is only few 10 seconds. However, when fitting the powder magnetization with a 10 parameter model, which is typical for this type of molecules, ca 10^7 diagonalizations need to be performed, resulting in an impractical total time for completing the fit of several years. In this talk our approaches to tackle this challenge are demonstrated.

CPP 25.6 Mon 16:15 HSZ 101

Dy2O-clusterfullerenes: Strong magnetic anisotropy and fullerene-dependent single molecule magnetism — •Georgios Velkos[1], Wei Yang[2], Stanislav Avdoshenko[1], Ning Chen[2], Bernd Büchner[1], and Alexey Popov[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]College of Chemistry, Soochow University, Suzhou, China

The exceptional ability of fullerenes to stabilize species which can hardly exist otherwise has been extensively used to create a number of endohedral metallofullerene families. Among them, there is a great interest in Dy-metallofullerenes, caused by their robust magnetic properties. In this work, we report on the synthesis and in-depth magnetic study of the first Dy2O-clusterfullerenes. The compact geometry of Dy2O cluster leads to both strong axial ligand field and unprecedentedly strong antiferromagnetic exchange coupling between Dy ions. We demonstrate that Dy2O-clusterullerenes are excellent molecular magnets exhibiting broad magnetic hysteresis and the strongest super-exchange coupling between Dy ions ever reported for non-radical bridged compounds.

CPP 25.7 Mon 16:30 HSZ 101

Dynamic magnetic response of a single Magnetite nanoparticle chain detected by Scanning Transmission X-Ray Microscopy Ferromagnetic Resonance — •Thomas Feggeler[1], Benjamin Zingsem[1,2], Ralf Meckenstock[1], Michael Winklhofer[3], Detlef Spoddig[1], Hendrik Ohldag[4], Michael Farle[1], Heiko Wende[1], and Katharina Ollefs[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, Duisburg, Germany — [2]ERC and PGI, Fz. Jülich GmbH, Jülich, Germany — [3]School of Mathematics and Science, University of Oldenburg, Oldenburg, Germany — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

The dynamic magnetization of a single nanoparticle chain of 19 Magnetite particles (diameter of about 50 nm) embedded in a bacterium Magnetospirillum Magnetotacticum is measured using Scanning Transmission X-Ray Microscopy detected Ferromagnetic Resonance (STXM-FMR) [1]. A resonant response of the segments of the nanoparticle chain is identified and confirmed by micromagnetic simulations. STXM-FMR features the element specific detection of magnetization dynamics with a spatial resolution $<$ 50 nm and a time resolution in the ps regime. The manipulation of the genetic code of the bacteria allows to control the arrangement of the nanoparticles leading to the creation of magnonic logic devices as a future concept for magnonic computing [2]. [1] S. Bonetti, et al., Rev. Sci. Instrum. 86 (2015). [2] B. W. Zingsem, et al., Nat. Commun. 10 (2019). Financial support: FWF Project I-3050, ORD-49, DFG Project 321560838.

CPP 25.8 Mon 16:45 HSZ 101

Biologically encoded magnonics — •Benjamin Zingsem[1], Thomas Feggeler[1], Ralf Meckenstock[1], Michael Farle[1], and Michael Winklhofer[1,2] — [1]University Duisburg-Essen — [2]Universität Oldenburg

We report on the spectral properties of spin-waves (magnons) in individual chains of dipolar coupled magnetite nanoparticles. The particle-chains are biologically produced in magnetotactic bacteria. Straight chains where obtained from wild-type, curved and looped chains form mutant bacteria. A strong link between distinct spectral properties of the chains and their geometrical arrangement is identified, paving the way towards genetically engineered spin-wave computing on the nanoscale. Each chain consists of ca. 12 nanoparticles with a diameter of about 30 nm, separated by a spacing of about 8 nm. Ferromagnetic resonance spectroscopy was employed to measure the magnonic Eigenstates of each single particle in the chain as a function of the magnitude and direction of an applied magnetic field. The measurements are supplemented with micromagnetic simulations, which reveal the origin of spectral features such as band repulsion and attraction in resonant eigenstates. The emergent topology of the spin-wave band structure exhibits functional properties such as band deflection and band deformation, which may be harnessed in energy efficient magnon computing [1] and neuro-inspired magnonic networks. Future nanomagnonic devices may be self-assembled via genetic engineering of magnetotactic bacteria.

[1] B. Zingsem, et al. Nat Commun 10, 4345 (2019)

CPP 26: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)

Time: Monday 15:00–17:30 Location: GER 38

CPP 26.1 Mon 15:00 GER 38

Satellites in optical and loss spectra — •Pier Luigi Cudazzo — Faculty of Science, Technology and Communication, RU Physics and Materials Science, Campus Limpertsberg, Université du Luxembourg, 162 A, avenue de la Faïencerie, L-1511 Luxembourg

Coupling of excitations leads to intriguing effects on the spectra of materials. We propose a cumulant formulation for neutral electronic excitations which opens the way to describe effects such as double plasmon satellites or exciton-exciton and exciton-phonon coupling. Our approach starts from the GW plus Bethe-Salpeter approximation to many body perturbation theory which is based on a quasiparticle picture, and it adds coupling of excitations through a consistent inclusion of dynamically screened interactions. This requires to consider scattering contributions that are usually neglected. The result is formulated in a way that highlights essential physics, that can be implemented as a post processing tool in first principles codes, and that suggests which kind of materials and measurements should exhibit strong effects. This is illustrated using a model.

CPP 26.2 Mon 15:15 GER 38

The XPS limit within the one-step model of photoemission: temperature and photon energy effects — •Laurent Nicolaï[1], Vladimir Strocov[2], Juraj Krempaský[2], Federico Bisti[2], Jürgen Braun[3], Hubert Ebert[3], Charles Fadley[4], Ajith Kaduwela[5], Nicholas Pike[6,7], Matthieu J. Verstraete[7], and Ján Minár[1] — [1]Univiversity of West Bohemia, Plzeň, Czech Rep. — [2]Paul Scherrer Institut, Villigen, Suisse — [3]Ludwig-Maximilians-Universität, Germany — [4]Berkeley, California, USA — [5]University of California, USA — [6]University of Oslo, Norway — [7]Université de Liège & European Theoretical Spectroscopy Facility, Belgium

Angle-Resolved Photoemission Spectroscopy (ARPES) is the method of choice for characterising the electronic structure of a given material. A complete understanding of the experimental spectra requires theoretical analyses as well. However, the development of theoretical tools in order to reproduce experimental conditions remains, to this day, a challenge. Using the one-step model of photoemission[1] as implemented in the SPRKKR package[2], our calculations incorporate temperature- and phonon energy-dependent effects via inclusion of both bulk[3] and surface phonons. We also investigate the photon energy range over which the Angle-Integrated PhotoEmission (AIPES) spectra can be compared to the corresponding Weighed Density of States (WDOS).

[1] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996), [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011), [3] L. Nicolaï and J. Minár, AIP Conf. Proc. 1996, 020033 (2018)

CPP 26.3 Mon 15:30 GER 38

Ab Initio Linear and Pump-Probe Spectroscopy of Naphthalene Crystals — •Alan Lewis[1] and Tim Berkelbach[2,3] — [1]MPSD, Hamburg, Germany — [2]Columbia University, New York City, USA — [3]Flatiron Institute, New York City, USA

Linear and non-linear spectroscopies are powerful tools used to investigate the energetics and dynamics of electronic excited states of both molecules and crystals. While highly accurate ab initio calculations of molecular spectra can be performed relatively routinely, extending these calculations to periodic systems is challenging. Here, we present calculations of the linear absorption spectrum and pump-probe two-photon photoemission spectra of the naphthalene crystal using equation-of-motion coupled-cluster theory with single and double excitations (EOM-CCSD). Molecular acene crystals are of interest due to the low-energy multi-exciton singlet states they exhibit, which have been studied extensively as intermediates involved in singlet fission. Our linear absorption spectrum is in good agreement with experiment, predicting a first exciton absorption peak at 4.4 eV, and our two-photon photoemission spectra capture the behavior of multi-exciton states, whose double-excitation character cannot be captured by current methods. The simulated pump-probe spectra provide support for existing interpretations of two-photon photoemission in closely-related acene crystals such as pentacene.

CPP 26.4 Mon 15:45 GER 38

All-electron real-time TDDFT implementation with Ehrenfest molecular dynamics — •Ronaldo Rodrigues Pela[1,2] and Claudia Draxl[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]European Theoretical Spectroscopy Facility (ETSF)

Linearized augmented planewaves with local-orbitals (LAPW+lo) are arguably the most precise basis set to represent Kohn-Sham states. When employed within real-time time-dependent density functional theory (RT-TDDFT), they promise ultimate precision achievable for exploring the evolution of electronic excitations in time scales ranging from attoseconds to picoseconds. In this work, we present the implementation of RT-TDDFT in the full-potential LAPW+lo code exciting [1]. For relaxing the nuclear degrees of freedom, we include Ehrenfest molecular dynamics [2]. We benchmark our implementation by analyzing the electric current density and the ion dynamics of Si, C, SiC, and two dimensional BN under the exposure to laser pulses. We compare our results with those obtained using the octopus code [3] and find a satisfactory level of agreement.

References

[1] A. Gulans et al. J. Phys.: Condens. Matter **26**, 363202 (2014).

[2] G. Kolesov et al. J. Chem. Theory Comp. **12**, 466 (2015).

[3] X. Andrade et al. Physical Chemistry Chemical Physics **17**, 31371 (2015).

CPP 26.5 Mon 16:00 GER 38

Ab initio study of nonradiative recombination for defects in MoS2 via multiphonon emission — •Simone Manti[1], Lukas Razinkovas[2], Audrius Alkauskas[2], and Kristian Thygesen[1] — [1]Computational Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark — [2]Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania

Carrier capture at point defects determines the lifetime of charge carriers and is therefore a very important process for both electronic and opto-electronic devices. The general theory of nonradiative recombination via the so-called multiphonon emission is rather well established, but most studies to date have mainly focused on the description in bulk materials. In this work, we investigate nonradiative carrier capture for a prototypical 2D material, molybdenum disulphide MoS2. Multiphonon emission is governed by (i) electron-phonon coupling between the band edge states and defect states and (ii) the change in the defect geometry upon carrier capture. Our results provide a preliminary description for nonradiative electron capture at sulphur vacancies in monolayer MoS2. In particular, we reveal the important role of the Jahn-Teller effect on the capture process.

CPP 26.6 Mon 16:15 GER 38

Phonon-induced electronic relaxation in a strongly correlated system: the Sn/Si(111) $(\sqrt{3}\times\sqrt{3})$ **adlayer revisited** — •Peter

Kratzer and Maedeh Zahedifar — Faculty of Physics, University Duisburg-Essen

The ordered adsorbate layer Sn/Si(111) $(\sqrt{3} \times \sqrt{3})$ with coverage of one third of a monolayer is considered as a realization of strong electronic correlation in surface physics. Our theoretical analysis shows that electron-hole pair excitations in this system can be long-lived, up to several hundred nanoseconds, since the decay into surface phonons is found to be a highly non-linear process. We combine first-principles calculations with help of a hybrid functional (HSE06) with modeling by a Mott-Hubbard Hamiltonian coupled to phononic degrees of freedom. The calculations show that the Sn/Si(111) $(\sqrt{3} \times \sqrt{3})$ surface is insulating and the two Sn-derived bands inside the substrate band gap can be described as the lower and upper Hubbard band in a Mott-Hubbard model with U=0.75eV. Furthermore, phonon spectra are calculated with particular emphasis on the Sn-related surface phonon modes. The calculations demonstrate that the adequate treatment of electronic correlations leads to a stiffening of the wagging mode of neighboring Sn atoms; thus, we predict that the onset of electronic correlations at low temperature should be observable in the phonon spectrum, too. The deformation potential for electron-phonon coupling is calculated for selected vibrational modes and the decay rate of an electron-hole excitation into multiple phonons is estimated, substantiating the very long lifetime of these excitations.

CPP 26.7 Mon 16:30 GER 38

Spectral properties of the interacting homogeneous electron gas — •Tommaso Chiarotti[1], Nicola Marzari[1], and Andrea Ferretti[2] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Centro S3, CNR–Istituto Nanoscienze, 41125 Modena, Italy

Despite its simplicity, the interacting homogeneous electron gas (HEG) is a paradigmatic test case in the study of the electronic structure of condensed matter. Beside being a model for valence electrons in simple metals, it also provides the basic ingredients for key electronic-structure theories. Here, we propose to study it with many-body perturbation theory (MBPT) using one shot, partial self-consistent, and full self-consistent GW, and analyze the description of its spectral function. For this, a novel numerical implementation of MBPT for the 3D non-relativistic HEG has been developed, with a special focus on the treatment of the full-frequency dependence of the Green's function and self-energies. Results for a broad range of densities (going from r_s from 1 to 10) are presented with particular attention to the calculated density-of-states and the spectral potential.

CPP 26.8 Mon 16:45 GER 38

Multipole Polarizabilites of Positronium and Its Interaction with Atoms and Molecules — •Jorge Charry, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Positron – the antiparticle of the electron – has many intriguing fundamental properties and it is also useful in many applications for probing matter. Besides electron-positron annihilation, metastable states of atomic and molecular systems involving binding between electrons and positrons are of great interest [1]. In addition, electrons and positrons can form positronium (Ps) atoms and even larger clusters. The polarization of positron by a residual ion is one of possible mechanisms for the formation of bound states for positron-based chemistry [2]. An accurate description of the polarizability of Ps and its bound state with atoms and molecules is essential to understand such interactions. Here, we extend the direct transition-matrix approach, proposed by Kharchenko to determine the multipole polarizabilities of the hydrogen atom [3], to the case of finite nuclear mass. The obtained analytical results, which are in agreement with our numerical calculations performed by means of the molecular orbital based method [4], show that Ps has unique properties in comparison to other normal atoms. Our results shed light into the fundamental interactions between matter and antimatter. [1] Gribakin *et al.*, Rev. Mod. Phys. **82**, 2557 (2010); [2] Bromley and Mitroy, J. Phys.: Conf. Series **199**, 012011 (2010); [3] Kharchenko, Annal. Phys. **355**, 153 (2015); [4] Reyes *et al.*, Int. J. Quant. Chem. **119**, 1 (2019)

CPP 26.9 Mon 17:00 GER 38

Energy gap closure of crystalline molecular hydrogen with pressure — •Vitaly Gorelov[1], Markus Holzmann[2,3], David M. Ceperley[4], and Carlo Pierleoni[5,1] — [1]Maison de la Simulation, CEA-Saclay, Gif-sur-Yvette, France — [2]Univ. Grenoble Alpes, CNRS, LPMMC, Grenoble, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Physics, University of Illinois Urbana-Champaign, USA — [5]Department of Physical and Chemical Sciences, University of L'Aquila, L'Aquila, Italy

We study the gap closure with pressure in Phases III and IV of molecular crystalline hydrogen. Nuclear quantum and thermal effects are considered from first principles with Coupled Electron Ion Monte Carlo. The fundamental electronic gaps are obtained from grand-canonical Quantum Monte Carlo methods properly extended to quantum crystals. Nuclear zero point effects cause a large reduction in the gap ($\sim 2eV$). As a consequence the fundamental gap closes at 530GPa for ideal crystals while at 360GPa for quantum crystals. Since the direct gap remains open until ∼450GPa, the emerging scenario is that upon increasing pressure in phase III (C2/c-24 crystal symmetry) the fundamental (indirect) gap closes and the system enters into a bad metal phase where the density of states at the Fermi level increases with pressure up to ∼450GPa when the direct gap closes. Our work partially supports the interpretation of recent experiments in high pressure hydrogen.

CPP 26.10 Mon 17:15 GER 38

Using the powerful electronic structure theory to identify single photon emitters in h-BN. — •Sajid Ali — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In recent years two-dimensional Van Der Walls material h-BN have gained a considerable interest due to the discovery of single photon emission (in both visible and UV region) from the colour centres in this material. This emission is bright, owing to the natural proximity of the centres to the surface, showing promise for high quantum efficiency applications, linearly polarized and strain tuneable. However, the exact chemical nature of the emitting centres is still unknown.

Here, we have performed first principle calculations to obtain observables that can be directly compared with electron paramagnetic resonance (EPR), Optically Detected Magnetic Resonance (ODMR), photoluminescence spectroscopy (PL) and Raman spectroscopy techniques performed on these h-BN emitters. We identify, based on the comparison of our calculations with the experimental data, the defect centres responsible for single photon emission from hexagonal boron nitride.

CPP 27: Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar II (joint session HL/CPP)

Hybrid halide perovskites are by now well established solar absorber and emitter materials, with power conversion efficiencies of single cell devices exceeding 20

Organizers: Linn Leppert (Universiät Bayreuth) and Felix Deschler (TU Munich)

Time: Monday 15:00–17:00 Location: POT 251

Invited Talk CPP 27.1 Mon 15:00 POT 251

Double perovskite electronic structures: A chemical perspective — •Adam Slavney[1], Hemamala Karunadasa[2], Linn Leppert[3], and Bridget Connor[2] — [1]Department of Chemistry, Harvard University, Cambridge, Massachusetts, USA — [2]Department of Chemistry, Stanford University, Stanford, California, USA — [3]Institute of Physics, University of Bayreuth, Bayreuth, Germany

Halide double perovskites, of the formula A2BB'X6, are close analogs to the APbX3 lead halide perovskites and have attracted significant interest as possible non-toxic alternatives to the lead materials in perovskite photovoltaics. Double perovskites divide the formally +2 charge on the octahedral B site unevenly over two B sites, allowing for cations with charges from +1 - +4 to be incorporated into the perovskite lattice. I will discuss the results of our experimental and theoretical investigations into double perovskites over the last several years, with a particular emphasis on understanding the differences in electronic structure between single and double perovskites. The double perovskite electronic structure is largely dictated by the combination of the B and B* cations rather than either cation individually and I will provide simple rules which accurately predict the band structure from the chemical formula in nearly every case. Double perovskites electronic structures have features not available in single perovskites including symmetry-forbidden bandgaps and unusually small bandgaps generated by metal-metal charge transfer transitions. Finally, I will discuss some of the defect chemistry of double perovskites and how those lessons can be applied to halide perovskites more broadly.

Invited Talk CPP 27.2 Mon 15:30 POT 251

Solid state ionics of hybrid halide perovskites: equilibrium situation and light effects — •Alessandro Senocrate[1,2], Gee Yeong Kim[1], Tae Youl Yang[1], Giuliano Gregori[1], Michael Graetzel[1,2], and Joachim Maier[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]École polytechnique fédérale de Lausanne

In recent years, hybrid halide perovskites have been attracting great attention due to their exceptional photo-electrochemical properties. When used as light-harvesters in solar cells, device efficiencies exceeding 25% can be realized. We showed that a deeper understanding of (i) functionality, (ii) stability, as well as (iii) the possibility to improve the performance require a thorough insight into non-stoichiometry and ion transport.

In this contribution, we study the nature of the ionic conductivity in methylammonium lead iodide (MAPbI$_3$), the archetypal halide perovskite, by means of a great number of electrochemical and nuclear magnetic techniques. To aid the experimental investigation, we include detailed defect chemical modelling describing the effects of varying iodine partial pressure (stoichiometry) and dopant content. By extending this study to the situation under illumination, we observe a striking enhancement of ionic conductivity by more than 2 orders of magnitude in MAPbI$_3$, alongside the expected increase in electronic conductivity. We provide a mechanistic explanation of this astonishing phenomenon and discuss its relevance for the photo-stability of this class of materials.

CPP 27.3 Mon 16:00 POT 251

Looking beyond the surface: The band gap of bulk methylammonium lead iodide — Oskar Schuster[1], Peter Wientjes[1], Shreetu Shrestha[2], Ievgen Levchuk[2], Mykhailo Sytnyk[3], Gebhard Matt[2], Andres Osvet[2], Miroslaw Batentschuk[2], Wolfgang Heiss[3], Christoph Brabec[2], Thomas Fauster[1], and •Daniel Niesner[1] — [1]Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7, 91058 Erlangen, Germany — [2]Materials Science Department (I-MEET), FAU, Martensstrasse 7, 91058 Erlangen, Germany — [3]Materials Science Department, FAU, Energy Campus Nürnberg, 90429 Nürnberg, Germany

Reported optical properties of lead halide perovskites as basic as the absorption onset and the band gap vary significantly. To unambiguously answer the question whether the discrepancies are a result of differences between bulk and "near-surface" material, we perform bulk-sensitive two-photon absorption with an information depth in the millimeter range on single crystals. In the application-relevant room-temperature tetragonal phase (170 K) we find a bulk band gap of 1.55 ± 0.01 eV. Reference measurements on the surface-near region in a reflection geometry show excitonic transitions at 1.59 ± 0.01 eV, consistent with the literature. The small band gap of the bulk material explains the extended infrared absorption of crystalline perovskite solar cells, the narrow bandwidth of crystalline perovskite photodetectors making use of the spectral filtering at the surface, and the low-energy bands which carry optically driven spin-polarized currents.

CPP 27.4 Mon 16:15 POT 251

Double Peak Emission in Lead Halide Perovskites by Self-Absorption — •Konstantin Schötz[1], Abdelrahman M. Askar[2], Wei Peng[3], Dominik Seeberger[1], Tanaji P. Gujar[1], Mukundan Thelakkat[1], Sven Huettner[1], Osman M. Bakr[3], Karthik Shankar[2], Anna Köhler[1], and Fabian Panzer[1] — [1]Universität Bayreuth, Bayreuth, Germany — [2]University of Alberta, Edmonton, Canada — [3]King Abdullah University of Science and Technology (KAUST), Thuwal, Kingdom of Saudi Arabia

Despite the rapidly increasing efficiencies of perovskite solar cells, the optoelectronic properties of this material class are not completely understood. Especially when measured photoluminescence (PL) spectra consist of multiple peaks, their origin is still debated. In this work, we investigate in detail double peak PL spectra of halide perovskite thin films and single crystals with different material compositions. By different optical spectroscopic approaches and quantitative models, we demonstrate that the additional PL peak results from an extensive self-absorption effect, whose impact is intensified by strong internal reflections. This self-absorption accounts for the unusual temperature dependence of the additional PL peak and it implies that absorption until far into the Urbach tail of the perovskite is important. The strong internal reflections entail that even for thin films self-absorption can have a significant contribution to the PL spectrum. Our results allow for a clear assignment of the PL peaks by differentiating between optical effects and actual electronic transitions, which is necessary for understanding the optoelectronic properties of halide perovskites.

CPP 27.5 Mon 16:30 POT 251

Surface atomic and electronic structure of CsPbBr$_3$ inorganic perovskite — •Janek Rieger, Felix Trunk, Thomas Fauster, and Daniel Niesner — Lehrstuhl für Festkörperphysik, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Staudtstr. 7, D-91058 Erlangen, Germany

The crystallographic orientation of the surface has a strong impact on the performance of solar cells built from lead-halide perovskites [1]. For a systematic study of the surface carrier-dynamics, we prepare atomically well-defined (001) surfaces of the inorganic perovskite CsPbBr$_3$ by epitaxial growth in ultra-high vacuum. Low-energy electron diffraction was carried out to analyze the resulting samples.
The measured surface unit cell as well as the corresponding phase transitions differ from the bulk-terminated ones. Angle-resolved photoelectron spectroscopy finds a valence-band structure in line with data we obtained from single crystals. Finally, we also investigated the energetics of the conduction-band electrons using two-photon photoelectron spectroscopy. From the positions of the valence-band maximum and the conduction-band minimum we conclude that our CsPbBr$_3$ samples are intrinsic.
[1] S. Y. Leblebici et al., Nat. Energy **1.8**, 16093 (2016).

CPP 27.6 Mon 16:45 POT 251

Finite temperature effects on the excited states in layered BiI$_3$ — •Ivona Bravic and Bartomeu Monserrat — TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Over the last decade layered BiI$_3$ has been matter of investigation in the optoelectronics community as it exhibits a fundamental band gap similar to that of silicon but behaves like a direct band gap semiconductor. However, the excited state properties of this system remained poorly understood, which is mostly a consequence of the extremely flat band structure and the arising low robustness with respect to dynamical distortions, volume expansion and stacking faults. In order to determine its potential performance in an optoelectronic device at finite temperature, it proves invaluable to establish a fundamental understanding of its excited states and how the aforementioned properties effect those. In this study we reveal the effect of spin-orbit coupling, electron-phonon coupling, exciton-phonon coupling, stacking faults and volume expansion on the optical response and photoluminescence properties of this materials using DFT as well as GW-BSE, proving that it is crucial to account for all these effects to provide a comprehensive understanding of the optoelectronic performance of layered BiI$_3$, and in general layered van-der Waals materials.

CPP 28: Microscopy and Spectroscopy with X-rays, Ions and Positrons (joint session KFM/CPP)

Chair: Enrico Langer (TU Dresden)

Time: Monday 15:00–17:40 Location: TOE 317

CPP 28.1 Mon 15:00 TOE 317

Single-Shot Phase-Contrast Microscopy of Laser-induced Cavitation at MID/EuXFEL — •Johannes Hagemann[1], Malte Vassholz[2], Hannes Höppe[2], Markus Osterhoff[2], Juan Rosello[3], Robert Mettin[3], Andreas Schropp[1], Christian Schroer[1,4], and Tim Salditt[2] — [1]DESY, Notkestraße 85, 22607 Hamburg — [2]Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [3]Drittes Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen — [4]Department Physik, Universität Hamburg,Luruper Chaussee 149, 22761 Hamburg

X-ray free electron lasers offer unique opportunities for imaging of ultra-fast processes on smallest length-scales paired with the penetration power of hard X-rays. One of these processes is laser-induced cavitation in water. The dynamic nature of the processes under study is incompatible to scanning schemes for image acquisition thus we chose propagation-based near-field imaging as full-field imaging scheme. The illumination with high intensity, fs-short X-ray pulses enables imaging with single pulses which yield a still image of the cavitation bubble without motion blur. In this contribution we will present a pump-probe imaging experiment conducted at the MID instrument at the European XFEL. The experiment has been carried out at 14/17.8 keV photon energy. The X-rays have been focused by aberration corrected Be-compound refractive lenses down to 100 nm focus-size. The fluctuating nature of the SASE-process poses some challenges for the data analysis. We present our approach to the data-processing, phase-retrieval and results.

CPP 28.2 Mon 15:20 TOE 317

Latest developments in multi-modal scanning X-ray microscopy — •Michael Stuckelberger — DESY, 22607 Hamburg, Germany

Scanning X-ray microscopy is challenged not only by the ever-smaller structures requiring higher resolution, but also by the increasing complexity of in-situ and operando environments of functional materials. Given that relevant information about micro- and nanostructures is typically extracted from the point-by-point correlation of different properties, the same spot needs to be in the same condition for all measurements. Often, this is not possible without the simultaneous evaluation of all critical measurement modalities.

At the leading X-ray nanoprobe endstations in the US and in Europe, we have set up experiments for multi-modal X-ray microscopy. Involving up to 5 different modalities, the measurements allow the simultaneous evaluation of composition by X-ray fluorescence, structure by X-ray diffraction and ptychography, and of the electrical and optical performance by X-ray beam induced current and X-ray excited optical luminescence.

In this contribution, we will demonstrate the application of multi-modal scanning X-ray microscopy to nanoscale semiconductors and electronic devices, and discuss detector arrangement and compatibility with different scan modes and samples. Beyond state-of-the-art measurements, we will give an outlook to new opportunities and challenges at X-ray nanoprobe endstations of 4th generation synchrotrons that will see light in the coming years.

CPP 28.3 Mon 15:40 TOE 317

Experimental optimization of geometry for propagation based phase contrast X-ray imaging — •Hanna Dierks and Jesper Wallentin — Synchrotron Radiation Research, Lund University, Sweden

Propagation-based phase contrast imaging (PB-PCI) with an X-ray lab source is a powerful technique to study low-absorption samples, e.g. soft tissue or plastics, on the micrometer scale. The choice of the propagation distance and magnification is crucial for the performance, and a trade-off in terms of resolution, contrast and noise is always necessary. Theoretical optimization strategies based on Fresnel propagation have been reported, and here we systematically test these experimentally using a setup with a Cu X-ray tube and a detector with 0.55um effective pixel size. The source-detector distance was between 25 and 40cm and magnification ratios were varied from 1 to 1.3. We verify the key conclusions from the proposed models. The experiments show that the theoretical optimization approach is very sensitive to system parameters such as the X-ray source spot size and detector resolution. Moreover, the energy dependence of the refractive index needs to be taken into account when modelling the polychromatic illumination of an x-ray tube. Finally, the sensitivity of TIE based phase retrieval algorithms on the image noise and contrast are studied.

CPP 28.4 Mon 16:00 TOE 317

Multiscale Mapping and Quantification of Elastic Stress and Domain Size in Bulk Ferroelastic Systems by Dark-Field X-Ray Microscopy — •Jan Schultheiss[1,2], Lukas Porz[1], Lalitha Kodumudi Venkataraman[1], Marion Höfling[1], Semen Gorfman[3], Jürgen Rödel[1], and Hugh Simons[4] — [1]Department of Materials and Earth Sciences, TU Darmstadt, Germany — [2]Department of Materials Science and Engineering, NTNU Trondheim, Norway — [3]Department of Materials Science and Engineering, Tel Aviv University, Israel — [4]Department of Physics, DTU, Denmark

Twinned domains in ferroelastic systems are intimately coupled to local strain fields. Problematically, in complex oxides this coupling often spans over several orders of magnitude of length scale. State-of-the art characterization techniques, however, either lack spatial resolution or their sensitivity is limited to the surface.

Here we use Dark-field X-Ray Microscopy to map and quantify spatial variations of elastic stress and domain size from nm to several μm in a grain of a polycrystalline ferroelectric/ferroelastic (Ba,Ca)(Zr,Ti)O_3 model system as a function of the applied electric field. We find, that the electric field narrows the distribution of elastic stresses by 60%, while the domain size increases by 35%. The suggested methodology can be applied to multiscale correlations in emerging fields in complex oxides and twinned systems.

CPP 28.5 Mon 16:20 TOE 317

Soft X-ray Laminography adds a third dimension to STXM — Katharina Witte[1], •Andreas Späth[2], Simone Finizio[1], Claire Donnelly[1,3], Michal Odstrcil[1], Manuel Guizar-Sicairos[1], Mirko Holler[1], Benjamin Watts[1], Rainer H. Fink[2], and Jörg Raabe[1] — [1]Paul Scherrer Institut, Villigen, Switzerland — [2]FAU Erlangen-Nürnberg, Germany — [3]Department of Physics, University of Cambridge, United Kingdom

Scanning Transmission X-ray microscopy is a powerful tool for spectromicroscopic analysis of nanostructured thin-film specimens. While developments focused on organic soft matter for many years, STXM has meanwhile also contributed to imaging of magnetic nanostructures based on (XMCD) contrast. However, 3D imaging is so far limited to a narrow selection of suitable specimens and constraint experimental conditions. This is especially true for the implementation of tomography, since the full sample rotation perpendicular to the optical axis is usually not possible for geometric reasons. Laminography overcomes this limitation by inclining the sample rotation axis by the laminography angle $\theta < 90°$ so that it is no longer perpendicular to the incident X-ray beam. The major advantage is that the sample (and its support) can be laterally extended without further modification and without risking collisions during rotation. A new setup combines laminography and STXM using soft X-rays. We will present first 3D reconstructions of nanostructured objects from material science, biology and functional magnetic materials. Funding: BMBF grant 05K19WE2 and EU Marie Skłodowska-Curie grant No. 701647.

20 min. break

CPP 28.6 Mon 17:00 TOE 317

Detection system for transmission imaging in helium ion microscope — •Eduardo Serralta[1], Nico Klingner[1], Olivier De Castro[2], Serge Duarte Pinto[3], Cecilia Bebeacua[4], Stefan Findeisen[1], Olivier Bouton[2], Tom Wirtz[2], and Gregor Hlawacek[1] — [1]Helmholz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg — [3]Photonis Netherlands B.V, Ro-den, Netherlands — [4]Eidgenössische Technische Hochschule, Zürich, Switzerland

Transmission imaging in the helium ion microscope allows to measure mass-thickness contrast and reveal crystallographic information. We recently customized a microchannel plate followed by a delay line readout structure especially for this application. This system can correlate the scanning transmission ion image to the angular distribution of the transmitted ions. An in-vacuum linear support is used to place the detector at different distances from the sample, adjusting the maximum collection angle. Post-processing allows the reconstruction of images for selected scattering angles. The first results show images with nanometer resolution, material contrast, and identification of subsurface features in biological tissues. This work has been supported by the H2020 Project npSCOPE under grant number 720964.

CPP 28.7 Mon 17:20 TOE 317

Positron Annihilation Studies using a Superconducting Electron Linac — •Maik Butterling[1], Andreas Wagner[1], Maciej Oskar Liedke[1], Eric Hirschmann[1], Ahmed G. Attalah[1], Reinhard Krause-Rehberg[2], and Kay Potzger[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Martin-Luther-Universität Halle, Institut für Physik, 06099 Halle, Germany

The Helmholtz-Center at Dresden-Rossendorf operates several user beamlines for materials research using different techniques for positron annihilation spectroscopy. Two of them are being operated at a superconducting electron linear accelerator producing positrons via pair production from electron-bremsstrahlung. While one of the sources uses bremsstrahlung to directly generate positrons inside the sample of interest, in the second source (MePS), monoenergetic positrons with energies up to to 25 keV are used for thin-film studies of porosity and defect distributions. The MePS beam line is currently complemented by a new in-situ end station (AIDA-2), where defect studies can be performed in a wide temperature range during thin film growth and ion irradiation. Developments as well as examples of recent experimental results at all facilities will be presented. The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). The AIDA facility was funded by the Impulse- und Networking fund of the Helmholtz-Association (FKZ VH-VI-442 Memriox) and through the Helmholtz Energy Materials Characterization Platform.

CPP 29: Plasmonics and Nanooptics III: Ultrafast and Nonlinear Phenomena (joint session O/CPP)

Time: Monday 15:00–18:00 Location: WIL A317

Invited Talk CPP 29.1 Mon 15:00 WIL A317

Probing Nanophotonic Modes and Optical Phase Shaping of Electron Beams in Ultrafast Transmission Electron Microscopy — •Armin Feist — IV. Physical Institute, University of Goettingen, 37077 Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) combines the versatile imaging, diffraction and spectroscopy capabilities of state-of-the-art TEM with femtosecond temporal resolution achieved by a laser-pump/electron-probe scheme [1,2]. The novel applications of UTEM include the study of coherent inelastic electron-light scattering (IELS) at laser-excited nanostructures [3,4].

Here, I will briefly introduce the UTEM methodology and show recent results of the Göttingen UTEM instrument, which features high coherence electron pulses generated from nanoscale field emitter tips [2]. Besides nanometer mapping of chiral optical near-fields and local plasmonic modes, IELS enables the transverse and longitudinal phase control of the free-electron wavefunction [4,5], with applications for coherent electron beam splitters and generating attosecond electron pulse trains. Furthermore, the phase-matched interaction of electrons with optical whispering gallery modes (WGMs) enables a strongly enhanced coupling and traces the ring-down of a dielectric microresonator [6].

[1] A. H. Zewail, Science **328**, 187 (2010). [2] A. Feist *et al.*, Ultramicroscopy **176**, 63 (2017). [3] Barwick *et al.*, Nature **462**, 902 (2009). [4] A. Feist *et al.*, Nature **521**, 200 (2015). [5] K. E. Priebe *et al.*, Nat. Photonics **11**, 793 (2017). [6]. O. Kfir *et al.*, arXiv:1910.09540 (2019).

CPP 29.2 Mon 15:30 WIL A317

Time-resolved and spatially-resolved mode dynamics within a plasmonic nanoslit cavity investigated by coherent two-dimensional nanoscopy — Sebastian Pres[1], Daniel Friedrich[2], Daniel Fersch[1], Enno Krauss[2], Bernhard Huber[1], Victor Lisinetskii[1], •Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Recently, we revealed the impact of off-resonant eigenmodes on the local field dynamics of plasmonic hot-spots within a single nanoslit cavity with a spatial and temporal resolution of 10 nm and 20 fs, respectively, by combining photoemission electron microscopy and interferometric two-pulse sequences [1]. Here, we extend the excitation scheme of the nanoslit cavity to a three-pulse sequence using an LCD-based pulse shaper to perform two-dimensional spectroscopy with unprecedented spatial resolution [2]. Due to the nonlinearity of the photoelectron emission process higher-order signals are easily disclosed. These results are supported by quantum dynamical simulations in which the plasmonic nanoslit is modelled as a quantized harmonic oscillator instead of classical fields. Detecting such signal contributions will be helpful in future experiments to reveal the impact of many-body interactions in molecular or solid-state systems with nanometer resolution.

[1] M. Hensen et al., *Nano Lett.* 19, 4651 (2019)
[2] B. Huber et al., *Rev. Sci. Intrum.* 90, 113103 (2019)

CPP 29.3 Mon 15:45 WIL A317

Coherent two-dimensional nanoscopy on coupled plasmonic nanostructures — •Lysanne Monika Dietrich[1], Daniel Friedrich[2], Jessica Meier[2], Enno Krauss[2], Daniel Fersch[1], Raphael Wichary[1], Victor Lisinetskii[1], Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]NanoOptics & Biophotonics Group, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Two-dimensional (2D) nanoscopy combines the femtosecond time resolution of coherent 2D spectroscopy with nanoscale selectivity: Instead of measuring optical diffraction-limited light fields, we detect photoemitted electrons with a spatial resolution < 5 nm utilizing aberration-corrected photoemission electron microscopy (AC-PEEM) [1]. Since 2D spectroscopy provides direct insights into couplings between single system constituents, we investigate coupled plasmonic nanostructures (i.e. "dolmen" structures) as a model system [2,3] to demonstrate the additional spatial resolution. We complement our experimental findings by simulated 2D spectra using the local response function as retrieved from finite-difference time-domain (FDTD) method.

[1] B. Huber et al., *Rev. Sci. Instrum.*, **90**, 113103 (2019).
[2] H. Yu et al., *ACS Nano*, **10**, 10373-10391 (2016).
[3] J.-S. Huang et al., *Nano Lett.*, **10**, 2105-2110 (2010).

CPP 29.4 Mon 16:00 WIL A317

THz streaking spectroscopy for mapping the transformation from far-fields to nanostructure near-fields — •Felix Sommer and Georg Herink — Physikalisches Institut EP VIII, Universität Bayreuth

Field-driven experiments at the nanoscale require the precise characterization of local ultrafast transients. We apply THz near-field streaking spectroscopy [1,2] to metallic nanotips to map the enhanced near-field at the apex.

The local waveforms are critical to various emerging ultrafast instruments for nanoscopic imaging and spectroscopy. The transformation of focused far-fields to nanoscale near-fields sensitively depends on either the individual nano- and macroscopic geometry and structure, involving effects of antenna resonances, plasmon excitations and excitation geometries [3,4]. In order to study the THz-response in the time-domain, we developed an optimized near-field streaking setup based on a strong-field THz source and present experimental data on the THz-waveform transformation.

[1] Wimmer et al., Nat. Phys. 10, 432-436 (2014).
[2] Wimmer et al., APL 111(13), 131102 (2017).
[3] Talebi et al., ACS nano 9(7), 7641-7648 (2015).
[4] Schröder et al., PRB 92(8), 085411 (2015).

CPP 29.5 Mon 16:15 WIL A317

Tunable strong coupling — •Daniel Friedrich, Benedikt Schurr, Heiko Gross, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Using a scanning plasmonic nano resonator we have shown recently how to achieve tunable strong coupling to colloidal CdSe quantum dots at ambient conditions. The developed system provides an elegant method to tune the coupling strength and can also be used as high resolution optical microscope. [1]

In the presentation we highlight the possibility to establish strong coupling with different kinds of emitters that can be placed on any (transparent) substrate. The emitters include a variety of colloidal semiconductor nanoparticles and platelets as well as TMDCs.

[1] H. Groß et al., Science Adv. 4, 3, eaar4906 (2018)

CPP 29.6 Mon 16:30 WIL A317

Strong coupling in planar metamaterials — •Manuel Gonçalves[1], Hayk Minassian[2], and Armen Melikyan[3] — [1]Ulm University, Ulm, Germany — [2]A. Alikhanyan National Laboratory (YerPHI), Yerevan, Armenia — [3]Russian-Armenian University, Yerevan, Armenia

Strong coupling is a regime of matter-radiation interaction in a resonant cavity where both the decay rate of the excited state of the matter and the loss rate of the radiation in the cavity are smaller than the coupling strength of matter with radiation. This is a special case of modified spontaneous emission. Fast decay of excited matter state and large cavity loss lead to the more probable Purcell enhancement of spontaneous emission. However, there is strong coupling beyond the quantum optical realm. In classical systems an interaction regime of coupled resonators with similar properties to the quantum case can be produced.

We show how coupled planar optical resonators can be fabricated and present their optical properties. For some configurations the classical analogue of the quantum strong coupling is achieved. Furthermore, higher degrees of interaction between resonators can be achieved and an analogy with the ultrastrong coupling regime of quantum optical systems can be established.

CPP 29.7 Mon 16:45 WIL A317

Quantum Coherent Interference Paths in Interaction of Single-Electron Wavepackets with Light — •Nahid Talebi[1] and Christoph Lienau[2] — [1]Institute für Experimentelle und Angewandte Physik, Christian Albrechts Universität zu Kiel, D-24118 Kiel, Deutschland — [2]Institut für Physik and Center of Interface Science, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg, Germany

Ultrafast coherent processes imposed by laser beams into a traveling electron wavepacket in an electron microscope modulate the phase and amplitude of the electron wavefunction (Near-Field Mediated Electron-Light Interactions, Springer Nature, Switzerland (2019)). As a result, electrons can be either accelerated (Nat. Phys. 14 121-5 (2018)), or diffracted (Proc. Camb. Phil. Soc. 29 297-300 (1923)). Particularly the latter, the so-called Kapitza-Dirac effect (KDE), is within the scope of current work. Here, with the aid of first-principle numerical calculations, we describe the physics of KDE. Moreover, we generalize the KDE into a combination of standing-wave and travelling-wave platforms (New J. Phys. 21 093016 (2019)). We show that by virtue of such generalizations, novel quantum-coherent interference paths are formed. Two competing parts of the interaction Hamiltonian, i.e., photon-absorption and emission processes as well as ponderomotive potential, contributes to these interference effects. These interference paths can be controlled by means of either laser or electron wavepacket parameters. Our investigations open up new directions in the domain of matter-wave interferometry.

CPP 29.8 Mon 17:00 WIL A317

Strong-Field Angle-Resolved Plasmoemission Spectroscopy — •Pascal Dreher, David Janoschka, Jan-Henrik Herrig, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty of Physics, University of Duisburg-Essen, Germany

Photoemission in strong fields has received a lot of attention in the past and the coherent interaction of electrons with the field after the emission process has been revealed, i.e. using plasmonic near-field enhancement at nanotips. The behavior of electrons within the solid, however, can as well become dominated by the influence of strong fields, and the respective electron dynamics is expected to be fundamentally different from the electronic equilibrium. Clarifying the dominant interaction processes in this case ultimately requires electronic state resolution as well as precise control over the exact field.

We combine nanofocusing of femtosecond surface plasmon polariton (SPP) pulses on flat surfaces with photoemission electron microscopy to achieve angle-resolved plasmoemission spectroscopy (ARPLES) in the strong-field regime. The emission of electrons from the Au(111) Shockely surface state into SPP-dressed electron final states by the absorption of up to seven SPP quanta is observed. The ponderomotive energy that the emitted electrons acquire within the strong plasmonic nanofocus is determined and provides us with a direct measure for the transient SPP field strength in the focus point.

CPP 29.9 Mon 17:15 WIL A317

Nonlinear plasmon-exciton coupling enhances sum-frequency generation from a Au/ZnO nanohybrid — •Jin-Hui Zhong[1], Jan Vogelsang[2], Jue-Min Yi[1], Dong Wang[3], Lukas Wittenbecher[2], Sara Mikaelsson[2], Anke Korte[1], Abbas Chimeh[1], Cord L. Arnold[2], Peter Schaaf[3], Erich Runge[3], Anne L'Huillier[2], Anders Mikkelsen[2], and Christoph Lienau[1] — [1]Carl von Ossietzky University, 26111 Oldenburg, Germany — [2]Lund University, SE-221 00 Lund, Sweden — [3]Technische Universität Ilmenau, 98693 Ilmenau, Germany

Nanohybrids of plasmon/quantum emitter system can dramatically enhance coherent harmonic generation, often resulting from the coupling of fundamental plasmonic fields to higher-energy, electronic or excitonic transitions of quantum emitters. The ultrafast optical dynamics of such hybrids have been rarely explored. Here, we study those dynamics by interferometrically probing nonlinear optical emission from individual porous gold nanosponges infiltrated with zinc oxide (ZnO) emitters. Few-femtosecond time-resolved photoelectron emission microscopy reveals multiple long-lived localized plasmonic hot spot modes at the surface of single nanosponges, resonant in a broad spectral range. The hot spot near-field couples to the ZnO excitons, enhancing sum-frequency generation, and boosting resonant excitonic emission. The quantum pathways of the coupling are further uncovered from a two-dimensional spectrum correlating fundamental plasmonic excitations to nonlinearly driven excitonic emissions.

CPP 29.10 Mon 17:30 WIL A317

fluctuation-modulated third harmonic deep ultraviolet emission from randomly disordered Si nanograss — •Juemin Yi[1], Dong wang[2], Jinhui Zhong[1], Peter Schaaf[1], Erich Runge[3], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Institut für Physik and Center of Interface Science, 26129 Oldenburg — [2]TU Ilmenau, Institut für Werkstofftechnik und IMN MacroNano, 98693 Ilmenau — [3]TU Ilmenau, Institut für Physik und IMN MacroNano, 98693 Ilmenau

It is well known that Si nanograss or black Si greatly enhances light absorption in a broad spectral range and thus is of relevance for solar cell application. Very little is known about their nonlinear optical properties. For that, we have utilized a broadband and few-cycle ultrafast laser to generate coherent third harmonic (TH) emission from randomly disordered Si nanograss. The TH signal is two-order-of-magnitude stronger than that from bulk Si surfaces. For individual hot spots, the TH enhancement even reaches a factor of the order of 1000. A statistical analysis of the TH intensity fluctuations demonstrates that multiple light scattering within the randomly disorder medium is the cause of those fluctuations. A phase-locked and collinear pulse pair excitation proves the coherent nature of the deep ultraviolet emission. The interferometric frequency-resolved autocorrelation (IFRAC) microscopy shows that the deep ultraviolet pulse is around 10fs. Our findings identify random Si nanograss as the most promising candidates for generating ultrashort deep ultraviolet pulses.

CPP 29.11 Mon 17:45 WIL A317

Electron-Driven Photon-Sources for Spectral Interferometry using Electron Microscopes — Nika van Nielen[3], Mario Hentschel[2], Harald Giessen[2], Albert Polman[3], and •Nahid

Talebi[1] — [1]Institute für Experimentelle und Angewandte Physik, Christian Albrechts Universität zu Kiel, D-24118 Kiel, Deutschland — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [3]Center for Nanophotonics, AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

Electron beams can inelastically interact with matters, and as a result, photons are emitted to the far-field. Mechanisms of electron-induced radiations are numerous, covering Cherenkov radiation, transition radiation, and plasmon-induced radiation, to name a few (Rev. Mod. Phys. 82, 209 (2010)). Here, we report on metamaterial- and photon-sieve-based structures for tailoring the electron-induced emission (Nature communications 10 (1), 599 (2019)). By engineering the dispersion of the interface optical modes, radiation relaxation channels for the plasmon polaritons supported by our engineered thin film are formed, leading to an enhanced electron-induced radiation. We also particularly emphasize on the generation of chiral light using plasmonic chains of nanohole arrays. Moreover, we outline our efforts towards realization of combined electron-photon spectroscopy techniques for investigating nanooptical systems in electron microscopes, using electron-driven photon sources (Scientific Reports 6, 33874 (2016)).

CPP 30: 2D Materials II: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)

Time: Monday 15:00–18:15 Location: WIL C107

CPP 30.1 Mon 15:00 WIL C107

Unfolding and analysis of a defect band structure using doped $MoSe_2$ and MoS_2 — •Stefan Rost, Christoph Friedrich, Irene Aguilera, Beata Kardynal, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We investigate substitutional doping of chromium and phosphorus in $MoSe_2$ and MoS_2 monolayers, as they are promising candidates for single photon emission. The systems are characterized by density-functional-theory (DFT) studies of structural relaxation, projected density-of-states, and band structure, all calculated with the Jülich FLAPW code family (www.flapw.de). Different sizes of super-cells are necessary to calculate the doped system depending on the strength of interaction between the dopants. The super-cells contain between 3×3 and 5×5 monolayer unit cells. Compared to the pristine material, the band structure of the defect system is backfolded in **K**-space, which complicates a straightforward interpretation, in particular for low doping concentrations. We have implemented a method for unfolding the bands obtained from the super-cell calculation. The resulting band structure resembles the one of the pristine material, but it contains additional information about the defect system, which, in this sense, can be regarded as a perturbed host system. – The authors gratefully acknowledge the computing time granted through JARA-HPC on the supercomputer JURECA at Forschungszentrum Jülich, (project cjpgi10) as well as the support through „Integration of Molecular Components in Functional Macroscopic System“ initiative of VW Stiftung.

CPP 30.2 Mon 15:15 WIL C107

Geometry, electronic structure, and bonding of single-domain h-BN on Pt(110) — •Marco Thaler[1], Dominik Steiner[1], Alexander Menzel[1], Florian Mittendorfer[2], and Erminald Bertel[1] — [1]Physikalische Chemie, Universität Innsbruck, Österreich — [2]Institut für Angewandte Physik, TU Wien, Österreich

Recently we reported single-domain growth of hexagonal Boron Nitride (h-BN) on Pt(110)[1]. This is a peculiar system, where the substrate adapts to the h-BN adlayer by forming a (1xn) missing-row reconstruction (n = 5 or 6). The bandstructure was investigated by angle-resolved UV photoemission (ARPES) and is very similar to that of a free-standing h-BN monolayer except for the appearance of umklapp bands reflecting the periodicity of the Moiré pattern and testifying for the perfect film quality. Binding energies agree with other h-BN/transition metal systems if referenced to the vacuum level. Additionally, we studied the local density of states (LDOS) for differently positioned atoms in the h-BN film by DFT calculations. For N atoms on top of Pt atoms a small LDOS maximum appears at the Fermi level, indicating a weak covalent contribution to the h-BN-Pt bonding. This, the mean h-BN-Pt(110) distance, and the workfunction change place the present system at the borderline between purely dispersive and chemisorptive bonding[2]

[1] Steiner, D., Mittendorfer, F., Bertel, E. ACS Nano 13, 7083-7090(2019)

[2] Bokdam, M., Brocks, G., Kelly, P. J. Phys. Rev. B 90, 085415(2014)

CPP 30.3 Mon 15:30 WIL C107

Photoinduced band renormalization in the nodal-line semimetal ZrSiSe — •Gianmarco Gatti[1], Alberto Crepaldi[1], Nicolas Tancogne-Dejean[2], Michele Puppin[3], Angel Rubio[2], Majed Chergui[3], and Marco Grioni[1] — [1]Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Laboratory of Ultrafast Spectroscopy, ISIC, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

ZrSiSe is a layered material that is classified as a nodal-line semimetal. Its low-energy bandstructure is composed by linearly dispersing surface and bulk bands whose crossing points creates a one-dimensional contour in the momentum space with vanishing density of states close to the Fermi level. We investigate its equilibrium and out-of-equilibrium electronic structure by the means of angle- and time-resolved photoemission spectroscopy and compare the results with ab initio calculations. Our analysis indicates that the dispersion of the Dirac quasiparticle can be correctly reproduced by density functional theory with the inclusion local and non-local electronic correlations. Moreover, we observe a transient renormalization of the bands velocity above the Fermi level under the photoexcitation produced by ultrashort infrared pulses. We associate the microscopic origin of this effect to the increased screening of the non-local Coulomb interaction due to the presence of high-energy and non-thermalized carriers.

CPP 30.4 Mon 15:45 WIL C107

Micro-focus ARPES on a twisted graphene/hBN field-effect device — •Alfred Jones[1], Ryan Muzzio[2], Davide Curcio[1], Deepnarayan Biswas[1], Jill A. Miwa[1], Philip Hofmann[1], Simranjeet Singh[2], Chris Jozwiak[3], Eli Rotenberg[3], Aaron Bostwick[3], Roland J. Koch[3], Søren Ulstrup[1], and Jyoti Katoch[2] — [1]Aarhus University, Aarhus, Denmark — [2]Carnegie Mellon University, Pittsburgh, Pennsylvania, USA — [3]Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, Berkeley, California, USA

Graphene/ hBN heterostructures are an ideal testing ground for functional 2D devices owing to the atomically smooth surface and weak screening offered by hBN. On top of the record mobilities this structure offers, controlling the twist angle between layers creates a superlattice effect from which exotic electronic properties can occur.

Here, I present a study of the ARPES spectrum of graphene integrated in a device architecture with a hBN dielectric and graphite gate electrode. Micron-scale ARPES based on an X-ray capillary was used to collect the Dirac spectrum at different gate-voltages. A clear, reversible doping effect up to $5*10^{12}$ cm^{-2} is observed, providing access to the doping dependent quasiparticle dynamics in graphene on hBN.

Simultaneous measurements of this gate-dependent Dirac cone dispersion and the electrical resistance of the device enables extraction of electronic mobility and lifetimes. Our approach thereby demonstrates the tantalizing prospect of combining electron transport measurements with a spectroscopic probe of the electronic structure.

CPP 30.5 Mon 16:00 WIL C107

Final-State Effects in Photoemission from Black Phosphorus — •Charlotte E. Sanders[1], Irene Aguilera[2], Klara Volkaert[3], Deepnarayan Biswas[3], Marco Bianchi[3], and Philip Hofmann[3] — [1]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell OX11 0QX, UK — [2]Institute of Energy Research - Photovoltaic, Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Department of Physics and Astronomy, Aarhus University, 8000-C Aarhus, Denmark

Intrinsically doped bulk black phosphorus, although a van der Waals layered crystal, has nontrivial interlayer interactions and out-of-plane dispersing (k_z) electronic states, with a direct bandgap at the Z point of the three-dimensional (3D) Brillouin zone. The material's 3D character is related to key properties such as the thickness dependence of the bandgap in thin films and the tunability of the bandgap by strain and electric field. Interestingly, studies from angle-resolved photoemission spectroscopy (ARPES) of the k_z dispersion reveal intensity modulations near the Fermi level that are difficult to interpret in terms of the valence band dispersion predicted by theory. They have been attributed to surface-resonant states [1,2]. However, on the basis of density functional theory calculations and ARPES data acquired across a broad photon energy range, we suggest here an alternative interpretation based on final-state effects. The results call attention to the meaning of the free-electron-like final-state assumption and to the limits of its applicability. [1] *PRB* **90** (2014) 085101. [2] *PRB* **93** (2016) 075207.

Invited Talk CPP 30.6 Mon 16:15 WIL C107

Atomic scale neural circuitry capable of self-adaptation — •Brian Kiraly — Radboud University, Nijmegen, The Netherlands

Driven by the rise of artificial intelligence and its potential for reduced energy consumption, there have been expanded efforts directed toward investigating materials which can perform pattern recognition directly in hardware. This requires a step away from physical systems which show simple bistability, toward complex, stochastic systems, which are inherently tunable. At the moment, however, the state of the art in neuromorphic computing still struggles with fundamental issues, such as scaling or adaptability, often referred to as on-chip learning. In this talk, I will show a ground-breaking example, in which as few as 7 cobalt dopants on the surface of anisotropic semiconducting black phosphorus [1,2] can be utilized for pattern recognition. For this demonstration, we illustrate that controlled coupling between Co atoms [3] leads to a stochastic system which is well described using the concept of a Boltzmann machine. Both probing and reading the system with a scanning tunneling microscope, I will demonstrate how we realize an atomic scale synaptic memory and how the stochastic dynamics adapt and learn, depending on the input stimulus. The main aspects of this work have been carried out in the Scanning Probe Microscopy department at Radboud University. [1] Kiraly, Knol, Volckaert, Biswas, Rudenko, et. al., Phys. Rev. Lett. 123, 216403 (2019). [2] Kiraly, Hauptmann, Rudenko, Katsnelson, Khajetoorians, Nano Lett. 17, 3607 (2017). [3] Kiraly, Rudenko, Weerdenburg, Wegner, Katsnelson, Khajetoorians, Nature Commun. 9, 3904, (2018).

CPP 30.7 Mon 16:45 WIL C107

Diffusion of magnetic dopants in pristine and defected phosphorene — •Rohit Babar[1] and Mukul Kabir[1,2] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune, India — [2]Centre for Energy Science, Indian Institute of Science Education and Research, Pune, India

The incorporation of transition metal atoms is a robust way to imprint magnetism in non-magnetic 2D materials. In this regard, phosphorene has emerged as a versatile host for spintronic applications. Combining first-principles calculations with kinetic Monte Carlo simulations, we study the binding, magnetism, and diffusion of TM (TM = Cr, Fe, Co) atoms in pristine and defected phosphorene. The TM migration is highly anisotropic and favorable along the zigzag axis due to the puckered structure of phosphorene. While TM adsorption on pristine surface induces a local moment, the TM diffusion is uncontrolled at room temperature. We further show that vacancy defects exert an attractive potential beyond 1 nm and act as trapping centers for magnetic dopants. Our findings will assist in overcoming the practical limitations of surface decoration in phosphorene.

CPP 30.8 Mon 17:00 WIL C107

Ab-initio structural dynamics of laser-excited graphene — •Sergej Krylow[1], Felipe Valencia Hernandez[2], Bernd Bauerhenne[1], and Martin E. Garcia[1] — [1]University of Kassel, 34132 Kassel, Germany — [2]National University of Colombia, 111321 Bogota, Colombia

We calculate the response of graphene to an ultrafast laser pulse using ab initio density functional molecular dynamics simulations. Our results show a biexponential decay of the Bragg peak intenities of the (100) and (110) peaks. We are able to show that the fast decay is caused by the equilibration between the electrons and a few strongly coupled optical phonons (SCOPs). The slower decay can be attributed to the equilibration of the SCOPs to the other phonon modes. Furthermore, we analyze the decay pathways from the SCOPs to the other phonon modes.

CPP 30.9 Mon 17:15 WIL C107

Tailoring the opto-electronic response of graphene nanoflakes by size and shape optimization — •Raquel Esteban-Puyuelo[1], Rajat Sonkar[2], Bhalchandra Pujari[2], Oscar Grånäs[1], and Biplab Sanyal[1] — [1]Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box-516, SE 75120, Sweden — [2]Centre for Modeling and Simulation, Savitribai Phule Pune University, Ganeshkhind, Pune 411007, India

The long spin-diffusion length, spin-lifetime and excellent optical absorption coefficient of graphene provide a promising platform for building opto-electronic devices as well as spin-based logic in the nanometer regime. We have used time-dependent density functional theory to study how the magnetic structure and optical properties of graphene nanoflakes depend on their size and shape. We optimize the magnetic ground state and the exchange coupling between the edges of the flakes to tailor the external fields needed to switch the magnetic ordering. Finally it's shown that the magnetic state alters the optical response of the flake leading to the possibility of opto-spintronic applications.

CPP 30.10 Mon 17:30 WIL C107

Electronic and optical properties of two-dimensional magnets (CrI_3) and their effects on adjacent material (WSe_2/CrI_3) — •Marie-Christin Heissenbüttel, Michael Rohlfing, and Peter Krüger — Institut für Festkörpertheorie WWU, Münster, Deutschland

For the development of novel opto-electronic devices the access and manipulation of the spin degree of freedom is of fundamental importance. The recently discovered 2D magnets provide a great opportunity to study the delicate interplay of spin, orbital, charge and lattice degree of freedom and the manipulation of other non-magnetic 2D materials, as for example TMDCs, by proximity effects. In this talk I will demonstrate our results from ab-initio calculations for the magnetic monolayer of chromium triiodide (CrI_3). The electronic and optical properties are analyzed as well as the effects of magnetism on the optics of WSe_2 within the heterobilayer tungsten diselenide (WSe_2) on CrI_3 are shown. The investigation of CrI_3 by many body perturbation theory (MBPT) within the LDA+GdW approximation reveals a ferromagnetic and insulating behavior and the optical absorption obtained from the solution of the BSE shows large exciton binding energies up to 1.04 eV. Furthermore due to the impact of ferromagnetic proximity effects on the TMDC WSe_2 in the heterosystem WSe_2 / CrI_3 a lifting of the energy degeneracy in the K-valleys of WSe_2 is found. Both the electronic band gap at ±K as well as the corresponding excitons in WSe_2 are affected.

CPP 30.11 Mon 17:45 WIL C107

Engineering intrinsic π-magnetism in nanographenes — •Shantanu Mishra[1], Doreen Beyer[2], Kristjan Eimre[1], Shawulienu Kezilebieke[3], Reinhard Berger[2], Oliver Gröning[1], Peter Liljeroth[3], Carlo Pignedoli[1], Xinliang Feng[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]Technical University of Dresden, Dresden, Germany — [3]Aalto University, Espoo, Finland

Among the multitude of properties realized in organic compounds due to the chemical versatility of carbon, magnetism remains one of the most challenging. The electronic structure of polycyclic aromatic hydrocarbons (nanographenes) depends critically on the topology of the underlying π-electron network, which provides a tunable platform to realize all-carbon magnetism at the nanoscale.

Combining rational design principles with on-surface synthesis, we engineer and probe emergent magnetism in elusive magnetic nanographenes, namely, Clar's goblet [1] and extended triangulenes [2], and their covalently-bonded assemblies. Our experimental approach follows low-temperature scanning tunneling microscopy and inelastic electron tunneling spectroscopy, with further insights provided by mean-field and many-body perturbation theory calculations.

[1] S. Mishra et al., Nature Nanotech. (in press)

[2] S. Mishra et al., J. Am. Chem. Soc. 141, 10621 (2019)

CPP 30.12 Mon 18:00 WIL C107

Theoretical study on the magnetic structure of few-layer TMPS3 — •Tae Yun Kim[1,2,3] and Cheol-Hwan Park[1,2,3] —

[1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Gwanak-Gu Hoam-Ro 519 101-1205 — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Transition metal phosphorus sulfides (TMPS3) are a family of the layered magnetic materials. Due to the layered structure and the rich spectrum of the magnetic structure [1], TMPS3 has been thought to be a good playground for testing two-dimensional magnetism in real world experiments [2]. It was found that the antiferromagnetic order in FePS3 remains down to the monolayer limit [3, 4], which was soon followed by the discovery of two-dimensional ferromagnetism in CrI3 [5] and Cr2Ge2Te6 [6]. More recently, the existence of the magnetic ordering in few-layer TMPS3 has been investigated in experiments [7, 8]. In this contribution, we present an in-depth investigation of the magnetic structure of few-layer TMPS3 based on the results of our first-principles calculations.

[1] R. Brec, Solid State Ionics 22, 3 (1986).
[2] K. S. Burch et al., Nature 563, 47-52 (2018).
[3] X. Wang et al., 2D Materials 3, 031009 (2016).
[4] J.-U. Lee et al., Nano Letters 16, 7433 (2016).
[5] B. Huang et al., Nature 546, 270-273 (2017).
[6] C. Gong et al., Nature 546, 265-269 (2017).
[7] K. Kim et al., Nature Communications 10, 345 (2019).
[8] K. Kim et al., 2D Materials 6, 041001 (2019).

CPP 31: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Monday 15:00–17:30 Location: ZEU 250

CPP 31.1 Mon 15:00 ZEU 250

Reptation of DNA nanotube tracers in semiflexible polymer networks — •Tina Händler[1,2], Cary Tutmarc[1,2], Martin Glaser[1,2], Josef Käs[1], David Smith[2], and Jörg Schnauss[1,2] — [1]University of Leipzig, Soft Matter Physics Division — [2]Fraunhofer Institute for Cell Therapy and Immunology, DNA Nanodevices Unit, Leipzig

Over many decades, actin has been the gold standard for exploring the theories about mechanics and dynamics of semiflexible polymers. Unfortunately, naturally occurring biopolymers are limited in their properties such as stiffness and interaction strengths. Programmable polymers enable us to study parameters otherwise unavailable in natural systems and therefore expand theoretical approaches. Nanotubes formed from synthetic DNA strands are ideal model polymers: they are semiflexible and can be hybridized to have characteristics such as a persistence length which is similar to actin filaments or can be varied in a controllable way. Additionally, DNA nanotubes are extremely stable, making them both favorable for polymer physics experiments and material science applications. We visualize the dynamics of nanotube tracer filaments in entangled and crosslinked semiflexible biopolymer networks. The results can be used to measure the networks' tube width and mesh size. Scaling laws concerning the parameter persistence length that have been beyond reach before are accessible now. Furthermore, reptation analysis with our programmable filaments enables the test of latest predictions about the dynamics of single filaments inside entangled solutions vs. crosslinked networks.

CPP 31.2 Mon 15:15 ZEU 250

Dynamics during thermal gelation of egg-white studied using X-ray photon correlation spectroscopy — •Nafisa Begam[1], Anita Girelli[1], Anastasia Ragulskaya[1], Hendrik Rahmann[2], Fabian Westermeier[3], Christian Gutt[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]DESY, Germany

Gelation of proteins is a fundamental topic in food industry as well as in condensed matter physics [1]. We report a systematic time dependent study of the dynamics of hen egg-white during its gelation at 80°C using X-ray photon correlation spectroscopy in the ultra-small angle X-ray scattering mode. Two distinct regimes of dynamics are identified. The initial growth of the aggregates, as expected for heat-induced coagulation of egg-proteins, results in an early stage non-equilibrium dynamics. Interestingly, at the later stage (after $\sim$ 30 min of heating), the system reaches an equilibrium dynamical state with an average characteristic time scale of few tens of seconds. The intermediate scattering function changes from an exponential to a compressed exponential decay, indicating gel formation. The aggregates eventually show correlated temporally heterogenous dynamics. Such dynamical fluctuations are further quantified in terms of a fourth order intensity correlation function. The monotonic increase in heterogeneity as a function of wave vector transfer observed here is similar to the behavior of strongly attractive colloidal gels [2].

[1] Croguennec et al., *J. Food. Sci.*, **67**, 2, (2002)
[2] Fluerasu et al., *Phys. Rev. E*, **76**, 010401(R), (2007)

CPP 31.3 Mon 15:30 ZEU 250

Reversible Underwater Adhesion in Beetles — •Pranav Sudersan, Thomas Endlein, Michael Kappl, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

Many animals are able to climb smooth surfaces using adhesive pads on their feet. Unlike artificial glues, animals can adhere reversibly i.e. attach and detach easily to a wide variety of surfaces. Insects such as beetles have hairy pads on their feet and also secrete an adhesive fluid resulting in capillary forces for strong attachment. In contrast to adhesion in air, reversible adhesion underwater is particularly challenging. Insects drawing their adhesive force from the capillary action of the air-fluid interface would not stick underwater as such an interface is usually abolished. Some terrestrial beetles are however able to easily adhere and walk underwater by using an entrapped air bubble around their hairy pads to de-wet the surface upon entering water. But it is unclear as to what extent the air bubble influences adhesion. In our study, we measure adhesion and friction forces in live ladybug beetles (Coccinella septempunctata) under controlled conditions. The effect of surface hydrophobicity, pad attachment/detachment speeds and de-wetted area on adhesion and friction performance is examined and compared for dry and wet surfaces. Our study aims to draw inspiration from an animal model in order to fabricate artificial adhesives which would work in a similar way.

CPP 31.4 Mon 15:45 ZEU 250

Visco-elastic properties of albumin films upon periodical mechanical loading — •Lukas Böttcher[1], Sven Kraft[1], Regina Lange[1], Ingo Barke[1], Jessica Hembus[2], Carmen Zietz[2], Rainer Bader[2], and Sylvia Speller[1] — [1]Institute of Physics, University of Rostock, 18059 Rostock — [2]Biomechanics and Implant Technology Research Laboratory, University Medical Center Rostock, 18057 Rostock

The synovial fluid in human natural and endoprosthetic joints usually implies outstanding lubrication and low wear. The question is how this fluid or its components, such as albumin and hyaluronic acid, participate in this performance. The high periodic forces acting on the protein in hips and knees during walking lead to changes in protein structure and visco-elastic-plastic behavior. Therefore, we mimic the situation in the joint using a tapping nanoprobe-sample junction in a force microscope. Films from albumin and synthetic synovial fluid are prepared and maintained wet in a humidifying chamber during treatment and data acquisition. Upon applying 200000 cycles at high force of several hundred nN the albumin film has swollen by about 5 nm in height. With increasing mechanical load the film gets softer and ropier. This may be explained in terms of loosening the protein secondary structure and incorporating additional fluid in the pores.

CPP 31.5 Mon 16:00 ZEU 250

Towards transparent living tissues — •Kaushikaram Subramanian[1,2,3], Heike Petzold[1], Lena Hersemann[1,2], and Moritz Kreysing[1,2,3] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence, Physics of Life, Technische Universität Dresden, Germany

Most biological tissues are optically opaque, largely precluding access by light microscopy. In stark contrast, some living tissues and organisms have evolved to be highly transparent. Examples include many deep-sea fish and your retina that enables you to read this text. We asked the question if directed evolution can be used to change the optical phenotype of cells. For this we used a mutation, selection, and replication scheme, in which we favoured the growth of genetic mutant cells that showed reduced light scattering. After only few rounds of selection we gained mammalian cells with upto 2-fold reduced side scattering. Further analysis revealed that the induced partial transparency goes along with last changes of the transcriptome and frequently a reduction of nuclear substructure, a phenotype similar to the photoreceptor cells in the mouse retina. Our results encourages the possibility that deep microscopy on genetically cleared living tissues might one day become reality.

15 min. coffee break

Invited Talk CPP 31.6 Mon 16:30 ZEU 250

Optoregulated force application to individual cellular receptors using molecular motors — •Aránzazu del Campo — INM-Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany — Chemistry Department, Saarland University

Inspired by cellular mechanisms for force application, a unique molecular machine that can apply forces at cell-matrix and cell-cell junctions using light as energy source will be presented. The key actuator is a light-driven rotatory molecular motor linked to polymer chains, which is intercalated between a membrane receptor and an engineered biointerface. The light-driven actuation of the molecular motor is converted in mechanical twisting of the polymer chains, which will in turn effectively *pull* on engaged cell membrane receptors (integrins, cadherins*) within the illuminated area. Applied forces have the adequate magnitude and occur at time scales within the relevant ranges for mechanotransduction at cell-friendly exposure conditions. The presnetation will provide experimental demonstrations of force-dependent focal adhesion maturation and T cell activation in vitro using the rotary motor.

CPP 31.7 Mon 17:00 ZEU 250

Experimental setups to mimic the Peritoneal Dialysis in humans — •Bernd Eberle[1,2], Christian Wagner[1], and Thomas John[1] — [1]Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — [2]Fresenius Medical Care Deutschland GmbH, St. Wendel, Germany

Peritoneal dialysis (PD) uses the peritoneum as a semipermeable dialysis membrane to clear the patient's blood. Therefore, dialysate solution gets filled into the abdominal cavity through an implanted catheter. Due to the osmotic concentration gradient between the blood capillarys and the dialysate, excess water and uremic toxins are removed from the blood by diffusing through the pores in the peritoneum into the dialysate. In contrast to Hemodialysis, the artificial filter membrane is well characterized, properties of the peritoneum are divers and vary for each patient. Consequently, a better understanding of membrane parameters is a crucial step for optimization treatment conditions. At present, commercially available software tools are used to simulate the membrane characteristics of the peritoneum but are lacking the precision to predict the ultrafiltration behavior in vivo. Hence, we present experiments which mimic the diffusion, convection and ultrafiltration through the peritoneum with artificial membranes allowing a patient-tailored PD-therapy with higher efficiency. Various osmotic agents and membrane compositions were investigated, and characteristic membrane parameters were extracted from the measurements.

CPP 31.8 Mon 17:15 ZEU 250

Characterization of microstructures obtained by the cryoprinting method for rapid microfluidic chip fabrication — •Sebastian Ronneberger, Ales Charvat, Claudia Hackl, Christian Elsner, and Bernd Abel — Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany

Cryo-printing is a non-conventional rapid prototyping method for microfluidic devices in which liquid state (aqueous) micro-droplets are deposited onto a cooled substrate surface like glass or silicon which immediately undergo transition to the frozen solid state. By a controlled motion between the substrate surface and the microdrop printing head microstructures of ice can be scribed. After coverage of the microstructures with an UV-cured polymer coating thawing releases an *inverse imprint* in the covering coating which is still bonded to the substrate forming a microfluidic device. The talk presents off-line characterization methods for the topological analysis of cryo-printed ice microstructures by using datasets obtained from a laser-scanning profilometer. The datasets were automatically analyzed applying self-coded Python3 scripts to obtain channel parameters such as channel widths and channel depths at different positions. Analysis of crafted microchannels shows that this method can be used for optimizing the printing parameters which have an influence on the shape of the created microchannel structures. Furthermore, the reproducibility of the printing process was assessed. This might enable cryo-printing of microfluidic channels with variable and customized channel parameters which could be applied in advanced cryo-printed microfluidic chips.

CPP 32: Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)

Time: Monday 15:30–18:15 Location: HÜL 186

CPP 32.1 Mon 15:30 HÜL 186

Funnel Hopping Monte Carlo: An efficient method to overcome broken ergodicity — •Jonas Alexander Finkler and Stefan Goedecker — University of Basel, Switzerland

Monte Carlo simulations are a powerful tool in the investigation of thermodynamic properties of atomic systems. In practice however sampling of the complete configuration space is often hindered by high energy barriers between different regions of configuration space which can make ergodic sampling completely infeasible within accessible simulation time.

We present a novel method called Funnel Hopping Monte Carlo (FHMC) to overcome broken ergodicity in Monte Carlo simulations. The method requires a priory knowledge of the funnel structure of the potential energy surface. This information does not have to be obtained from expensive Monte Carlo simulations but can be obtained very cheaply from a Minima Hopping [1] run. By approximating the Boltzmann distribution around local minima using Gaussian mixtures high quality Monte Carlo moves can be proposed that allow the simulation to directly jump between different funnels, circumventing the energy barriers in between.

The methods performance is demonstrated on the example of the 38 and 75 atom Lennard-Jones clusters which are well known for their double funnel energy landscapes that completely prevent ergodic sampling with conventional Monte Carlo simulations.

[1] S. Goedecker, J. Chem. Phys. 120, 9911 (2004)

CPP 32.2 Mon 15:45 HÜL 186

Second-principles investigation of the electrocaloric properties of $PbTiO_3$ — •Monica Graf[1] and Jorge Iñiguez[1,2] — [1]Luxembourg Institute of Science and Technology - LIST — [2]University of Luxembourg

Electrocaloric effects attract increasing attention as they provide an ecologically-friendly alternative for solid-state cooling [1] . Here we investigate the electrocaloric response of prototype ferroelectric $PbTiO_3$, using a second-principles approach that has already proved its ability to reproduce qualitatively the properties of this compound in bulk [2] and when embedded in various heterostructures [3]. More precisely, we perform Monte Carlo simulations at finite temperature and under applied electric field to obtain the first- and second-order electrocaloric tensor of $PbTiO_3$, in a temperature range including the ferroelectric transition. The first-order electrocaloric tensor can be computed from the thermal fluctuations of polarization and energy, as obtained from simulations in absence of electric field, taking advantage of Maxwell's relations in the same way that is done in "indirect" experimental measurements of the electrocaloric effect. To access the second-order tensor, we simulate the material subject to electric fields of varying magnitude, parallel and perpendicular to the polarization. In this talk we will present and discuss our results.

References:
1. Nat Commun 9, 1827 (2018)
2. Phys. Rev. Lett. 112, 247603 (2014)
3. Nature 534, 524 (2016)

CPP 32.3 Mon 16:00 HÜL 186

Exploring Chemical Reaction Space with Machine Learning — •Sina Stocker[1], Gábor Csányi[2], Karsten Reuter[1], and Johannes T. Margraf[1] — [1]Chair of Theoretical Chemistry, Technical University Munich, Germany — [2]Department of Engineering, University of Cambridge, United Kingdom

Reaction networks are essential tools for the analysis, visualization and understanding of chemical processes in such diverse fields as catalysis, combustion and the origin of life. For complex processes, the number of individual reaction steps in such a network is so large that an exhaustive first-principles calculation of all reaction energies and rates becomes prohibitively expensive. In this contribution, we use machine learning (ML) to accelerate the exploration of chemical reaction space, in analogy to the more established ML-based exploration of chemical space. To this end, we generated a new *reactive* reference database of open- and closed-shell organic molecules. This allows us to apply "chemical space" ML methods to predict the thermochemistry of reaction networks. We also develop explicitly "reaction space" based ML approaches to directly predict reaction properties. The performance of these methods confirms the potential of ML for the high-throughput screening of large reaction networks.

CPP 32.4 Mon 16:15 HÜL 186

Kernel-based machine learning for efficient molecular liquid simulations — •Christoph Scherer[1], René Scheid[1], Tristan Bereau[1,2], and Denis Andrienko[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]University of Amsterdam, Netherlands

Most current force fields based on machine learning (ML) techniques result in high computational cost at every integration time step of an MD simulation. We describe a number of practical and computationally-efficient strategies to parametrize force fields for molecular liquids with kernel-based ML. We employ a particle decomposition ansatz to two- and three-body force fields and covariant kernels. Binning techniques allow to incorporate significantly more training data. Tabulation of the kernel predictions lead to MD simulations with the same computational cost than analytic three-body potentials. Results are presented for model molecular liquids: pairwise Lennard-Jones and three-body Stillinger-Weber systems, as well as an example from bottom-up coarse-graining of liquid water [1]. Many-body representations, decomposition, and kernel regression schemes are implemented in the open-source software package VOTCA [2].

[1] Scherer, Andrienko, PCCP, 20, 22387 (2018); [2] Rühle, Junghans, Lukyanov, Kremer, Andrienko, JCTC, 5, 3211 (2009)

CPP 32.5 Mon 16:30 HÜL 186

Anharmonic phonons sampled from large scale molecular dynamics based on on-the-fly machine- learning force fields — •Jonathan Lahnsteiner and Menno Bokdam — Computational materials physics University of Vienna, Sensengasse 8/12 1090 Wien

The phonon spectrum for complex dynamic solids at elevated temperatures is often ill-described by the harmonic approximation. In this talk, I will present a molecular dynamics (MD) study of the Caesium Lead Bromide perovskite (CsPbBr3) in its orthorhombic and cubic phase. In the cubic phase, the Cs cation displays 'rattling' motion and (surrogate) structures are dynamically unstable, as indicated by imaginary phonon modes obtained in the harmonic approximation. For high accuracy and efficiency, the on-the-fly machine-learning force field (MLFF) method [1] is applied. This method generates a force-field with near first-principles accuracy and is trained to mimic the potential energy surface described by the SCAN density functional. Large scale microcanonical ensembles are generated with the MLFF and the finite-temperature dynamic structure factors are computed from the Fourier transform of the ionic density-density correlation functions. The intensities of the dynamic structure factor directly give insight in the phonon properties by taking into account phonon scattering events up to infinite order. These fully dynamic phonon spectra are compared to the phonons in the harmonic approximation. With this we are able to discuss the importance of anharmonic lattice vibrations to the stabilization of CsPbBr3 perovskite phases at finite temperature.

[1] Jinnouchi et.al. Phys.Rev.Let.10.1103/PhysRevLett.122.225701

15 min. break.

CPP 32.6 Mon 17:00 HÜL 186

Edgy and Parallel – Efficient Equilibration of Anisotropic Hard Particulate Systems — •Marco Klement and Michael Engel — Institute for Multiscale Simulation, FAU Erlangen, Erlangen, Germany

Particle simulations are an important method to study the phase behavior of fluids and solids. A common task is structure prediction via thermal equilibration. Examples are crystallization or melting and the aging of glasses. Near the liquid-solid phase transition of hard spheres event driven molecular dynamics (EDMD) is known as most efficient. Correlated movement of particles in EDMD aids the equilibration. For Monte Carlo methods event-chains [1] introduce a correlation of particle updates. Particles move until the next collision. One of several collision rules determines the new particle to continue the chain and the new direction of the chain. The recently published Newtonian event-chain (NEC) algorithm [2] is an advanced statistical methodology that assigns velocities to particles and performs collisions elastically. It is a close competitor in efficiency to EDMD. In this contribution we present the extension of NEC to polyhedral particles. We also discuss how parallelization strategies [3] can be adapted to this algorithm. Our implementation has been added to the software package HOOMD-blue. [4]

[1] Bernard et al., Phys. Rev. E 80, 056704 (2009)
[2] Klement et al., J. Chem. Phys. 150, 174108 (2019)
[3] Kampmann et al., J. Comput. Phys. 281, 864-875 (2015)
[4] http://glotzerlab.engin.umich.edu/hoomd-blue/

CPP 32.7 Mon 17:15 HÜL 186

Machine-learning force fields trained on-the-fly with bayesian inference — Ryosuke Jinnouchi[1,2], Jonathan Lahnsteiner[1], Ferenc Karsai[3], Georg Kresse[1], and •Menno Bokdam[1] — [1]University of Vienna, Vienna, Austria — [2]oyota Central R&D Labs, Inc., Aichi, Japan — [3]VASP Software GmbH, Vienna, Austria

Realistic finite temperature simulations of matter are a formidable challenge for first principles methods. Long simulation times and large length scales are required, demanding years of compute time. We present an on-the-fly machine learning scheme that generates force fields automatically during molecular dynamics simulations[1]. This opens up the required time and length scales, while retaining the distinctive chemical precision of first-principles methods and minimizing the need for human intervention. The method is widely applicable to multi-element complex systems and implemented in the VASP code. We demonstrate its predictive power on the entropy-driven phase transitions of hybrid perovskites (CH3NH3PbI3), which have never been accurately described in simulations.

[1] R. Jinnouchi et al., Phys. Rev. Lett. 122, 225701 (2019)

CPP 32.8 Mon 17:30 HÜL 186

Learning effective collective variables for biasing via t-distributed stochastic neighbor embedding — •Omar Valsson[1] and Jakub Rydzewski[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland

A common strategy to overcome the time scale problem of molecular dynamics (MD) simulations is to employ collective variable (CV) based enhanced sampling methods [1]. However, the efficiency of such approaches depends critically on the quality of the chosen CVs that must describe all the slow degrees of freedom. While physical and chemical intuition has proven generally successful in achieving this, there is a growing need for methods that can automatically find good CVs. An appealing option to accomplish this is to use ideas from the field of machine learning.

Here we show how dimensionality reduction via t-distributed stochastic neighbor embedding (t-SNE) [2] can be employed to learn effective CVs for biasing. We have implemented t-SNE directly in the PLUMED plug-in, which allows us to use it directly in numerous MD codes.

[1] O. Valsson, P. Tiwary, and M. Parrinello, Ann. Rev. Phys. Chem. 67, 159 (2016)

[2] L. van der Maaten and G. Hinton, J. Mach. Learn. Res. 9, 2579 (2008)

CPP 32.9 Mon 17:45 HÜL 186

Variational autoencoders as a tool to learn collective variables from simulation snapshots — •Miriam Klopotek and Martin Oettel — Institut für Angewandte Phsyik, Eberhard Karls Universität Tübingen, Tübingen, Germany

Variational autoencoders (VAEs) are powerful neural-network architectures capable of learning abstract representations of data (distributions of latent variables) in an unsupervised fashion. We apply a standard formulation of VAEs [1,2] to equilibrium configurations obtained by grand canonical Monte Carlo simulations and formulate a probabilistic model for the VAE which shows that the latent variables are collective variables, and their variances are generalized susceptibilities. Upon application to a lattice model with sticky rods which shows competing gas, liquid and nematic phases we find that the leading collective variables are akin to the two order parameters of the model. Furthermore, the collective variables define coarse-grained configurations. Increasing the number of latent variables leads to finer spatial resolution of the coarse-grained configurations and increasingly preciser physical observables obtained from them. Finally, we discover there is an optimal hyperparameter β in so-called β-VAEs [3] where the collective variables become disentangled with respect to structural correlation length-scales: These disentangled collective variables hence form a hierarchy of different levels-of-detail.

[1] Kingma, D. P. & Welling, M. (2013). arXiv:1312.6114. [2] Rezende, D. J., Mohamed, S., & Wierstra, D. (2014). arXiv:1401.4082. [3] Higgins, I. et al. (2017). ICLR, 2(5), 6.

CPP 32.10 Mon 18:00 HÜL 186

Adversarial Reverse Mapping of Equilibrated Condensed-Phase Molecular Structures — •Marc Stieffenhofer[1], Michael Wand[2], and Tristan Bereau[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]JGU Mainz, Institute of Computer Science, Staudingerweg 9, 55128 Mainz

Coarse-grained molecular dynamics simulations circumvent prohibitively long equilibration times by averaging out degrees of freedom. However to consistently link the scales a reverse mapping scheme is needed to reintroduce higher resolution details. Traditional schemes propose a rough coarse-to-fine mapping and rely on further energy minimization and molecular dynamics simulations to re-equilibrate the system. In this study we introduce DeepBackmap: A deep neural network based approach to predict equilibrated molecular structures without running molecular dynamics simulations. We use generative adversarial networks to learn the Boltzmann distribution from training data and realize reverse mapping by using the coarse-grained structure as a conditional input. Our method can be used for condensed-phase systems of arbitrary sizes. The model uses only local information and reconstructs the atomistic structure autoregressively. We test our method on syndiotactic polystyrene molecules and show that the model trained in a melt shows remarkable transferability to the crystalline phase. The learned local correlations appear to be temperature independent indicating a separation of the scales.

CPP 33: Glasses and Glass Transition (joint session DY/CPP)

Time: Monday 15:00–18:00 Location: ZEU 118

Invited Talk CPP 33.1 Mon 15:00 ZEU 118

Shearing of glasses: new insight from studying model glasses of different system sizes — •Andreas Heuer, Markus Blank-Burian, Lawrence Smith, and Moumita Maiti — Inst. Phys. Chemie, WWU Muenster, Germany

Upon shearing of glasses a large variety of different phenomena can be observed. This includes, e.g., the stress overshoot and the emergence of shear bands. Many properties have been related to the presence of shear transformation zones (STZs).

In previous work on quiescent glasses important information about the physical mechanisms could be extracted from studying the dependence of dynamical properties on the system size. Here it was essential to study system sizes between approx. 60 and a few thousand [1]. Furthermore, an appropriate discretization of the dynamics in terms of metabasins was essential.

Here we study the properties of sheared systems in an analogous setting. Formally, shearing corresponds to a time-dependent energy landscape, requiring a generalization of the metabasin concept [2]. Interestingly, when studying the size dependence upon shearing at low temperatures, it turns out that macroscopically relevant behavior starts to be observed for system sizes above (approx.) 10.000. Important properties of the dynamic heterogeneities as reflected, e.g., by the emergence of shear bands, is extracted from these dependencies and related to the STZs.

[1] C. Rehwald, A. Heuer, Phys. Rev. E, 86, 051504 (2012). [2] M. Blank-Burian. A. Heuer, Phys. Rev. E 98, 033002 (2018).

CPP 33.2 Mon 15:30 ZEU 118

Nonlinear dielectric response: molecular reorientation models — •Gregor Diezemann — Institut für Physikalische Chemie, JGU Mainz, Duesbergweg 10-14, 55128 Mainz

The nonlinear dielectric response of supercooled liquids has been intensively studied, both experimentally and theoretically during the last decade. Since an analogue of the well known fluctuation dissipation theorem for nonlinear responses is missing, one has to rely on the results of model calculations. A number of different models have been used for the calculation of the nonlinear (third order) response and some of them exhibit features also observed experimentally.

I will present the results of calculations of the third order and the fifth order response for models of molecular reorientations. Sofar, one important point in the interpretation of the peaks observed in the modulus of the nonlinear response was that rotational Brownian motion does not give rise to such a peak. However, it is well known that this model of isotropic rotational diffusion is also not able to reproduce important features of the linear dielectric response of glassforming systems.

Here, I will show that very simple models like the model of random rotational jumps or anisotropic rotational diffusion also exhibit a so-called hump in the modulus of the nonlinear response functions. Also the relation between the third order response and the fifth order repsonse is obeyed to some extent. What is missing in this kind of models is a temperature dependence of the features observed. I will discuss the results in the context of recent experimental observations.

CPP 33.3 Mon 15:45 ZEU 118

Efficient algorithm to study dynamics in the transition between quasiperiodic and disordered environments — •Alan Rodrigo Mendoza Sosa and Atahualpa Kraemer — Universidad Nacional Autónoma de México, Mexico City, Mexico

Crystals have translational and rotational symmetries while quasicrystals have rotational symmetry in a single point, and glasses have none. This is revealed in the diffraction pattern, where crystals and quasicrystals have a discrete pattern, but quasicrystals exhibit forbidden symmetries, while glasses have a continuous pattern. Increment the rotational symmetry of quasicrystals should produce a denser diffraction pattern, closer to the continuous pattern exhibit in glasses. Motivated with the previous arguments we propose to study the structure of a quasiperiodic array and the dynamics of particles in quasiperiodic environments when the folding symmetry increases. However, the usual techniques to produce quasiperiodic arrays are aimed at producing arrays of low symmetries and near to the center of symmetry, then it becomes time expensive to perform simulations. In this work, we present an algorithm to produce quasiperiodic arrays with arbitrary symmetry around any point in the space, based on the generalized dual method. Also, using the Voronoi tessellation of the quasiperiodic array, and the incremental algorithm to track particles, we made an algorithm to perform simulations of particles moving in a quasiperiodic potential with arbitrary symmetry. We apply this algorithm to a quasiperiodic Lorentz gas with high symmetry to study diffusion and compare it with the random Lorentz Gas.

CPP 33.4 Mon 16:00 ZEU 118

Interpreting the Types of Derivatives in Fractional Relaxation Models — •Tillmann Kleiner and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

The excess wing of α-relaxation peaks and the phenomenon of nearly constant loss that have been observed in dielectric spectra of glass forming materials [1] are predicted by susceptibility functions that involve stretching exponents derived from fractional dynamics [2,3]. The relaxation motions predicted by such models can be described by initial value problems involving fractional derivatives with a type parameter. Special choices for the type parameter yield Liouville-Caputo and Riemann-Liouville derivatives.

Using a translation invariant fractional derivative the fractional ini-

tial value problems are reformulated as linear response equations. The influence of the type parameter is then described by additional fractional derivative expressions. The reformulation brings the advantage that the mathematical external force term coincides with the physical external force term which is not guaranteed for all types in the initial value problem formulation. Further, predictions for realistic spectroscopy and relaxation experiments are now described in a unified way and physical predictions depend continuously and more transparently on the parameters of the model.
[1] F. Kremer and A. Loidl, The Scaling of Relaxation Processes, Springer, (2018)
[2] R. Hilfer, Analysis **36**, 49-64 (2016)
[3] R. Hilfer, J. Stat. Mech. (2019) 104007

CPP 33.5 Mon 16:15 ZEU 118

Dynamic properties of quasi-confined colloidal hard-sphere liquids near the glass transition — •Lukas Schrack, Charlotte Petersen, and Thomas Franosch — Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, 6020 Innsbruck, Austria

The complex behavior of confined fluids arising due to a competition between layering and local packing can be disentangled by considering quasi-confined liquids with translational invariance along the confined direction. We provide a mode-coupling theory (MCT) for quasi-confined liquids using multiple relaxation channels and elaborate an efficient method for the numerical implementation.

Investigating both the collective and tagged-particle motion near the glass transition we focus on the non-monotonic behavior of the glass-form factor as well as of the intermediate scattering functions comparing numerical MCT results and simulations. We also provide a non-equilibrium state diagram as a function of the confinement length.

CPP 33.6 Mon 16:30 ZEU 118

Broadband Dielectric and Nuclear Magnetic Resonance Spectroscopy Studies on Dynamics of Ethylene Glycol in Soft and Hard Confinement — •Melanie Reuhl, Max Weigler, and Michael Vogel — Institut für Physik kondensierter Materie, Technische Universität Darmstadt

As hydrogen-bond networks are often restricted or confined in nature and technology, we investigate the influence of the type of confinement on hydrogen-bonded systems. Using nuclear magnetic resonance (NMR) and broadband dielectric spectroscopy (BDS), we analyse the dynamics of ethylene glycol (EG) in nanoporous silica, elastin and Ficoll matrices over broad temperature ranges. For all investigated systems, BDS and NMR results consistently indicate a slowdown and an enhanced heterogeneity of dynamics due to confinement. For EG in silica pores, calorimetric studies reveal partial freezing at temperatures below the bulk freezing point, indicating substantial freezing point suppression. We study changes in the dynamical behaviour when the confined liquid evolves into coexisting liquid and solid phases upon cooling. The dynamical behaviour of both EG phases in silica confinement is independent of pore size for diameters below 6 nm. In the studied soft confinements, fractional freezing does not occur. Still, two dynamically distinguishable EG species occur, which can be assigned to free EG and interfacial EG at elastin/sugar surfaces.

15 min. break.

CPP 33.7 Mon 17:00 ZEU 118

Dynamics of Ethylene Glycol Water Mixtures in Bulk and Mesoporous Silica Studied by Nuclear Magnetic Resonance and Dielectric Spectroscopy — •Philipp Monnard, Melanie Reuhl, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Hydrogen bonds remain a topic of scientific interested because of their key role in countless chemical systems. Aqueous solutions of ethylene glycol (EG) create complex networks of hydrogen bonds, because of EGs ability to form both intramolecular and intermolecular bonds. Those solutions are also widely used in heating, cooling and deicing applications, since their freezing point is significantly lower than that of their components. Using nuclear magnetic resonance (NMR) and dielectric spectroscopy (DS), we analyze the effect of silica confinement on the dynamics of EG-water mixtures with different concentrations. In particular, we determine the dependence of correlation times on the pore diameter over a broad temperature range. In doing so, we exploit the isotope selectivity of NMR to observe only the partially deuterated EG-d4(C2D4(OH)2) molecules. Further, we prepared solutions, with heavy water and EG-d2(C2H4(OD)2) to measure the dynamics of the counterpart. We found that the dynamics depend on the mixing ratio, explicitly there is a slowdown with higher concentrations of EG. Moreover, we observe strong dynamical heterogeneity and, for solutions of 30 wt.% EG, the relaxation is even bimodal at intermediate temperatures.

CPP 33.8 Mon 17:15 ZEU 118

Aging of SiO_2: Scaling of Dynamic Heterogeneities and Cluster Analysis of Single Particle Jumps — •Katharina Vollmayr-Lee[1], Horacio E. Castillo[2], Christopher H. Gorman[3], and Taylor S. Cookmeyer[4] — [1]Bucknell University, Lewisburg, PA, USA — [2]Ohio University, Athens, OH, USA — [3]University of California, Santa Barbara, CA, USA — [4]University of California, Berkeley, CA, USA

We study the aging dynamics of the strong glass former SiO_2 via molecular dynamics simulations. We quench the system from a high to a low temperature, and then investigate the dynamics of the system as a function of waiting time, the time elapsed since the quench. For a system of 336 atoms, we find that both the dynamic susceptibility and the probability distribution of the local incoherent intermediate scattering function can be described by simple scaling forms in terms of the global incoherent intermediate scattering function. We also find for the scaling of these dynamic heterogeneities that the aging dynamics is controlled by a unique aging clock which is the same for Si and O atoms. Furthermore, we present results for a system of 115248 atoms for which we use single particle trajectories to identify single particle jump events when a particle escapes its cage formed by its neighbors. To study how these jump events are correlated in space and time, we find clusters of jumping particles. We will present cluster size distributions of both simultaneously jumping particles, as well as space-time clusters (jump events which are neighbors in space and time).

CPP 33.9 Mon 17:30 ZEU 118

Residual stress distributions and mechanical noise in athermally deformed amorphous solids from atomistic simulations — •Céline Ruscher[1,2] and Jörg 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

The distribution $P(x)$ of local residual stresses in amorphous packings governs the statistical properties of global collective failure events at the yielding transition. We reveal the evolution of $P(x)$ upon deformation by combining atomistic simulations with the frozen matrix approach. 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 plateau p_0 in the small x limit, where $p_0 \sim L^{-p}$ with L the system size. A direct comparison with the system size scaling of the stress drops shows that the distribution of avalanche sizes are controlled by θ in the transient regime and the plateau exponent p in the steady state flow. The broad distribution of mechanical noise $P(\Delta x) \sim |\Delta x|^{-1-\mu}$ is characterized by a Levy-exponent μ and can be related to the behavior of $P(x)$ via a mean-field description.

CPP 33.10 Mon 17:45 ZEU 118

AGE-INDEPENDENT PROCESS IN AGING HARD-SPHERE SUSPENSIONS: THE BETA PROCESS AND ITS RAMIFICATIONS — •Hans Joachim Schöpe[1] and William van Megen[2] — [1]Universität Tübingen — [2]RMIT University Melbourne

We consider the dynamics of a suspension of hard sphere-like particles in the proximity of its glass transition, the region where the intermediate scattering functions show significant aging. The time correlation function of the longitudinal particle current shows no dependence on age and reveals behaviour of ideal super-packed fluid and glass. The power laws of the beta process of the idealised mode coupling theory are exposed directly without reliance on fitting parameters. We proffer a mechanism linking the reversible/ageless dynamics, which constitutes the beta-process, and the irreversible aging dynamics.

CPP 34: Microswimmers (joint session DY/CPP)

Time: Monday 15:00–17:45 Location: ZEU 160

Invited Talk CPP 34.1 Mon 15:00 ZEU 160

Microswimmers in (semi-)dilute suspensions: binary mixtures, trapping, orientational ordering, collective motion, and imposed shear flows — Christian Hoell, Giorgio Pessot, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Active microswimmers self-propel while setting the surrounding fluid into motion. This leads to hydrodynamic swimmer interactions and can enable emergent collective behavior. Extending our corresponding statistical characterization of (semi-)dilute microswimmer suspensions, we have derived a dynamical density functional theory to describe binary microswimmer mixtures [1]. First, we address mixtures of pushers and pullers of otherwise identical properties [1]. We find that the majority species hydrodynamically imposes its behavior onto the minority species, both under spherical confinement and for unbounded planar motion [1,2]. Particularly, this concerns emergent polar orientational order. Second, we consider trapped active microswimmers confined by a ring of driven passive particles [1]. Through resulting imposed hydrodynamic fluid flows, the enclosed microswimmers concentrate in a centered spot, mimicking the behavior of active circle swimmers [3]. Since frequently in nature many active species interact with each other under confinement, we consider our extensions essential on the path of statistically characterizing corresponding biological systems.

[1] C. Hoell et al., *J. Chem. Phys.* **151**, 064902 (2019).
[2] G. Pessot et al., *Mol. Phys.* **116**, 3401 (2018).
[3] C. Hoell et al., *New J. Phys.* **19**, 125004 (2017).

CPP 34.2 Mon 15:30 ZEU 160

Fine balance of chemotactic and hydrodynamic torques: When microswimmers orbit a pillar just once — •Chenyu Jin[1,2], Jérémy Vachier[1], Soumya Bandyopadhyay[3], Tamara Macharashvili[4], and Corinna Maass[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany. — [2]University of Bayreuth, Bayreuth, Germany — [3]Purdue University, West Lafayette, USA — [4]Princeton University, Princeton, USA

Self-propelling liquid crystal droplets in an aqueous surfactant solution is an excellent model system for biological microswimmers: they exhibit chemotaxis and negative autochemotaxis, and they interact with boundaries. Here we study the detention statistics of these droplet microswimmers attaching to microfluidic pillars. The repulsive trail of spent fuel shed by themselves biases them to detach from pillars in a specific size range after orbiting the pillars just once. We have designed a microfluidic assay recording microswimmers in pillar arrays of varying diameter, derived detention statistics via digital image analysis, and interpreted these statistics via the Langevin dynamics of an active Brownian particle model. By comparing data from orbits with and without residual chemical field, we can independently estimate quantities such as hydrodynamic and chemorepulsive torques, chemical coupling constants and diffusion coefficients, as well as their dependence on environmental factors such as wall curvature. This type of analysis is generalizable to many kinds of microswimmers.

CPP 34.3 Mon 15:45 ZEU 160

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.

CPP 34.4 Mon 16:00 ZEU 160

Percolation transition of pusher-type microswimmers — •Fabian Jan Schwarzendahl[1,2] and Marco G. Mazza[2,3] — [1]Department of Physics, University of California, Merced,5200 N. Lake Road, Merced, California 95343, USA — [2]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [3]Interdisciplinary Centre for Mathematical Modelling and Department of Mathematical Sciences,Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom

In this talk I will present the presence of a continuum percolation transition in model suspensions of pusher-type microswimmers. The clusters dynamically aggregate and disaggregate resulting from a competition of attractive and repulsive hydrodynamic and steric interactions. As the microswimmers' filling fraction increases, the cluster size distribution approaches a scale-free form and there emerge large clusters spanning the entire system. We characterize this microswimmer percolation transition via the critical exponents, analytical arguments, and scaling relations known from percolation theory. This finding opens new vistas on microswimmers' congregative processes.

CPP 34.5 Mon 16:15 ZEU 160

Self-assembling complex and functional structures at the (sub)millimeter scale — •Nicolas Vandewalle — GRASP, Institut de Physique B5a, Sart Tilman, Universite de Liege, B4000 Liege, Belgium

When soft ferromagnetic particles are suspended at air-water interfaces in the presence of a vertical magnetic field, dipole-dipole repulsion competes with capillary attraction such that structures self-assemble. The complex arrangements of such floating bodies are emphasized. By adding a horizontal and oscillating magnetic field, periodic deformations of the assembly are induced. We show herein that collective particle motions induce locomotion at low Reynolds number. The physical mechanisms and geometrical ingredients behind this cooperative locomotion are identified. These physical mechanisms can be exploited to much smaller scales, offering the possibility to create artificial and versatile microscopic swimmers. Moreover, we show that it is possible to generate complex structures that are able to capture particles, perform cargo transport, fluid mixing, etc...

15 min. break.

CPP 34.6 Mon 16:45 ZEU 160

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 [3]. 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. 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.*, PRL 110.22 (2013): 228102.
[2] Wensink *et al.*, PNAS 109.36 (2012): 14308-14313.
[3] Downton *et al.*, J. of Ph.: Cond. Mat. 21.20 (2009): 204101.

CPP 34.7 Mon 17:00 ZEU 160

Chemokinesis causes trapping and avoidance by dynamic scattering — •Justus Kromer — Stanford University, Stanford, United States of America

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. Interestingly, these agents violate a mean-chord-length theorem. 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. arXiv:1904.11020

CPP 34.8 Mon 17:15 ZEU 160

Feedback Control of Multiple Active Microswimmers — •Alexander Fischer and Frank Cichos — Uni Leipzig

Collective motion created by the interaction of autonomous individuals plays a major role in flocks of birds, bacterial growth or the motion of robotic swarms. Sensing and reacting to signals is a fundamental issue of life. Microswimmers, which are artificial objects that mimic the active motion of biological systems, do not have such sensing and response features built in yet, but may gain them through an external control of their propulsion. Here we explore the emergent collective behavior as a result of an information exchange between artificial microswimmers by computer-controlled feedback processes. We have created a setup where multiple active microswimmers can react to their position in space or their distance to other microswimmers [1]. Our system consists of autonomous agents performing directed motion in a plane and their orientation is subject to noise. We study in particular the delayed response of the swimmers to environmental signals, where the swimmers remember previous information on a signaling landscape or infer future signals from the experience. We find that this type of delayed response is changing the collective behavior.

[1] U. Khadka, V. Holubec, H. Yang, F. Cichos, Nat. Commun. 9, 3864 (2018)

CPP 34.9 Mon 17:30 ZEU 160

Viscosity destabilizes the propulsion dynamics of active droplets — •Babak Vajdi Hokmabad[1], Maziyar Jalaal[2], Ranabir Dey[1], Kyle Baldwin[1,3], Detlef Lohse[1,2], and Corinna Maass[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Physics of Fluids Group, Max Planck Center for Complex Fluid Dynamics, Enschede, The Netherlands — [3]Nottingham Trent University, Nottingham, United Kingdom

Biological micro-organisms have developed sophisticated swimming behaviors such as run-and-tumble or switch-and-flick. These complex functions depend on their complicated biophysical machinery. In efforts to develop artificial micro-swimmers, the aim is to build a minimal system based on the principles of out-of-equilibrium physics that is able to mimic such complex behaviors. In this work, we show that an active droplet, undergoing micellar solubilization, experiences unsteady self-propulsion in response to an increase in the viscosity of the swimming medium. The origins of this seemingly counterintuitive behavior is explained using theory in conjunction with a novel experimental technique to simultaneously visualize the hydrodynamic and chemical fields around the droplet. By varying the viscosity we can tune the propulsion dynamics and observe behaviors reminiscent of natural micro-swimmers.

CPP 35: Topical Session: Data Driven Materials Science - Machine Learning for Production (joint session MM/CPP)

Time: Monday 17:00–17:30 Location: BAR 205

Topical Talk CPP 35.1 Mon 17:00 BAR 205

First-principle infused machine learning models allowing digital twins to self-organise production processes — •Marcus Neuer — Sohnstr. 65, 40237 Düsseldorf

For European process industries, optimization of the production route plays an increasingly important role for keeping a competitive edge in a tough market. New concepts like digital twins arrived recently in real-world applications. They allow an agent-based, active self-organisation of the route and introduced the ability to apply models live, during the processing. These models may be analytically derived, data-based or a combination of both: first-principle infused machine learning models. Herein, the stochasticity of the process is modelled by the machine learning approach, while an analytical first-principle backbone acts as basis. With the ability to forecast its potential future, materials and products have new degrees of freedom. They optimize their future path with respect to energy consumption, order matching and material homogeinety. The presented concepts are shown in real-world production environments, where they have already reached technical readiness to sustain continuous production.

CPP 36: Focus: Exploitation of Anisotropy in Organic Semiconductors I (joint session CPP/HL)

Molecular glasses and semi-crystalline thin films play a key role in organic semiconductor devices, particularly organic light-emitting diodes and solar cells. Surprisingly, some of these materials exhibit considerable anisotropies regarding their molecular orientation which leads to non-isotropic electronic properties. In spite of the importance for optoelectronic devices, however, this phenomenon is not fully understood yet. This focus session will bring together concepts from the physics of glasses, structure formation in soft matter as well as applications of such anisotropic molecular solids in organic electronics. Organized by: Wolfgang Brütting (University Augsburg), Sebastian Reineke (TU Dresden); Wolfgang Wenzel (Karlsruher Institut für Technologie).

Time: Tuesday 10:00–12:30 Location: ZEU 222

Invited Talk CPP 36.1 Tue 10:00 ZEU 222

Anisotropic packing in vapor-deposited glasses — •Mark Ediger — University of Wisconsin-Madison, USA

Glasses are generally regarded as highly disordered and the idea of controlling molecular packing in glasses is reasonably met with skepticism. However, as glasses are non-equilibrium materials, a vast array of amorphous structures are possible in principle, even for a single component system. Physical vapor deposition (PVD) allows a surprising amount of control over anisotropic molecular packing in glasses. For organic semiconductors, glasses can be prepared in which the molecules have a substantial tendency to stand-up or lie-down relative to the substrate, and molecular layering can also be achieved. The high density and anisotropic packing of PVD glasses can be explained by a mechanism that is "anti-epitaxial" as structure is templated by the top surface rather than by the underlying substrate. This mechanism implies that similar structures can be prepared by increasing substrate temperature and by decreasing deposition rate, and this has recently been experimentally verified.

CPP 36.2 Tue 10:30 ZEU 222

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 36.3 Tue 10:45 ZEU 222

Application of polar molecules to electret for vibrational energy generator: Improvement of device productivity and output power by utilizing spontaneous orientation polarization — •Yuya Tanaka[1,2], Noritaka Matsuura[1], and Hisao Ishii[1] — [1]Chiba University, Chiba, Japan — [2]Japan Science and Technology Agency, PRESTO, Saitama, Japan

Electret-based vibrational energy generator (E-VEGs) have attracted much attention because they can generate electrical power from ambient vibrations. The challenges for E-VEGs are to: (i) simplify charging process for making electret and (ii) enhance output power (P) of the device. Recently, we developed polar molecules (PM), such as Alq3 and TPBi, based VEGs that do not require any charging process by utilizing spontaneous orientation of the molecules. To increase P of the device, enhancement of surface potential (SP), namely, order parameter of the molecule, is required. In this study, we prepared PM films with various deposition rate (r). We found that the SP becomes larger in the case of high r, suggesting that molecular orientation can be controlled by r. Further, the estimated surface charge density was comparable to conventional polymer-based electret after charging (typically, 2 mC/m2). We believe that the realization of PM-VEGs will open up the novel ways for supplying electrical energy to the various devices.

CPP 36.4 Tue 11:00 ZEU 222

Post processing temperature dependence of the emitter molecule orientation in organic thin films — •Christian Hänisch, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany

One of the main loss channels reducing the efficiency of organic light-emitting diodes is optical trapping of already generated photons due to total internal reflection and coupling to plasmonic modes. Aligning the transition dipole moment of the emitter molecules parallel to the interface planes of the stratified device structure can drastically decrease the unusable power fraction.

In this work, the long term, post processing stability of the molecular orientation of two well-known phosphorescent emitters is investigated for different storage temperatures up to 95% of the glass transition temperature (Tg) of the host material. Both, photoluminescent samples and electroluminescent devices are analyzed. In the first case, the emission layers are embedded between two layers of higher Tg in order to avoid crystalization of bare emission layers.

It is shown that the orientation keeps unchanged for several months as long as Tg is not exceeded but changes immediately as soon as the samples are exposed to temperatures above Tg for only a few minutes. The latter is demonstrated exemplarily for selected samples after the long term storage period.

15 min. break

Invited Talk CPP 36.5 Tue 11:30 ZEU 222

Influence of stability and molecular orientation on the properties of stable glasses — •Javier Rodríguez-Viejo — Physics department, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Stable glasses have attracted great interest since their discovery in 2007. Their superior behavior, compared to liquid-cooled glasses, includes higher kinetic and thermodynamic stability, higher density, sound velocity and elastic moduli or the modification of the low-temperature properties. The origin of the high thermodynamic and kinetic stability of these vapor-deposited glasses is related to the high mobility of surface molecules that enables them to settle into energetic favorable positions during the deposition process. Besides, depending on the molecular shape PVD glasses exhibit packing anisotropies that depend on the deposition temperature. Although molecular orientation does not seem to play a substantial role in the observed stability enhancement, it can have a significant impact in many properties of vapor-deposited glasses. For instance, we have previously shown that molecular orientation may induce variations of the growth front velocity during the heterogeneous transformation of a glass into the supercooled liquid state. In addition, molecular anisotropy plays a key role in charge and thermal transport. We will describe the impact of the deposition process and the molecular orientation on the thermal properties and on electronic and heat propagation. We also explore the benefits of using stable glasses grown at temperatures around 85% Tg to increase device efficiency and operational stability of OLEDs.

CPP 36.6 Tue 12:00 ZEU 222

Infrared organic light-emitting diodes with horizontally oriented carbon nanotube emitters — •Caroline Murawski[1,3], Arko Graf[2,3], Jana Zaumseil[2], and Malte C. Gather[3] — [1]Kurt-Schwabe-Institut Meinsberg — [2]Universität Heidelberg — [3]University of St Andrews, UK

Semiconducting single-walled carbon nanotubes (SWCNT) have shown great potential as electrodes and transport layers in organic light-emitting diodes (OLEDs) and field-effect transistors. Here, we incorporate polymer-wrapped SWCNTs as emitter into OLEDs and achieve narrowband pure infrared emission between 1000 and 1200 nm. Due to the 1D nature of CNTs, the transition dipoles exhibit strong horizontal orientation, which results in an exceptionally high outcoupling efficiency of 49%.

CPP 36.7 Tue 12:15 ZEU 222

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.

CPP 37: Interfaces and Thin Films II (joint session CPP/O/DY)

Time: Tuesday 9:30–13:00 Location: ZEU 260

Invited Talk CPP 37.1 Tue 9:30 ZEU 260
Phospholipid membranes as model systems for fundamental soft matter research — •Sebastian Jaksch — Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science, Garching, Germany

Phospholipid membranes play an important role as interfaces in virtually all biological systems. By their interplay between structure and dynamics they provide the basic functions necessary to support living organisms, such as stability for the cells and trans-membrane transport for nutrients and drugs. Using SoyPC as an example, this presentation will give an overview of grazing incidence neutron techniques for structure and dynamics measurements of phospholipid membranes.[1] We investigated the structure with grazing incidence small-angle neutron scattering (GISANS) at extremely low background conditions [2] and correlated that data with grazing incidence neutron spin-echo spectroscopy [3] (GINSES). These investigations revealed thermally excited modes in the plane of the membrane and its corresponding structures. This modes could be frozen in at temperatures below room temperature and reappeared after reheating to physiological temperatures.

[1] Jaksch, S., Gutberlet, T., Müller-Buschbaum, P. (2019). Grazing Incidence Scattering - Status and Perspectives in Soft Matter and Biophysics. Current Opinion in Colloid & Interface Science.

[2] Jaksch, S., et al. (2019). Long-range excitations in phospholipid membranes. Chemistry and physics of lipids, 225, 104788.

[3] Jaksch, S., et al. (2017). Nanoscale rheology at solid-complex fluid interfaces. Scientific reports, 7(1), 4417.

CPP 37.2 Tue 10:00 ZEU 260
Brownian motion in near-surface pressure driven flows with 3D-nanometric spatial resolution — •Joshua McGraw[1], Alexandre Vilquin[1,2], Pierre Soulard[1], Vincent Bertin[1], Gabriel Guyard[1,2], David Lacoste[1], Elie Raphael[1], Frederic Restagno[2], and Thomas Salez[3] — [1]ESPCI Paris — [2]Université Paris Sud — [3]Université de Bordeaux

In near-surface flows, interfaces play a major role by imposing (typically) no-slip boundary conditions, greatly reducing the fluid velocity compared to the central part of a channel. With total internal reflection fluorescence (TIRF), a flow is illuminated with an evanescent field decaying over a few hundred nanometers into the channel; this decay allowing a determination of nanoparticle altitudes. Combined with particle tracking, experimental determination of the velocity profile and local velocity distributions in three dimensions are possible. Here we present a detailed look at the statistics of near-surface particle motions in pressure-driven water for which diffusion is important compared to advection. The distribution of displacements in the invariant flow direction is Gaussian as for normal diffusion. Significant anomalies are however observed for both of the other spatial dimensions. Combining experiments and simulations, we disentangle contributions from so-called Taylor-Aris dispersion, nanoparticle polydispersity and the optical measurement system. This description of TIRF allows for the study of many Brownian motion problems, such as near-surface polymer solution dynamics or particle motion near soft boundaries.

CPP 37.3 Tue 10:15 ZEU 260
Relation between stability and interfacial structure of polyelectrolyte containing foam films — •Larissa Braun and Regine von Klitzing — TU Darmstadt, Darmstadt, Germany

For many industrial applications foams of oppositely charged polyelectrolyte/surfactant-mixtures are of high impact, as they form surface active complexes.

Extensive research on such mixtures was already performed[1,2] but the influence of the ionic strength is still unclear.

This work focuses on the influence of added LiBr on foam films of mixtures of the anionic polyelectrolyte sPSO$_2$-220 (similar to PSS but stiffer) with the cationic surfactant C$_{14}$TAB. Therefore, disjoining pressure isotherms were measured with a fixed C$_{14}$TAB concentration and a variable polyelectrolyte concentration.

Different stability regimes were identified. Already a low salt concentration of 10^{-4} M leads to a considerably less stable foam films regarding the maximum disjoining pressure. An unexpected formation of an unstable Newton Black Film was found at this low salt concentration. Higher salt concentrations will also be considered. These findings will be correlated with the surface excesses of both compounds which can be separated from each other by neutron reflectometry measurements.

[1] N. Kristen, A. Vüllings, A. Laschewsky, R. Miller, R. v. Klitzing, Langmuir, 2010, 12, 9321-9327. [2] M. Uhlig, R. Miller, R. v. Klitzing, Phys. Chem. Chem. Phys., 2016, 18, 18414-18423

CPP 37.4 Tue 10:30 ZEU 260
Near-surface dynamics of semidilute polymer solutions: diffusion, nonlinear rheology, and the hydrodynamic boundary condition — •Gabriel Guyard[1,2], Alexandre Vilquin[1,2], Frederic Restagno[2], and Joshua McGraw[1] — [1]ESPCI Paris — [2]Université Paris Sud

The near-surface dynamics of polymer solutions challenge both experimental and theoretical efforts – especially in the case of semi-dilute solutions for which chains overlap – yet evanescent wave microscopy allows for the characterization of such interfacial flows. Here we report molecular-size-resolution particle motions in microfluidic channels for pressure-driven flows of semidilute polymer solutions. The results using polymer-free water are in good agreement with Stokes-flow hydrodynamic and diffusive theory. Experiments using polyacrylamide at different volume fractions close to and above the overlap concentration are done in the same chips as for the water experiments. In contrast to Newtonian fluid behaviour, the shear-rate/pressure drop relation is non-linear for the polymer solution flows, suggesting nanometrically-resolved, shear-thinning effects, accompanied with a non-trivial hydrodynamic boundary condition. The diffusive motion of the tracer particles is also distinguished from that of the water experiments, and such motions detailed here. These results set the basis for a study of near-wall hydrodynamic flow and diffusion in complex fluids, notably including semidilute polymer solutions.

CPP 37.5 Tue 10:45 ZEU 260
AFM Force-Distance-Curves on Different Lubricants — •Sebastian Friedrich and Brunero Cappella — Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, D-12205 Berlin

AFM force-distance-curves have been recorded on thin films of nine different lubricant liquids. Those lubricants wet the AFM-tip, which causes a capillary force. This force depends on the tip shape, as well as on liquid properties like surface tension, contact angle, and viscosity. Those liquid properties have been measured independently with other methods, so their influence on the shape of the force-distance-curves can be discussed. This study provides a tool for the characterization of thin lubricant films and contributes to the understanding of tribology on the nanoscale.

CPP 37.6 Tue 11:00 ZEU 260
Revealing the formation of sputter deposited copper nanolayers on functional polymer thin films for lithium-ion batteries — •Simon J. Schaper[1], Franziska C. Löhrer[1], Senlin Xia[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2,4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, Photon Science, 22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel — [4]KTH, Department of Fibre and Polymer Technology, 100 44 Stockholm, Sweden

Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-film morphologies on the nanoscale and offers a superior adhesion of the deposited material. We use in-situ grazing incidence small angle X-ray scattering (GISAXS) to investigate the formation, growth and, self-assembled structuring of copper on polymer thin films and composites used in LIBs. The growth of copper on polymer thin films is described based on a model approach.

15 min. break

CPP 37.7 Tue 11:30 ZEU 260

Insight into ion transport across polypyrrole-electrolyte interfaces by in situ X-ray reflectivity and electrochemistry — •Pirmin H. Lakner[1,2], Manuel Brinker[3], Christoph Seitz[1], Sergey Volkov[1], Patrick Huber[3], and Thomas F. Keller[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Physics Department, Universität Hamburg, Germany — [3]Institute of Materials Physics and Technology, Technische Universität Hamburg-Harburg, Germany

Polypyrrole (PPy) is a conducting polymer with actuatoric and pseudocapacitive properties due to potential-induced ion incorporation/expulsion. Electrical potentials were applied to a perchlorate-doped PPy thin film ($\sim$ 30 nm) in an aqueous perchloric acid electrolyte and the associated changes in thickness and electron density were recorded by X-ray reflectivity (XRR). Assuming a sole perchlorate anion transfer carrying 50 electrons, a ratio of 50:1 is expected between electrons crossing the PPy-substrate interface and electrons crossing the electrolyte-PPy interface. By correlating the XRR data and the electrochemical data, a ratio of 10:1 was obtained, which indicates that water movement takes place as an anion counter-flow. The recorded low strain-charge coefficient supports this assumption. One explanation is the high stability and the low porosity of the PPy film due to its fast potentiodynamic deposition method. The properties of the analyzed PPy film make it a suitable choice for supercapacitor applications.

CPP 37.8 Tue 11:45 ZEU 260

Revealing Lithium Transport Processes in Lithium-Ion Battery Anodes Using Neutron Depth Profiling — •Markus Trunk[1,2], Fabian Linsenmann[3], Philip Rapp[3], Jamie Weaver[4], Lukas Werner[1], Roman Gernhäuser[1], Ralph Gilles[2], Bastian Märkisch[1], Zsolt Revay[2], and Hubert Gasteiger[3] — [1]TUM, Physik-Department, Garching — [2]TUM, Heinz Maier-Leibnitz Zentrum, Garching — [3]TUM, Lehrstuhl für Technische Elektrochemie, Chemie Department, Garching — [4]Material Measurement Laboratory, NIST, Gaithersburg, Maryland

Neutron Depth Profiling (NDP) is a non-destructive, isotope-specific, high-resolution nuclear analytical technique, which is often used to probe lithium or boron concentration profiles in different thin substrates. NDP provides depth sensitivities up to a few ten nanometers and the maximum viewing depth is limited to tens of micrometers. The non-destructive nature of the measurement is of special interest for lithium-ion batteries, where the lithium transport processes can be studied during operation. However, due to the limited viewing depth a special battery cell design is required, which is transparent for the charged particles while ensuring an undisturbed battery performance even at low ambient pressures. We present NDP measurements on lithium-ion batteries performed using a newly developed cell design and discuss insights into the lithium transport processes occurring in the anode material during battery operation.

CPP 37.9 Tue 12:00 ZEU 260

Comparison of the effects of solvent additives on the morphology development of printed PPDT2FBT:PC71BM films — •Dan Yang[1], Sebastian Grott[1], Xinyu Jiang[1], Kerstin S. Wienhold[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1,3] — [1]TU München,Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Lichtenbergstr. 1, 85748 Garching, Germany

The morphology and crystallinity of bulk heterojunction (BHJ) films have profound effects on the performance of organic photovoltaics. Currently, most morphological studies on BHJ films are based on spin-coating as deposition technique. However, to commercialize organic photovoltaic products, large-scale fabrication processes such as printing must be taken into consideration. In the present study, the effects of solvent additives on the morphology formation and polymer crystallinity growth of printed BHJ films are investigated by in-situ grazing incidence small/wide-angle X-ray scattering (GISAXS/GIWAXS). The results show that the solvent additives with different boiling points lead to different film drying behaviors, and the phase demixing is changing in the forming BHJ film along with solvent evaporation. These findings provide valuable insights into the film morphology and crystallinity developments of printed BHJ films, which determines the future design of BHJ film printing for large-scale fabrication.

CPP 37.10 Tue 12:15 ZEU 260

Functionalization of Metalloxid surfaces with Porphyrins — •Klaus Götz[1,2], Annemarie Prihoda[1,2], and Tobias Unruh[1,2] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 — [2]Interdisziplinäres Zentrum für Nanostrukturierte Filme, Cauerstr. 3, 91058 Erlangen

Porphyrins are widely studied for their use as catalysts and in dye sensitized solar cells. In these systems the porphyrins are bound to metal oxide surfaces as a functionalizing layer.

We study the binding mechanism in the porphyrin - metal oxide interface on TiO_2 and Co_3O_4. Special emphasis of our work is focused on the exchange process of organic stabilizing molecules with porphyrins. This process is studied using a variation of different scattering techniques. The talk will focus on the characterization of the exchange reaction on the surface of nanoparticles.

Therefore, the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments will be a key element. These measurements are well suited to study core/shell systems. X-rays interact mainly with electrons and therefore SAXS yields information about the inorganic core of the nanoparticles. Neutrons on the other hand are very sensitive to hydrogen and therefore SANS is well suited to get information about the organic stabilizer shell.

The talk will focus on SAXS/SANS measurements and give an overview over complimentary technique. Furthermore, their usage in the characterization of the morphology of the produced particles and the ligand exchange to porphyrins will be presented.

CPP 37.11 Tue 12:30 ZEU 260

Atomistic modelling of confined molecules between atomically flat surfaces — •Jose D. Cojal Gonzalez and Jürgen P. Rabe — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

The contact interface created between an atomically flat cleavage plane of a layered crystal and a 2D material forms a flexible slit or nano pore which can be occupided by (macro)molecules. This arrangement offers a versatile platform for the study of structural, vibrational, elastic and electrical properties of those highly confined molecules. Using molecular dynamics simulations of a graphene-mica slit pore filled with small solvent molecules such as water and ethanol, we provide an instructive model to establish structure and dynamics, i.e. nature and interactions of the molecular layers, mica and graphene. Furthermore, it provides the first step towards the incorporation of larger molecules, such as Rhodamine 6G and dendronized polymers (denpols) in order to complement and better understand the results obtained from Raman spectroscopy and scanning force microscopy measurements.

CPP 37.12 Tue 12:45 ZEU 260

Exploring the Resistive Switching Properties of HfO2 Nanoparticle Assemblies — •Sonam Maiti[1], Chen Liu[1], Thorsten Ohlerth[2], Ulrich Simon[2], and Silvia Karthäuser[1] — [1]Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich GmbH, Germany — [2]Institute of Inorganic Chemistry (IAC), RWTH Aachen University, Germany

Hafnium oxide nanocrystals (NCs) can be considered as possible candidates for further miniaturization of future resistive random access memories. The switching properties of NC assemblies remain under-explored due to difficulties in fabricating ordered structures. Here, we use a facile, low-cost method to prepare highly ordered assemblies of 6 nm HfO2 NCs capped with TOPO via evaporation based self-assembly. X-ray photoelectron spectroscopy is applied to investigate the oxidation state of near surface HfOx under various conditions. Electrical transport measurements were performed on devices with micrometer and nanometer sized gaps to determine the resistive switching character of NCs arrays. They enable the observation of cyclic voltammograms with redox reaction peaks when used with micrometer sized gaps. We discuss the electronic properties of these devices in the light of varying contributions of electronic vs ionic transport and highlight the effect on the device stability. We especially focus on the resistive switching behaviour of the NP assemblies which is dependent on the oxygen vacancy formation under the influence of the capping ligand.

CPP 38: Organic Electronics and Photovoltaics I

Time: Tuesday 9:30–10:45 Location: ZEU 255

CPP 38.1 Tue 9:30 ZEU 255

Exploring the Design Space of Organic Semiconductors — •Christian Kunkel, Johannes T. Margraf, Karsten Reuter, and Harald Oberhofer — Chair for Theoretical Chemistry, Technical University Munich

Improving charge carrier mobilities of organic semiconductors is usually tackled by empirical structural tuning of promising compounds. Computational methods can greatly accelerate such local exploitation of knowledge -namely by exploration-, providing an overview of the problem-specific design space. Here, we intend to provide such an overview for organic semiconductors. In a first approach, we apply data mining strategies to an in-house database of >64.000 organic molecular crystals, annotated with charge-transport descriptors (electronic coupling and the reorganization energy) that are calculated from first principles. Analysing the design space regions in this dataset by a chemical space network hints at already explored or promising regions. From the dataset, we further derive general design principles by evaluating the performance of molecular scaffold and sidegroup clusters of compounds. For these, we find certain scaffolds (sidegroups) to consistently improve charge-transport properties. Functionalizing promising scaffolds with favorable sidegroups then results in molecular crystals with improved charge-transport properties. Secondly, we test algorithms for chemical space exploration, that demonstrate a high efficency in the detection of useful candidate compounds. Both approaches highlight the usefulness of data-based strategies for a targeted design of organic electronics materials.

CPP 38.2 Tue 9:45 ZEU 255

Thiophene based Semiconductors for Organic Solar Cells — •Roy Schaffrinna[1,2], Martina Schwager[2], Julian E. Heger[1], Nian Li[1], Calvin J. Brett[3], Matthias Schwartzkopf[4], Stephan V. Roth[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Hochschule München, Fakultät für Angewandte Naturwissenschaften und Mechatronik, 80335 München — [3]Königliche Technische Hochschule, Mechanik-Department, Teknikringen 8, SE-100 44 Stockholm — [4]Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg

Polythiophene homo- and copolymer derivatives are synthesized by chemical oxidative polymerization and are characterized with optical spectroscopy and grazing-incidence small-angle X-ray scattering (GISAXS). The molecules differ in their inner morphological behavior but also in their optoelectronic properties, which are both designable during polymerization. The organic materials are electrically conductive due to their extended conjugated π-electron system and therefore require neither heavy metals / heavy metal complexes nor dopants for charge transport and can be easily deposited via spin-coating from the liquid phase. The synthesized electron donors are used together with the polymer acceptor PNF222 as active layer in fullerene free full organic solar cells. The devices are fabricated at air conditions, are resistant to illumination and the electrodes require no evaporation of metals from the gas phase.

CPP 38.3 Tue 10:00 ZEU 255

Factors Determining Charge Transfer Energetics for Organic Photovoltaics — Shahidul Alam[1,2], Ulrich S. Schubert[1,2], and •Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), FSU Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), FSU Jena, Germany

Recently, non-fullerene acceptors have received increasing attention for use in polymer-based bulk-heterojunction organic solar cells, as they have demonstrated considerably improved photovoltaic performances over classical polymer-fullerene blends. One part of the success of these materials has been attributed to an increased contribution to the overall absorption of the solar cells, thanks to relatively low bandgaps in these materials. Another part may be related to lower energy or voltage losses through closer adaptation to todays common donor polymers for organic photovoltaics. Since we like to learn more about the general applicability of non-fullerene acceptors as well as about the energy level alignment at the donor-acceptor heterojunction, we studied the latter and consequences thereof for three different donors in conjunction with classical fullerene-derivatives [6,6]-phenyl-C61/C71-butyric acid methyl ester (PCBM/PC70BM) and the exemplari non-fullerene-acceptor 2,2*-[[6,6,12,12-Tetrakis(4-hexylphenyl)-6,12-dihydrodithieno[2,3-d:2*,3*-d*]-s-indaceno[1,2-b:5,6-b*]dithiophene-2,8-diyl]bis[methylidyne(3-oxo-1H-indene-2,1(3H)-diylidene)]]bis[propanedinitrile] (ITIC). We find that rather specific properties of ITIC control the solar cell performance and limit its general application.

CPP 38.4 Tue 10:15 ZEU 255

Bimodal Electronic Interactions in Molecular-doped Conducting Polymers — •Vandana Tiwari[1,2], Ajay Jha[1], Hong-Guang Duan[1], Michael Thorwart[3], and R. J. Dwayne Miller[1,4] — [1]MPSD, Hamburg — [2]Department of Chemistry, University of Hamburg (UH), Germany — [3]I. Institut für Theoretische Physik, UH, Germany — [4]University of Toronto, Canada

Doping is an extremely important process where intentional insertion of impurities in semiconductors controls their electronic properties. Unraveling the favorable electronic interaction between dopant and polymer is the key to the success of molecular doping in organic semiconductors. Here we use two-dimensional electronic spectroscopy to explore the electronic dynamics of F4TCNQ-doped conducting polymers, P3HT and PBTTT in precursor solution mixtures. The electronic interactions among the ion-pairs formed in precursor solutions are captured in the form of off-diagonal peaks connecting the electronic states of polymer and dopant radicals. This electronic interaction represents a well resolved electrostatically bound state, as opposed to a random distribution of ions. We have theoretically modeled our system to simulate the experimental data and achieve a quantitative picture of the Coulombic interaction between cation and anion radicals in solution. Our study reveals the heterogeneous electronic interactions that possibly serve as a seed for the structures in the spin-casted films. This new insight will help pave the way towards rational tailoring of the electronic interactions to improve doping efficiencies in processed organic semiconductor thin films.

CPP 38.5 Tue 10:30 ZEU 255

Excitation lifetime reduction in ensembles of oligoacene molecules attached to argon clusters — •Matthias Bohlen, Moritz Michelbach, Rupert Michiels, and Frank Stienkemeier — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg

The energy conversion efficiency of solar cells is generally limited by the Shockley-Queisser limit [1]. One way to circumvent this limit is through the use of organic photovoltaics (OPV), for which specific charge and energy transfer processes can lead to higher conversion efficiencies. Polyaromatic hydrocarbons, such as oligoacene molecules are promising candidates for OPV applications. In addition to that, these molecules exhibit interesting quantum effects, such as singlet fission, triplet-triplet annihilation or superradiance. Recently anthracene, tetracene and pentacene molecules attached to the surface of neon clusters have been shown to provide interesting model systems for detailed studies of such effects [2]. We have extended these measurements by spectroscopy of oligoacenes deposited onto the surface of argon clusters. The results indicate similar processes as observed for neon clusters, but different magnitudes and timescales of the effects.

[1] W. Shockley and H. J. Queisser, J. Appl. Phys. 32, 510 (1961)
[2] S. Izadnia et al., J. Phys. Chem. Lett. 8,2068 (2017)

CPP 39: Charged Soft Matter, Polyelectrolytes and Ionic Liquids

Time: Tuesday 9:30–12:15 Location: ZEU 114

CPP 39.1 Tue 9:30 ZEU 114

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 39.2 Tue 9:45 ZEU 114

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.

CPP 39.3 Tue 10:00 ZEU 114

Transport properties of two water-in-salt electrolytes: LiTFSI and LiOTF — •Maedeh Zahedifar and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Over the past two decades, “solvent-in-salt” electrolytes have gained attention as a promising electrolyte concept for safer energy storage applications. Water is in principle an ideal solvent, but it has only a small range of electrochemical stability, which does not allow it to be used in high-voltage batteries. However, this limitation can be overcome by using highly concentrated aqueous electrolytes together with LiTFSI and LiOTF [1], so-called water-in-salt electrolytes. In order to better understand the properties of solvent-in-salt electrolyte, we have performed molecular dynamics simulations [2] of mixtures of water molecules with either LiTFSI or LiOTF salts. SPC/E and Lennard-Jones parameters are used for the desription of water molecules and anions, respectively [3]. Values of the viscosity for both LiTFSI and LiOTF salts in water have been derived from the time integral of the stress tensor auto-correlation function. Besides the viscosity, we will discuss further properties of the electrolytes such as radial distribution functions and mean-square displacements, and we will also present results of first-principles electronic structure calculations addressing these electrolytes.
[1] L. Suo et al., Angew. Chem. Int. Ed. **55**, 7136-7141 (2016).
[2] S. Plimpton, J. Comp. Phys. **117**, 1 (1995).
[3] J. Chandrasekhar et al., J. Am. Chem. Soc. **106**, 903 (1984).

CPP 39.4 Tue 10:15 ZEU 114

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 39.5 Tue 10:30 ZEU 114

Helical twist of dsDNA depends on cation type and concentration — •Sergio Cruz-Leon[1], Willem Vanderlinden[2], Jan Lipfert[2], and Nadine Schwierz[1] — [1]Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Max-von-Laue-Str. 3 60438 Frankfurt am Main, Germany — [2]Department of Physics, Nanosystem Initiative Munich and Center for Nanoscience, LMU Munich, Amalienstr. 54, 80799 Munich, Germany

The structural properties of double-stranded (ds)DNA determine many of its biological functions and are central for the development of precise artificial structures in nanotechnological applications. One of the most fundamental and iconic properties of DNA is its helicity, which depends on environmental factors such as temperature and salt concentration. While it has been known that DNA twist changes in a salt-dependent manner, the molecular origin of the effect remains unexplained. Here, we quantify the changes of dsDNA helical properties with ion type and concentration for a set of mono- and divalent cations. We combine single-molecule magnetic tweezers, molecular dynamics simulations, and theoretical modeling, and find that dsDNA changes its helical twist in a unique form depending on both ion type and concentration. Furthermore, we propose a mechanical model that captures the dependence on salt conditions for the changes in the dsDNA structure. Our structural insights and the mechanistic model facilitate the use of ion type and concentration as a tool to delicately manipulate DNA structures, for example, in the growing field of DNA origami technology.

CPP 39.6 Tue 10:45 ZEU 114

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 39.7 Tue 11:00 ZEU 114

The Kinetic Pathway for Polyelectrolyte Coacervate Formation revealed by Time-resolved Synchrotron SAXS — Matthias Amann[1], Jakob Diget[1], Jan-Skov Pedersen[2], Theyencheri Narayanan[3], and •Reidar Lund[1] — [1]Department of Chemistry, University of Oslo, Norway — [2]Aarhus University, Denmark — [3]ESRF, France

The kinetic pathways for coacervation and micelle formation are still not fully understood. Driven by electrostatic interactions and entropically driven counter-ion release, complexation of oppositely charged macromolecules lead to the formation of micellar nanostructures. Here we study the coacervation process, from initial formation and growth of stable micelles, on a nanometric length scale using time-resolved small-angle X-ray scattering (TR-SAXS). The micellar coercevates are formed through the complexation of anionic polyelectrolyte (PSSS) and cationic block copolymer (PEO-b-PVBTA). The results reveal that the formation polyelectrolyte coacervates follows a two-step process; i) first, metastable large-scale aggregates are formed upon a barrier-free complexation immediately after mixing; ii) Subsequently the clusters undergo charge equilibration upon chain rearrangement and exchange processes yielding micellar-like aggregates with net neutral charge that are pinched off to yield the final stable micelle-like coacervates. Interestingly, the overall kinetic process was essentially concentration independent, indicating that the rearrangement process is mainly accomplished via noncooperative chain rearrangement and chain exchange processes.

15 min. break

CPP 39.8 Tue 11:30 ZEU 114

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 39.9 Tue 11:45 ZEU 114

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.

CPP 39.10 Tue 12:00 ZEU 114

Environmental controlled Molecular Plasmon Resonance of Anthracene — •Woldemar Niedenthal[1,2], Dennis Pietruschka[2,3], Doreen Mollenhauer[2,3], and Sangam Chatterjee[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany. — [2]Center for Materials Research, Justus-Liebig-University, Giessen, Germany. — [3]Physikalisch-Chemisches Institut, Justus-Liebig-Universität, Gießen, Germany.

Within the last years polycyclic hydrocarbons (PHCs) were investigated as materials for electrochromic applications. It was proposed that the underlying processes of the color change are based on purely electronic excitation processes, i.e. photon absorption and the formation of molecular plasmons. This mechanisms predict an ultrafast switching speed between the charged and the neutral state. We studied the absorption behavior of charged and neutral anthracene by changing the liquid electrolyte and in devices with polymer-gel-electrolytes by cyclo-voltametric measurements. The experiments show a clear dependence of the color changing process on the electrolyte and polymer surrounding. The results show that the color changing processes of the electrochromic devices are more complex than considered so far. Further investigations are needed to uncover the full effect of the surrounding medium on the colorization processes.

CPP 40: Polymer and Molecular Dynamics, Friction and Rheology

Time: Tuesday 10:45–12:45 Location: ZEU 255

CPP 40.1 Tue 10:45 ZEU 255

Exploring the Properties of Ionomers Through the Use of Coarse Grained Molecular Dynamic Simulations — •Nicholas Michelarakis[1], Konstantinos Gkagkas[2], and Frauke Gräter[1] — [1]Heidelberg Institute for Theoretical Studies, Heidelberg, Germany — [2]Toyota Motor Europe NV/SA, Zaventem, Belgium

The mechanical and structural properties of the Nafion membrane in the core of a Proton Exchange Membrane Fuel Cell (PEMFC) are controlled by the molecular interactions within the Nafion molecules and with the dispersion solvent. The effect of the dispersion solvent on the Nafion membrane assembly process, and on the final Nafion membrane properties (structural morphology, water/solvent content, ion exchange capacity, membrane stability), remains an area of intense study. Here we present a non-equilibrium Coarse Grained Molecular Dynamics method, based on the MARTINI force field, for calculating the dynamic shear viscosity of the Nafion 'ink' used in PEMFC membrane printing; a trait closely correlated to the properties of the final Nafion membrane. In this method, two stationary walls are introduced in the simulation box. A pulling force along the z-axis is then applied to the bottom wall allowing for the simulation of a Couette flow. Using water as an initial test-case we demonstrate that this method has the ability to accurately predict the dynamic shear viscosity of this solvent. This is subsequently extended to a collection of other solvents and Nafion solutions, simulated under PEMFC printing conditions, indicating that this approach has the ability to recapitulate the dynamic viscosity values calculated experimentally.

CPP 40.2 Tue 11:00 ZEU 255

Polymer electrolytes: how do they react upon application of an external electric field? — Alina Wettstein, Diddo Diddens, and •Andreas Heuer — Inst. Phys. Chemie, WWU Muenster, Germany

Polymer electrolytes are of utmost relevance for many applications of lithium ion batteries. Close to the electrodes they are exposed to high electric fields. Here we present extensive molecular dynamics simulations of a standard polymer electrolyte (poly(ethylene oxide) with a lithium salt) for different applied electric fields up to a few Volt per nanometer. We observe a prominent dependence of structural and dynamical properties on the electric field, reflecting nonlinear effects. It is shown that studying the field dependence allows one to characterize the motional mechanisms for the lithium transport in these electrolytes. Furthermore, several key questions can be answered: (1) Does the strong increase of the mobility upon increasing electric field result from the corresponding change of structural features? (2) Is it possible to identify the underlying reasons for structural field dependencies? Finally, the results are compared with corresponding experimental studies of the same system [1].

[1] M. Rosenwinkel and M. Schönhoff, J. Electrochem. Soc. 166, A1977-A1983 (2019).

15 min. break

CPP 40.3 Tue 11:30 ZEU 255

dynamics of ring on polymer in polyrotaxane investigated by quasi-elastic neutron scattering and MD simulation — •koichi mayumi[1], yusuke yasuda[1], takeshi yamada[2], kazushi fujimoto[3], susumu okazaki[3], hideaki yokoyama[1], and kohzo ito[1] — [1]The University of Tokyo, Chiba, Japan — [2]CROSS, Ibaraki, Japan — [3]Nagoya University, Aichi, Japan

We study molecular dynamics of polyrotaxane (PR), composed of alpha-cyclodextrins (CDs) and a poly(ethylene glycol) (PEG) axis chain, in solution by means of quasi-elastic neutron scattering (QENS) measurements and full-atomistic molecular dynamics (MD) simulations [1]. From the QENS experiments on PR with hydrogenated PEG (hPR) and that with deuterated PEG (dPR), we separately estimated the translational diffusion coefficients of CD and PEG monomers in PR solutions. For further analysis, we performed full-atomistic MD simulations on PR solutions. By analyzing the simulation results, we succeeded for the first time in observing and quantifying the sliding motion of CD along PEG chain. The sliding diffusion coefficient is formulated by a combination of Brownian diffusion term and Arrhenius-like jump diffusion term with an energy barrier along the axial chain.

[1] Y. Yasuda, Y. Hidaka, Y., K. Mayumi, T. Yamada, K. Fujimoto, S. Okazaki, H. Yokoyama, K. Ito, J. Am. Chem. Soc., 141, 9655 (2019).

CPP 40.4 Tue 11:45 ZEU 255

Local polymer chain mobility under shear — Benjamin Kohn[1], Roland Vogel[1], Petrik Galvosas[2], and •Ulrich Scheler[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V — [2]Victoria University of Wellington

The NMR transverse relaxation T2 is sensitive to the slow motion of polymer chain segments. In entangled polymers at least two components are observed, a short one for chain segments with restricted motion due to entanglements and a longer component originating from the more free chain segments. Here the effect of external shear in a Searle cell as used in rheological experiments is studied. For short polymer chains little effect of shear is observed while for high molecular weight with clear signs of entanglement both components become longer. This is indicative of longer chain segments between entanglements, which results from loss of entanglements or rearrangement resulting in longer chain segments between entanglements. A new experimental setup permits measuring NMR relaxation under oscillatory shear varying both amplitude and frequency. The resulting strain-rate dependence shows that the prolongation of the relaxation time indicating longer chain segments between entanglements starts at a strain of at least 100 for entangled PDMS.The combination of PFG NMR with NMR imaging in the same setup allows to measure flow pattern. At the turning point of the oscillation for low-viscosity fluids a counterflow is observed.

CPP 40.5 Tue 12:00 ZEU 255

The instability onset behavior of viscoelastic Taylor-Couette flow as a combined function of flow geometry and rheological parameters: purely elastic versus thermo-elastic instabilities — •Reza Ghanbari[1,3] and Bamin Khomami[1,2] — [1]MRAIL (Material Research and Innovation Lab), Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, USA — [2]Sustainable Energy and Education Research Center (SEERC), University of Tennessee, Knoxville, USA — [3]Present: Adolphe Merkle Institute, University of Fribourg, Chemin des Verdiers 4, CH-1700 Fribourg, Switzerland

Linear stability analysis of Taylor-Couette flow (TCF) of dilute polymer solutions has been performed by using prototypical constitutive equations for polymeric solutions, namely, the Oldroyd-B & the FENE-P models. The hydrodynamic stability characteristics of the flow in the presence & absence of thermal effects & in the limit of vanishing fluid inertia have been determined using an eigenvalue analysis. Particular attention has been paid to determine the instability onset conditions as a function of fluid thermal sensitivity & gap ratio. We observed a reduction in the critical Weissenberg (Wic) for the instability onset as the gap ratio & fluid thermal sensitivity are enhanced. In particular, under non-isothermal conditions, Wic was reduced by almost an order of magnitude for all gap ratios. Our results suggest that recent experimental observations of purely elastic turbulence in the TCF at order (1) Wi were not performed under isothermal conditions. Hence, this new flow state should be labeled as thermo-elastic turbulence.

CPP 40.6 Tue 12:15 ZEU 255

Rheological and diffusion properties of solutions of polyethersulfone and poly(N-vinyl pyrrolidone) for membrane fabrication — •Ulrich A. Handge[1], Oliver Gronwald[2], Martin Weber[2], Joachim Koll[1], Clarissa Abetz[1], Birgit Hankiewicz[3], and Volker Abetz[3] — [1]Helmholtz-Zentrum Geesthacht, Institute of Polymer Research, Max-Planck-Strasse 1, 21502 Geesthacht, Germany — [2]BASF SE, Advanced Materials & Systems Research, Performance Polymer Blends & Membranes RAP/OUB, Carl-Bosch-Strasse 38, 67056 Ludwigshafen, Germany — [3]University of Hamburg, Institute of Physical Chemistry, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Membranes of polyethersulfone (PESU) and poly(N-vinyl pyrrolidone) (PVP) are commonly used for ultrafiltration applications. We investigate the rheological and diffusion properties of solutions which are used for membrane fabrication via a non-solvent induced phase separation process. The polymer solutions are composed of PESU and PVP as well as a mixture of the solvent N-methyl-2-pyrrolidone (NMP) and the non-solvent glycerol. In this work, the influence of glycerol is studied. The addition of glycerol leads to a larger viscosity, a larger average relaxation time and a stronger tendency of demixing. The increase of viscosity is explained by the increase of the monomeric friction coefficient with increasing glycerol concentration. Dynamic light scattering data reveal the existence of two diffusive processes with different time scales in the presence of glycerol. This result is discussed taking into account the phase behaviour of the solution and the solvent quality.

CPP 40.7 Tue 12:30 ZEU 255

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 41: Organic Thin Films, Organic-Inorganic Interfaces I (joint session DS/CPP)

Time: Tuesday 9:30–11:00 Location: CHE 91

CPP 41.1 Tue 9:30 CHE 91

Shape controlled assembly of carboxylic acids: intercalation into molecular nanotunnels — Rodrigo Ortiz de la Morena[1], Andika Asyuda[2], Hao Lu[2], Hannah Aitchison[1], Kelly Turner[1], Stephen M. Francis[1], •Michael Zharnikov[2], and Manfred Buck[1] — [1]EaStCHEM School of Chemistry, University of St Andrews, North Haugh, St Andrews KY16 9ST, United Kingdom — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Binary self-assembled monolayers (SAMs) combining a Y-shaped aromatic carboxylic acid (CA), 1,3,5-benzenetribenzoic acid (H3BTB), and a cage-type alicyclic CA, adamantane CA (AdCA), were prepared by molecular adsorption from solution on Au substrates modified by underpotential deposition of Ag. These SAMs exhibit a pronounced dependence of their structure on the assembly protocol. Exposing an AdCA SAM to H3BTB results in the disordered arrangements. In contrast, exposing an H3BTB SAM to AdCA doesn't seemingly affect the highly regular row structure of the native H3BTB layer, with no signs (STM) of AdCA adsorption. However, spectroscopic analysis reveals its presence, suggesting that the AdCA molecules are hidden in the nanotunnels of the H3BTB monolayer. Additional evidence for this hypothesis is provided by appearance of densely packed and highly ordered AdCA monolayer upon local removal of H3BTB. Formation of such a compact layer is explained by expulsion of AdCA from the H3BTB nanotunnels of the surrounding intact mixed SAM, driven by release of stress in the nanotunnels built up when AdCA is intercalated.

CPP 41.2 Tue 9:45 CHE 91

Reestablishing odd-even effects in anthracene-derived monolayers by introduction of a proper symmetry — Christoph Partes[1], Eric Sauter[2], Michael Gärtner[1], Martin Kind[1], Andika Asyuda[2], Michael Bolte[1], Andreas Terfort[1], and •Michael Zharnikov[2] — [1]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

A series of anthracene[2,3-d]oxazolyl-2-alkylthioacetates (AOxCnSAc) with n = 2-6 methylene groups in the alkyl chain were designed and synthesized to investigate the influence of the substitution along the long axis of the molecule on the structural behavior of the respective self-assembled monolayers (SAMs) on Au(111). While in previous work anthracene-terminated alkanethiols, in which the alkyl group was attached to the off-axis 2-position of the acene, showed an exceptionally small influence of the number of methylene groups (n) in the aliphatic linker, the new system exhibits a strong dependence of almost all monolayer properties on the length of the aliphatic linker, with the parity of n being the decisive parameter - so-called odd-even effects. The high quality and well-defined character of these SAMs, along with a low band gap of only 3.0 eV, make them relevant for application in organic and molecular electronics.

CPP 41.3 Tue 10:00 CHE 91

Exploring Electron Beam Induced Processing on Porphyrin Multilayers for the Fabrication of Nanostructured Ultrathin Membranes — •Christian Preischl, Elif Bilgilsoy, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II Friedrich-Alexander Universität Erlangen-Nürnberg

We investigate two gas-assisted electron beam lithography methods, i.e. Electron-Beam-Induced-Deposition and Electron-Beam-Induced-Surface-Activation (EBISA) on porphyrin multilayers. In EBISA, a surface is irradiated by a focused electron beam, resulting in an activation of the exposed area. The activated areas can then lead to the decomposition of suitable precursor gases.[1] Here we show that EBISA on thin layers of a free-base porphyrin (2HTPP) is compatible with the precursors $Fe(CO)_5$ and $Co(CO)_3NO$[2]. Remarkably, the latter exhibited no EBISA-reactivity on other activated organic substrates like Self-Assembled-Monolayers or Surface-Anchored Metal-Organic Frameworks[3]. We also demonstrate that thin layers of 2HTPP can be cross-linked to form a 2D carbon membrane via low energetic electron irradiation. This membrane is stable enough to transfer the metallic nanostructures onto any desirable substrate.

[1] H. Marbach, Appl.Phys. A 117 (2014) 987 [2] M. Drost et al., Small Methods 1 (2017) 1700095 [3] M. Drost et al., ACS Nano 12 (2018) 3825

CPP 41.4 Tue 10:15 CHE 91

Fabrication of metallic nanostructures via FEBIP on top of ultrathin organic membranes — •Alexander Wolfram, Christian Preischl, Elif Bilgilsoy, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, GER

We report a novel method to fabricate ultrathin organic membranes with metallic nanostructures. In a first step, clean iron nanostructures were prepared on a self-assembled-monolayer (SAM) of 1,1',4',1"-terphenyl-4-thiol (TPT) via Electron-Beam-Induced-Deposition (EBID) by using $Fe(CO)_5$ as precursor.[1] In a next step, the SAM is converted into a carbon nanomembrane (CNM) by using low energetic electron-induced crosslinking.[2] In a third step, the membrane was then transferred onto SiO_2 or a TEM grid. We demonstrate that the nanostructures maintain their shape and the membrane remains intact during the transfer. In this way, metallic nanostructures on a free-standing CNM can be fabricated. We also show the influence of the underlying substrate (Ag or Au) of the SAM and the associated wet chemical process on the appearance of the transferred nanostructures.

[1] M. Walz et al., *Angew. Chem. Int. Ed.*, 49 (2010) 4669 [2] A. Turchanin, A. Gölzhäuser, *Advanced Materials*, 28 (2016) 6075.

CPP 41.5 Tue 10:30 CHE 91

Interfaces between Tetraphenylporphyrin and Low-Work Function Metals: Interphase Formation Studied with HAXPES — •Maik Schöniger, Stefan R. Kachel, Jan Herritsch, Philipp Schröder, Claudio K. Krug, Mark Hutter, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Fabrication of organic electronic devices often involves the electrical contacting of organic semiconductors by vapor deposition of metals, resulting in the formation of metal-organic interfaces. These interfaces are crucial for the device's performance in terms of e.g. charge-carrier injection. However, especially metals with low work function can diffuse into and react with the organic material, leading to extended interphases consisting of the reaction products. The question then is: How thick is the formed interphase? As well-defined model systems, we investigated metalloporphyrin (M_xTPP) interphases formed through reaction of tetraphenylporphyrin (H_2TPP) with different vapor-deposited metals M, including earth alkalines (Mg, Ca) and the alkali metal Li. The non-destructive depth-profiling technique of choice is hard X-ray photoelectron spectroscopy (HAXPES), because H_2TPP and M_xTPP can be distinguished by their N 1s signals. Compared to earlier work with Fe and Co, Mg and Ca show increased reaction depths up to few nanometers. In the case of Li, complete reaction to Li_2TPP was observed in a 24 nm thick H_2TPP film. TPD-MS results showed that even thicker H_2TPP layers fully react.

CPP 41.6 Tue 10:45 CHE 91

Extended Interphase Formation at a Metal/Organic Interface: Lithium on Tetraphenylporphyrin — •Stefan Renato Kachel, Maik Schöniger, Jan Herritsch, Philipp Schröder, Mark Hutter, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Porphyrins are versatile model compounds for organic semiconductors (OSC) in application-related studies of metal/organic interfaces. The properties of such interfaces strongly influence the performance of organic electronic devices. To study processes at the interface between an OSC and a low work-function metal, lithium was deposited onto tetraphenylporphyrin (H2TPP) layers and the product composition was analyzed with temperature-programmed desorption mass spectrometry (TPD-MS) and X-ray photoelectron spectroscopy (XPS). With sufficient amounts of Li, we found complete conversion of H2TPP into dilithium tetraphenylporphyrin (Li2TPP). The depth range of this reaction exceeds several 10 nm, contrasting previous findings for transition metals. Even a 50 nm thick layer of H2TPP fully reacted with an excess of Li. For substoichiometric amounts of Li, singly metalated LiHTPP was found. This study shows that the metal/organic interface can be very diffuse with a thick reacted interphase layer separating the metal from the pristine OSC.

CPP 42: Data analytics for dynamical systems I (joint session SOE/DY/CPP/BP)

Data analytics is often focussed on (generalized) regression to create models of the structure of complex systems. Here we focus on data-driven approaches of data analytics for complex systems that take into account their intrinsic nonlinear dynamics. Applications to natural and human-made systems, from cardiac dynamics to human mobility, illustrate recent progress and current methodological challenges. (Session organized by Marc Timme)

Time: Tuesday 9:30–13:15 Location: GÖR 226

Topical Talk CPP 42.1 Tue 9:30 GÖR 226
One model to rule them all — •Jens Timmer — Institute of Physics, University of Freiburg, Germany

A major goal in systems biology is to reveal potential drug targets for cancer therapy. A common property of cancer cells is the alteration of signaling pathways triggering cell-fate decisions resulting in uncontrolled proliferation and tumor growth. However, addressing cancer-specific alterations experimentally by investigating each node in the signaling network one after the other is difficult or even not possible at all. Here, we use quantitative time-resolved data from different cell lines for non-linear modeling under L1 regularization, which is capable of detecting cell-type specific parameters. To adapt the least-squares numerical optimization routine to L1 regularization, sub-gradient strategies as well as truncation of proposed optimization steps were implemented. Likelihood-ratio tests were used to determine the optimal penalization strength resulting in a sparse solution in terms of a minimal number of cell-type specific parameters that is in agreement with the data. The uniqueness of the solution is investigated using the profile likelihood. Based on the minimal set of cell-type specific parameters experiments were designed for improving identifiability and to validate the model. The approach constitutes a general method to infer an overarching model with a minimum number of individual parameters for the particular models.

CPP 42.2 Tue 10:00 GÖR 226
Volatility and Fractionality in Power-Grid Frequency — •Leonardo Rydin Gorjão[1,2], Anton Yurchenko-Tytarenko[3], and Dirk Witthaut[1,2] — [1]Forschungszentrum Jülich, Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), 52428 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — [3]Department of Mathematics, University of Oslo, P.O. Box 1053 Blindern, N-0316 Oslo

Power-grid frequency is a key indicator of stability in power grids. The trajectory of power-grid frequency embodies several processes of different natures: the control systems enforcing stability, the trade markets, production and demand, and the correlations between these. In this article, we study power-grid frequency from Central Europe, the United Kingdom, and Scandinavia under the umbrella of fractional stochastic processes. We introduce an estimator of the Hurst index for fractional Ornstein–Uhlenbeck processes. We show that power-grid frequency exhibits time-dependent volatility, driven by daily human activity and yearly seasonal cycles. Seasonality is consistently observable in smaller power grids, affecting the correlations in the stochastic noise. The United Kingdom displays daily rhythms of varying volatility, where the noise amplitude consistently doubles its intensity, and displays bi- and tri-modal distributions. Both the Scandinavian and United Kingdom power-grids exhibit varying Hurst indices over yearly scales. All the power grids display highly persistent noise, with Hurst indices above $H > 0.5$.

Topical Talk CPP 42.3 Tue 10:15 GÖR 226
Gaming the system - Analyzing Uber price data reveals anomalous supply shortages — •Malte Schröder[1], David Storch[1], Philip Marszal[1], and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden — [2]Lakeside Labs, Klagenfurt

Dynamic pricing schemes are ubiquitously employed across industries to balance demand and supply. One well-known example is the ride-hailing platform Uber and their *surge pricing* intended to incentivize drivers to offer their service during times of high demand. However, recent reports [WJLA, Uber, Lyft drivers manipulate fares at Reagan National causing artificial price surges (2019)][Möhlmann and Zalmanson, ICIS 2017 Seoul (2017)] indicate that this surge pricing may instead cause demand-supply imbalances by incentivizing drivers to switch off their app to increase their revenue. Analyzing price estimate time series for trips from 137 locations in 59 urban areas across six continents, we identify locations with strong, repeated price surges. Correlations with demand patterns demonstrate that the observed price surges are indeed driven by supply anomalies instead of demand fluctuations. Moreover, we capture the minimal incentives driving the supply dynamics in a simple game-theoretic model, illustrating that such incentives constitute generic consequences of dynamic pricing schemes.

CPP 42.4 Tue 10:45 GÖR 226
Estimation of Langevin equations with correlated noise for signals of complex systems — •Clemens Willers and Oliver Kamps — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Germany

Over the last years, the estimation of stochastic evolution equations of complex systems has been applied in many scientific fields ranging from physics to biology and finance. Especially, Langevin models with delta-correlated noise terms, which realize a Markovian dynamic, have been used successfully in this context [1]. However, many real world data sets exhibit correlated noise and a non-Markovian dynamic, for example data sets from turbulence [2].

To tackle this problem, we use Langevin models containing an added hidden component which realizes a driving correlated noise. We develop two methods for the systematic estimation of the drift- and diffusion functions, parameterized through spline functions. The first method is based on a likelihood function which is constructed by a short-time propagator for the measured values of the visible component. For the second method, we use a comparison of transition probabilities via Jensen-Shannon divergence. Both methods are demonstrated using real world data sets as the turbulent air flow of a free jet [3], stock market prices [4] and wind energy production [5].

[1] Friedrich et al., Phys. Rep. 506, 87 (2011) [2] Friedrich et al., Phys. Rev. Lett. 78, 863 (1997) [3] Renner et al., J. Fluid Mech. 433, 383 (2001) [4] Nawroth et al., Eur. Phys. J. B 50, 147 (2006) [5] Kamps, in Wind Energy-Impact of Turbulence, Springer 2014, p. 67.

CPP 42.5 Tue 11:00 GÖR 226
Hyper-Parameter Optimization for Identification of Dynamical Systems — •Tobias Wand[1], Alina Steinberg[1], Tim Kroll[2], and Oliver Kamps[2] — [1]Institut für Theoretische Physik, Universität Münster, Deutschland — [2]Center for Nonlinear Science, Universität Münster, Deutschland

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. If more than one hyper-parameter has to be fine-tuned, simple methods like grid search are computationally expensive and due to this, sometimes not feasible. In this talk, we will introduce different approaches to optimally select the hyper-parameters for the identification of sparse dynamical systems.

[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

Topical Talk CPP 42.6 Tue 11:15 GÖR 226
Data driven modelling of spatio-temporal chaos in extended dynamical systems — •Ulrich Parlitz[1,2], Sebastian Herzog[1,3], Florentin Wörgötter[3], Roland S. Zimmermann[1,2], Jonas Isensee[1,2], and George Datseris[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institut für Dynamik komplexer Systeme, Georg-August-Universität

Göttingen, Germany — [3]Drittes Physikalische Institut, Georg-August-Universität Göttingen, Germany

Many spatially extended nonlinear systems, an example being excitable media, exhibit complex spatio-temporal dynamics. We shall present machine learning methods to predict the temporal evolution of these systems or estimate their full state from limited observations. The applied techniques include Reservoir Computing [1] and a combination of a Convolutional Autoencoder with a Conditional Random Field [2,3], whose perfomance will be compared to Nearest Neighbours Prediction based on dimension reduced local states [4]. Examples for demonstrating and evaluating the methods employed include the Lorenz-96 model, the Kuramoto-Sivashinsky equation, the Barkley model, and the Bueno-Orovio-Cherry-Fenton model, describing cardiac (arrhythmia) dynamics.
[1] R. S. Zimmermann and U. Parlitz, Chaos 28, 043118 (2018)
[2] S. Herzog et al., Front. Appl. Math. Stat. 4, 60 (2018)
[3] S. Herzog et al., Chaos (to appear) (2019)
[4] J. Isensee, G. Datseris, U. Parlitz, J. of Nonlinear Sci. (2019)

CPP 42.7 Tue 11:45 GÖR 226

Predicting Spatio-Temporal Time Series Using Dimension Reduced Local States — •Jonas Isensee[1,2], George Datseris[1,2], and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institut für Dynamik komplexer Systeme, Georg-August Universität Göttingen, Germany

Understanding dynamics in spatially extended systems is central to describing many physical and biological systems that exhibit behaviour such as turbulence and wave propagation. Correctly predicting dynamics is advantageous in experimental settings and data-driven approaches are useful, particularly when no adequate mathematical models are available. We present an approach to iterated time series prediction of spatio-temporal dynamics based on local delay coordinate states and local modeling using nearest neighbour methods [1]. A crucial step in this process is to find predictive yet low-dimensional descriptions of the local dynamics . We discuss how imposing symmetries on the dynamics can be used to increase the predictiveness of our approach. The efficacy of this approach is shown for (noisy) data from a cubic Barkley model, the Bueno-Orovio-Cherry-Fenton model.

[1] J. Isensee, G. Datseris, U. Parlitz, J. of Nonlinear Sci. (2019)

Topical Talk CPP 42.8 Tue 12:00 GÖR 226

Limits to predictability of complex systems dynamics — Jonathan Brisch and •Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Motivated by the challenges of weather forecasting and the well known fact that atmospheric dynamics takes place on many temporal and spatial scales, we discuss the possibility of scale dependent error growth and its consequences for predictions. In case that the growth rate of small errors depends on the error magnitude as an inverse power law, we can explain why forecasts of macroscopic observables can be successful on time scales which are orders of magnitude longer than the (estimated) Lyapunov time, and at the same time we find a strictly finite prediction horizon even for arbitrary accuracy of the initial condition. We propose a hierarchical model class, which is able to generate such an error growth behaviour, and finally we re-analyze published data of error-growth in a numerical weather forecast system to present evidence that the error growth rate there is indeed consistent with a power law with diverging growth rate for infinitesimal errors. It is plausible that the same mechanism is active in other complex phenomena which live on a variety of spatial and temporal scales.

CPP 42.9 Tue 12:30 GÖR 226

Network inference from event sequences: Disentangling synchrony from serial dependency — •Reik Donner[1,2], Forough Hassanibesheli[2,3], Frederik Wolf[2,3], and Adrian Odenweller[4,5] — [1]Magdeburg-Stendal University of Applied Sciences, Magdeburg — [2]Potsdam Institute for Climate Impact Research — [3]Department of Physics, Humboldt University, Berlin — [4]Center for Earth System Research and Sustainability, University of Hamburg — [5]Max Planck Institute for Meteorology, Hamburg

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.

CPP 42.10 Tue 12:45 GÖR 226

Reconstruction of nonlinear correlations and dynamical laws — Mirko Rossini, Konstantin Schmitz, and •Jürgen Stockburger — ICQ, Ulm University, Germany

Time series taken from a stationary process may feature dependencies far more subtle than linear correlations. We introduce a method based on non-linear feature extraction which can uncover and quantify such dependencies. Its utility is demonstrated using both synthetic and real-world data.

CPP 42.11 Tue 13:00 GÖR 226

Collective Response of Reservoir Networks — •Arash Akrami, Fabio Schittler Neves, Xiaozhu Zhang, Malte Schröder, and Marc Timme — Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden

Reservoir Computing constitutes a paradigm of bio-inspired machine learning relying on dynamical systems theory, that exploits high dimensionality of a large network of processing units (reservoir). However, as the collective dynamics of artificial neural networks is far from understood, their learning outcome is hardly predictable or transparent.

In Reservoir Computing systems, learning occurs exclusively in a read-out layer, with the intrinsic reservoir dynamics freely evolving.

Here we study reservoirs of processing units with linear activation functions, i.e., linear reservoirs and analytically predict the dynamic responses of all network units as a function of general, distributed and time-dependent input signals. These insights may help identifying nodes especially suitable for receiving input signals, and finding minimal reservoirs capable of performing a given task.

CPP 43: Active Matter II (joint session BP/DY/CPP)

Time: Tuesday 9:30–13:00 Location: HÜL 386

CPP 43.1 Tue 9:30 HÜL 386

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. The relevant parameters are the ratio of swimming to bulk sedimentation velocity and the normalized torque.

In the state diagram of these parameters, for neutral squirmers we observe sedimentation at strong gravitational forces and inverted sedimentation at finite torques, when activity dominates. In between, we identify plumes of collectively sinking squirmers that feed convective rolls of circling squirmers at the bottom of the simulation cell. At velocity ratios slightly above one and large torques squirmers form a spawning cluster, which floats above the bottom wall and 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] J.-T. Kuhr, *et al.*, Soft Matter **13**, 7548 (2017).
[3] H. Jeckel, *et al.*, PNAS **116**, 1489 (2019).
[4] T.J. Pedley, and J.O. Kessler, Annu. Rev. Fluid Mech. **24**, 313 (1992).

CPP 43.2 Tue 9:45 HÜL 386

Sculpting vesicles with active particles — Masoud Hoore[1], Clara Abaurrea-Velasco[1], Hanumantha Rao Vutukuri[2], Thorsten Auth[1], Jan Vermant[2], Gerhard Gompper[1], and •Dmitry Fedosov[1] — [1]Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Materials, ETH Zürich, 8093 Zürich, Switzerland

Biological cells are able to generate intricate structures and respond to external stimuli, sculpting their membrane from inside. Simplified biomimetic systems can aid in understanding the principles which govern these shape changes and elucidate the response of the cell membrane under strong deformations. We employ a combined simulation and experimental approach to investigate different non-equilibrium shapes and active shape fluctuations of vesicles enclosing self-propelled particles. Interestingly, the most pronounced shape changes are observed at relatively low particle loadings, starting with the formation of tether-like protrusions to highly branched, dendritic structures. At high volume fractions, globally deformed vesicle shapes are observed. The obtained state diagram of vesicles sculpted by active particles predicts the conditions under which local internal forces can generate dramatic cell shape changes, such as branched structures in neurons.

CPP 43.3 Tue 10:00 HÜL 386

Diffusing Activity: Active Particles in Evolving Environments — •Nima H. Siboni, S. Mohsen J. Khadem, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

We study the dynamics of a single active Brownian particle (ABP) and the collective behavior of interacting ABPs in a heterogeneous medium. We apply the idea of the diffusing diffusivity model [1] to mimic the environmental heterogeneity in the equation of motion of the ABPs via a time-dependent activity and diffusivities. In our model, the fluctuations of the environment affect simultaneously and similarly the motility and diffusion coefficients. We obtain analytically the probability distribution function of the particle displacement and its moments and support our results via particle-based simulations. We finally investigate the impact of the introduced fluctuations on the collective behavior of ABPs. We obtain the phase diagram of motility-induced phase separation [2,3] for a wide range of noise strength and compare our results with that for the conventional ABPs [4].

[1] M. V. Chubynsky and G. W. Slater, Phys. Rev. Lett. **113**, 098302 (2014).
[2] I. Buttinoni, J. Bialké, F. Kümmel, H. Löwen, C. Bechinger, and T. Speck, Phys. Rev. L. **110**, 238301 (2013).
[3] J. Stenhammar, A. Tiribocchi, R. J. Allen, D. Marenduzzo, and M. E. Cates, Phys. Rev. L. **111**, 145702 (2013).
[4] S. M. J. Khadem, N. H. Siboni, and S. H. L. Klapp, in preparation.

CPP 43.4 Tue 10:15 HÜL 386

Phoretic interactions of two chemically-active particles — •Babak Nasouri[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Catalytically-coated active particles in a viscous medium interact with one another by altering the chemical and hydrodynamic fields in their surroundings. Such phoretic interactions may drive particles in motion and are strongly dependent on the physico-chemical properties of the system, namely: the response of the particles to the interaction fields, and geometric factors such as inter-particle distances and particle sizes. In this work, we discuss an analytical approach which can accurately capture the dynamical behaviour of two phoretic spherical particles, for any given configuration.

CPP 43.5 Tue 10:30 HÜL 386

Axisymmetric spheroidal squirmers and self-diffusiophoretic particles — Ruben Poehnl[1], •Mihail Popescu[2], and William Uspal[1] — [1]Dept. of Mech. Eng., Univ. of Hawai'i at Manoa, 2540 Dole St., Honolulu, HI 96822, USA — [2]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany

By using previously published analytical solutions for Stokes flow around a spheroid, here we investigate the motion of a spheroidal, axisymmetric squirmer in an unbounded fluid and the low Reynolds number hydrodynamic flow induced by the squirmer.

In contrast to the case of a spherical squirmer, for the spheroidal squirmer each slip mode either contributes to the velocity, or contributes to the stresslet. Additionally, and also distinct from the case of a spherical squirmer, each slip mode excites either all of the fore-aft symmetric or fore-aft asymmetric components of the flow field, respectively. Accordingly, with small modifications of the squirming pattern, a microrganism could maintain its velocity unchanged but dramatically alter the topology of the flow around it. This raises the interesting speculative question as whether the spheroidal shape is providing an evolutionary advantage, i.e., a spheroidal squirmer possesses simple means – not available to a spherical one – for acting in hydrodynamic disguise, which can be advantageous as either predator or prey.

The results are straightforwardly extended to the self-phoresis of axisymmetric, spheroidal, chemically active particles with phoretic slip.

CPP 43.6 Tue 10:45 HÜL 386

Active particle penetration through a planar elastic membrane — •Abdallah Daddi-Moussa-Ider[1], Benno Liebchen[1,2], Andreas M Menzel[1], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Theorie Weicher Materie, Fachbereich Physik, Technische Universität Darmstadt, Germany

Active penetration of nanoparticles through cell membranes is an important phenomenon which has various biomedical and clinical applications. Using particle-based computer simulations and theory, we study the penetration mechanism of an active or externally driven particle through a planar elastic membrane. We model the membrane as a self-assembled sheet of particles embedded in a viscous fluid. We introduce a coarse-grained model to describe the mutual interactions between the membrane particles. We identify three distinct scenarios, including trapping of the active particle, penetration through the membrane with subsequent self-healing, in addition to penetration with permanent disruption of the membrane. The latter scenario may be accompanied by a partial fragmentation of the membrane into bunches of isolated or clustered particles. Our approach might be helpful for the prediction of the transition threshold between the trapping and penetration states in real-space experiments involving motile swimming bacteria or artificial self-propelling active particles. Reference: Daddi-Moussa-Ider *et al.*, Theory of active particle penetration through a planar elastic membrane, *New J. Phys.* **21**, 083014 (2019).

30 min. coffee break

Invited Talk CPP 43.7 Tue 11:30 HÜL 386

Physics of Growth: Another Form of Active Matter — •Jens Elgeti — Foschungszentrum Jülich, Germany Theoretical Soft Matter and Biophysics

Active matter is matter, driven out of equilibrium by its microscopic constituents. Growing mater is also active matter, but activity does not enter via the stress, but in material conservation. The material generates itself – think cells dividing or a tumor growing. Growth implies a change in volume. In physical terms, the conjugate force to volume is pressure. Thus, in order to grow, cells must exert mechanical pressure. In turn, pressure influences growth. This yields to interesting novel phenomena like infinite compressibility, self contracting materials and steady tread-milling states.

We use particle based simulations to study mechanical properties and effects in growing matter. These simulations have been helpful in understanding, interpreting and designing experiments. I will present an overview of the simulation technique, and several examples of how this model helped to gain insight in mechanical processes underlying tissue growth, ranging from growth of cancer spheroids under pressure [1], to *in silico* competition experiments [2-5] and tumor evolution [6].

[1] Montel et al., PRL **107**, 188102 (2011)
[2] Podewitz et al., EPL **109**, 58005 (2016)
[3] Basan et al., Phys. Biol. **8**, 026014 (2011)
[4] Podewitz et al., New J. Physics **18**, 083020 (2016)
[5] Ganai et al., New J. Phys. **21** 063017 (2019)
[6] Büscher et al., arxiv:1910.03263 (2019)

CPP 43.8 Tue 12:00 HÜL 386

The effect of hydrodynamic interactions on self-propulsion of multiple swimmers — •Sebastian Ziegler[1], Maxime Hubert[1], Thomas Scheel[2], Jens Harting[2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Friedrich-Alexander-Universität 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, such models, however, underestimate the impact of one swimmer's stroke on the stroke of all others, reducing the problem of hydrodynamic interactions to a purely geometric one. Furthermore, a number of experimental systems are associated with imposing the forces driving each of the devices. This situation is, from a theoretical point of view, significantly more demanding and has not been investigated so far for multiple swimmers. This issue is addressed in this presentation where we employ a recently developed perturbative calculation and numerical modeling to study the effects of nearby swimmers on the stroke, swimming speed and direction. Notably, we find that for two swimmers, a significant fraction of the parameter space results in both swimmers experiencing a boost from one another. We identify the key characteristics that yield this effect.

CPP 43.9 Tue 12:15 HÜL 386

Active particle scattering in structured and random 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 pillars of sufficiently small radius, self-propelled particles can slide along the surface of a pillar without becoming trapped over long times. Using simulations and theory, we study the impact of different modes of obstacle interaction on the diffusive transport of active particles in a lattice of such obstacles. We find that sliding along obstacles can result in large diffusivities even at high obstacle density, unlike particles that undergo classical specular reflection, as in the Lorentz gas. We introduce a microscopically derived run-and-tumble model, which describes the macroscopic transport for different scattering rules very well, and test it in microfluidic channels for E.coli. Finally, we discuss the role of tumbling in structured and random environments.

CPP 43.10 Tue 12:30 HÜL 386

Swimming behavior of squirmer dumbbells and polymers — •Judit Clopés Llahí, Gerhard Gompper, and Roland G. Winkler — Theoretical Soft Matter and Biophysics, Institute for Advanced Sim- ulation 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 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.: [1] J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. 78, (2015). [2] R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, (2017). [3] A. Martin-Gomez, T. Eisenstecken, G. Gompper, R. G. Winkler, Soft Matter 15, (2018).

CPP 43.11 Tue 12:45 HÜL 386

The step-wise induction of transcription drives morphological changes in aggregates of RNA polymerase II — Agnieszka Pancholi[1], Roshan Prizak[1], Tim Klingberg[2], Weichun Zhang[1], Amra Noa[1], Gerd Ulrich Nienhaus[1,3], Vasily Zaburdaev[2], and •Lennart Hilbert[1] — [1]Karlsruhe Institute of Technology — [2]Friedrich-Alexander University Erlangen-Nuremberg — [3]University of Illinois at Urbana-Champaign

In eukaryotic cells, a main control point of transcription is the transient pausing of engaged RNA polymerase II (Pol II) just before transcript elongation. Paused Pol II forms transient polymeric aggregates that exhibit diverse morphologies. Here, we use super-resolution microscopy in embryonic zebrafish cells to show how entry into and exit from Pol II pausing determines these aggregate morphologies. Instant structured illumination microscopy (iSIM) in live embryos revealed that aggregates initially are morphology complex, round up as they grow, and unfold again when actual transcript elongation begins. Using transcription inhibitors, we confirm that Pol II pausing indeed drives aggregate rounding. Further resolving aggregates by STimulated Emission Double Depletion (STEDD) microscopy, we found a granular fine-structure that suggests clustering aggregation rather than liquid-liquid compartmentalization. We currently develop a theoretical model to explain what underlying macro-molecular interactions could result in the observed morphologies.

CPP 44: Functional semiconductors for renewable energy solutions I (joint session HL/CPP)

Time: Tuesday 9:30–12:00 Location: POT 151

Invited Talk CPP 44.1 Tue 9:30 POT 151

Ionic Defects in Hybrid Perovskite Solar Cells — •Carsten Deibel[1], Sebastian Reichert[1], Qingzhi An[2], and Yana Vaynzof[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany — [2]Technische Universität Dresden, Institut für Angewandte Physik and Centre for Advancing Electronics Dresden (cfaed), Nöthnitzer Straße 61, 01069 Dresden

Hybrid perovskite semiconductors are an interesting material system to build low-cost solar cells with high efficiency. However, processing them can be challenging: minimal and unintentional sample-to-sample variations during the fabrication process affect the ionic defects and thus the device performance. Here, I will present a joint study on the defect properties in perovskite solar cells consisting of methylammonium lead iodide (MAPbI$_3$) in dependence of the precursor solution stoichiometry. We applied impedance spectroscopy and deep-level transient spectroscopy. Our results show different ion species, and each of them features a distribution of the diffusion coefficients. The ion migration activation energies vary systematically with stoichiometry, which might explain the wide range of activation energies in the literature. I will show that the ionic defect properties we observed can be categorised using the Meyer–Neldel rule.

CPP 44.2 Tue 10:00 POT 151

Ferroelectric Materials for Photocatalytic Water Splitting - Strained Mixed Anion Perovskites — •Nathalie Vonrüti and Ulrich Aschauer — University of Bern, Switzerland

Polarity, for example in ferroelectric materials, can significantly increase a catalyst's performance by improving charge-carrier separation. However, polar distortions also increase the band gap as shown for epitaxially strained SrTiO3 (1). While this band-gap increase is small for oxides, our density functional theory calculations show a much larger increase for oxynitrides: The enhanced covalency due to reduced electronegativity of nitrogen compared to oxygen results in larger strain-induced polar distortions and therefore more strongly increased band gaps by up to 1.5 eV. The reduced electronegativity, which leads to a higher valence band in oxynitrides and therefore a band gap in the visible that is attractive for photocatalysis, thus also has a detrimental effect on photo absorption when polar distortions are present. This results in a trade-off between small band gaps and polarity. We will discuss different strategies on how to overcome this trade-off with mixed anion perovskite compounds, which have not yet been considered for photocatalytic water-splitting. (1) RF Berger et al. PRL 107.14(2011):146804

Funding Acknowledgement: Swiss National Science Foundation PP00P2_157615

CPP 44.3 Tue 10:15 POT 151

Preparation of $Mg_xZn_{1-x}O$ Photoanodes for Increased Photovoltage in Dye-sensitized Solar Cells — •Andreas Ringleb[1], Tsukasa Yoshida[2], and Derck Schlettwein[1] — [1]Justus Liebig University Gießen, Institute of Applied Physics — [2]Yamagata University (Yonezawa, Japan), Graduate School of Science and Engineering

ZnO is an n-type semiconductor and a promising candidate for applications in various types of optoelectronic devices due to its wide direct bandgap of about 3.3 eV and a high electron mobility. The targeted substitution of Zn with magnesium enables a tunable band gap of $Mg_xZn_{1-x}O$ in the ZnO wurtzite structure between 3.3 and 4.0 eV through control of the Mg-content. The tunability of the bandgap can be used to minimize losses during electron injection in dye-sensitized solar cells (DSCs). $Mg_xZn_{1-x}O$ nanoparticles have been prepared from acetate precursors in ethanol through a wet chemical route. Thin films have been deposited on quartz and FTO-coated glass substrates by screen-printing of pastes and subsequent annealing. SEM has been used to study the morphology of these films, while XRD was used to detect changes in the crystal lattice caused by Mg. The modulation of the band gap has been confirmed by UV-Vis spectroscopy. A focus has been put on the homogeneity and porosity of the resulting films. DSCs were prepared and analyzed to investigate the effect of the shifted band edge on the solar cell characteristics.

15 min. break.

CPP 44.4 Tue 11:00 POT 151

Reactive sputtering of tantalum nitride for photoelectrochemical energy conversion — •Laura Wagner, Chang-Ming Jiang, and Ian Sharp — Walter Schottky Institut, Technische Universität München

Nitride semiconductors have gained increasing attention for photoelectrochemical (PEC) energy conversion. Traditionally, oxides have been widely investigated as photoelectrodes due to their chemical stability and versatile synthesis pathways; however oxide materials that simultaneously fulfill the efficiency and stability requirements have yet to be found. Many nitrides compounds are theoretically predicted to be semiconducting, though only a small fraction of these materials have been synthesized. Given their higher covalency compared to oxides, these nitrides may be promising candidates for PEC applications. Among transition metal nitrides, Ta3N5 has 2.1 eV bandgap and suitable valence band position for driving the water oxidation. While most studies perform nitridation on Ta or TaOx in order to obtain Ta3N5 thin films, we prepare Ta3N5 on various substrates by reactive magnetron sputtering deposition, which allows a wide range of control of chemical composition, crystallinity, and defect concentration. Additional to Ta3N5, this work also obtained a rarely reported Ta2N3 phase that adopts the Bixbyite structure. Detail characterization of structural, optical, and electrical properties of Ta2N3 are reported. Optimization of PEC performances of Ta3N5 and Ta2N3 thin films as photoanodes is achieved by adjusting deposition parameters. Improvement strategies for these emerging nitrides will also be discussed.

CPP 44.5 Tue 11:15 POT 151

Atomic-Layer-Deposited TiO_2 protection layers for InP photocathodes — •Matthias Kuhl[1], Oliver Bienek[1], Alex Henning[1], Agnieszka Paszuk[2], Thomas Hannappel[2] und Ian D. Sharp[1] — [1]Walter Schottky Institut, Technische Universität München — [2]Institut für Physik, Technische Universität Ilmenau

InP has gained increased interest as a photocathode for solar fuels generation due to its suitable band gap of 1.34 eV, a conduction band edge slightly above the water reduction potential and a high incident photon to charge conversion efficiency (IPCE). While it has been found that a TiO_2 passivation layer, grown by atomic layer deposition (ALD), improve the InP/TiO_2 photocathode stability, the influence of the TiO_2 optoelectronic properties on surface reactions and interfacial charge transfer is not yet understood.

Here we investigate the role of ultrathin TiO_2 (<10nm), grown by plasma-enhanced ALD, its phase, as well as defect type and concentration for the photoelectrochemical (PEC) performance of InP/TiO_2 photocathodes. Tetrakis(dimethylamino)titanium (TDMAT) and titanium isopropoxide (TTIP) as precursors as well as H_2O and O_2-Plasma as oxidants are used to grow ALD TiO_2 films with different oxidation states and defect levels. X-Ray photoelectron spectroscopy of TiO_2 grown by PE-ALD revealed only trace amounts of impurities and stoichiometric TiO_2 consistent with a lower defect density measured by photothermal deflection spectroscopy. This work provides insights into how electronic properties of photocathode protection layers affect interfacial charge injection.

CPP 44.6 Tue 11:30 POT 151

Photoanode protection by atomic-layer-deposited TiO_2 thin films — •Oliver Bienek, David Silva, and Ian D. Sharp — Technische Universität München, Walter Schottky Institut, Germany

In the development of artificial photosystems, significant effort has been devoted to preventing the degradation of photoanodes under harsh electrochemical reaction environments. A promising solution is the deposition of highly conformal protective coatings by atomic layer deposition (ALD). While the application of TiO_2 protection layers to improve the stability of photoanodes has been demonstrated successfully, questions remain regarding the mechanisms of charge carrier transport across the interface and the critical role of defects on performance characteristics. In this work, TiO_2 thin films are fabricated by plasma-enhanced ALD using different precursors and oxidizing agents on n-type Si substrates to vary both defect concentration and crystallinity of the films. In addition, the defect concentration, which is typically dominated by oxygen vacancies, is manipulated by post-annealing treatments in oxidizing atmosphere. The successful removal of defects is confirmed by analysis of sub-bandgap absorption using photothermal deflection spectroscopy. Grazing incidence X-ray diffractometry and Raman spectroscopy further prove changes in the film structure from amorphous to anatase phase upon annealing. Supplementing the optical and structural characteristics, the role of film structure and defect concentration on charge injection across the interface into the electrolyte during water oxidation is investigated using photoelectrochemical methods.

CPP 44.7 Tue 11:45 POT 151

Pseudo-dreidimensionales schwerioneninduziertes Single-Event-Effect Mapping an Hochvolt Silizium Super-Junction-MOSFETs (SJ-MOS) — •Marcel Gerold[1], Michael Rüb[1], Günther Dollinger[2], Judith Reindl[2], Matthias Sammer[2] und Andreas Bergmaier[2] — [1]Ernst-Abbe-Hochschule Jena, SciTec, Carl-Zeiss-Promenade 2, 07747 Jena — [2]Universität der Bundeswehr München, LRT 2, Werner-Heisenberg-Weg 39, 85577 Neubiberg

Vertikale SJ-MOS sind weit verbreitete Halbleiterbauelemente, die in der Energiewandlung eingesetzt werden. SJ-MOS zeichnen sich durch eine komplexe drei dimensionale innere Struktur aus, welche einen niedrigen Einschaltwiderstand bei gleichzeitig hoher Spannungsfestigkeit ermöglichen. Dabei zeigt sich durch eine breite Driftzone, eine Empfindlichkeit gegenüber Partikelstrahlung. Bereits die Wirkung eines einzigen Partikels kann zu Single Event Burnout führen. Wir berichten über Ergebnisse zur Analyse der Empfindlichkeit von SJ-MOS auf Höhenstrahlung durch orts- und tiefenaufgelöste Bestrahlung mit hochenergetischen Kohlenstoffionen (E<=55 MeV, Mikrostrahlanlage "SNAKE", Maier-Leibnitz-Laboratorium, Garching). Während der Bestrahlung wird eine definierte Sperrspannung eingestellt und die Bauelementreaktion erfasst. Es werden Ladungs-Positions-Maps mit einer Auflösung von ca. 1 μm erstellt. Es zeigen sich charakteristische, mit dem Bauelementlayout korrelierbare Bereiche unterschiedlicher Sensitivität. Diese Arbeit demonstriert die Abbildung sensibler Volumina auf mikroskopischer Skala, mit dem Ziel das Verständnis von Ausfallsmechanismen bei Single-Event-Effekten zu verbessern.

CPP 45: Perovskite and photovoltaics I (joint session HL/CPP)

Time: Tuesday 9:30–12:30 Location: POT 251

CPP 45.1 Tue 9:30 POT 251

Properties of In_2S_3:V epitaxially grown on *p*-Si for Intermediate Band Solar Cell Applications — •Tanja Jawinski[1], Michael Lorenz[1], Roland Scheer[2], Marius Grundmann[1], and Holger von Wenckstern[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Germany

The Shockley Queisser limit of single junction solar cells can be overcome by introducing an intermediate band (IB) in wide band gap materials. Thus thermalization losses can be reduced [1]. Furthermore sub-bandgap photons can be absorbed by valence band to IB and IB to conduction band transitions. According to theoretical calculations In_2S_3 hyper-doped with vanadium is a suitable candidate to realize such an IB solar cell [2].

Undoped and V-doped In_2S_3 layers are epitaxially grown by physical co-evaporation of the elements on *p*-type Si wafers. Using a combinatorial approach, we can cover a wide range of doping concentrations of up to 14 at-% V. Heterostructure *pin* solar cells are completed using *n*-ZnO:Al grown by pulsed laser deposition as transparent top electrode. Improved structural properties can be attributed to the epitaxial growth mechanism even for V-doped samples. We compare diode and solar cell parameters of undoped and V-doped sample by analyzing dark and illuminated current-voltage characteristics. Furthermore we use thermal admittance spectroscopy to investigate defect states, that are induced by V-doping. [1] Luque and Martí, *Phys. Rev. Lett.*, 1997, **78**, 5014. [2] Palacios *et al.*, *Phys. Rev. Lett.*, 2008, **101**, 046403.

CPP 45.2 Tue 9:45 POT 251

Time resolved spin dynamics in lead halide hybrid organic perovskite $\mathrm{Fa}_0.9\mathrm{Cs}_0.1\mathrm{PbI}_{2.8}\mathrm{Br}_{0.2}$ — •Erik Kirstein[1], Eiko Evers[1], Vasilli V. Belykh[1,2], Evgeny A. Zhukov[1], Dennis Kudlacik[1], Ina V. Kalitukha[3], Olga Nazarenko[4], Maxim V. Kovalenko[4,5], Dmtri R. Yakovlev[1,3], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44227 Dortmund, Germany — [2]P.N. Lebedev Physical Institute, Russian Academy of Sciences, 119991 Moscow, Russia — [3]Ioffe Institute, Russian Academy of Sciences,194021 St. Petersburg, Russia — [4]Laboratory of Inorganic Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland — [5]Laboratory for Thin Films and Photovoltaics, Empa-Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Lead halide hybrid organic perovskites attract increased attention due their promising applications, related to high quantum efficiency and easy synthesis. Spin dynamics in perovskite materials is not studied in detail so far, but shows promising results. The studied $\mathrm{Fa}_{0.9}\mathrm{Cs}_{0.1}\mathrm{PbI}_{2.8}\mathrm{Br}_{0.2}$ bulk sample was grown out of solution of respective ions in polar solvents. Its bandgap of 1.51 eV makes this material well-suited for the resonant excitation with Ti:Sapphire laser. We study the coherent spin dynamics of electrons and holes by means of time-resolved pump-probe Kerr rotation technique at cryogenic temperatures and magnetic fields up to 6 T. We measure longitudinal spin relaxation times T_1, transverse dephasing times T_2^*, g-factor values and their spread Δg.

CPP 45.3 Tue 10:00 POT 251

Ultrafast Charge Carrier Relaxation in Inorganic Halide Perovskite Single Crystals Probed by Two-Dimensional Electronic Spectroscopy — Xuan Trung Nguyen[1], •Daniel Timmer[1], Yevgeny Rakita[2], David Cahen[2], Alexander Steinhoff[3], Frank Jahnke[3], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Institut für Physik, Carl von Ossietzky Universität, Germany — [2]Weizmann Institute of Science, Israel — [3]Institut für Theoretische Physik, Universität Bremen, Germany

In recent years, halide perovskites have become one of the most intensely studied semiconductors for the development of optoelectronic devices. Regardless, the fundamental understanding of their optical and electronic properties still remains limited. To investigate the ultrafast dynamics of optical excitations we performed pump-probe and two-dimensional electronic spectroscopy (2DES) on CsPbBr3 single crystals with 10 fs time resolution [1]. While pump-probe spectra show a single bleaching feature near the band edge at 2.4 eV, 2DES maps reveal a more rich structure. In addition to a diagonal exciton bleaching peak, free carrier signatures in form of an elongated cross peak along the excitation axis appear. The separation of exciton and free carrier contributions allows to derive a rapid cooling rate of ~3 meV/fs, indicating a strong electron-phonon coupling. The experimental findings are supported by theoretical simulations based on semiconductor Bloch equations. Our results suggest that strong electron-phonon couplings may substantially contribute to the unusual optoelectronic properties of perovskites. [1] Nguyen, X.T., et al., JPCL, 10, p. 5414-5421, 2019.

CPP 45.4 Tue 10:15 POT 251

Two-Dimensional Perovskite Solar Cells with 14.1% Power Conversion Efficiency and 0.68% External Radiative Efficiency — •Weifei Fu[1,2], Alex K.-Y Jen[1], and Michael Saliba[2] — [1]University of Washington, Seattle, Washington 98195, United States — [2]Technical University of Darmstadt, Darmstadt, Germany

Quasi-2D perovskites are attractive due to their improved stability compared to 3D counterparts but they suffer from reduced performance. Here we report an efficient quasi-2D perovskite (PEA)2(MA)4Pb5I16 based optoelectronic device processed with NH4SCN and NH4Cl additives, showing a stabilized photovoltaic power conversion efficiency as high as 14.1 % (average value 12.9+_0.8 %), among the highest performing quasi-2D perovskite solar cells. These additives increase the perovskite crystallinity and induce a preferred orientation with the (0k0) planes perpendicular to the substrate, resulting in improved transport properties hence increased short-circuit current density. Furthermore, the NH4Cl treatment enriches the Cl-concentration near the PEDOT:PSS/perovskite interface, which passivates the electron traps leading to an enhanced electroluminescence external quantum efficiency (0.68% at +2.5 V bias). As a result, high open-circuit voltages of 1.21+_0.01 V with a record-low non-radiative VOC loss of only ~ 0.16 V could be achieved for the quasi-2D perovskite system.

CPP 45.5 Tue 10:30 POT 251

Structural Influence on the Exciton Fine Structure of Cesium Lead Halide Quantum Dots — •Torben Steenbock and Gabriel Bester — Institute of Physical Chemistry, University of Hamburg, Grindelallee 117, 20146 Hamburg, Germany.

Cesium lead halide quantum dots (QDs) show a bright emission, which makes them interesting for applications in optoelectronics. The origin of the bright emission is still under debate. One suggestion [1] is based on a theoretical effective mass model assuming a very strong Rashba effect, which would leads to an unusual bright exciton ground state. Another explanation is based on the idea of a phonon bottleneneck, wich leads to an efficient emission from the higher-energy bright state [2] without dark ground state.

We calculate the exciton fine structure splitting (FSS) based on abinitio density functional theory combined with a screened configuration interaction approach for small $CsPbX_3$ (X=Cl,Br,I) QDs. We find that the bright-dark splitting for Cl, Br, and I $CsPbX_3$ perovskites amount to 17, 12 and 5 meV, respectively, with only small changes due to the symmetry (cubic, tetragonal, orthorhombic) so that we always obtain a dark ground state. The FSS (splitting between the bright states) is sensitive to the symmetry with splittings of up to 5 meV for the lowest symmetry orthorhombic structures.

[1] P.C. Sercel *et al.*, *Nano Lett.* **2019**, *19*, 4068–4077.

[2] P. Tamarat *et al.*, *Nat. Mater.* **2019**, *18*, 717–724.

30 min. break

CPP 45.6 Tue 11:15 POT 251

Understanding the Role of Antisolvent Quenching in Film Formation, Device Performance, and Reproducibility of Triple Cation Perovskite Solar Cells — •Alexander Taylor[1,2], Qing Sun[1,2], Katelyn Goetz[1,2], Maximillian Litterst[1,2], Fabian Paulus[1,2], and Yana Vaynzof[1,2] — [1]Integrated Center for Applied Physics and Photonics, TU Dresden — [2]cfaed, TU Dresden

Organic-inorganic perovskite materials are promising candidates for high-efficiency solar cells, quickly approaching the performance of current state-of-the-art materials. However, irreproducibility between devices made by different research labs, even world leading labs, continue to plague the field. The causes of this issue seem to be related to small, hard to control details, such as stoichiometry variations of fractions of a percent. Herein, we seek to further the understanding of the irreproducibility in cutting edge "triple cation" perovskite solar cells by examining the minute technical differences exhibited by different researchers. We reveal that subtle differences during the crucial antisolvent step dramatically affect the resulting film microstructure, and therefore the final PV performance. By simulating this device-to-device variation, we can reliably produce devices with widely disparate power conversion efficiencies * as low as 15% and as high as 21%. Crucially, these devices would currently be reported in the literature with the exact same recipe. These results challenge some of the prevailing beliefs currently held by the research community, regarding not only what the highest performing antisolvents are, but also the general role of the antisolvent in fabricating high performance perovskite solar cells.

CPP 45.7 Tue 11:30 POT 251

Efficient and Stable Hybrid Triple-Cation Perovskite/PbS Quantum Dot Solar Cells — •Miguel Albaladejo-Siguan[1], David Becker-Koch[1], Alex Taylor[1], Qing Sun[2], Vincent Lami[2], Pola Goldberg-Oppenheimer[3], Fabian Paulus[1], and Yana Vaynzof[1] — [1]Integrated Centre for Applied Physics and Photonic Materials and cfaed, Technical University Dresden — [2]Kirchhoff Institute for Physics, Heidelberg University — [3]School of Biochemical Engineering, University of Birmingham, United Kingdom

Solution-processed quantum dots (QDs) are promising for fabricating flexible, low cost and large-scale solar cells. Researchers have shown that QD devices employing a single monovalent cation perovskite shell exhibit an increased PCE when compared to standard ligand passivation. Herein we demonstrate that the use of a triple cation Cs_0.05(MA_0.17FA_0.83)_0.95Pb(I_0.9Br_0.1)_3 perovskite composition for surface passivation of the QDs results in highly efficient solar cells, which maintain 96 % of their initial performance after 1200h shelf storage. We trace the perovskite shell formation around the core by a range of spectroscopic techniques as well as high-resolution TEM. We find that the triple cation shell results in a favorable energetic alignment to the core of the dot, resulting in reduced recombination due to charge confinement without limiting transport in the active layer. Consequently, photovoltaic devices reached a maximum AM1.5G power conversion efficiency of 11.3 % surpassing previous reports of PbS solar cells employing perovskite passivation.

CPP 45.8 Tue 11:45 POT 251

Microscopic Insights into the Ionic Defect Migration in Metal Halide Perovskites — •Nga Phung[1], Amran Al-Ashouri[1], Simone Meloni[2], Alessandro Mattoni[3], Steve Albrecht[1], Eva L. Unger[1], Aboma Merdasa[1], and Nga Phung[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstr. 5, Berlin D-12489, Germany — [2]Dipartimento di Scienze Chimiche e Farmaceutiche (DipSCF), Università degli Studi di Ferrara (Unife), Via Luigi Borsari 46, I-44121, Ferrara, Italy — [3]Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, CNR-IOM, Cagliari, Cittadella Universitaria, Monserrato 09042-I (CA), Italy

Halide perovskites are emerging as revolutionary materials for optoelectronics. Their ionic nature and the presence of mobile ionic defects have a dramatic influence on the operation of thin-film optoelectronics. This study combines photoluminescence (PL) experiments and molecular dynamics simulations to demonstrate that the grain boundaries within a perovskite film inhibit the movement of ions. Based on experimental observation and theoretical calculation, we find that the diffusion of ions is inhibited by grain boundaries, at the same time, the simultaneous removal of methylammonium and iodine causes a blue-shift of the PL spectrum. This blue-shift is reproduced by simulations, revealing that it is caused by a structural distortion of the perovskite*s Pb-I octahedral network induced by an increased concentration of ionic defects. These findings provide critical information for modeling and explaining the dynamic behavior of perovskite-based optoelectronics.

CPP 45.9 Tue 12:00 POT 251

Highly stable perovskite nanocrystals in polymer micelles — •Juri G. Crimmann, Carola Lampe, and Alexander S. Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Halide perovskite nanocrystals (NCs) have been synthesized through many approaches. Comprising a variety of geometrical shapes, these NCs exhibit excellent optoelectronic qualities, such as near-unity quantum yields and tunable photoluminescence emission. However, perovskite nanocrystals suffer from stability problems as well as extremely mobile halide ions, both resulting in shifts of the photoluminescence emission and instant degradation in water. By using a polymer-templated synthesis we massively improve the stability and suppress halide ion migration by encapsulating NCs individually instead of entire devices. During our synthesis perovskite NCs are formed inside diblock copolymer micelles. The micelles act not only as nanoreactors, but also encapsulate and passivate the NCs, protecting them from the environment. The stability against water degradation increases significantly. Accordingly, even after 75 days of complete submersion in water, characteristic photoluminescence is observable. Furthermore, we have shown that halide ion migration through the polymer shell is nonexistent. We explore the extension of this synthesis to other perovskite compositions, comparing efficiencies and stability. And finally, we explore strategies for incorporating these highly stable NCs into working optoelectronic devices, such as light-emitting diodes (LEDs).

CPP 45.10 Tue 12:15 POT 251

Optical Printing of Single Perovskite Nanoparticles — •Andreas Niklas Rank, Carola Lampe, Moritz Gramlich, and Alexander Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

The investigation of single perovskite nanocrystals in different temperature regimes can reveal the fundamental optical properties of the individual nanocrystals and enable further improvement for optical applications. Spin-coating diluted dispersions is the typical approach to obtain films with single, separated nanocrystals. Another versatile method is optical printing, an already established approach for gold, silver and silicon nanoparticles. In this method, the optical forces of a focused laser beam are utilized to localize nanoparticles at specific positions on a substrate. A specific surface coating prevents unwanted binding of other nanoparticles. The remaining solution can be washed away, leaving only the printed nanoparticles bound to the substrate via Van der Waals forces. Here, we investigate the applicability of this method to perovskite nanocrystals. We look into different nanocrystal morphologies and compositions as well as important laser parameters and substrate materials. Adapting this method to perovskite nanocrystals would not only unlock facilitate the investigation of single perovskite nanocrystals but could also lead to complex, nanostructured substrates.

CPP 46: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 9:30–13:00 Location: ZEU 160

CPP 46.1 Tue 9:30 ZEU 160

Topological states of hard rods in extreme annular confinement — •René Wittmann[1], Louis Cortes[2], Dirk Aarts[2], and Hartmut Löwen[1] — [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 a system 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 map out a full phase diagram. Then we focus on 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.

CPP 46.2 Tue 9:45 ZEU 160

Phase Field Crystal Model of patchy colloids in two dimensions — Robert Weigel and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 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).

CPP 46.3 Tue 10:00 ZEU 160

Relations between angular and Cartesian orientational expansions* — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Orientational expansions, which are widely used in the natural sciences, exist in angular and Cartesian form. Although these expansions are orderwise equivalent, it is difficult to relate them in practice. Moreover, the standard expansion has to be modified for particles with asymmetric shape, where a description in terms of spherical harmonics or symmetric traceless tensors is not sufficient. We discuss various methods for orientational expansions and their application for the definition of orientational order parameters in liquid crystal physics. In particular, we explain how conversion tables between angular and Cartesian expansions can be constructed, which we have done up to third order. This is important, e.g., for the comparison of theoretical and experimental results in liquid crystal physics.

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

CPP 46.4 Tue 10:15 ZEU 160

Dynamic wrinkling of thin liquid crystal films — •Dominik Mnich, Torsten Trittel, Kirsten Harth, Christoph Klopp, and Ralf Stannarius — Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany

We demonstrate spontaneous wrinkling as a dynamical pattern in freely floating liquid-crystalline films. These films behave liquid-like with respect to flow within the film plane. The adjustment of the film shape to quick changes often requires the formation of additional layers. Centimeter-sized freely floating smectic bubbles are studied during the excitation with acoustic waves. We show that such films develop an undulation instability under acoustic excitation. The results of parabolic flight and ground lab experiments are presented. The observed "wrinkles" show charactistic wavelengths in the submillimeter range. We introduce a basic model of the wavelength selection mechanism.

CPP 46.5 Tue 10:30 ZEU 160

Thermally driven material transport in thin freestanding films — •Torsten Trittel, Christoph Klopp, Kirsten Harth, and Ralf Stannarius — Otto von Guericke University, Institute for Physics, 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.

[1] Trittel et al., Marangoni Flow in Freely Suspended Liquid Films, Phys. Rev. Lett., 122 (2019)

CPP 46.6 Tue 10:45 ZEU 160

Defect annihilation 2D using free-standing smetic films — •Kirsten Harth[1], Amine Missaoui[1], Peter Salamon[2], and Ralf Stannarius[1] — [1]Institut für Physik, Otto-von-Guericke Universität Magdeburg — [2]Department of Complex Fluids, Wigner Research Center, Budapest, Hungary

Interacting defects in quasi-2D geometries occur in manifold systems, from strings in cosmology over spin systems in Bose-Einstein condensates or thin magnetic films to liquid crystals. Free-standing smecti C films (smC FSF) represent a quite simple sytem for studying fluid mechanics and pattern formation in 2D. They are particularly easy to handle and orientational patterns are directly observable using polarizing microscopy, but few experiments exist so far. Theory is either fully numerical or focuses on very simplified situations. Orientational problems among the defects and with the far director field were only recently noticed.

With a special method, we are able to prepare isolated pairs of +1 and -1 defects in homogeneous smC FSF, and we study their annihilation. Aligned defect pairs qualitatively follow expectations from theory and approach on straight paths. Misoriented defects pairs display curved trajectories, and their dynamics quantitatively disagrees with theoretical predictions[1]. We discuss experimental findings and possible explanations for the discrepancies.

[1] X. Tang and J. V. Selinger, Soft Matter 13, 5481 (2017)
[2] A. Missaoui, K. Harth, P. Salamon, R. Stannarius, arXiv:1911.05224

15 min. break.

CPP 46.7 Tue 11:15 ZEU 160

Static properties of modulated hard-spheres liquid. — •Michele Caraglio, Charlotte F. Petersen, and Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria

The structure of a liquid can be manipulated with externally applied fields. This can be achieved experimentally with interfering lasers and has been implemented with colloidal particles [1, 2]. This possibility also paves the way to a better understanding of confined liquids [3], which are prevalent in nature and necessary in many industrial applications.

We investigate static properties in a hard-sphere liquid with modulated density profile obtained by applying an external periodic field. In this system we will control three dimensionless parameters: the packing fraction, the amplitude of the potential relative to temperature and its wavelength relative to particle diameter. For this purpose, the Ornstein-Zernike integral equation using Percus-Yevick closure relation is solved numerically. The theory requires the density profile as input, which can be obtained from density functional theory. Similar to a liquid confined in a slit, a non-monotonic evolution of the static structure factor peak and the pressure is observed upon variation of the potential wavelength.

[1] C. Bechinger, M. Brunner and P, Leiderer, PRL 86, 2001. [2] F. Evers, et al., PRE 88, 2013. [3] S. Saw and C. Dasgupta, J. Chem. Phys. 145, 2016.

CPP 46.8 Tue 11:30 ZEU 160

Analytical classical density functionals from an equation learning network — •Shang-Chun Lin[1], Georg Martius[2], and Martin Oettel[1] — [1]Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, 72076 Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems Tübingen, 72076 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 the 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. If time allow, we will show the result that forgo the idea gas contribution.

[1]G. Martius and C. H. Lampert, arXiv:1610.02995 (2016).

[2]S.-C. Lin, G. Martius and M. Oettel, arXiv:1910.12752 (2019).

CPP 46.9 Tue 11:45 ZEU 160

First order phase transitions: From bifurcation diagrams to the thermodynamic limit — •Uwe Thiele[1], Tobias Frohoff-Hülsmann[1], Sebastian Engelnkemper[1], Edgar Knobloch[2], and Andrew J. Archer[3] — [1]Institut für Theoretische Physik and Center of Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK

We consider simple mean field continuum models for first order liquid-liquid demixing and solid-liquid phase transitions and show how the Maxwell construction at phase coexistence emerges on going from finite-size closed systems to the thermodynamic limit [1]. The theories considered are the Cahn-Hilliard model of phase separation, which is also a model for the liquid-gas transition, and the phase field crystal model of the solid-liquid transition. Our results show that states comprising the Maxwell line depend strongly on the mean density with spatially localized structures playing a key role in the approach to the thermodynamic limit. [1] U. Thiele et al., New J. Phys., at press (2019), doi: 10.1088/1367-2630/ab5caf.

CPP 46.10 Tue 12:00 ZEU 160

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).

CPP 46.11 Tue 12:15 ZEU 160

Universal properties of creep flow — •Marko Popović[1], Tom de Geus[1], Wencheng Ji[1], Alberto Rosso[2], and Matthieu Wyart[1] — [1]Institue of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]LPTMS, CNRS, Univ.Paris-Sud, Universite Paris-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 it, while 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 eventually yield at fluidisation time τ_f. In recent years various numerical values and/or laws have been suggested for the exponent μ and time τ_f in particular experimental or numerical studies. We propose that mechanism underlying creep flow is the same as that of the steady state flow, which allows us to predicts parameters μ and τ_f of creep flow 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.

CPP 46.12 Tue 12:30 ZEU 160

Formation of networks from attractive particles under shear — •Sebastian Bindgen[1], Dieter Diels[1], Pierre de Buyl[2], Joost de Graaf[3], and Erin Koos[1] — [1]Department of Chemical Engineering, KU Leuven, Celestijnenlaan 200f - box 2424, 3001 Leuven, Belgium — [2]Institute for Theoretical Physics, KU Leuven, Celestijnenlaan 200d - box 2415, 3001 Leuven, Belgium — [3]Institute for Theoretical Physics, Utrecht University, Princetonplein 5, 3584 CC Utrecht, The Netherlands

Simulations give access to physical quantities at the particle-level, which are not readily accessible via experimental techniques. Lees-Edwards boundary conditions replicate in-vitro conditions and have seen significant use in the polymer community. We have implemented and tested a version of this algorithm in the MD simulation package ESPResSo. The implementation, which is based on pair-wise thermostating using the dissipative particle dynamics technique, can also mimic non-linear effects such as shear banding. We demonstrate that our implementation captures the enhanced diffusion of particles coupled to the fluid. Furthermore, we use our implementation to study the dynamic properties of depletion gels including their formation and breakup under shear flow. Recent investigations have shown that hydrodynamics affects the time scales on which these gels form under quiescence, while leaving the final structure unaltered. We aim to show these processes under dynamic conditions. Our study is of clear interest for industrial systems such as ink or pastes as they can experience various complex flow fields during processing and application.

CPP 46.13 Tue 12:45 ZEU 160

Tactoids, membranes and fribrils – finite assemblies of rod-like particles — •Anja Kuhnhold, Nils Göth, Nadja Helmer, Victor Tänzel, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Systems composed of rod-like particles and spherical depleting agents show a variety of self-assembled shapes and structures. We discuss a few of them and present corresponding Monte Carlo simulation results. The model system ingredients are hard spherocylinders as rod-like component and implicit Asakura-Oosawa spheres as depletants. In addition we study the effect of a chiral pair interaction between the rods.

This work got inspired by experiments using viruses as rod-like particles and polymer coils as depleting agents, see e.g. [1,2]. The monodispersity of viruses makes them a nice model system to compare simulations to. Beyond the comparison simulation results can be used to direct the self-assembly for specific structure-function relationships, e.g. templating or sensing.

[1] T. Gibaud, J. Phys.: Condens. Matter **29**, 493003 (2017).

[2] B. Sung et al., Soft Matter **15**, 9520 (2019).

CPP 47: Focus: Phase Separation in Biological Systems II (joint session BP/CPP)

Stem cells have the remarkable capacity to differentiate into multiple cell types and therefore play pivotal roles in our understanding of tissue maintenance and disease. Theoretical and experimental approaches from physics have advanced our understanding of stem cell dynamics, while at the same time stem cell biology has led to questions at the frontier of non-equilibrium physics. In this session, we will show how mechanical signalling influences cell fate and how concepts from physics can yield understanding of the collective phenomena underlying stem cell behaviour on the molecular and cellular scales.

Time: Tuesday 9:30–12:45 Location: ZEU 250

CPP 47.1 Tue 9:30 ZEU 250

Salt-dependent rheology and surface tension of protein condensates using optical traps — Louise Jawerth[1], Mahdiye Ijavi[1], Martine Ruer[1], Shambaditya Saha[1], Marcus Jahnel[1,4], Anthony Hyman[1], Frank Jülicher[2,3], and •Elisabeth Fischer-Friedrich[4,5] — [1]MPI CBG, Pfotenhauerstr. 108, 01307 Dresden, Germany — [2]MPI PKS, Nöthnitzerstr. 38, 01187 Dresden, Germany — [3]Center for Systems Biology Dresden, Pfotenhauerstraße 108, 01307 Dresden, Germany — [4]Biotec, TU Dresden, Tatzberg 47-49, 01307 Dresden, Germany — [5]Excellence Cluster Physics of Life, TU Dresden, Dresden, Germany

An increasing number of proteins with intrinsically disordered domains have been shown to phase separate in buffer to form liquid-like phases. These protein condensates serve as simple models for the investigation of the more complex membrane-less organelles in cells. To understand the function of such proteins in cells, the material properties of the condensates they form are important. However, these material properties are not well understood. Here, we develop a novel method based on optical traps to study the frequency-dependent rheology and the surface tension of PGL-3 condensates as a function of salt concentration. We find that PGL-3 droplets are predominantly viscous but also exhibit elastic properties. As the salt concentration is reduced, their elastic modulus, viscosity and surface tension increase. Our findings show that salt concentration has a strong influence on the rheology and dynamics of protein condensates suggesting an important role of electrostatic interactions for their material properties.

CPP 47.2 Tue 9:45 ZEU 250

Protein condenstates as aging Maxwell fluids — •Louise Jawerth[1], Elisabeth Fischer-Friedrich[2], Anthony Hyman[3], and Frank Julicher[1] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Biotec, TU Dresden, Tatzberg 47-49, 01307 Dresden, Germany — [3]Max Planck Institute of Molecular Cell Biology and Genetics

Protein condensates (PC) are intracellular compartments that segregate material without the use of a membrane. The liquid-like behavior of the condensates is a defining characteristic and the material properties of condensates are tuned to their biological function. It has become increasingly clear that some condensates do not have time-independent material properties, but can, instead, transition to more solid, gel-like materials. Here, we present our efforts to quantify these new materials as they age in vitro. We measure the visco-elastic material properties of several proteins by means of a combination of active and passive microrheology. At early times, we find that the droplets behave much like simple liquids but gradually become more elastic. Surprisingly, the changing mechanical properties can all be scaled onto a single master curve using one characteristic time scale which grows as the sample ages. We consider protein condensates as soft glassy materials with age dependent material properties that we call Maxwell glasses. To gain insight into the molecular origins of this behavior, we present electron microscopy images of the condensates at different ages. Furthermore, we demonstrate how salt concentration tunes the characteristics of the aging process.

CPP 47.3 Tue 10:00 ZEU 250

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.

CPP 47.4 Tue 10:15 ZEU 250

Phase Separation of Active Polymers — •Antoine Deblais[1], Daniel Bonn[1], and Sander Woutersen[2] — [1]Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, 1098XH Amsterdam, The Netherlands. — [2]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands.

Here, we investigate the aggregation and phase separation of thin, living T.Tubifex worms that behave as active polymers. Randomly dispersed active worms spontaneously aggregate to form compact, highly entangled blobs, a process similar to polymer phase separation, and for which we observe power-law growth kinetics. We find that the phase separation of active polymer-like worms does not occur through Ostwald ripening, but through active motion and coalescence of the phase domains. Interestingly, the growth mechanism differs from conventional growth by droplet coalescence: the diffusion constant characterizing the random motion of a worm blob is independent of its size, a phenomenon that can be explained from the fact that the active random motion arises only from the worms at the surface of the blob. This leads to a fundamentally different phase-separation mechanism, that may be unique to active polymers.

Invited Talk CPP 47.5 Tue 10:30 ZEU 250

Could the cytoskeleton influence liquid-liquid phase separation? — •Eric Dufresne — ETH Zürich, Department of Materials

We have recently demonstrated using synthetic polymers that mechanical stresses can have a dramatic impact on the phenomena of liquid-liquid phase separation [1-3]. Shin *et al* [4] recently revealed a coupling of condensation to chromatin density, suggesting that similar effects may play a role in the condensation of liquid droplets in the nucleoplasm.

Here, I will describe our new experiments exploring the interaction of phase-separated domains to elements of the cytoskeleton.

[1] Style, R. W. *et al*, *Phys. Rev. X*, **8**, 011028 (2018)
[2] Kim, J.-Y. *et al*, *arXiv:*1811.00841 (2019)
[3] Rosowski, K. A. *et al*, *arXiv:*1907.08465 (2019)
[4] Shin, Y. *et al*, *Cell* **175** 1481 (2018)

30 min. coffee break

CPP 47.6 Tue 11:30 ZEU 250

Theory of dissolution front dynamics predicts droplet distribution in stiffness gradients — •Estefania Vidal-Henriquez and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Liquid-liquid phase separation is an important mechanism for compartmentalizing the cell's cytoplasm, allowing the dynamic organization of the components necessary for survival. However, it is not clear how phase separation is affected by the complex viscoelastic environment inside the cell. Here we study theoretically how stiffness gradients influence droplet growth and arrangement. Since elastic gradients imply concentration gradients in the dilute phase, droplet material is transported from stiff to soft regions. This process drives a dissolution front invading the stiff region. Using a mean-field theory, we predict how the front emerges and how it propagates. This elastic ripening occurs at a rate much faster than classical Ostwald ripening, thus driving the dynamics. Our work shows how spatial differences in elastic properties could control liquid compartments inside cells.

CPP 47.7 Tue 11:45 ZEU 250

Structure and development of patterned silica in the diatom frustule. — •Maria Feofilova and Eric Dufresne — ETH Zurich, Zurich, Switzerland

Diatoms are single-celled organisms, which make an amazing multi-scale silica structure called the frustule as their cell wall. While much is known about the biochemistry involved, currently it is not clear what is the physical mechanism by which the structure is achieved. One of the proposed models is templating by phase separation.

In this work, we observe both the developing structure in living cells and the completely formed structure in extracted frustules of the diatom *Coscinodiscus granii*. By characterizing the development of structural features over time, we hope to gain insight into the mechanism by which ordering of the structure occurs.

CPP 47.8 Tue 12:00 ZEU 250

Formation of pilus induced cellular aggregates and their rheological properties — •Hui-Shun Kuan[1,3], Frank Jülicher[2], and Vasily Zaburdaev[1,3] — [1]Department of Biology, Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Aggregates of living cells are an example of active materials with unconventional material properties. The rheological properties of cellular aggregates can, therefore, be markedly different from those exhibited by passive soft systems. Motivated by colonies of Neisseria gonorrhoeae bacteria, we develop a continuum theory to study cellular aggregates formed by attractive pili–pili intercellular interactions which introduce active stresses in the system. The formation of cellular aggregates can be explained by an active phase separation process, and the activity-induced viscoelastic properties of such aggregates are coupled with pili–pili interactions. By studying the behaviour of aggregates under oscillatory shear, the loss and storage moduli of the aggregates can be linked to the dynamics of the active intercellular forces. Due to the turnover of pili, the aggregates show a liquid-like behaviour at large times and strong shear-thinning effect under the large amplitude oscillatory shear. Our theory provides an essential insight on how pilus mediated intercellular forces in cellular aggregates govern their material properties which in the future could be tested experimentally.

CPP 47.9 Tue 12:15 ZEU 250

Active growth and degradation of coacervate droplets controlled by enzymatic reactions — •Karina Nakashima, Alain André, Merlijn van Haren, and Evan Spruijt — Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

Liquid-liquid phase separation plays an important role in the organization of biochemical processes in the cell. Control over phase separation by enzymatic reactions and the localization of biomolecules inside different droplet compartments is essential for many cellular functions. To elucidate the physicochemical principles that govern the nucleation, growth and coarsening of droplet organelles, we use coacervate droplets that we control by enzymatic reactions. Here, we present two experimental model systems, in which we achieve dynamic control over condensation and dissolution of coacervate droplets by changing either the charge density or the length of the constituent biomolecules. We track the coacervates by microscopy and follow their active growth and degradation at a single-droplet level. Our results indicate that droplets grow faster with increasing reaction-diffusion rate, while degradation of droplet material leads to a gradual dissolution of all droplets simultaneously. We also find that Ostwald ripening is suppressed in complex coacervates. We quantify the partitioning of all components in our system by HPLC and fluorescence labelling to support our results with a kinetic model. Our findings suggest that controlling phase separation in biological systems through enzymatic reactions may lead to a wide variety of droplet growth and degradation behaviours.

CPP 47.10 Tue 12:30 ZEU 250

Protein storage vacuoles and autophagosomes form by similar physical mechanisms — •Roland L. Knorr — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — The University of Tokyo, Tokyo 113-0033, Japan — Max Planck Institute of Molecular Plant Physiology, Potsdam, Germany

Proteins are components and nutrients essential for the growth and maintenance of the human body. The most important protein source worldwide are plants and the majority of plant protein consumed is packed in protein storage vacuoles (PSVs) of seeds in all major crops including wheat and soy. How highly fragmented PSVs storing protein derive from a single, vegetative vacuole functioning in protein degradation is little understood. Here, we investigate the mechanisms of PSV generation. We find in living embryos that vacuolar phase separation generates storage protein droplets with liquid-like properties. A physical model combined with reconstituted droplet-membrane interactions shows that partial wetting of proteinaceous droplets on membranes determines droplet engulfment by a process we call liquid scaffolding. We thus demonstrate that phase separation and engulfment are the mechanisms underlying the formation of physically separated droplets of storage proteins, which may be important to reprogram degradative vacuoles into storage vacuoles by restricting the access of vacuolar proteases to developing protein reservoirs. Further, we demonstrate that the autophagosomal sequestration of cytosolic droplets underlies similar physical principles.

References: Fujioka, Y; Alam, J.M.D.; Noshiro, D.; Mouri, K.; Ando, T.; Okada, Y.; May, A.I.; Knorr, R. L.; Suzuki, K.; Ohsumi, Y; Noda, N.N.; Nature, accepted. Knorr, R. L.*; Franzmann, T.; Feeney, M.; Kittelmann, M.; Frigerio, L.; Dimova, R.; Hyman, A. A.; Lipowsky, R.; submitted. Agudo-Canalejo, J.; Schultz, S.W.; Chino, H.; Migliano, S.; Saito, C.; Koyama-Honda, I.; Stenmark, H.; Brech, A.; May, A.I.; Mizushima, N.; Knorr, R. L.*; submitted.

CPP 48: Organic Thin Films, Organic-Inorganic Interfaces II (joint session DS/CPP)

Time: Tuesday 11:15–12:45 Location: CHE 91

CPP 48.1 Tue 11:15 CHE 91

Strong coupling of exciton polaritons in laterally structured organic microcavities — •Tony Henseleit[1,2], Markas Sudzius[1,2], Harmut Fröb[1,2], and Karl Leo[1,2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials — [2]Technische Universität Dresden

Strong coupling in inorganic semiconductor materials has been investigated for many years with rising interest in strong coupling in organic materials. The realization of strong coupling at room temperature leads to possible applications as for example polariton lasing and enables investigation of many other interesting physics such as polariton blockade effects.

A polariton is a quasi particle comprising of a photon coupled to an exciton. We are focusing on exciton polaritons in layered resonator structures with organic active materials. We investigate organic materials at room temperature in strong coupling regime and can report to see a reasonable large splitting of the cavity mode in our spectroscopic studies. Furthermore we are especially examining the influence of lateral periodic submicrometer structures on strongly coupled polaritons. This results in an additional confinement of the particles in the system and forms for example waveguide modes in the structure.

CPP 48.2 Tue 11:30 CHE 91

Electrochemical Deposition of Polyelectrolytes — •Felix Plamper[1], Sabine Schneider[2], and Olga Mergel[2] — [1]TU Bergakademie Freiberg, Germany — [2]RWTH Aachen University, Germany

Charged polymers (polyelectrolytes) interact with oppositely charged counterions. In case of redox-active counterions, their charge can be changed by electrochemical means, allowing a solubility change of these complexes at the electrode (electrochemically-induced film formation). Hence, we address polycations of various architectures made of quaternized poly(dimethylaminoethyl methacrylate) and derivatives to assess their influence on the electrodeposition with help of hexacyanoferrates. A rotating ring disk electrode (RRDE) used during hydrodynamic voltammetry is a powerful method to learn about the interactions of polymers and electroactive species. The RRDE allows a quantification of the deposition efficiency DE. The DE assigns the ratio of charge which was used to produce the deposited electroactive species compared to the total charge. It complements Quartz Crystal Microbalance QCM measurements, which is sensitive to the deposited mass, providing information on the water contents in the films. Different linear polyelectrolytes are investigated and a comparison between other architectures, like star-shaped polymers and microgels, was obtained. The results demonstrate that linear polymers of moderate molar mass are most efficient in the deposition due to pronounced intermolecular physical crosslinking (by help of the hexacyanoferrates), while hydrophilic side groups weaken the deposition by water uptake.

CPP 48.3 Tue 11:45 CHE 91

Tuning the electronic properties of graphene with periodically arranged metal-organic coordination networks — •Qiankun Wang, Brian D. Baker Cortés, Joris de la Rie, Mihaela Enache, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Here, we investigate by means of scanning tunneling microscopy and photoelectron spectroscopy how the electronic properties of graphene are modified upon deposition of 5,10,15,20-tetra(4-pyridyl)porphyrin (2HTPyP) with and without coordination to Co atoms. Graphene was prepared on two different substrates, namely Cu(111) and CuOx, and it has been reported to be n-type doped on Cu(111) and quasi-freestanding on CuOx. Thereby, a comparison how the molecular adsorption changes the electronic properties of doped/undoped graphene could be done. We will discuss (i) the transition of the H-bonded self-assembled 2HTPyP network into a long-range ordered metal-organic coordination network (MOCN) upon Co deposition and (ii) the electronic level alignment at the graphene/MOCN interface and how this is influenced by the underlying substrate. Our study provides a viable possibility for the usage of graphene as a charge and spin transport material in future electronic and spintronic applications.

CPP 48.4 Tue 12:00 CHE 91

Growth of Extended DNTT Fibers on Metal Substrates by Suppression of Step-Induced Nucleation — •Maximilian Dreher, Dayeon Kang, Tobias Breuer, and Gregor Witte — Philipps-Universität Marburg, 35032 Marburg, Germany

Due to their anisotropic optoelectronic properties, crystalline organic fibers constitute an interesting class of nanoscale materials with great potential for integration into future optoelectronic devices based on organic-inorganic hybrid systems. While chemical synthesis allows for flexible tailoring of electronic molecular properties, structural control of hybrid structures is hampered by the incompatibility of traditional structuring methods. Here we examine the formation of crystalline fibers of dinaphthothienothiophene (DNTT), a recently synthesized organic semiconductor with high charge carrier mobility, upon film growth on noble metal substrates. Based on a comparison of the film growth on a regularly stepped, vicinal surface, we show by STM measurements that substrate steps affect the azimuthal molecular orientation in the seed layer. In particular, they induce a fiber orientation which competes with that of fibers formed on flat terraces and thereby strongly limits the fiber dimensions. We demonstrate a strategy to suppress this parasitical step-induced fiber nucleation by first exposing Ag(111) surfaces to oxygen, which causes a selective saturation of the active step sites, while subsequent deposition of DNTT yields strongly enlarged fibers that are epitaxially aligned on the (111) surface [1,2]. [1] M. Dreher et al., Adv. Mater. Interfaces 5, 1800920 (2018) [2] M. Dreher et al., Nanoscale Horiz. 4, 1353-1360 (2019)

CPP 48.5 Tue 12:15 CHE 91

Epitaxial Growth of PEN and PFP Thin Films on hBN(0001) — •Darius Günder[1], Tobias Breuer[1], Takashi Taniguchi[2], and Gregor Witte[1] — [1]Philipps University, Marburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Hexagonal boron nitride (hBN) has gained considerable attention because it is an insulating 2D material, which is frequently used as gate dielectric in transistor applications [1]. Combining XRD, AFM, UV/Vis spectroscopy and polarization resolved optical microscopy we demonstrate that pentacene (PEN) and perfluoropentacene (PFP) form epitaxial films on exfoliated hBN(0001) substrates where molecules adopt a lying orientation on highly ordered hBN surfaces, while they grow in an upright molecular fashion on defective surfaces. We demonstrate in particular that PEN does not crystallize in a new polymorph as reported by Zhang et al. [2]. Based on our azimuthal analyses, the epitaxial relation between PEN and PFP films and hBN substrates is resolved and compared to the similar growth behavior on graphite substrates [3,4].

[1] M. Kratzer et al., J. Journal of Physics D 52, 383001 (2019).
[2] Y. Zhang et al., Phys. Rev. Lett. 116, 016602 (2016).
[3] J. Götzen et al., Phys. Rev. B 81, 085440 (2010).
[4] R. Felix et al., Cryst. Growth Des 16, 6941 (2016).

CPP 48.6 Tue 12:30 CHE 91

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 49: Poster Session II

Topics: Exploitation of Anisotropy in Organic Semiconductors (49.1-49.4); Hybrid and Perovskite Photovoltaics (49.5-49.20); In-situ probes toward better understanding of hybrid halide perovskites (49.21-49.24); Molecular Electronics and Excited State Properties (49.25-49.32); Organic Electronics and Photovoltaics (49.33-49.54).

Time: Tuesday 14:00–16:00 Location: P1A

CPP 49.1 Tue 14:00 P1A

The Influence of Side Chain Linkage on Bulk Structure and Orientation in Thin Films of Ethylene Glycol Substituted Polythiophenes — •Robert Kahl[1], Oleksandr Dolynchuk[1], Philip Schmode[2], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

Polythiophenes with ethylene glycol side chains exhibit ionic as well as electronic charge transport, making them promising materials for application in organic electrochemical transistors (OECTs). In the present study, we investigated the effect of linkage of diethylene glycol side chains in polythiophenes on the structure formation and orientation in thin films. Three polythiophenes in which the diethylene glycol side chain is either directly linked to the thiophene backbone (P3MEET) or attached via a methylene (P3MEEMT) or an ethylene (P3MEEET) spacer were investigated in bulk (DSC, WAXS) and in thin films on Si/SiO$_2$ (GIWAXS, AFM). As seen in DSC and WAXS measurements, the molecular order in the bulk significantly decreases with decreasing spacer length. In confirmation to this, a clear lamellar morphology is only visible in AFM measurements of thin films of P3MEEET. GIWAXS measurements show, that all samples have a strong preference for edge-on orientation in thin films. From these results we conclude, that the length of the alkyl spacer has a significant influence on the molecular order, but little influence on the orientation in thin films.

CPP 49.2 Tue 14:00 P1A

Morphology Study of self-assembled Supramolecular Structures — •Asena Cerhan[1], Christopher Greve[1], Michael Buchhorn[1], Richard Kellnberger[1], Bernd Wittmann[2], Felix Wenzel[3], Hans-Werner Schmidt[3], Richard Hildner[2,4], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — [2]Lehrstuhl für Spektroskopie weicher Materie, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — [3]Makromolekulare Chemie I, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — [4]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4 9747 AG Groningen, Netherlands

Organic, supramolecular systems can exhibit extraordinary transport properties [1]. Here we investigate the self-assembly of a carbonyl-bridged triarylamine (CBT) small molecule into helical supramolecular nanostructures [2]. The self-assembly is sensitive to environmental parameters like solvent type and temperature. Using x-ray scattering on the system in various solvents we are able to study the morphology of supramolecular nanostructures formed from CBT molecules. Examining the morphology further with temperature resolved measurements, as well as comparisons of behaviour in solution versus thin films, allows us to learn more about the intermolecular interactions, that are key for their functional properties. [1] Brixner, T., Hildner, R., Köhler, J., Lambert, C. & Würthner, F. Adv. Energy Mater. 7, 1700236 (2017).[2] Haedler, A. T. et al. Nature 523, 196-199 (2015).

CPP 49.3 Tue 14:00 P1A

Rotary Kelvin probe system to efficiently measure the giant surface potential ofpolarized organic films in completely dark condition — •Masahiro Ohara[1], Tatsuya Watanabe[2], Yuya Tanaka[2,3], and Hisao Ishii[2,3,4] — [1]Fac. Eng. Chiba Univ. — [2]GSSE Chiba Univ. — [3]CFS Chiba Univ. — [4]MCRC Chiba Univ.

Amorphous organic films often show orientation polarization with giant surface potential (GSP). The polarization due to GSP often affects device performance; however, the origin of anisotropic orientation is still not well understood. One of the factors that hinders understanding this phenomenon is the difficulty in Kelvin probe (KP) experiment. GSP have been investigated by using conventional KP method. In this method, the repeated cycles of KP measurements and film depositions are quite time-consuming. In addition, ambient light illumination to sample film cannot be avoided at the switching between measurement and deposition, and it reduces the GSP more or less due to the compensation by photo-generated carriers. In this study, we have developed a surface potential measurement apparatus using the "Rotary KP method". It can solve the above problems by rotating the reference electrode. Since the reference electrode does not always cover the sample, the surface potential can be measured continuously even during the film deposition. Thus, GSP values free from light illumination can be efficiently measured. We will report on the details of our apparatus with the results of the surface potential of TPBi film prepared from its methanol solution to compare with the GSP of the vacuum evaporated film.

CPP 49.4 Tue 14:00 P1A

Structure Formation and Optical Emission of Organic Binary Mixed Thin Films — •Oleg Vladimirov, Nadine Russegger, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Tübingen 72076, Germany

We present a comprehensive investigation of the charge transfer (CT) effect in weakly interacting organic semiconductors by means of planar heterostructures and mixtures. The donor-acceptor pairs diindenoperylene (DIP) with N,N*-Dimethyl-3,4,9,10-perylenetetracarboxylic diimide (PTCDI-C1), 2,9-Dipropylanthra[2,1,9-def:6,5,10-d*e*f*]diisoquinoline-1,3,8,10(2H,9H)tetrone (PTCDI-C3) and N,N*-Dipentyl-3,4,9,10-perylenedicarboximide (PTCDI-C5) have been chosen for this purpose in order to investigate the structure and CT characteristics in dependence of the chain length of the respective molecules. The binary mixtures of PTCDI derivatives have already been studied for different mixing ratios in reference [V.Belova J. Am. Chem. Soc. 2017, 139, 25, 8474-8486]. A wide range of experimental methods, for instance atomic force microscopy, x-ray reflectometry, photoluminescense spectroscopy, UV-Vis spectroscopy and ellipsometry were used in order to characterize the structural, optical, electronic, and device properties of the intermolecular interactions. We observed that the mixtures with PTCDI-C1 phase separate due to their short chain length and form crystal structures when grown at high temperature, whereas mixtures with PTCDI-C3 show the formation of a co-crystal with pronounced CT.

CPP 49.5 Tue 14:00 P1A

Investigation of polymer templated silicon-germanium nanostructures for hybrid photovoltaics — •Christian L. Weindl[1], Michael A. Giebel[2], Matthias Schwartzkopf[3], Thomas F. Fässler[2], Stefan V. Roth[3,4], 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

Latest research in the field of hybrid photovoltaics focuses on the benefits of inorganic and organic materials. Flexibility, low cost, and large-scale production are the most valuable properties of organic components whereas the inorganic components add chemical and physical stability. In this work, we analyze thin films with optical, electrical and morphological measurement techniques to understand and control the corresponding properties. An amphiphilic diblock copolymer templating with polystyrene-b-polyethylene oxide (PS-b-PEO) and a potassium-semiconductor-semiconductor precursor is used to prepare porous thin films via sol-gel synthesis. The focus is to implement these mesoporous nanostructures into hybrid photovoltaics.

CPP 49.6 Tue 14:00 P1A

Key factors study in amphiphilic block copolymer-oriented porous SnO2 synthesis process — •Shanshan Yin[1] and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, D-85748 Garching, Germany

SnO2, as a crucial material in the field of energy storage, has always been the focus of scientific research. For organic-inorganic halide perovskite solar cells (PSCs) or dye-sensitized solar cells (DSSCs), SnO2 contributes a high electron mobility and superior chemical stability amongst the various metal oxides. Moreover, as an alternative anode material for lithium ion battery, it possesses a decent theoretical specific capacity of 1494 mAhg-1. Compared with conventional bulk materials, mesoporous SnO2 with high specific surface area affords more advantages when applied on either solar cells or lithium-ion batteries. In the present work, a novel amphiphilic block copolymer assisted sol-gel chemistry is used for the synthesis of porous SnO2 nanostructure. Different kinds of solvent are used as good solvent for both PS and PEO polymer chains, HCl is utilized as a selective poor solvent for PS chains and catalyst for the hydrolytic condensation reaction of SnCl4 precursor. For removing the organic polymer template, the composite thin films are calcined at 500 °C for two hours under ambient condition. The obtained nanostructures are characterized by scanning electron microscope (SEM), X-ray dffraction (XRD) and grazing-incidence small-angle X-ray scattering (GISAXS) measurement.

CPP 49.7 Tue 14:00 P1A

In situ morphology study of printed ZnO photoanodes templated by block polymer for scalable fabrication of hybrid

solar cells — •Ting Tian[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, Photon Science, 22607 Hamburg — [3]KTH, Department of Fibre and Polymer Technology, 100 44 Stockholm, Sweden — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, D-85748 Garching, Germany

Hybrid solar cells have attracted great attention due to the advantages of their short payback time, high stability and flexibility, which results from the combination of inorganic and organic materials. As photoanodes, mesoporous ZnO with a large surface area were widely employed to host the light-harvesting dyes and the organic molecular hole-transporters. For the synthesis of nanostructured ZnO, diblock copolymer assisted sol-gel approach has been corroborated by countless reports to be powerful in morphology tunability. The amphiphilic diblock copolymer assisted sol gel method and suitable printing parameters are used to fabricate nanostructured ZnO films. In situ grazing-incidence small-angle X-ray scattering (GISAXS) monitors continuously the inner film morphology in a destruction free manner. Based on printed nanostructured ZnO films, hybrid dye-sensitized solar cells are prepared and photovoltaic performance is investigated.

CPP 49.8 Tue 14:00 P1A

Quantification of Phase Purity in Formamidinium Based Multiple-Cation Perovskites by X-ray Scattering — •Lena Merten, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

During the last decade, the material class of hybrid organic-inorganic perovskites aroused huge interest in the solar cell community, leading to a substantial rise in photovoltaic efficiency and a promising perspective for relatively cheap and easy to manufacture solar cell materials. Formamidinium (FA) used as a central cation has the advantage of enhanced light harvesting due to a relatively small band gap, however, α-FAPbI$_3$ is unstable at room temperature and decays into hexagonal δ-FAPbI$_3$. Mixing various organic and inorganic cations within the perovskite material is investigated as one means to achieve enhanced phase purity of the photoactive cubic perovskite phase.

We used grazing incidence x-ray diffraction[1] to examine mixed cation perovskite thin films on mesoporous TiO$_2$ substrates with regard to their ability to stabilize FA based perovskite.

Addition of the inorganic cations Cs and Rb to mixed MA:FA hybrid perovskites was found to significantly reduce the amount of hexagonal phases and excess lead iodide phase. By varying the probing depth, differences in phase composition between the film surface and the bulk material could be observed. The presence of inorganic cations also affected the degree of orientational order, crystallite size and the lattice constant of the perovskite crystal structure.

[1] A. Greco et al.,J. Phys. Chem. Lett. 2018, 9, 23, 6750-6754

CPP 49.9 Tue 14:00 P1A

Influence of Different Organic Cation and Halide Combinations on the Crystallization Dynamics of Perovskite Thin Films — •Ekaterina Kneschaurek, Alexander Hinderhofer, and Frank Schreiber — Institute for Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Understanding the kinetic and energetic effects during organic-inorganic perovskite film growth is very important, since they determine how ions distribute in the structure, which affects the optoelectronic properties of the perovskite film. By tuning the composition of the perovskite films, the growth and formation of perovskite crystals and the extraordinary photophysical properties of perovskite materials can be significantly improved. The initial composition and formation mechanism define crystallization dynamics and structural properties of the resulting thin film. Samples with different compositions of MPbX$_3$ (M = CH$_3$NH$_3{}^+$, CH(NH$_2$)$_2{}^+$, Cs$^+$ or Rb$^+$ and X= Br$^-$, I$^-$ or a mixture) were produced using one-step conversion, a common fabrication technique. The perovskite crystal formation was induced by annealing. We applied in situ grazing incidence wide angle X-ray scattering (GIWAXS) to determine the reaction rate, intermediate phases during growth and perovskite unit cell parameter change in several perovskite thin films over time.[1] We discuss how combining lead halide precursors with different organic and inorganic halide solutions can impact the quality and time scale of the structural and morphological development of the spin-coated perovskite thin films.

1. A. Greco *et. al.*, J. Phys Chem Lett., **2018**, 6750

CPP 49.10 Tue 14:00 P1A

Fabrication on plasmonic nanostructures as light trapper in perovskite and organic solar cells — •Tianfu Guan, Renjun Guo, Xinyu Jiang, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Photovoltaic technology that can converting sunlight directly into electricity is one of the most promising technologies to harvest solar energy for renewable electricity supply. For photovoltaics, such as organic solar cells (OSCs) and perovskite solar cells (PSCs), the light management is an essential issue for achieving higher efficiency and the utilization of plasmonic metal nanostructures has been demonstrated as a promising approach for enhancing light harvesting. In view of this point, to regulate the plasmonic spectral of gold nanoparticles (Au NPs) for maximizing the enhancement in light-absorption of active layer, we assembly the metal NPs onto the electron collecting layer to broaden absorption band of photoactive layer of OSCs and PSCs 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 metallic NPs will influence the crystallinity of the photoactive film and charge transportation of the device. In addition, grazing incidence wide angle x-ray scattering (GIWAXS) is used to probe the crystalline structure of the polymer/perovskite active layers. Grazing incidence small angle x-ray and neutron scattering (GISAXS and GISANS) is used to study the quality of the interface in terms of contact area between the materials.

CPP 49.11 Tue 14:00 P1A

Time-Resolved Microwave Conductivity: Temperature Dependent Dielectric Constant and Charge Carrier Dynamics of Methylammonium Lead Iodide — •Patrick Dörflinger, Julian Höcker, Philipp Rieder, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Perovskite solar cells are one of the most promising new photovoltaic technologies with steadily rising efficiencies. To further improve their potential performance, it is essential to understand their optoelectronic properties as well as to develop novel, not yet established, perovskite materials. With Time-Resolved Microwave Conductivity (TRMC) the mobility and lifetime of photogenerated charge carriers in a perovskite layer, e.g. methylammonium lead iodide (CH$_3$NH$_3$PbI$_3$), can be determined in a non-contact way. Besides the well known data handling in TRMC, one crucial parameter exhibits a strong dependency with temperature. The dielectric constant is not yet experimentally reported in literature for any perovskite material at 9 GHz, the frequency at which TRMC is measured. Considering the behaviour of the dielectric constant of the perovskites and its variation with temperature, one can estimate the temperature dependent mobility with better accuracy. We perform temperature dependent measurements for MAPbI$_3$ from different preparation routes and discuss the power-law behaviour of the mobility in the context of temperature dependence of dielectric constant and the phase transitions of these materials.

CPP 49.12 Tue 14:00 P1A

In-situ GISAXS and GIWAXS measurements during slot-die printing of perovskite thin-films — •Manuel A. Scheel[1], Lennart K. Reb[1], Renjun Guo[1], Sebastian Grott[1], Volker Körstgens[1], Wei Chen[1], Nian Li[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]Technische Universität München, Physik Departement, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]DESY, Notkestr. 85, 22607 Hamburg — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

Organic-inorganic metal halide perovskite based solar cells (PSCs) are currently intensely researched for their potential as cheap and highly efficient next generation solar cells applicable for industrial scale production. In principle, industrial requirements can be met by roll-to-roll slot-die coating. Highly crystalline and uniform films with low defect concentrations are paramount in reaching high power conversion efficiencies in PSCs. In order to better understand morphology evolution and crystallization kinetics during printing deposition in-situ GISAXS and in-situ GIWAXS measurements were done on methyl ammonium lead iodide (MAPI) thin films also covering the wet film stage during the printing process. Printing was carried out at ambient conditions with a self-built slot-die coater equipped with a meniscus guiding blade and temperature controlled sample stage on glass/ITO/PEDOT:PSS.

CPP 49.13 Tue 14:00 P1A

***In-situ* Observation of Perovskite Formation Upon Deposition of Tin Iodide onto Formamidinium Iodide** — •Jonas Glaser, Jonas Horn, and Derck Schlettwein — Justus Liebig University Gießen, Institute of Applied Physics

As lead-based organic-inorganic halide perovskite solar cells have emerged as promising technology for low-cost and highly efficient photovoltaics, issues such as upscaling the manufacturing process and the toxicity of lead are put into focus of interest. Substituting lead by tin, originated in the same main-group with similar properties, yielded solar cell devices with power conversion efficiencies close to 10 %. Usually, tin-based perovskites are prepared via spin-coating from a precursor solution containing formamidinium iodide (FAI) and tin iodide (SnI$_2$). A different approach consists in the interdiffusion method, which combines spin-coating of the organic part with subsequent physical vapor deposition of SnI$_2$ and final annealing [1]. In order to study the formation of the perovskite phase in detail, an experimental setup for in-situ optical characterization of formamidinium tin iodide (FASnI$_3$) has been established, in order to study the transformation of the organic base-layer into the target perovskite through stepwise evaporation of SnI$_2$ and/or annealing.

1. J. Xi, Z. Wu, B. Jiao, H. Dong, C. Ran, C. Piao, T. Lei, T.-B. Song, W. Ke, T. Yokoyama, X. Hou, M. G. Kanatzidis, *Adv. Mater.* **29**, 1606964 (2017).

CPP 49.14 Tue 14:00 P1A

Morphological effects of cesium incorporation in mixed organic mixed halide perovskites — Lennart Klaus Reb, •Manuel Andree Scheel, Renjun Guo, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Sunlight is one of the most promising energy source towards a sustainable future power generation. In the emerging field of new-generation thin-film photovoltaics, perovskite solar cells recently surpassed a power conversion efficiency of 25 % and are therefore a promising complement or even alternative for the commercially established silicon-based solar cells. Especially the highly tunable chemical composition of the perovskite layer allows optimizing the hybrid crystal structure in a way to profit from its unique optoelectronic properties. The incorporation of the alkali metal cation cesium (Cs) into the perovskite lattice has been shown to be beneficial for properties of the perovskite layer by influencing the crystal size and orientation in thin-films. Understanding and controlling the bulk film morphology is therefore essential for highly stable and efficient perovskite solar cells. In this work, we apply statistically relevant grazing-incidence wide-angle X-ray scattering (GIWAXS) to investigate the effect of Cs incorporation on the film morphology. In particular, we investigate the popular (FAPbI$_3$)$_{83}$(MAPbBr$_3$)$_{17}$ perovskite composition in thin-films with different Cs contents and discuss the influence of Cs on their bulk film morphology with focus on the crystallinity.

CPP 49.15 Tue 14:00 P1A

Influence of the optical microcavity effects on the emission and absorption of perovskite solar cells — •Jakob Wolansky, Christian Wolff, Lorena Perdigón-Toro, and Dieter Neher — University of Potsdam, Institute of Physics and Astronomy, Germany

Perovskite solar cells are thin-film devices with usual thicknesses of some hundred nanometres, comparable with the wavelength of absorption and emission of light. Therefore, microcavity effects can influence the device emission and absorption properties, and finally its photovoltaic response.

In this work several parameters of the device stack are varied (e.g. thickness of the perovskite and the transport layers) and their influence on the luminescence and absorption spectra are consequently investigated. This is complemented by a detailed study of the electroluminescence and external quantum efficiency and their correlation via the reciprocity relation by U. Rau[1]. Finally, angular dependent measurements are performed and compared to the results of optical modelling.

[1] U. Rau, Physical Review B 76, 085303 (2007)

CPP 49.16 Tue 14:00 P1A

Pathways towards 30% efficient single-junction perovskite solar cells — •Jonas Diekmann[1], Pietro Caprioglio[1], Daniel Rothhardt[1], Malavika Arvind[1], Thomas Unold[2], Thomas Kirchartz[3,4], Dieter Neher[1], and Martin Stolterfoht[1] — [1]University of Potsdam — [2]Helmholtz-Zentrum-Berlin — [3]Forschungszentrum Jülich — [4]University of Duisburg-Essen

Perovskite semiconductors have demonstrated outstanding external luminescence quantum yields, therefore potentially allowing power conversion efficiencies (PCE) close to the thermodynamic limits. In this work, we establish a simulation model that well describes efficient p-i-n type perovskite solar cells (PCE = 20%) and a range of different experiments helping to quantify the efficiency-limiting processes in state-of-the-art devices. Based on these results, we studied the role of important device and material parameters with a particular focus on chemical doping, carrier mobilities, energy level alignment and the built-in potential across all stack layers. We demonstrate that an efficiency regime of 30% can be unlocked by optimizing the built-in potential across the perovskite layer by using either highly doped thick transport layers (TLs) or ultrathin undoped TLs, e.g. self-assembled monolayers. Importantly, we only consider parameters that have been already demonstrated in recent literature, that is a bulk lifetime of 0.01 ms, interfacial recombination velocities of 100 cm/s, a perovskite bandgap of 1.47 eV and an EQE of 95%. A maximum efficiency of 31% is obtained for a bandgap of 1.4 eV using doped TLs.

CPP 49.17 Tue 14:00 P1A

Enhancing the Open-Circuit Voltage of Inverted Perovskite Solar Cells via Post Treatment Precursor Engineering — •Zekarias Teklu, Shahidul Alam, Steffi Stumpf, Ulrich S. Schubert, and Harald Hoppe — Friedrich Schiller University Jena, Germany

We develop a method of precursor engineering to prepare high-quality perovskite film and its stable PSC with enhanced Voc based on PbAc2 and MAI. The precursor engineering process is done through simple post-treating on pure MAPbI3 host film with (MABr, FABr and FAIsolutions resulted in the formation of mixed cation and or mixed anion of MAPbI3-xBrx, FAxMA1-xPbI3-xBrx,and FAxMA1-xPbI3 perovskites respectively. This post treatment step leads to increased crystal grain dimension, compact and uniform morphology. The dipolar molecules of MABr, FABr, and FAI can simultaneously passivate both cationic and anionic defects of MAPbI3 perovskite films and reduced the defects density, non-radiative recombination and electronic disorder, which are responsible for the Voc reduction. With the post engineering precursor modification, we have developed, the device Voc is enhanced markedly from 0.5 V to 1.08 V of average. The optimized device based on the FAxMA1-xPbI3 obtained from the cation intermixing engineering of FAI on MAPbI3 film shows a promising power conversion efficiency of 16%. As compared to conventional passivation approaches, by using anti-solvent engineering and fast crystallization, which are typically carried out at difficult and short time windows. Our post-treatment process can be easily done on the already crystallized perovskite film.

CPP 49.18 Tue 14:00 P1A

Role of Additives in Perovskite film formation for large area semi-transparent devices — •Gopinath Paramasivam[1], Janardan Dagar[1], Florian Mathies[1], Chandra Shakher Pathak[3], Iris Visoly-Fisher[3], and Eva Unger[1,2] — [1]Helmholtz Zentrum Berlin, Germany — [2]Lund University, Sweden — [3]Ben Gurion University, Israel

Organic-Inorganic Hybrid perovskites have seen a profound interest over the last decennary. Perovskite solar cells (PSC) have reached a record power conversion efficiencies of over 25%. Its accessibility for large-area processing has seen applications in building-integrated photovoltaics. Perovskite Tandems have been realized to surpass the Shockley Quiesser Limit which limits the efficiency of the single-junction solar cells. Semitransparent solar cells make it a wider prospect for the PSCs to be witnessed in the tandem and building-integrated photovoltaics. Herein, we aim to present a detailed role of the additives in controlling the morphology of the films and in the chemical stability of the perovskite. We deployed various polymer hybrids into the perovskite precursor to improve the performance of the perovskites, where we see a change in the morphology with different polymers and performance is enhanced. We also intend to show our results on how the polymer additives tuned our inks for large area deposition through Slot die coating and Inkjet printing. We have achieved 16% power conversion efficiency on semitransparent devices in n-i-p architecture and 19% in opaque devices through spin coating.

CPP 49.19 Tue 14:00 P1A

Orders of Recombination in Perovskite Solar Cells — •Christian Wolff[1], Sean Bourelle[2], Sascha Feldmann[2], Felix Deschler[2,3], and Dieter Neher[1] — [1]Institute für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Cavendish

Laboratory, Department of Physics, University of Cambridge, Cambridge, UK. — [3]Walter Schottky Institut, Technische Universität München, Garching, Germany

Understanding the mechanism and order of recombination in solar cells is of great importance to advance device performance. Pump-probe measurements on neat perovskite layers showed that the rate of recombination is in accordance with $dn/dt = -a \cdot n - b \cdot n \cdot (n + p_0) - c \cdot n^3$, which has been explained as the superposition of SRH, free-carrier, and Auger recombination. The situation in the full devices is more difficult, because charges recombine furthermore at surfaces, within other layers or across interfaces. Different measurements have been applied & reported, but thus far rendered an inconsistent picture of the dominant recombination orders and corresponding lifetimes. Combining multiple spectroscopic and electronic experiments, we provide a consistent picture of the dominating processes. We find that recombination under 1 sun illumination is dominated by a first-order process, while at higher intensities radiative recombination is prevailing. Therefore, the recombination in full devices can be well described by a simple rate equation, without the need to employ mixed-order processes. With this, we are able to reconstruct all device characteristics from dynamic variables.

CPP 49.20 Tue 14:00 P1A

Optical properties of electrons interacting with rotating molecules — •Volker Karle, Areg Ghazaryan, and Mikhail Lemeshko — Institute of Science and Technology Austria (IST Austria), Am Campus 1 3400 Klosterneuburg, Österreich

Recently solar panels based on halide perovskites have seen a tremendous increase in efficiency. However, the key mechanism responsible for this efficiency remains obscure [1]. In this project we theoretically investigate the interactions between electrons and molecules and calculate the resulting change in the absorption coefficient, which can be related to quantum efficiency. The main idea is based on the fact that rotating molecules can exchange angular momentum with the electrons [2]. Furthermore, electrons can decrease their ground-state energy by building up correlations with the molecules. This changes their absorption and mobility properties and could be used for tuning material properties.

[1] T. Chen, W.-L. Chen, B. J. Foley, J. Lee, J. P. Ruff, J. P. Ko, C. M. Brown, L. W. Harriger, D. Zhang, C. Park, and others, Proceedings of the National Academy of Sciences 114, 7519 (2017).

[2] D. H. Fabini, T. A. Siaw, C. C. Stoumpos, G. Laurita, D. Olds, K. Page, J. G. Hu, M. G. Kanatzidis, S. Han, and R. Seshadri, Journal of the American Chemical Society 139, 16875 (2017).

CPP 49.21 Tue 14:00 P1A

Magneto-Optical Properties of magnetically-doped Perovskite Semiconductors — •Timo Neumann[1,2], Jonathan Zerhoch[2], Sascha Feldmann[1], Martin Brandt[2], and Felix Deschler[2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Dilute magnetic semiconductors (DMS) constitute a material class which combines semiconducting and magnetic properties by introducing magnetic impurities to an otherwise non-magnetic host semiconductor. Fully inorganic DMS have been known for decades and advanced material processing techniques have enabled control over various functionalities like spin injection and the control of magnetism by electric fields and currents. Due to their outstanding optoelectronic properties and high defect tolerance, organo-metal halide perovskites form an ideal system for efficient magnetic doping. We perform temperature and magnetic field dependent magnetometry to characterise the magnetic properties of magnetically-doped perovskite semiconductors and employ polarisation-dependent, low temperature magneto-photoluminescence measurements to reveal the coupling between localised magnetic impurities and optically excited charge carriers.

CPP 49.22 Tue 14:00 P1A

Stabilizer-assisted tin-lead perovskite solar cells for high efficiency and stability — •Rui Wang, Renjun Guo, and Peter Müller-Buschbaum — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Lead-based perovskites have proven to exhibit high photovoltaic performance and power conversion efficiency of over 20%. FA-stabilized perovskites show high long-term stability and are thermally endurable where other perovskite devices do not continue to function and lose their perovskite phase. Important is to further improve perovskite-based solar cells as a goal by reducing or removing the use of the heavy metal lead. To stabilize more the perovskite solar cell, PEA (phenethylammonium) is mixed with FA to achieve better stability. Thus, we systematically investigate the performance of FA(1-x)PEAI(x)Pb(1-x)Sn(x)I3 mixed metal halide perovskites. Adding Sn leads to the stabilization of the black perovskite phase and the low formation temperature of 100*C is sufficient to reach of the formation of the perovskite phase. The efficiency we aimed at is over 10% with Sn content of x=0.5, 0.8, 0.3. The higher amount of Sn is expected to not enhance device performance.

CPP 49.23 Tue 14:00 P1A

GI/T-XPCS for slot-die coated perovskite thin films — •Christopher Greve[1], Michael Buchhorn[1], Dinesh Kumar[2], Alexander Hexemer[2], Lutz Wiegart[3], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Advanced Light Source, Lawrence Berkeley National Lab, 1 Cyclotron Road, Berkeley Ca 94720, USA — [3]NSLSII, Brookhaven National Lab, Brookhaven Avenue, Upton NY, USA

X-Ray Correlation Spectroscopy (XPCS) is a useful tool to investigate the dynamics and the morphology of hard and soft condensed matter. Via XPCS, it is possible to probe length scales $<$ 100nm and time scales $>$10-4s. To obtain information about the underlying dynamics, the correlations of the scattered intensity (speckles) in a time series are investigated. We use XPCS to investigate slot-die coated thin films in situ in gracing incident (GI) and gracing incident transmission (GT) geometry to gain insights in the underlying processes of thin film formation. For printing, an up-scalable printer setup is used and as a system methylammonium lead iodide (MAPI) is featured. MAPI is known for its solar cells applications, but the underlying processes of thin film formation are poorly understood. XPCS offers the possibility to investigate the dynamics in the evolving MAPI thin film. In our approach the optimized GT geometry allows to model the data in the born approximation, thus to ignore multiple scattering events from the thin film and the need to consider their impact on extracted dynamics.

CPP 49.24 Tue 14:00 P1A

The effect of surfactant doping on the crystallization kinetics and stability of perovskite solar cells — •Yuqin Zou and Peter Müller-Buschbaum — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) have gained high attention within the last years. They have achieved a remarkable development due to their excellent optical properties and the power conversion efficiency of PSCs has meanwhile crossed the 25% border. However, the efficiency, hysteresis and stability of PSCs are still the main obstacles to their commercial application. The existing challenges are largely attributed to the presence of defect states. Tailoring functional ligands to passivate the defects in perovskite films and interfacial traps is an effective way to improve the performance of PSCs. In the present study, a small amount of surfactants (SDBS) is introduced to modify the perovskite interface, so that a high efficiency and stability of the PSCs can be obtained by crystallization control and defect passivation. The crystal structure, phase and orientation are studied with grazing incidence wide angle X-ray scattering (GIWAXS).

CPP 49.25 Tue 14:00 P1A

Electrical transport through DNA templated metallic nanowires and ds-DNA. — •Archa Jain[1,2], Türkan Bayrak[1], Jingjing Ye[3], Bilal Khan[1], Ralf Seidel[3], Artur Erbe[1], and Stefan Schulz[2] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany — [2]Technische Universität Chemnitz, 09107 Chemnitz, Germany — [3]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, 04103 Leipzig, Germany

Here we investigate self-assembled devices using DNA as excellent constructive and self-organizing material for nanoelectronics. So-called DNA origamis have been used as molds to build metallic nanowires in any shape and size, in contact with double stranded (ds) DNA segments. The combination with electron beam lithography as top down process allows for attaching metallic wires to the DNA origamis of smallest dimensions.

We investigate the charge transport through self-assembled, DNA templated metallic nanowire- ds-DNA- metallic nanowire structures.

The ds-DNA structures between the Au nanowires are about 15 nm long (˜30bp). We characterize the charge transport through these structures by current-voltage measurements. This electrical measurement through ds-DNA demonstrate the feasibility to use DNA for electron transport in nanodevices (Molecular electronics) and also increase the potential to use this bio- molecule for future applications.

CPP 49.26 Tue 14:00 P1A

Energy transfer mechanism in fluorescent carbon nanoparticle/dye composite — •Sumesh Sofin R. G[1], Abey Issac[1], Malik R. S. Al Naabi[1], Myo T. Zar Myint[1], Htet H. Kyaw[2], and Osama K. Abou-Zied[3] — [1]Department of Physics, College of Science, Sultan Qaboos University, Al Khoud, Muscat, Sultanate of Oman. — [2]Nano Chair, College of Science, Sultan Qaboos University, Al Khoud, Muscat, Sultanate of Oman. — [3]Department of Chemistry, College of Science, Sultan Qaboos University, Al Khoud, Muscat, Sultanate of Oman.

The photoluminescence of carbon nanoparticles (CNPs) is fascinating due to its application potential though the PL mechanism is not completely understood. Energy transfer between fluorophores and CNPs is also an important aspect in the field of green energy harvesting. In this work, we studied the energy transfer process between CNPs Rhodamine 6G dye molecules. CNPs were prepared using microwave assisted green synthesis method. The prepared particles were characterized using various tools to understand the structure and morphology. UV-Vis absorption/emission spectroscopy and time-resolved fluorescence decay measurements were done on particles and particle/dye composites. The results were analysed using Stern-Volmer quenching and Fluorescence resonance energy transfer models. Deconvolution analysis were performed on all the emission peaks to get in-depth details of energy transfer mechanism. Quantum yield and molar extinction coefficient of CNPs were estimated in this work. These studies may shine some light on the emission mechanism of CNPs.

CPP 49.27 Tue 14:00 P1A

What is the role of planarity and flexibility for aggregation in organic semiconductor materials? — •Stefan Wedler[1], Axel Bourdick[2], Stavros Athanasopoulos[3], Stephan Gekle[2], Fabian Panzer[1], Caitlin McDowell[4], Guillermo C. Bazan[4], and Anna Köhler[1,5] — [1]Soft Matter Optoelectronics, U Bayreuth — [2]Biofluid Simulation and Modeling, U Bayreuth — [3]Universidad Carlos III de Madrid — [4]Center for Polymers and Organic Solids, UC Santa Barbara — [5]BIMF, U Bayreuth

Planarity and flexibility play an important role for the aggregation process in organic semiconductors. Stiff and planar molecules seem to aggregate more easily. However, it is not clear whether these factors are a prerequisite or just a side effect of aggregation. We have investigated their influence on the aggregation properties using two similar conjugated molecules, with benzothiadioazole donor moieties and thiophene acceptor units. They differ only by their central unit, where a bithiophene unit either allows for flexible twists (TT), or where it is bridged to provide a rigid planar connection (CT). Temperature dependent absorption and luminescence spectroscopy in solution shows that both molecules can readily form aggregates. However, CT exhibits only weak aggregation signatures. MD simulations and DFT calculations reveal that although TT planarizes upon aggregation, its flexibility prevents the formation of excimer-like states, which seems to be the case for CT.

CPP 49.28 Tue 14:00 P1A

Photophysics of Pentacene Blends with Weakly Interacting Spacer Molecules — •Frederik Unger, Clemens Zeiser, and Katharina Broch — Institute of Applied Physics, University of Tübingen, Germany

One of the main interests in pentacene (PEN) arises from its ability to undergo singlet fission (SF), a process where absorption of a single photon results in the generation of two triplet excitons [1]. Although being used as a prototypical model system, the details of the SF mechanism in PEN are still not fully understood. It is therefore crucial to understand and enable controlled tuning of the absorption behavior of PEN.

We mixed PEN with weakly interacting spacer molecules ([5]-phenacene [2] and [6]-phenacene) and investigated the PEN Davydov splitting as function of mixing ratio. Subsequent exciton behavior was investigated by temperature dependent photoluminescence spectroscopy. The comparison of the two systems is of special interest as the chemical and physical properties for both spacer molecules are similar, except for the difference in molecule length.

[1] Smith, M. B., and Michl, J., Chemical Reviews 110 (2010), [2] Dieterle, J., et al., J. Phys. Chem. C (2015).

CPP 49.29 Tue 14:00 P1A

Directly probing the singlet-triplet dynamics in organic semiconductors by high intensity step-function photoexcitation — •Jonas Gehrig[1], Ulrich Müller[1], Lena Roos[2], Anke Krueger[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute of Organic Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — [3]ZAE Bayern, 97074 Würzburg

The excitonic singlet-triplet dynamics of organic semiconductors play a crucial role for their efficient implementation in opto-electronic devices. We present a compact setup to probe the relevant time-dependent processes like inter-system crossing, singlet fission (SF) or thermally activated delayed fluorescence (TADF). Unlike single molecule spectroscopy or pump-probe techniques, we utilize step-function photoexcitation at high excitation intensities in combination with time correlated single photon counting. Applying this technique to neat single crystals of tetracene (Tc) and its 2,2'-ditetracene dimer (DTc) we observed a sub-ns SF in Tc while this process is efficiently suppressed in DTc. X-ray diffraction analysis in combination with theoretical coupled-cluster calculations attribute this striking difference to the respective crystal structure being slightly modified by the covalent linking at the DTc 2,2'-position. On the molecular level, represented by doped anthracene single crystals, the fluorescent properties of Tc and DTc are almost identical and the absence of SF in both host-guest-systems emphasizes the role of inter- rather than intramolecular interactions for this non-radiative decay process.

CPP 49.30 Tue 14:00 P1A

Theoretical study of p-type double-doping in a conjugated polymer — •Thomas Bathe[1], Chuan-Ding Dong[1], and Stefan Schumacher[1,2] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP),Paderborn University, Warburger Strasse 100, 33098 Paderborn, Germany — [2]College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

Efficient molecular doping is essential for achieving the charge carrier densities needed for applications of conjugated polymers in electronic devices. Recent studies [1] have demonstrated the possibility to induce two charges in a conjugated polymer blend for each individual small dopant molecule. Dopants with sufficiently high electron affinity have to be used and those were shown to form di-anions upon successful transfer of two charges, increasing the efficiency of molecular p-type doping without increasing the concentration of doping molecules. Here, the formation of di-anions in charge-transfer complexes is studied theoretically. A single dopant molecule (CN6-CP and F6TCNNQ, respectively) is investigated in the vicinity of two conjugated oligomers based on density functional theory calculations [2]. For certain configurations, double-doping is indeed found and evidenced by an integer charge transfer from both oligomers onto the dopant molecule, leading to di-anion formation for the dopant molecule. Signatures of double doping are also found in the calculated optical and vibrational spectra.

[1] Kiefer et al., Nature Materials 18, 149-155 (2019).

[2] Dong, Schumacher, ChemRxiv (2019).

CPP 49.31 Tue 14:00 P1A

Adsorption of the photochromic diarylethene CMTE on a diamond surface — •Fabian Bauch[1], Chuan-Ding Dong[1], Christian Wiebeler[2], Cedrik Meier[1], and Stefan Schumacher[1] — [1]Department Physik, Universität Paderborn, Deutschland. — [2]Institut für Analytische Chemie, Universität Leipzig, Deutschland.

Photochromic materials bear great potential for electronic devices such as optical switches and optical memories due to their reversible photoisomerization mechanism [1]. The photochromic cis-1,2-dicyano-1,2-bis(2,4,5trimethyl-3- thienyl)ethene (CMTE) exhibits particularly high fatigue resistance and thermal stability [2]. In particular, the CMTE undergoes a pericyclic cyclization reaction upon irradiation with UV light while visible light triggers the cycloreversion reaction [2]. In realistic applications the molecular material or molecule would typically reside on or be bound to a substrate surface. To investigate the influence of such a surface on the structural and electronics properties of the molecular photoswitch, here we perform detailed density functional theory (DFT) calculations for CMTE in free gas-phase and adsorbed on different diamond surfaces saturated with hydrogen. We also calculate the optical absorption of CMTE in a single-particle approach for different molecule orientations on the surfaces. We find that the electronic and optical properties of CMTE are very similar to the gas-phase results for the case, when the molecule is only physisorbed on the surface but not chemically bound.

[1] M. Irie and M. Mohri. J. Org. Chem. 1988, 53, 4, 803-808. [2] C. Wiebeler, C. Bader. et.al. Phys.Chem.Chem.Phys., 2014, 16, 1453.

CPP 49.32 Tue 14:00 P1A

Light-Induced Electron Transfer in the MOF-Based Noble-Metal-Free Photocatalyst Ni/CdS@MIL-101 as Studied with Fluorescence Lifetime Imaging Microscopy (FD-FLIM) — SEBASTIAN FEULNER[1], •LOTHAR KADOR[1], MARA KLARNER[2], and RHETT KEMPE[2] — [1]University of Bayreuth, Institute of Physics, 95440 Bayreuth, Germany — [2]University of Bayreuth, Institute of Inorganic Chemistry, 95440 Bayreuth, Germany

Particles of the semiconductor CdS on size-optimized colloidal metal-organic framework (MOF) crystallites act as a photo-catalyst for the H_2 liberation from amines. This acceptorless process is of great interest, since imine derivatives serve as intermediates to synthesize aromatic N-heterocycles which are highly desirable products for the fine chemical industry. The catalytic activity is strongly enhanced when co-catalytic Ni nanoparticles are present. We demonstrate that the photoluminescence lifetime of the CdS is shortened in the presence of Ni nanoparticles, so the improved catalytic activity can be related to electron transfer from the conduction band of the CdS to the Ni. The effect of Ni was found to be stronger than that of the noble metals Pt and Pd. The experiments were performed with a custom-built fluorescence lifetime imaging microscope operating in the frequency domain (FD-FLIM). It is based on a diode laser at 488 nm which was amplitude-modulated in the range 110 - 160 MHz. The data are evaluated with the polar-plot (or Cole-Cole plot) technique.

CPP 49.33 Tue 14:00 P1A

A new sample for coherent multidimensional spectroscopy: Preparation of molecules on cold rare gas clusters — •ELENA LEISSLER, LUKAS BRUDER, ULRICH BANGERT, MARCEL BINZ, FRIEDEMANN LANDMESSER, DANIEL UHL, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

The recent advances of coherent multidimensional spectroscopy towards the gas phase made new samples accessible, featuring low internal temperatures and minimal environmental perturbation [1]. In particular, matrix isolation on rare gas clusters is of interest, as it provides a high degree of control over molecule-molecule and molecule-solvent interactions. Doping the rare gas clusters with variable numbers of different molecules directly dictates the interaction strength. Here we present a cluster beam apparatus with a highly flexible doping unit. The unit features high dopant densities and the possibility to simultaneously dope with various molecules out of the gas and solid phase.

[1] Lukas Bruder et al, J. Phys. B: At. Mol. Opt. Phys. 52 183501 (2019).

CPP 49.34 Tue 14:00 P1A

Recent advances in materials and modelling of organic electrochemical transistors — •FLORIAN GÜNTHER, RENAN COLUCCI, HENRIQUE F. P. BARBOSA, GERMÁN GÓMEZ, PRISCILA CAVASSIN, and GREGÓRIO C. FARIA — Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil

Organic electrochemical transistors (OECTs) have been successfully used as a transducer in applications requiring conversion of ion fluxes to electronic current. To fully understand and optimize them, it is mandatory to develop in-depth theoretical predictions of experimental data that fits both modes of operation: depletion and accumulation. Moreover, it is imperative to count with a vast palette of semiconducting polymers that can be efficiently used as active layers in electrochemical devices. Here, we present a universal method and accompanying guidelines for fabricating OECTs using water-insoluble hydrophobic semiconducting polymers. By taking advantage of the interactions of semiconducting polymers in certain organic solvents and the formation of a stable liquid-liquid interface between such solvents and water, we fabricated accumulation mode OECTs with high transconductance and enhanced stability. Additionally, we present an extension of the well-known Bernard-Malliaras model for the steady-state response of OECTs to describe electrical responses of accumulation mode OECT. We have fit output-curves of accumulation mode OECT, fabricated with the universal method previously mentioned. In all cases we got good agreements between experimental data and theoretical fittings.

CPP 49.35 Tue 14:00 P1A

Modelling of anharmonic properties and thermal conductivity in organic semiconductors — •FABIAN HAUPTMANN[1], SANDRO WIESER[1], TOMAS KAMENCEK[1], NATALIA BEDOYA-MARTINEZ[2], ROCHUS SCHMID[3], JOHANNES PETER DÜRHOLT[3], and EGBERT ZOJER[1] — [1]Institute for Solid State Physics, Graz University of Technology, NAWI Graz, Petersgasse 16, 8010 Graz, Austria — [2]Materials Center Leoben, Roseggerstraße 12, 8700 Leoben, Austria — [3]Computational Materials Chemistry group, Ruhr-Universität Bochum, Universitätsstraße 150, Bochum 44801, Germany

Thermal transport is important for most practical applications of functional materials. In (opto)electronic devices, it is typically desirable that materials dissipate heat as efficiently as possible. Conversely, for special purposes, like thermoelectric energy conversion, a low thermal conductivity is crucial. Organic semiconductors(OSC) are particularly relevant for optoelectronic applications, which is exemplified by their commercially successful use in displays for many devices. Moreover, OSCs have also been explored as promising candidates for thermoelectric applications. A central aspect for understanding thermal transport in OSCs is to realize, how the thermal conductivity and the structure of an OSC material are interrelated. In this work we parametrize advanced, system-specific force fields analogous to MOF-FF for a range of different acene-based OSC materials, to study their thermal expansion and thermal transport properties by using MD simulations. Our results, where available, are compared to experimental data.

CPP 49.36 Tue 14:00 P1A

Influence of morphology on the work function reduction by polyethylenimine — SUJITKUMAR BONTAPALLE[1,2], •ANDREAS OPITZ[2], RAPHAEL SCHLESINGER[2], SETH R. MARDER[3], SUSY VARUGHESE[1], and NORBERT KOCH[2,4] — [1]Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India — [2]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [3]School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics (COPE), Georgia Institute of Technology Atlanta, Atlanta, USA — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Polyethylenimine (PEI) layers are used to reduce the work function of electrode materials and are frequently applied to organic or perovskite opto-electronic devices. Intermixing of PEI from water-based solution with the conductive polymer poly(3,4-ethylenedioxythiophene):polystyrene sulfonate mixture can be avoided by the usage of anhydrous butanol as solvent for PEI. This preserves also the transparency of the polymer mixture. Heating of inhomogeneous PEI films in ultra-high vacuum ensures the removal of residual solvent and the homogeneous coverage. Thus, the work function of PEI film is reduced to about 1.65 eV below the original substrate work function, which gives 2.3 eV as lowest observed value for zinc oxide.

CPP 49.37 Tue 14:00 P1A

Influence of Morphology on the Density of Charge-Transfer States in Organic Donor/Acceptor Blends — •ANNA-LENA HOFMANN[1], THOMAS ZECHEL[1], THERESA LINDERL[1], ALEXANDER HOFMANN[1], TOMOYA SATO[3], KOHEI SHIMIZU[2], HISAO ISHII[3], and WOLFGANG BRÜTTING[1] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg — [2]Graduate School of Science and Engineering, Chiba University, Chiba, Japan — [3]Center for Frontier Science, Chiba University, Chiba, Japan

Charge-transfer (CT) states are considered as precursors for charge generation and their energy (E_{CT}) as the upper limit for the open-circuit voltage (V_{OC}) in organic donor/acceptor (D/A) solar cells. In this study the morphological influence of using a crystalline donor diindenoperylene (DIP) versus an amorphous donor tetraphenyldibenzoperiflanthene (DBP) with almost identical ionization energy is investigated. As acceptor material the widely used fullerene C_{60} is used. Reduced electroluminescence (EL) and reduced external quantum efficiency (EQE) spectra in the visible and near infrared spectrum are used to determine E_{CT} and the character of the CT density of states (CT DOS). This is then related to the morphology of the different D/A systems. In this context we try to verify the necessity of static disorder in the description of CT emission and absorption spectra of small molecule solar cells. Remarkably, the more crystalline donor DIP shows a significant contribution of static disorder, whereas for the amorphous DBP a description without static disorder soley based on Marcus theory is sufficient.

CPP 49.38 Tue 14:00 P1A

Effect of thiophene- and benzothiadazole-based non-fullerene acceptors in organic solar cells — •Jannis Klotz, Hannah Lindl, Stefanie Dietz, Maria Kotova, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic bulk heterojunction solar cells based on small molecule non-fullerene acceptors (NFA) received a lot of attention in the past few years due to a rapid increase in the device efficiencies up to 16%. This breakthrough, being highly promising, was mostly driven by empirical material engineering rather than by device-physics design. In this work we compare the already well established thiophene-based acceptor molecule ITIC and a novel benzothiadiazole-based acceptor molecule Y6. We studied optical and electrical properties of pure materials and blends as well as working devices. The acceptor ITIC was combined with the donor polymer PBDB-T and Y6 with a fluorinated version of PBDB-T: PM6. The redshifted and increased absorption of the PM6:Y6 blend in comparison to PBDB-T: ITIC lead to substantially increased short circuit currents and thus to higher device efficiencies. Nevertheless, fluorinated materials have shown to have limited solubility and faster device degradation. We investigated device preparation and degradation of both to evaluate their prospects for organic solar cells.

CPP 49.39 Tue 14:00 P1A

The mechanism of doping low band gap polymers with a Lewis acid — •Simon Biberger[1,2], Viktor Brus[2], David Cao[2], Brett Yurash[2], Dirk Leifert[2,3], Thuc-Quyen Nguyen[2], and Anna Köhler[1] — [1]Softmatter Optoelectronics (EP2), University of Bayreuth, Germany — [2]Center for Polymers and Organic Solids, UCSB, Santa Barbara, USA — [3]Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Münster, Germany

To p-dope organic semiconductors F4TCNQ is commonly used. This doping mechanism relies on the electron transfer from the HOMO of the semiconductor to the LUMO of the dopant. This occurs by a match of those energy levels. For a solution-processed semiconductor this approach suffers from the differential solubility of the dopant, the charge-transfer complex and of the polymer what ultimately limits the processability of the doped semiconductor. In this study we use electrophilic Lewis acids to p-dope conjugated polymers. Work by Zalar et al. (Adv. Mat. 2014, 26, 727-727) showed an increased mobility after addition of Lewis acid. Yet the mechanism behind this doping approach is still elusive. To understand this approach we systematically investigate the effect of structural and electronic factors by varying, e.g., the donor and acceptor strength of the polymer. Optical and electrical characterization, using, e.g., optical spectroscopy and EPR, were performed to understand the influence of the adduct formation on the properties of the polymer.

CPP 49.40 Tue 14:00 P1A

Ground-state charge transfer and influence on charge carrier transport in organic donor-acceptor mixtures — Hongwon Kim, Marius Gebhardt, Domenik Vögel, and •Wolfgang Brütting — Experimental Physics IV, Institute of Physics, University of Augsburg, Augsburg Germany

In organic semiconductors, charge transfer states form at interfaces of electron accepting and donating molecules resulting in a partial or full transfer of electrical charges. This charge transfer doping is crucial to generate excess charges in (opto-)electronic devices. We have investigated charge transfer states and charge transport properties of organic semiconductor mixtures consisting of electron donating molecules, DIP, 6T, DBTTF, and DBP, doped by a strong acceptor, F6TCNNQ. Charge transfer effects are observed by optical absorption spectroscopy and electrical transport properties are characterized depending on field and temperature by current-voltage measurements and impedance spectroscopy. In this way, it is possible to distinguish between integer charge transfer states and charge transfer complex formation, and to explain high electrical conductivity at a certain doping concentration with morphology and derived design rules for efficient charge transfer.

CPP 49.41 Tue 14:00 P1A

Influence of solvent on the morphology and optical properties of printed active layers based on PBDB-T-SF:IT-4F for application in organic solar cells — •Daniel Maximilian Steger, Kerstin Sabrina Wienhold, and Peter Müller-Buschbaum — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

The morphology of the active layer of polymer-based organic solar cells (OSCs) greatly influences their efficiency. Therefore factors determining the structure such as the used solvents are highly relevant in current research. The active layer consist of a blend of the polymer donor material PBDB-T-SF and the non-fullerene small molecule acceptor material IT4F. In this work the active layer is, in contrast to most other studies, produced via thin film printing, as this technique is a very promising approach to increase the scalability of solar cell production. The influence of the solvent on the morphology is investigated by observing the optical properties via UV/VIS- and fluorescence spectroscopy, the surface structure via atomic force microscopy (AFM) and studying the inner morphology by using scattering methods such as grazing incidence wide angle x-ray scattering (GIWAXS) and grazing incidence small angle x-ray scattering (GISAXS).

CPP 49.42 Tue 14:00 P1A

Influence of printing temperature on the efficiency of organic solar cells — •Linus Fidelis Huber, Kerstin Sabrina Wienhold, and Peter Müller-Buschbaum — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Solar cells have been a prominent and successful concept for eco-friendly energy conversion for a long time, but in search for better efficiencies and cheaper production costs, new materials and production techniques need to be explored. Printable-thin-film solar cells could lower production-cost by means of a high scale-up potential and an easier production process. They can also yield high efficiencies, are of lighter weight, flexible and semitransparent. This suggests a wide variety of possible applications, where silicon-solar cells seem to be less applicable. Printing temperature is an important parameter and varying it, could lead to better efficiencies and a broader understanding of the polymers dependence on temperature. We focus on novel low band gap polymers in combination with non-fullerene acceptor molecules. Four different printing temperatures are studied and evaluated using UV-Vis, photoluminescence, AFM and GISAXS measurements.

CPP 49.43 Tue 14:00 P1A

Studying aggregation behavior of Conjugated Polyelectrolytes as a function of molecular weight for Poly(3-hexylthiophen-2,5-diyl) (P3HT) and Poly(6-(thiopene-3-yl)hexane-1-sulfonate) (PTHS) — •Sanwardhini Pantawane and Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth, Bayreuth, Germany

Aggregation of π conjugated polymers like Poly(3-hexylthiophen-2,5-diyl) (P3HT) and the improved P3HT substitute - Poly(6-(thiopene-3-yl)hexane-1-sulfonate) (PTHS) is important for their performance in optoelectronic devices. It is experimentally observed that the red shift in the UV-vis spectra with increasing molecular weight is much stronger for PTHS than for P3HT, even though both molecules are structurally very similar. To understand this, we prepared different polymer chains of P3HT and PTHS starting with 13 monomers each, as was done in the experimental studies, and carry out molecular dynamics simulation in water and sodium ions, to correlate the fluorescence spectra with difference in the aggregation conformation as a function of the polymer's molecular weight. We perform free energy calculations to pull the end rings of the polymer towards each other and investigate their potential of mean force (PMF). This study gives us an insight about the folding probability of the P3HT and PTHS chains with varying lengths.

CPP 49.44 Tue 14:00 P1A

Impact of Mixing on Coupling of Tranisition Dipole Moments in Pentacene: Dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene — •Arne Morlok[1], Clemens Zeiser[1], Daniel Lepple[1], Guillaume Schweicher[2], Yves Geert[3], and Katharina Broch[1] — [1]Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]University of Cambridge, Cavendish Laboratory, JJ Thompson Avenue 19, CB3 0HE Cambridge, UK — [3]Universite Libre de Bruxelles, Chemistry Departement, Avenue Franklin Roosevelt 50, 1050 Bruxelles, Belgium

The coupling of transition dipole moments (TDMs) strongly affects the optical properties of organic semiconductors (OSCs), for instance in H- or J-type coupling or Davydov-splitting [1].Despite changes in the unit cell parameters, in blends of pentacene (PEN) with the H-aggregate diindenoperylene (DIP) no significant changes in the H-type coupling have been observed, which is consistent with the orientation of the TDMs [2]. For J-aggregates however, the impact of mixing and the corresponding increase in intermolecular distances will be more pronounced but has so far not been discussed in detail in the literature.

Here, we report the optical properties of dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene, which shows the optical properties of a J-aggregate, in blends with PEN. We observe strong changes in the intensity of absorption peaks, which can be directly related to the increase in the lattice spacing and the reduced coupling of TDMs.

[1] F. C. Spano, Acc. Chem. Res. 43 (2010)

[2] K. Broch et al., J. Phys. Chem. C 117 (2013)

CPP 49.45 Tue 14:00 P1A

Der Einfluss von Elektrophorese auf die aktive Schicht organischer Solarzellen — •Fabian Eller, Stephan Pröller und Eva M. Herzig — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

Slot-die coating bietet die Möglichkeit, organische Dünnschichtsolarzellen effizient mit industrienahen Methoden herzustellen. Um einen hohen Wirkungsgrad zu erreichen, ist eine optimale Nanostrukturierung des Dünnfilms notwendig. Wir haben gezeigt, dass die Morphologie des gedruckten Filmes mit einem elektrisches Feld während des Druckprozesses beeinflusst werden kann [1].

Um den Effekt eines elektrischen Feldes auszunutzen, charakterisieren wir systematisch die elektrophoretischen Mobilitäten von halbleitenden Materialien für die Nutzung in OPV Systemen. Die Abhängigkeit von diversen externen Parametern und der Lösungsherstellung erlaubt es uns, die Mobilitäten gezielt einzustellen.

Unser Ziel ist es die Morphologie und damit den Wirkungsgrad von gedruckten Solarzellen in unterschiedlichen Materialsystemen durch Anlegen eines elektrischen Feldes zu steuern.

[1] paper, submitted

CPP 49.46 Tue 14:00 P1A

Donor-Acceptor Polymers with PDMS-Ur based crosslinkers: A Novel Hybrid Material for Stretchable Semiconductor Applications — •Florian Günther[1], Ubirajara P. Rodrigues-Filho[2], and Roberto M. Faria[1] — [1]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [2]Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, Brazil

The visions that we have for our future, especially the expectations we have on electronic devices, require the invention of new materials. In the past decades, organic semiconducting materials have been intensively studied since they show some advantages over bulk semiconductors. E.g., they offer the possibility to fabricate flexible devices. So far, however, flexibility has mainly been studied in terms of bendable and twistable thin films. The next stage on the road map towards higher functionality is therefore to focus on stretchability. Our work aims at combining the semiconducting properties of donor-acceptor polymers, especially those based on dithienyl-diketopyrrolopyrrole (TDPP), with the flexible properties of polydimethylsiloxane (PDMS). More specific, the TDPP-based DA backbones shall be crosslinked via PDMS by forming urethane (Ur) bonds between these two compounds. For this, the so-called Figovsky reaction can be used. The urethane bonds promise a higher chemically and mechanically stability due to additional hydrogen bonds. In this presentation, we are going to show our synthesis and fabrication strategies as well as our results on the semiconducting properties obtained so far.

CPP 49.47 Tue 14:00 P1A

Direct measurement of charge recombinationlosses in organic solar cells by transientspectroscopy — •Florian Günther, Daniel R. B. Amorim, Roberto M. Faria, and Paulo B. Miranda — Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil

Research on organic solar cells has increased significantly in the past decade, covering both applied and basic aspects. Improvements in their performances depend on a deep knowledge about the photophysical and electronic processes that occur in the materials. The dynamics of charge recombination within operating devices is one important issue being relevant for determining the charge recombination losses and the overall device efficiency. Inour work, we directly probe the dynamics of charge recombination and extraction in organic solar cells by combining transient photoinduced absorption spectroscopy (TAS) with transient photocurrent (TPC) measurements in the ns to ms time range after excitation of the device by a short laser pulse. TAS probes the dynamics of the charge density inside the organic active layer of the solar cell, while TPC measures the rate of charge extraction from the device. Comparing both measurements it is possible to determine how much photogenerated charge is lostwithin the active layer due to charge recombination, a major loss mechanism that limits the overall device efficiency. Using this technique,we have probed high-quality solar cells based on porphyrinderivatives and also traditional polymer-based (P3HT:PCBM) solar cells.

CPP 49.48 Tue 14:00 P1A

Improvement of hole transport layer selectivity for polymer solar cells — •Aurelien Sokeng Djoumessi[1,2], Jose Prince Madalaimuthu[1,2], Shahidul Alam[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [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

Since the device performance and stability strongly depend on the interfacial layers, the hole transport layer (HTL) is one of the crucial parameters of polymer solar cells. Specifically interesting for charge extraction is the selectivity of the HTL. Furthermore unfavorable interactions with electrodes or the photoactive layer should be screened. We investigated organic solar cells in conventional architecture by varying the HTL systematically between PEDOT:PSS and a sol-gel derived metal oxide. The impact of modified HTL in the solar cells were investigated by different optical and electrical characterizations. In order to observe the effect on the recombination mechanism of the solar cells, light intensity-dependent current-voltage (LID-IV) measurements and analysis of IV-characteristics were performed.

CPP 49.49 Tue 14:00 P1A

Qualification of Thieno-Quinoxaline Based Polymers for Application in Non-Fullerene Organic Solar Cells — •Md Moidul Islam[1,2], Shahidul Alam[1,2], Christos L. Chochos[4,5], Ulrich S. Schubert[1,2,3], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, 07743 Jena, Germany — [3]Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Jena, Germany — [4]Institute of Chemical Biology, National Hellenic Research Foundation, Athens, Greece. — [5]Advent Technologies SA, 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 49.50 Tue 14:00 P1A

Re-evaluation of the IV-Curve — •Rico Meitzner[1,2], Shahidul Alam[1,2], Aman Anand[1,2], Ulrich S. Schubert[1,2] und Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry, Friedrich-Schiller-Universität Jena, 07743 Jena — [2]Institute for Organische und Makromolekulare Chemie (IOMC), Friedrich-Schiller Universität, 07743 Jena

The most basic measurement performed on solar cells is an IV-characterization. Most commonly the basic solar cell parameters, like open circuit voltage, short circuit current density, fill factor and power conversion efficiency are extracted from these measurements. From further analysis of these curves, we found that they could actually reveal more than meets the eye normally. We want to present a new method to analyze these curves and how it could help getting a better view on what to look into with more depth for these devices.

CPP 49.51 Tue 14:00 P1A

IR Spectroscopic Investigation on Immobilization of organic dopants — •Rainer Bäuerle[1,2,3], Patrick Reiser[1,4], Frank Simon Benneckendorf[1,3,4], Marc-Michael Barf[1,5], Sebastian Beck[1,2], Annemarie Pucci[1,2], Uwe H. F. Bunz[1,3], and Wolfgang Kowalsky[1,5] — [1]InnovationLab, Heidelberg — [2]Kirchhoff Institute for Physics, University of Heidelberg — [3]Organisch-Chemisches Institut, University of Heidelberg — [4]Materials Science Department, Surface Science Division, TU Darmstadt — [5]Institute for High-Frequency Technology, TU Braunschweig

One challenge in doping of organic semiconductors lies in the unstable spatial distribution of dopants. The simple intermixing of dopants to a matrix semiconductor makes them subject to diffusion and drift. With a universal anchor group that covalently binds to most semiconductors this problem can be overcome. We investigate the influence of an azide group as such anchor in a semiconductor thin film on the diffusion of dopants via infrared spectroscopy.

A derivate of the literature known n-dopant DMBI without anchor leaves a film of PCBM under UHV conditions undoped in time. The same dopant anchored via an azide group remains in the film after days in UHV proofing a successfull suppression of diffusion. During UV activation of the anchor only the azide absorption band vanishes indicating no major disintegration of both dopant and matrix. Unaltered electric properties make this approach feasible for use in organic devices. The universal use is demonstrated by successfully anchoring in the n-type small molecule PCBM and in the p-type polymer P3HT.

CPP 49.52 Tue 14:00 P1A

Eficiency loss channel determination in colloidal InP-based quantum dot light emitting diodes — •Manuel Engelmayer[1], Yohan Kim[2], André Gessner[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Fraunhofer Institute for Applied Polymer Research IAP, 14476 Potsdam, Germany

Colloidal quantum dot light emitting diodes have gained huge interest in both academia and industry over the course of the last years. In order to enable high luminances at low voltages with a reasonable energy consumption, the origin of efficiency losses must be clarified and then suppressed. CdSe-based literature shows two major possible loss channels, one being current dependent Auger quenching and the other being field-induced quenching. Unfortunately, purely electrical characterisation is not able to fully specify the respective contributions to the overall efficiency loss.

To gain deeper insights into the loss mechanisms of such quantum dot light emitting diodes, we built an experimental setup for combined electro- and photoluminescent excitation of quantum dots, which allows to simultaneously monitor the electrical and optical device efficiency. By comparing these with the photoluminescent quantum efficiency at an applied reverse bias, we are able to seperate the superimposed effects of Auger and field-dependent efficiency loss.

First results for InP-based core-shell quantum dot light emitting diodes point towards Auger recombination being the dominant efficiency loss mechanism.

CPP 49.53 Tue 14:00 P1A

Charge Transfer at the Interface of Dye-sensitized Solar Cells with $\mathbf{Mg_xZnO_{1-x}}$ — •Nico Hofeditz[1], Andreas Ringleb[2], Derck Schlettwein[2], and Wolfram Heimbrodt[1] — [1]Department of Physics and Material Sciences Center, Philipps-University Marburg, Renthof 5, 35032 Marburg, Germany — [2]Institute of Applied Physics, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Dye-sensitized solar cells containing the indoline dye D149 have been prepared with an iodide/triiodide electrolyte. The mesoporous photoanode has been prepared from ZnO with different concentrations of Mg. Hereby the effect of Mg-doping on cell performance can be studied.

An important process in high efficient dye-sensitized solar cells is an optimized electron transfer, i.e., the electron injection yield from the dye into the conduction band of the $(Mg_x)ZnO_{1-x}$ at the organic-inorganic interface.

The desired effect of the Mg-doping is an increased open-circuit voltage of the cell through a change in the energy level alignment of the anode. Since this has an effect on the charge injection characteristicts, we use time-resolved photoluminescence spectroscopy to study this process in detail.

CPP 50: Poster Session III

Topics: Complex Fluids and Colloids, Micelles and Vesicles (50.1-50.15); Composites and Functional Polymer Hybrids (50.16); Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (50.17-50.19); Fundamentals of molecular liquids, ionic liquids and mixtures (50.20-50.23); Modeling and Simulation of Soft Matter (50.24-50.30); Nanostructures, Nanostructuring and Nanosized Soft Matter (50.31-50.33); Polymer and Molecular Dynamics, Friction and Rheology (50.34-50.37); Polymers under confinement (50.38-50.40); Responsive and Adaptive Systems (50.41-50.47); Wetting, Fluidics and Liquids at Interfaces and Surfaces (50.48-50.52).

Time: Tuesday 14:00–16:00 Location: P1C

CPP 50.1 Tue 14:00 P1C

Cluster of supracolloidal magnetic polymers in a flow — •Ekaterina Novak, Elena Pyanzina, and Pedro Sanchez — Ural Federal University, Ekaterinburg, Russia

The active study of nanoparticles has opened new perspectives in the soft matter physics. 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 suspension of magnetic polymers with ferromagnetic particles and central attraction in the absence of an applied field quasi-spherical clusters are formed. One of that clusters 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 deformation happens slower if the dipolar interaction is stronger.

CPP 50.2 Tue 14:00 P1C

Impact of microstructure on the flow behaviour of micellar systems - a theoretical approach — •Benjamin von Lospichl[1,2], Valentina Alberini[1], Michael Gradzielski[2], and Sabnine H. L. Klapp[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin — [2]Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin

It has been shown by various experiments that elongated or wormlike micelles exhibit a unique viscoelastic behaviour yielding a non-linear flow [1]. The theoretical descriptions for this phenomenon can be either of tensorial form [2] or they correspond to one-dimensional models including additional degrees of freedom, e.g. a coupling of the mechanical variables and the microstructure [3]. Such a coupling yields a destabilization in the high shear rate branch of the flow curve as well as interesting dynamical states such as oscillatory and/or chaotic states. To improve the performance of this specific model and for a better (quantitative) comparison to experimental results, we explore the possibilities of introducing additional terms to describe the high shear rate behaviour. We also include concentration effects which strongly influence e.g., branching in wormlike micellar systems.

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

[2] M. Johnson, D. Segalman, J. Non-Newton. Fluid Mech. **2**, 255, (1977)

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

CPP 50.3 Tue 14:00 P1C

The free-energy profile of a copolymer micelle fusing with a homopolymer interface — •Niklas Blagojevic und Marcus Müller — Georg-August Universität, Göttingen, Institut für Theoretische Physik

In a blend containing immiscible A and B homopolymers, the polymers will phase-separate and form domains. If the blend also contains the corresponding AB diblock copolymers, the copolymers will segregate to the interface between the immiscible homopolymers and reduce the interface tension. In order to deliver the copolymers to the interface, micelles that form in one phase have to move to the interface and fuse. The movement of the micelles is protracted, and the fusion of the micelles with the AB interface is characterized by a free-energy barrier. Here, we will focus on the fusion barrier and gain insight into the free-energy landscape, and its dependence on the system parameters, and the molecular asymmetry of the diblock copolymer. Explicitly, we will study the minimum free-energy path (MFEP), ie. the most probable transition pathway, that connects these two states on the free-energy landscape and obtain the concomitant free-energy profile along the pathway. To do so, we will use highly parallelizable particle-based SCMF (Single-Chain in Mean Field) simulations in conjunction with Umbrella-sampling and the String-method to calculate the MFEP. For this purpose, we will investigate the the accuracy of the Umbrella-sampling as a function of the simulation parameters, such that an optimal sampling takes place.

CPP 50.4 Tue 14:00 P1C

The role of non-adiabatic forces during the collapse of a 1D capillary system — •Anja Schreiber, Johannes Bleibel, and Martin Oettel — Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany

We study the behavior of a one-dimensional system of colloidal particles trapped at a fluid interface using Brownian Dynamics (BD) simulations. Inter-facially trapped, micrometer-sized colloidal particles interact via long-ranged capillary attraction. The interaction is formally analogous to screened Newtonian gravity with the capillary length λ as the tuneable screening length. For a certain range of parameters, the system exhibits clustering behavior. After a characteristic timescale the system collapses globally and collectively to a close-packed patch, similar to a self gravitating fluid, and thus reaches the equilibrium state. Within studies of the impact of noise and starting position on the density profile during the clustering process, a significant discrepancy between simulation and Dynamical Density Functional Theory (DDFT) was found. Hence, it was concluded that non-adiabatic forces may contribute considerably to the dynamics. We obtain these non-adiabatic forces from applying an iterative scheme, developed for short-range interactions [1]. In order to investigate possible modifications for the DDFT, this method is adapted and appropriately modified for our long-ranged attractive system.

[1] D. de las Heras, J. Renner, and M. Schmidt, Phys.Rev. E 99, 023306 (2019)

CPP 50.5 Tue 14:00 P1C

Structural properties of biaxial phases formed by mixtures composed of uniaxial liquid crystal particles — •Louis Lehmann[1], Robert Skutnik[1], Sergej Püschel-Schlotthauer[1], Martin Schoen[1,2], and George Jackson[2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin — [2]Imperial College London, United Kingdom

In previous work, we investigated the formation of biaxial nematic phases in a model system consisting of a binary mixture of uniaxial molecules. The model potential was set up such that like molecules of each mixture component prefer a parallel alignment whereas two unlike molecules align preferentially in a T-shaped configuration. By tuning the potential parameters, we avoid a decomposition of the mixture which has hampered earlier studies because of its competition with the formation of an ordered biaxial phase. In this work we study the local orientational structure in a binary, decomposed mixture of uniaxial liquid crystals, using the same model as for the mixed phases, but lowering the interaction potential between particles of different kinds.

CPP 50.6 Tue 14:00 P1C

Molecular theory of a ferromagnetic nematic liquid crystal — •Immanuel Sebastian Geier[1], Stefanie Wandrei[1], Robert Arnold Skutnik[1], and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Berlin, Straße des 17. Juni 115, 10623 Berlin, Germany — [2]Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom

We employ a version of classical density functional theory to study the phase behavior of a simple model liquid crystal in an external field. The uniaxially symmetric molecules have a spherically symmetric core with superimposed orientation-dependent attractions. The interaction between the cores consist of a hard-sphere repulsion plus an isotropic square-well attraction. The anisotropic part of the interaction potential allows for the formation of a uniaxially symmetric nematic phase. The orientation of the molecules couples to an external polar field. The external field is capable of rotating the nematic director in the x-z plane. The field is also capable of changing the topology of the phase diagram in that it suppresses the phase coexistence between an isotropic liquid and a nematic phase observed in the absence of the field. We study the transition from an unpolar to a polar nematic phase in terms of the orientation-distribution function (odf), nematic and polar order parameters, and components of the nematic director.

CPP 50.7 Tue 14:00 P1C

Nanoparticle dynamics in magnetic liquid crystal hybrid materials — •Joachim Landers[1], Damian Günzing[1], Karin Koch[2], Soma Salamon[1], Annette M. Schmidt[2], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [2]Department of Chemistry, Institute of Physical Chemistry, University of Cologne

By adding magnetic nanoparticles to liquid crystals and liquid crystal elastomers, promising hybrid materials can be prepared, inheriting self-organiziation as well as a strong response to external magnetic fields. We utilize the ability of Mössbauer spectroscopy to provide information on particle dynamics as well as their magnetic alignment to study particle-matrix interaction across liquid crystal phase transitions. Thereby, the effect of self-ordering across the transition to the nematic state on particle dynamics will be analyzed, as well as the possibility of matrix reorientation via a magnetic stimulus. Regarding the possibility to extract direction-resolved particle diffusion coefficients from Doppler line-broadening, preliminary results on aligned anisotropic nanoparticles are discussed, which could represent a valuable approach for the future analysis of these hybrid materials aligned via magnetic or electric fields and other anisotropic soft magnetic composites. Funding by the DFG through SPP 1681 (project WE 2623/7-3 and SCHM1747/10) is gratefully acknowledged.

CPP 50.8 Tue 14:00 P1C

Magnetic properties of Stcokmayer supracolloidal magnetic polymers — •Vladimir Zverev[1], Ivan Novikau[2], Pedro Sanchez[1,2], and Ekaterina Novak[1] — [1]URFU, Ekaterinburg, Russia — [2]UNIVIE, Vienna, Austria

This work is devoted to magnetic properties of aggregates formed in suspensions of supracolloidal magnetic polymer-like structures of different topology. We find that due to the formation of compact clusters, the overall initial magnetic susceptibility decreases dramatically for chain-, Y- and X-like topologies. However, this decrease for chain-like supracolloidal magnetic polymers is much stronger than that of other topologies, especially for systems with strong magnetic interactions [1]. If an external field is applied, clusters deform as a result of complex interplay between four forces: external filed tends to align each dipole, the dipole-dipole interaction between magnetic particles tend to prevent rotations, permanent crosslinking prevent translation and finally central attraction favours the overall spherical shape of the cluster. Range of parameters when clusters remain stable and do not disintegrate is identified.

[1] E. Novak et al, JMMM 497, 166025 (2020).

CPP 50.9 Tue 14:00 P1C

Translational and rotational dynamics of anisotropic colloids — •Lisa Rohde, Manuel A. Escobedo-Sanchez, Juan Pablo Segovia-Gutierrez, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Micron-sized colloids show many physical phenomena, also encountered in more complex environments. In contrast to molecular systems, they are experimentally more accessible due to their larger size and slower dynamics. For example, they can be observed by optical microscopy. This renders them powerful model systems. While spherical particles have been used in many studies, the interest now moves to more complex structures. Here, we present experiments with 'colloidal molecules', namely trimers formed by three fused spherical particles[1]. The dynamics of spherical particles has been investigated in dependence of the particle concentration[2]. With increasing concentration, the dynamics slows down and eventually dynamical arrest is observed. A non-spherical shape introduces more complex dynamics with translation and rotation. In our experiments, the particles are in quasi-2D confinement resulting in translational motion as well as rotation around (only) one axis. The dynamics of pure trimers as well as the dynamics of trimers in the presence of spherical particles are investigated. The translational and rotational motions are quantitatively studied using microscopy and particle tracking.

[1]Manoharan et al.,Science,301,483-487,2003. [2]Pusey:Liquids,Freezing and Glass Transition,Elsevier p.763-942,1991.

CPP 50.10 Tue 14:00 P1C

Thermal diffusion of a single colloidal particle — •Daniel Benjamin Mayer and Thomas Franosch — Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria

We tackle the problem of a single charged colloid immersed in an electrolyte solution in the presence of an external applied small temperature gradient. Consequently electrical body forces are no longer counter balanced by pressure gradients, thereby inducing solvent flow and a directed motion of the colloidal particle.

The associated linearized electro-kinetic equations are solved numerically by adapting an adjusted solution scheme, originally invented by O'Brien and White [1] for the electrophoresis problem. Thus the thermal diffusivity is determined from the velocity field of a force-free Stokes flow. In addition a decomposition of the thermophoresis problem in two auxilary ones simplifies the aim of calculating the thermal mobility considerably as it does not appear explicitly as a boundary condition. In the end we examine its dependence on the surface potential and the Soret coefficients of the different ions in the electrolyte for arbitrary Debye-layer thickness.

[1] R. W. O'Brien and L. R. White, J. Chem. Soc.,Faraday Trans. 2, 1978, 74, 1607.

CPP 50.11 Tue 14:00 P1C

Diffusion and thermodiffusion of polymers in mixed solvents — Jannik Kantelhardt, •Daniel Sommermann, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

We present first results of experiments on diffusion and thermodiffusion of polymers in mixed solvents. So far, most works on thermodiffusion have dealt with binary or, more recently, ternary mixtures of small molecules. While binary mixtures are readily characterized by one diffusion and one thermodiffusion coefficient, the number of coefficients increases to four plus two for ternaries. Hardly any experiments exist for highly asymmetric ternary systems, like a polymer in a binary solvent. Two-color optical beam deflection (2-OBD) and supporting single-color thermal diffusion forced Rayleigh scattering (TDFRS) experiments show three well separated modes that can be assigned to the thermal diffusivity and the two eigenvalues of the mass diffusion matrix. We are particularly interested in the question, to what extent the dynamics of the large entity, the polymer, is coupled to the solvent-solvent dynamics, both with respect to diffusion and thermodiffusion. A first analysis supports the picture of an effective solvent whose internal dynamics is decoupled from the one of the polymer. The investigations are supplemented by recent microgravity experiments on a similar system within the DCMIX project and by the planned investigation of non-equilibrium fluctuations within the GIANT FLUCTUATIONS program of ESA.

CPP 50.12 Tue 14:00 P1C

DCMIX-4: experiments on thermodiffusion in fullerene and solvent mixtures on ground and aboard the International Space Station ISS — •Marcel Schraml[1], Ane Errarte[2], Mohammed Mounir Bou-Ali[2], and Werner Köhler[1] — [1]Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany — [2]Mechanical and Manufacturing Department, MGEP Mondragon Goi Eskola Politeknikoa, Mondragon, Spain

Diffusive flows in a non-isothermal multicomponent fluid are characterized by complex cross-coupling phenomena between all concentration and temperature gradients. Beside the well known Fickian diffusion, a mass flux due to a concentration gradient, there is another contribution to the total mass flux, the so-called Soret effect or thermodiffusion. Since the number of unknown coefficients increases quadratically with the number of components, such multicomponent systems quickly become intractable, and today's research focuses mainly on ternary mixtures as multicomponent model systems. Within the ESA/Roscosmos DCMIX program, measurements are performed under microgravity conditions aboard the International Space Station ISS to generate a benchmark system for comparision with ground-based laboratory experiments. On the poster we will focus on the currently completed DCMIX-4 campaign which includes a sample of solvents and fullerene. We are going to explain the different measurement techniques on ground and aboard the ISS and present some first results of the experiments.

CPP 50.13 Tue 14:00 P1C

Particle sorting by Marangoni convection in microfluidic channels — •Roman Reh, Lorenz Kiel, Daniel Zapf, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

Thermosolutal and thermocapillary Marangoni convection at a liquid-gas interface in a T-shaped microchannel structure of approximately $100 \times 100\ \mu\mathrm{m}^2$ cross section creates localized vortices that can be used for particle trapping, steering, and sorting. Experiments have been performed with water-ethanol mixtures as carrier liquid and dispersed micrometer-sized polystyrene beads. Due to collisions with the meniscus, particles are displaced from streamlines that approach the interface closer than one particle radius. These streamlines feed liquid volumes that are entirely cleared of particles. Particle accumulations structures form inside the vortex, from where only small particles can escape by diffusion. Since the critical streamline, which separates the depletion from the accumulation region, depends on the particle radius, the mechanism can be used for particle sorting by superposition of a Poiseuille flow and splitting of the flow downstream from the meniscus. In the simplest case, the initially homogeneous flow is split into two arms, one where the particles are enriched and one where all particles are removed from the liquid. The microchannel structures consist of crosslinked PDMS and the dispersed particles are observed by video microscopy. Flow fields are constructed by means of image correlation techniques and numerical simulations are performed that almost perfectly match the experimental observations.

CPP 50.14 Tue 14:00 P1C

Photosensitive Surfactants at Hydrophilic and Hydrophobic Surfaces — •Maren Umlandt, David Feldmann, and Svetlana Santer — University of Potsdam, Potsdam, Germany

Here we report the adsorption kinetics of photosensitive azobenzene containing surfactants on different substrates under illumination with UV and green light. The work is motivated by the newly discovered phenomena of light driven diffusioosmosis (LDDO) where flow is generated at the solid/liquid interface [1]. Colloidal particles trapped at solid/liquid interface move passively within this LDDO flow, and can be arranged in different pattern, removed selectively or gathered on demand. The main ingredient of this process is photosensitive azobenzene containing surfactant which undergoes photo-isomerization reaction from trans- to cis- state with corresponding changes in physical properties such as dipole moment, shape and size. In trans-state the molecule is hydrophobic, while in cis-state hydrophilic. Here we perform analysis of the surfactant adsorption on a hydrophilic and a hydrophobic surfaces using Zeta potential and quartz crystal microbalance (QCM-D) measurements. We analyses the adsorption isotherms in terms of four and five step models. It has been shown that the adsorption of trans- and cis-isomers differs significantly on each type of surfaces.

1. D. Feldmann, S. S. Maduar, N. Lomadze, O. Vinogradova and S. Santer, Scientific Reports, 6, 36443 (2016).

CPP 50.15 Tue 14:00 P1C

Synthesis and characterization of charged and sterically stabilized optically transparent aqueous suspensions — •Kathrin Eitel and Hans-Joachim Schöpe — Universität Tübingen, Germany

We report the synthesis and characterization of monodisperse, highly charged and sterically stabilized colloidal particles with low index of refraction (n=1,38). The core shell particles consist of 1H-1H Heptafluorobutyl-methacrylate (core) and polyethylenelycolmethacrylate (shell). We characterize the particles using various methods to determine the particle size and the size polydispersity, the core and shell dimensions, the optical properties, the diffusion coefficients, the effective particle charge and structure formation. The fluorination of the core allows an optical index match using DMSO as a co-solvent. The interparticle interaction potential can in principle be tuned by the content of excess ions and by the addition of free polymer over an extremely wide range. These fluorinated particle core shell particles are excellently suited as model system to study structure, dynamics and rheology as function of the interaction potential in and out of thermodynamic equilibrium using optical methods.

CPP 50.16 Tue 14:00 P1C

Adsorption of Magnetic Nanoparticles onto PNIPAM Brushes and Structure of Composite Materials — •Philipp Ritzert[1], Dikran Boyaciyan[1], Luca Silvi[2], Olaf Solfwedel[1], Larissa Braun[1], and Regine v. Klitzing[1] — [1]TU Darmstadt, Department of Physics, Hochschulstrasse 8, D-64289 Darmstadt — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109, Berlin

End-grafted polymer chains, covalently bound to a substrate are commonly referred to as polymer brushes. In recent decades, great attention was paid to their investigation as thin surface coating, due to their versatile applicability, as well as, high mechanical and chemical stability. The usage of various monomer units enables sensitivity to external stimuli (e.g. temperature, pH value) [1]. Furthermore, polymer brushes can bind different kinds of material with a high selectivity, depending on the available functional groups. Recent studies demonstrate *in-situ* synthesis of magnetic nanoparticles in polymer brushes resulting in sensitivity to external magnetic fields [2].

In this work, the adsorption behaviour of citric acid-capped, magnetic nanoparticles (MNPs) onto Poly(N-isopropylacrylamide) brushes is investigated. Thereby, pH value and MNP concentration during the attachment are varied. Moreover, the structure of the resulting composite materials is investigated by neutron reflectometry.

[1] S. Christau et al. Macromolecules, 2017, 50, pp. 7333-7343
[2] W. Choi et al. Advanced Materials, 2008, 20, pp. 4504-4508

CPP 50.17 Tue 14:00 P1C

Unveiling the recombination processes of free carriers in high-efficient organic solar cells by steady-state photoinduced absorption and photocurrent spectroscopy — •Le Phuong[1,2], Seyed Mehrdad Hosseini[1], Chang Woo Koh[3], Han Young Woo[3], and Safa Shoaee[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, Potsdam-Golm 14476, Germany — [2]Institute of Materials Science, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Hanoi, Vietnam — [3]Department of Chemistry, College of Science, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 136-713, Republic of Korea

Coupling steady state photoinduced absorption (PIA) and photocurrent (PC) spectroscopy, we investigate the recombination dynamics of long-lived carriers in high-efficient PPDT2FBT/PC70BM bulk heterojunction (BHJ) solar cells. By comparing the PIA and PC data measured under open-circuit and short-circuit conditions, the absorption cross sections of free carriers can be evaluated. In addition, the excitation-fluence- and modulation-frequency-dependent PIA measurements enable to reveal the recombination mechanism of free carriers in the BHJ solar cells. Our results show that the PIAPC spectroscopy provides an alternative and versatile technique to understand the recombination and extraction processes of free carriers in BHJ solar cells [1].

[1]. L. Q. Phuong et al., J. Phys. Chem. C 123, 27417 (2019).

CPP 50.18 Tue 14:00 P1C

Mechanochemical synthesis and topology transformation in polymorphic Zr-MOF qubit candidates — •Bahar Karadeniz, Krunoslav Užarević, Dijana Žilić, and Senada Muratović — Division of Physical Chemistry, R. Bošković Institute, Zagreb, Croatia

Among the large family of metal organic frameworks (MOFs), highly stable Zr-based MOFs are one of the most interesting members with various application areas owing to their stability, high porosity, high density of metal centers included in the cluster nodes, and varied types of topologies. Herein we present rapid, clean, high yield mechanochemical synthesis of pure phase cubic MOF-525 and hexagonal PCN-223 polymorphs built on tetratopic porphyrin linker by liquid-assisted grinding technique.[1] In-situ powder X-ray diffraction monitoring performed at the DESY synchrotron source reveals that particular ball-milling conditions can induce the transformation from cubic to hexagonal phase, denoting MOF-525 to be a kinetic phase in this polymorphic system. Electron spin resonance (ESR) data of these polymorphic MOFs showed significant differences due to the different spatial arrangement and efficient separation of the metal centres (Cu(II), Mn(II) and Fe(III)) in the porphyrin rings, denoting them also as candidates for advanced spintronics applications.

[1] B. Karadeniz, K. Užarević et al. Journal of American Chemical Society (2019).

The authors acknowledge support from the European Social Fund and the Croatian Science Foundation (PZS-2019-02-4129) and the DAAD-MZO bilateral project.

CPP 50.19 Tue 14:00 P1C

Improved virtual orbitals for charge transfer excitations in time dependent DFT — •Rolf Würdemann[1] and Michael Walter[2,3] — [1]reiburger Materialforschungszentrum, Freiburg, Germany — [2]Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany — [3]Institut für Werkstoffmechanik, Freiburg, Germany

Charge transfer excitations (CTE) are of high importance in photovolatics, organic electronics and molecular and organic magnetism. Range separated funtionals (RSF) can be used to correctly determine the energetics of CTEs within linear response time dependent density functional theory (TDDFT).

TDDFT becomes numerically very demanding on grids if hybrid or RSF are used due to the inclusion of exact exchange derived from Hartree-Fock theory.

We present the implementation of RSF on real space grids and discuss a way to circumvent the problem mentioned above by utilizing Huzinagas improved virtual orbitals (IVOs) that form an improved basis for this type of calculations. The CTE energetics may be even obtained by means of DFT ground-state calculations using IVOs[1].

[1] R. Würdemann, M. Walter, J. Chem. Theory Comput. 2018, 14, 7, 3667-3676

CPP 50.20 Tue 14:00 P1C

Surfaces of ionic liquid mixtures studied by temperature-dependent ARXPS — •Ulrike Paap, Bettina Heller, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Ionic liquids (ILs) are characterized by a low melting point, low vapor pressure and low surface tension. Many ILs carrying fluorinated moieties exhibit high gas solubility together with chemical and thermal stability. Such properties are beneficial for a potential substitution of fluorinated organic compounds in many areas such as gas absorbents, refrigerants, lubricants and surfactants.

In this work, we studied various mixed IL systems in the liquid state at different temperatures with angle-resolved X-ray photoelectron spectroscopy (ARXPS). Thereby, we investigated the surface composition of the topmost nanometers of these mixtures. All ILs studied consist of the same hexafluorophosphate anion ($[PF_6]^-$) and feature a selection of different fluorinated and non-fluorinated imidazolium cations. Our results allows for a deeper understanding of enrichment and molecular orientation processes at the outermost surface of these mixed IL systems.

U.P., B.H., F.M. and H.P.S. thank the European Research Council (ERC) for financial support of this research in the context of an Advanced Investigator Grant to H.P.S. (693398-ILID).

CPP 50.21 Tue 14:00 P1C

Chasing Aqueous Biphasic Systems from Simple Salts by Exploring the LiTFSI/LiCl/H_2O Phase Diagram — •Chanbum Park[1] and Joachim Dzubiella[1,2] — [1]Research Group for Simulations of Energy Materials, Hahn-Meitner-Platz 1, D-14109, Berlin, Germany — [2]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104, Freiburg, Germany

Aqueous biphasic systems (ABSs), in which two aqueous phases with different compositions coexist as separate liquids, were first reported more than a century ago with polymer solutions. Recent observations of ABS forming from concentrated mixtures of inorganic salts and ionic liquids raise the fundamental question of how "different" the components of such mixtures should be for a liquid-liquid phase separation to occur. Here we show that even two monovalent salts sharing a common cation (lithium) but with different anions, namely, LiCl and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), may result in the formation of ABSs over a wide range of compositions at room temperature. Using a combination of experimental techniques and molecular simulations, we analyze the coexistence diagram and the mechanism driving the phase separation, arising from the different anion sizes.[1] The understanding and control of ABS may provide new avenues for aqueous-based battery systems.

[1] Dubouis, N.; Park, C.; Deschamps, M.; Abdelghani-Idrissi, S.; Kanduč, M.; Colin, A.; Salanne, M.; Dzubiella, J.; Grimaud, A.;

Rotenberg, B. ACS Cent. Sci. 2019, 5, 4, 640-643.

CPP 50.22 Tue 14:00 P1C

Electrolyte solvents for high voltage lithium ion batteries: ion correlation and specific anion effects in adiponitrile — •Anand Narayanan Krishnamoorthy[1,2], Kristina Oldiges[2], Martin WInter[2,3], Andreas Heuer[4], Isidora Cekic-Laskovic[2], Christian Holm[1], and Jens Smiatek[1,2] — [1]Institute for Computational Physics - University of Stuttgart — [2]Helmholtz Institute Muenster — [3]MEET - Battery research Muenster — [4]Institute for Physical Chemistry - University of Muenster

We studied dynamic and structural properties of two lithium conducting salts in the aprotic organic solvent adiponitrile by a combination of atomistic molecular dynamics (MD) simulations, quantum chemical calculations, and experimental findings. The outcomes of our simulations reveal significant differences between both lithium salts, namely lithium tetrafluoroborate (LiBF4) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) at various concentrations, which can be mainly attributed to the solvation behavior of the individual anions. The increased tendency of ion complex formation for LiBF4 is reflected by lower values regarding the measured and computed effective ionic conductivities when compared to LiTFSI. All findings highlight the crucial importance of specific anion effects in combination with molecular details of solvation, and advocate the use of adiponitrile as a beneficial solvent in modern lithium ion battery technology with high voltage electrodes.

CPP 50.23 Tue 14:00 P1C

Experimental Thermodynamics of NiPAM in Water — •Jakub Polak, Daniel Ondo, and Jan Heyda — University of Chemistry and Technology, Prague, Czechia

Unlike for thermoresponsive polymer PNiPAM, the knowledge of thermodynamic properties of aqueous N-isopropylacryl amide (NiPAM) is far from being complete.

In this contribution, the macroscopic thermodynamic properties of aqueous NiPAM are measured and the workflow towards Kirkwood-Buff integrals is presented. Namely, we report the experimental determination of partial molar volumes, osmotic coefficients, and excess partial molar enthalpies of NiPAM in water. These thermodynamic functions are subject to the Kirkwood-Buff inversion procedure. The concentration and temperature dependence of Kirkwood-Buff integrals is discussed and compared to other amides.

CPP 50.24 Tue 14:00 P1C

Competing chain extension between exchange and irreversible reactions — •Michael Lang and Frank Böhme — Leibniz-Institut für Polymerforschung Dresden Hohe Straße 6, 01069 Dresden

A co-polycondensation reaction is discussed analytically and by Monte-Carlo simulations where two reactive units compete for reactions with an alternating third reactive unit, whereby irreversible reactions replace bonds which are able to undergo exchange reactions. The resulting number average molar mass, M_n, exhibits only one distinct peak at the stoichiometric condition of both competitors with the alternating partner. The weight average molar mass, M_w, reaches an additional second peak at the stoichiometric condition between the dominating competitor and the alternating partner. Both peaks of M_w surround a range of compositions where a rather high and approximately constant M_w is obtained. The degree of polymerization of the dominating and alternating reaction partners is rather insensitive towards composition fluctuations if the reaction mixture remains within this composition window. This promotes high molecular weight species and more homogeneous weight distributions at incomplete mixing conditions. An ideal reference case (identical reaction rates for all reactions) is solved analytically to describe these reactions. The position of the stable composition window and the average molar masses inside this window can be tuned by choosing appropriate precursor molecules, reaction mixtures, or post-tuning steps at later times.

CPP 50.25 Tue 14:00 P1C

Generic hysteresis model for palpation in the elasto-capillary regime — •Paul Zech, Andreas Otto, Martin Dehnert, and Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

We develop a multisensory interface that allows humans to perceive and to explore interactively the mechanical response of soft materials and tissues on the nanometer scale. To this end, we use an atomic force microscope for measuring force–distance curves which inform about the material's viscoelastic properties as well as its deformation behavior and capillary forces. Humans explore a material in much more variable ways than an instrumented indentation experiment. Therefore, existing models do not describe an arbitrary user–material interaction. We present a generic hysteresis model that predicts the force (output) of a haptic device for a given indentation trajectory (input). The model uses built-in memory in form of a hysteretic play operator and allows the user to perceive dissipative as well as elastic nanomechanical properties equally well.

CPP 50.26 Tue 14:00 P1C

The physics of the adaptive resolution approach to open systems — •Abbas Gholami, Felix Höfling, Rupert Klein, and Luigi Delle Site — Department of Mathematics and Computer Science, Freie Universität Berlin

The Adaptive Resolution Simulation (AdResS) scheme in its recent formulation couples an open region of interest to a reservoir of non-interacting particles [1]. Building on the statistical mechanics of the grand-canonical ensemble, we relate the chemical potential of the simulated atomistic liquid to the ingredients of the AdResS setup. Numerical tests for Lennard-Jones liquids were carried out to corroborate the formal derivation. The obtained expression differs in structure from that for AdResS with smoothly interpolated forces [2] and permits an interpretation in the framework of stochastic thermodynamics and the Jarzynski equality.

[1] L. Delle Site, C. Krekeler, J. Whittaker, A. Agarwal, R. Klein, and F. Höfling, Adv. Theory Simul. **2**, 1900014 (2019).

[2] A. Agarwal, H. Wang, C. Schütte, and L. Delle Site, J. Chem. Phys. **141**, 034102 (2014).

CPP 50.27 Tue 14:00 P1C

Open systems approach to molecular dynamics simulations of liquids out of equilibrium — •Roya Ebrahimi Viand, Luigi Delle Site, Rupert Klein, and Felix Höfling — Department of Mathematics and Computer Science, Freie Universität Berlin

We discuss the simulation of Lennard-Jones liquids subject to thermal and/or density gradients. In particular, we employ Adaptive Resolution Simulations (AdResS) in their recent form [1] to realise open boundaries and grand-canonical reservoirs. The model is validated by comparing it with full non-equilibrium simulations of atomistic resolution. The combination of out-of-equilibrium systems with open boundaries prompts for the development of a theoretical framework that treats the boundary conditions in a physically consistent manner. In this perspective, our study represents a numerical implementation of the conceptual approach put forward by Bergman and Lebowitz [2] for such situations.

[1] L. Delle Site *et al.*, Adv. Theory Simul. **2**, 1900014 (2019).

[2] P. G. Bergman and J. L. Lebowitz, Phys. Rev. **99**, 578 (1955).

CPP 50.28 Tue 14:00 P1C

Ground- and excited-state properties of tetraphenyl compounds from first-principles calculations — •Kevin Eberheim, Dues Christof, and Sanna Simone — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Tetraphenyl compounds with formula $X(C_6H_5)_4$ (X being a tetravalent atom of the 14th group such as C, Si, Ge, Sn, Pb), crystallize either in a tetragonal crystalline structure or in an amorph phase [1]. Depending on their habitus, the compounds are characterized by very different optical properties. The molecular crystals are known for their second harmonic generation (SHG) properties, while the amorph phase is a white light emitter. Tetraphenyl molecules feature indeed the delocalized π-orbitals, which have been proposed as a prerequisite for the white-light generation [2]. In an attempt to understand the mechanisms related to the white light emission, we model the structural, electronic and vibrational properties of different $X(C_6H_5)_4$ structures within density functional theory. The calculated structural parameters closely reproduce the measured values, however vdW corrections are crucial for a correct description of the structural properties. This confirms that dispersion forces are responsible for the intermolecular bonds in the compound. Different implementations of the vdW forces lead to very similar results. Calculated vibrational properties are in agreement with measured Raman spectra. [1] A Kitaigorodsky, Molecular crystals and Molecules, Acad. Press (1973). [2] Nils W. Rosemann et al., J. Am. Chem. Soc. **138**, 16224 (2016), Science **352**, 1301 (2016).

CPP 50.29 Tue 14:00 P1C

Optical properties of adamantane based molecular clusters — •Christof Dues[1,2], Kevin Eberheim[1,2], and Simone Sanna[1,2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Zentrum für Materialforschung (ZfM/LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

A new class of molecular materials based on adamantane-type organotetrel chalcogenide clusters has recently attracted the attention of the scientific community due to its outstanding optical properties [1]. Depending on the composition (organic substiuents and tetrel atoms in the cluster core), these materials show either white-light generation or strong non-linear response upon IR radiation [2]. In order to determine the prerequisites for white light generation, different related clusters have been synthesized, which posses an additional ligand based on a coinage-metal atom [3]. To explore the optical response, we perform first-principles calculations within the density functional theory. Linear optical properties such as absorption and transmission are calculated based on the electronic structure for both single molecules and molecular crystals. Furthermore, the frequency dependent non-linear optical response is estimated calculating the second harmonic coefficients $\chi^{(2)}_{\mathrm{SHG}}$ and the photoluminescence is modeled by constrained total energy calculations.

[1] N. W. Rosemann et al., Science **352**, 1301 (2016).
[2] N. W. Rosemann et al., J. Am. Chem. Soc. **138**, 16224 (2016).
[3] E. Dornsiepen et al., Adv. Optical Mater. **7**, 1801793 (2019).

CPP 50.30 Tue 14:00 P1C

Noise-induced symmetry breaking of self-regulators: An asymmetric phase transition towards homochirality — •Rafna Rafeek[1] and Debasish Mondal[2] — [1]Department of Chemistry, Indian Institute of Science Education And Research Tirupati, Tirupati, India 517507 — [2]Department of Chemistry, Indian Institute of Technology Tirupati, Tirupati, India 517506

Studies on the origin of spontaneous chiral symmetry breaking have become a 'Holy Grail' in recent research developments related to the origin of life. The paradigm of Frank (1953) and its subsequent variants indicate that a self-regulatory process may result in such single handedness in different reaction conditions. We consider a collection of Brownian particles, which can stay in any of the three possible isomeric states: one achiral and two enantiomers. Isomers are undergoing self-regulatory reaction along with chiral inhibition and achiral decay processes. The time evolution of the isomeric states is guided by those of its neighbors as well as the temperature of the system. We find that the relative dominance of self-regulation, chiral inhibition and achiral decay processes results in asymmetric transition between four different population phases, namely three-isomer coexistence, enantiomeric coexistence, chiral-achiral coexistence and homochiral phase. We also report that a fast stochastic self-regulation and an optimally slow chiral inhibition reaction along with a threshold population of interacting neighbors suffice the requisite for transition towards a completely symmetry broken state i.e., homochirality.

CPP 50.31 Tue 14:00 P1C

The Removal of NPs After Accident - How to Avoid Skin Penetration? — •Jonas Schubert[1,2] and Max Schnepf[1,2] — [1]Functional Colloidal Materials, Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Germany — [2]Physical Chemistry of Polymer Materials, Technische Universität Dresden, D-01062 Dresden, Germany

In this contribution we present a novel gel that is able to remove NPs from the skin. This is getting more and more important as NPs are frequently used in research as well as in industry. After skin contact some of the NPs are able to penetrate the skin and are then potentially harmful for the human health.[1] Normal soap is insufficient for the removal of NPs. Compared to that, our gel removes the majority of the NPs from the skin.

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CPP 50.32 Tue 14:00 P1C

CdZnSe/ZnS quantum dots - gold nanoparticle nanostructured complexes and the influence of the ligand length on their optical properties — •Tatiana Kormilina[1,3], Irina Arefina[1], Evgeniia Stepanidenko[1], Danil Kurshanov[1], Aliaksei Dubavik[1], and Elena Ushakova[1,2] — [1]Center of Information Optical Technologies, ITMO University, Saint Petersburg, Russia — [2]Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR, PR China — [3]Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Hybrid systems formed from semiconductor nanocrystals and noble metal nanoparticles are widely utilized in development of multicomponent materials for the photonic applications, biological imaging, and solar cell technologies, where these materials can be used as colloidal solutions or solid thin films. Of great importance are not only the nanomaterials themselves, but also the nanostructure of their linkage. In this work we show how optical properties of a semiconductor quantum dot - noble metal nanoparticle complex can depend on the chain length of the binding molecule. We developed a formation procedure for the colloidal complexes based on alloyed CdZnSe/ZnS quantum dots and gold nanoparticles where various mercaptocarboxylic acids are used as the binding molecules. The QD photoluminescence enhancement (up to 3.1) can be achieved by the control of the interparticle distance in colloidal solutions. The influence of the linking molecules on the optical parameters of the nanoparticle complexes is analyzed and compared through the steady-state and time-resolved spectral measurements.

CPP 50.33 Tue 14:00 P1C

Fluorescence Quenching of Copper Indium Sulfide/Zinc sulphide Quantum Dot-Dye Assembly — •Abey Issac[1], Sumesh Sofin R.G[1], and Osama K. Abou-Zied[2] — [1]Department of Physics, College of Science, Sultan Qaboos University, Muscat 123, OMAN — [2]Department of Chemistry, College of Science, Sultan Qaboos University, Muscat 123, OMAN

Deep understanding of electronic transitions in semiconductor quantum dots (QDs) are crucial for the realization of QD-based applications. Though enormous works have been reported on cadmium based QDs such as CdSe or CdS at ensemble and single particle level, current research interest is devoted to cadmium free QDs due to the carcinogenic activity of cadmium. In this work, we study the fluorescence quenching of Copper Indium Sulfide/Zinc sulfide core/shell QDs (CIS/ZnS) in QD-dye complexes. Time resolved spectroscopy techniques such as fluorescence decay (ns) and fluorescence up conversion (sub ps) are employed in this work. Different quenching pathways are identified in this QD-Dye assembly.

CPP 50.34 Tue 14:00 P1C

Stress components in adhesive joints of micromechanical structures — •Rika Unkelbach[1,2], Jan Kuypers[1], and Christine Papadakis[2] — [1]Blickfeld GmbH, 80339 München, Germany — [2]TU München, Physik-Department, Physik weicher Materie, 85748 Garching, Germany

The use of adhesives as a joining technique in structural applications is widespread and on the rise. For simple geometries such as lap shear joints, stress components can be analytically predicted and are well understood. However, the stress distribution for unusual joints or loading conditions is more complex and requires a more detailed analysis.

We present an approach to identify the stress components that eventually will lead to a failure of the joint in a specific micromechanical structure under torsional loading that has motivated this research. The influence of peeling and shear stress components in regards to the joint stability is discussed based on experimental data and results obtained from finite element analysis (FEA).

CPP 50.35 Tue 14:00 P1C

Insights in Structure and Dynamics of PEO-LiTFSI Electrolytes near Graphene Electrodes from Molecular Dynamics Simulations — •Andreas Thum[1], Diddo Diddens[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

All-solid-state lithium-ion batteries gain increasing attention as potentially safe and cheap second generation batteries. Polymer electrolytes are – besides other materials like inorganic ceramics – a promising replacement for the currently used flammable liquid organic electrolytes. However, the electrode-electrolyte interphase (EEI) of polymer electrolytes is even more complex than that of liquid electrolytes. Since the EEI is considered to affect the cycling performance and cell safety seriously, it is crucial to get a better understanding of its formation process, its structure and the lithium ion transport therein. Here we present atomistic molecular dynamics simulations of poly(ethylene oxide) (PEO) doped with lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) near charged and uncharged graphene electrodes. We explore the structure and dynamics of the polymer electrolyte which are governed by anisotropic effects and strong local electric fields in the vicinity of the electrodes.

CPP 50.36 Tue 14:00 P1C

Tunable-slip boundary for the soft coarse-grained model of polymer fluid — •Pritam Kumar Jana, Ludwig Schneider, Veronica Chappa, and Marcus Müller — Institut für Theoretische Physik, Universität Göttingen, Germany

The rheological properties of composites derived from fillers in a polymer matrix depend on particle size, filler loading, and dispersion, as well as the interfacial interaction between the fillers and polymer matrix. For the coarse-grained modeling of such systems, it is crucial to pay attention to the fluid flows past the solid filler surface because classical no-slip hydrodynamic boundary condition does not hold on the micro- and nanoscopic length scale. Instead, the flow is characterized by a microscopically small but finite slip length. To tailor the hydrodynamic boundary condition, we have implemented a strategy by forming dynamic bonds between the solid filler surface and polymer beads, using a grand-canonical Monte Carlo approach. Polymers are modeled as highly coarse-grained segments with soft potentials, including reduced extensibility for strong elongations. Entanglements between polymers are represented by slip-springs [1]. We perform molecular dynamics simulations in conjunction with a dissipative particle dynamics (DPD) thermostat. We successfully demonstrate that the equilibrium properties, e.g., density profile close to the wall, are independent of the number of dynamic bonds and explore the relation between the density of dynamic bonds and hydrodynamic boundary condition.

References 1. Chappa et al., Physical Review Letters 109 148302 (2012)

CPP 50.37 Tue 14:00 P1C

Mircorheology of Newtonian fluid — •Pankaj Pandey[1], Patrick Galenschowski[2], Christian Wagner[3], and Thomas John[4] — [1]Saarland University Campus, building E2 6 Saarbrücken Germany — [2]Saarland University Campus, building E2 6 Saarbrücken Germany — [3]Saarland University Campus, building E2 6 Saarbrücken Germany — [4]Saarland University Campus, building E2 6 Saarbrücken Germany

We have studied polystyrene particle in Newtonian (deionized water and Sucrose solution) fluid by dark field microscopy (DFM). Trajectory of the particle is analyzed in terms of the mean squared displacement (MSD). We have recorded very long trajectories comprising 10000 number of frames with 10 frames per second at room temperature. This enabled a statistical analysis of the resulting MSD curves as a function of the time. We find that the relative error of the diffusion coefficient can be minimized by taking long trajectory lengths into account by fitting the time dependent MSD curves with power law. Finally, we found these results are very good qualitative and quantitative agreement between experiment and theory.

CPP 50.38 Tue 14:00 P1C

Polymer adsorption in a micro channel — •Tobias A. Kampmann, Björn Lindhauer, and Jan Kierfeld — TU Dortmund University, Germany

Two entangled semiflexible polymers such as actin or DNA filaments confined to a channel exhibit at least three distinct scaling regimes of entropic repulsion. If the persistence length L_p exceeds the channel width d the entropic repulsion is $\sim L_p^{-1/3}$ and governed by deflections from the channel walls. If the polymer is more flexible such that the persistence length is smaller than the channel width, the entropic repulsion is governed by polymer blobs forming in confinement and scales $\sim L_p^{-1}$. In the presence of attractive interactions we find a single transition into a bundled phase upon increasing the potential strength. An intermediate entangled phase, where polymers are drawn into parallel alignment without bundling is absent. We conclude that parallel alignment and bundling of two confined polymers happen in a single transition. The results shed light on the self-assembly process of filament bundles in confinement.

CPP 50.39 Tue 14:00 P1C

Rheology of Oligo- and Polymers in Oxidic Nanoporous Materials: Gravimetric and Optofluidic Experiments — •Guido Dittrich and Patrick Huber — Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH), Eißendorfer Str. 42, D-21073 Hamburg-Harburg, Germany

The rheology in nanometer sized pores is a research field with many open questions especially for complex molecules. Oxidic nanoporous materials offer a stiff scaffold with high specific surface area and confining geometries. Therefore, surface tension and capillarity are dominant and affect along with interface interactions and pure spatial restrictions the flow properties. From a scientific point of view oligo- and polymers add to the complexity by a rheology that depends on the chain length and chemistry. We investigate the transport dynamics of styrene-based oligo- and polymer melts in anodic aluminum oxide (AAO) and compare them with those in controlled porous glasses (CPG). These materials exhibit a cylindrical, hexagonally arranged and a sponge-like pore morphology, respectively. Due to the different morphologies AAO is investigated with an opto-interferometric [1] and CPG with a gravimetric technique [2].

[1] Cencha, Luisa G., et al.: "Nondestructive high-throughput screening of nanopore geometry in porous membranes by imbibition." Applied Physics Letters 115 (2019) 113701.

[2] Gruener, Simon, and Patrick Huber: "Imbibition in mesoporous silica: rheological concepts and experiments on water and a liquid crystal." Journal of Physics: Condensed Matter 23 (2011) 184109.

CPP 50.40 Tue 14:00 P1C

Low-resolution NMR investigations of polymer immobilization in nanocomposites — •Mozhdeh Abbasi[1], Sol Mi Oh[2], Alexander Eckert[3], So Youn Kim[2], Andreas Walther[3], and Kay Saalwächter[1] — [1]Inst. f. Physik - NMR, Martin-Luther-Univ. Halle-Wittenberg, Halle (Saale), Germany — [2]School of Energy and Chemical Engineering, UNIST, Ulsan, Republic of Korea — [3]Inst.f. Makromolekulare Chemie, Albert-Ludwigs-Univ. Freiburg, Germany

We used low-resolution 1H NMR spectroscopy to study the molecular dynamics of poly (ethylene oxide), mixed with spherical silica nanoparticles [1] as well as self-assembled clay sheets (NHT) forming nacremimetics [2] as model materials. The decomposition of time-domain signals (FIDs) reveals three different phases of PEO with different dynamics, based on different transverse relaxation behavior [3] which are related to the strength of the dipolar coupling between proton spin pairs. Therefore, fast initial decay on the time scale of microseconds corresponds to a rigid phase with strong dipolar couplings, attributed to the intercalated part of PEO within the clay sheets or adsorbed chains on the silica surface. The intermediate phase with residual dipolar couplings and a mobile phase with faster segmental motions and a rather long T2 corresponds to free polymer chains. This study addresses the different molecular dynamics of PEO chains subject to different constraints in the two different nanocomposite structures. [1] S. Y. Kim et. al., Macromolecules 2012, 45, 4225. [2] P. Das et al., Nat. Commun. 2015, 6, 1. [3] K. Schäler et. al., Macromolecules 2013, 46, 7818.

CPP 50.41 Tue 14:00 P1C

Isodesmic or cooperative? The self-assembly scenario of azobenzene stars unravelled in computer simulations — •Vladyslav Savchenko[1], Markus Koch[1], Aleksander S. Pavlov[2], Marina Saphiannikova[1], and Olga Guskova[1] — [1]IPF Dresden — [2]Department of Physical Chemistry, Faculty of Chemistry and Technology, Tver State University, Tver, Russia

Employing a number of computer simulation techniques, we quantify the intermolecular interactions between three-armed azobenzene stars with benzene-1,3,5-tricarboxamide core [1]. Our results suggest that during the formation of ordered phases [2, 3], these molecules prefer to build columns in which stars are held together via weak interactions whose strength growths with increasing the size of the aggregate. This phenomenon called cooperative self-assembly is proven for azobenzene stars in aqueous solution by calculating the binding energies, hydrogen bond lengths and macrodipoles. The simulations clearly attribute the cooperativity of the self-assembly to the development of a macrodipole, in other words, to the redistribution of the electronic density along the column. This, in turn, enhances the strength of the hydrogen bonds, and subsequently the intermolecular coupling in the stacks [4].

This work is funded by the DFG projects GU1510/3-1 and GU1510/5-1.

[1] M. Koch, et al. J. Phys. Chem. B 2017, 121, 8854. [2] S. Lee, et al. Langmuir 2013, 29, 5869. [3] M. Koch, et al. Langmuir 2019, 35, 14659. [4] V. Savchenko, et al. Molecules 2019, 24, 4387.

CPP 50.42 Tue 14:00 P1C

Do Columns of Azobenzene Stars Disassemble under Light Illumination? — Markus Koch, Marina Saphiannikova, and •Olga Guskova — Leibniz Institute of Polymer Research Dresden

The clustering properties of star-shaped molecules comprising three photochromic azobenzene-containing arms [1] are investigated with a specific focus on the influence of light on these structures. Previous experimental works report the self-assembly of azobenzene stars in aqueous solution into long columnar clusters that are detectable using optical microscopy. These clusters appear to vanish under UV irradiation, which is known to induce trans-to-cis photoisomerization of the azobenzene groups. We have performed MD simulations, density functional theory and density functional tight-binding calculations to determine conformational properties and binding energies of these clusters [2, 3]. Our simulation data suggest that the binding strength of the clusters is large enough to prevent a breaking along their main axis. We conclude that very likely other mechanisms lead to the apparent disappearance of the clusters.

This research was funded by the German Research Foundation (DFG), grant numbers GU1510/3-1, SA1657/13-1 and GU1510/5-1.

[1] M. Koch et al. J. Phys. Chem. B, 2017, 121, 8854.

[2] M. Koch et al. Langmuir, 2019, 35, 14659.

[3] V. Savchenko et al. Molecules, 2019, 24, 4387.

CPP 50.43 Tue 14:00 P1C

Spiropyran Sulfonates for Photo and pH Responsive Air-Water Interfaces and Aqueous Foam — •Marco Schnurbus[1], Malgorzata Kabat[2], Ewelina Jarek[2], Marcel Krzan[2], Piotr Warszynski[2], and Björn Braunschweig[1] — [1]Institute of Physical Chemistry, WWU Münster — [2]IKiFP PAN, Krakow

The photochromic reaction of a spiropyran sulfonate surfactant was used to render interfacial and foaming properties active to light stimuli. We have applied sum-frequency generation (SFG) spectroscopy which has provided information on the surface excess and the interfacial charging state as a function of light irradiation and solution pH. Under blue light irradiation, the surfactant forms a closed ring, spiro form (SP), whereas under dark conditions the ring opens and the merocyanine (MC) form is generated. The MC surfactants O-H group can be deprotonated as a function of pH, which is used to tune the molecules net charge at the interface. SFG spectroscopy shows that with increasing pH the intensity of O-H stretching band from interfacial water molecules increases, which we associate to an increase in surface net charge. At a pH of 5.3, irradiation with blue light leads to a reversible decrease of O-H intensities, whereas the C-H intensities were unchanged compared to the corresponding intensities under dark conditions. Measurements of the foam stabilities showed a higher foam stability under dark light conditions. At pH 2.7 this behavior is reversed as far as the surface tension and charging as well as the foam stability are concerned. The light-triggered changes at both pH values can be used to control foams and interfaces on a molecular level.

CPP 50.44 Tue 14:00 P1C

Cononsolvency-induced collapse transitions in thin PMMA-b-PNIPAM and PMMA-b-PNIPMAM films — •Julija Reitenbach[1], Christina Geiger[1], Cristiane Henschel[2], André Laschewsky[2], Christine M. Papadakis[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany — [3]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

Thin films of the thermoresponsive diblock copolymers PMMA-b-PNIPAM and PMMA-b-PNIPMAM both exhibit cononsolvency-induced collapse transitions when organic cosolvents are introduced into the surrounding atmosphere. The chemical structures of NIPAM (N-isopropylacrylamide) and NIPMAM (N-isopropylmethacrylamide) differ by a methyl functional group, which is able to influence the film collapse kinetics on a macroscopic scale. We reveal the solvent/cosolvent exchange taking place at the polymer functional groups with FTIR and attribute key changes in the local chemical environment to the macroscopic film collapse stages.

CPP 50.45 Tue 14:00 P1C

Mussel-inspired pNIPAM-microgels with adhesive potential — •Sandra Forg[1], Xuhong Guo[2], and Regine von Klitzing[1] — [1]Technische Universität Darmstadt, Institut für Festkörperphysik, Darmstadt, Germany — [2]ECUST, School of Chemical Engineering, Shanghai, China

The temperature-sensitivity of pNIPAM based hydrogels provides a huge potential for biologically motivated applications due to their phase transition close to the temperature of the human body (32°C). Combining this responsiveness with adhesive attributes would be of use for tissue engineering or medical purposes. Therefore hydrogels inspired by living marine organisms such as mussels have recently become highly attractive. Mussels can strongly adhere to other substrates even under harsh under water conditions, which is mainly determined by the protein 3,4-dihydroxyphenyl-L-alanine (DOPA). This DOPA-group can be incorporated into the hydrogel structure by the addition of a polymerizable group. However, most of these hydrogels are mechanically weak and / or possess a low elastic modulus, which remarkably limits their use in in vivo environments.

In this work, pNIPAM microgels are synthesized by free-radical precipitation polymerization. They are modified with DOPA to obtain adhesive properties. To get a closer insight into the polymerization process, time samples are taken during the synthesis. The monomer concentration of those time samples is analysed with mass spectrometry. By this knowledge, future synthesis can be controlled. The properties of these microgels are studied by DLS and Zetasizer measurements.

CPP 50.46 Tue 14:00 P1C

The thermoresponsive diblock copolymer PMMA-b-PNIPAM in aqueous solution: Influence of copolymer composition on micelle formation — •Nadir Aziz[1], Chia-Hsin Ko[1], Cristiane Henschel[2], Peter Müller-Buschbaum[1], André Laschewsky[2,3], and Christine M. Papadakis[1] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Institut für Chemie, University of Potsdam, Potsdam-Golm, Germany — [3]Fraunhofer Institute for Applied Polymer Research IAP, Potsdam-Golm, Germany

Amphiphilic diblock copolymers having a hydrophobic poly(methyl methacrylate) (PMMA) block and a thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) block form core-shell micelles in aqueous solution. The PNIPAM shell collapses at the cloud point of this block, and the micelles form large aggregates. We investigate the role of the block copolymer composition on the critical micellization concentration, the micellar size and shape as well as the collapse behavior at the cloud point. At this, we use fluorescence correlation spectroscopy and dynamic light scattering.

CPP 50.47 Tue 14:00 P1C

Minority Chains with Wall-Adsorbing End Groups Admixed to Polymer Brushes — •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 one of the most promising systems for the creation of surfaces with stimulus-responsive properties. It is highly desirable for applications to expose or hide specific chemical groups within the brush depending on changing system conditions. To this end, we investigate monodisperse polymer brushes, to which a small fraction of end-modified minority chains is admixed. The minority chains can be of a different length as compared to the brush chains and their terminal groups adsorb to the grafting surface at sufficient attraction energies. We study these systems combining Scheutjens-Fleer self-consistent field calculations [1], MD simulations and analytical theory. Firstly, the conformational changes of the admixed chains are explored, which depend on minority chain lengths as well as the attractivity between their end groups and the grafting wall. Furthermore, we analyze the free energy profiles of the end-group adsorption, from which transition energies are obtained. Lastly, we demonstrate that the adsorption barriers are predicted reasonably well by our theoretical approach and that they are strongly reduced under poor solvent conditions.

[1] Fleer, G. J., Cohen Stuart, M. A., Scheutjens, J. M., Cosgrove, T., Vincent, B., Polymers at Interfaces. London, Chapman and Hall, 1993.

CPP 50.48 Tue 14:00 P1C

Drying of shallow sessile droplets — •Swati Kaushik, Stefan Karpitschka, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The evaporation of sessile droplets on solid surfaces is an everyday phenomenon. The quantitative description of the evaporation dynamics is not only of interest from a fundamental perspective, but also highly relevant for practical applications such as coating technologies and inkjet printing. Here, we investigate the evaporation dynamics of shallow sessile droplets of pure n-Tetradecane on functionalized Si-wafers. We use an optical interference microscopy technique to construct the droplet profile over the course of drying process along with the dynamic measurement of the contact angle θ. The contact radius and droplet volume are also quantified taking into account the spherical cap approximation. This technique allows for measuring contact angles with a precision of 0.1°. The droplet dynamics are studied for different substrate temperatures and surface functionalization during the early stages of evaporation where the drop stays pinned to the substrate. We find a good agreement of the experimental results with theoretical models for diffusion-based evaporation. In addition, it is found that the depinning time varies with the initial contact angle and substrate temperature. We also report an interesting linear dependency of the rate at which the contact angle changes, $d\theta/dt$, on the inverse of the initial contact area in the limit of small contact angles.

CPP 50.49 Tue 14:00 P1C

Photo-Switchable Arylazopyrazole Phosphonic Acid SAMs on Al_2O_3 — •Christian Honnigfort and Björn Braunschweig — Institute of Physical Chemistry and Center for Soft Nanoscience SoN, University of Münster, Germany

The great interest in smart surfaces that can change their wetting behaviour on demand arises from their potential applications for self-cleaning surfaces, tunable lenses or microfluidics. Using light as a stimulus to change the wetting behaviour allows the spatio temporal confinement of the external stimulus. One way to exploit this is the decoration of surfaces with photo-responsive SAMs, e.g. phosphonic acids on Al_2O_3 surfaces. Here we used arylazopyrazole-functionalized phosphonic acids to induce the formation of photoresponsive SAMs on Al_2O_3. We show that the wetting behaviour can be changed reversibly with $\Delta\ \Theta = 8\ °$. The quantitative description of these wetting dynamics is still challenging. While contact angle measurements can quantify the changes in the macroscopic wetting behaviour the application of inherently interface specific sum-frequency generation spectroscopy can provide information on the wetting dynamics on a molecular level for instance by observing C-H and O-H stretching vibrations under different light irradiations. It allows to quantify the degree of ordering within the monolayer and to gain information on the interfacial water structure.

CPP 50.50 Tue 14:00 P1C

Simple model for drops on elastic substrates — •Christopher Henkel[1], Johannes Kemper[1], Jacco Snoeijer[2], and Uwe Thiele[1] — [1]Institut für Theoretische Physik, Münster, Germany — [2]Fac. of Science and Technology, Twente, Netherlands

The investigation of the wetting behaviour on viscoelastic or elastic substrates is of great interest. We present a simple model for steady liquid drops on fully compressible elastic substrates, and show that a double transition appears under variation of the substrate softness, similar to the one described in [1]. We further investigate how the transition depends on wettability and how it is amended by the Shuttleworth effect, i.e., the dependency of the interfacial tensions on local strain. 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.

CPP 50.51 Tue 14:00 P1C

Characterization of nano-particles with regard to hydrophobicity, size and emulsion-stabilizing capabilities — •Kai Luca Spanheimer[1], Sebastian Stock[1], Annika Schlander[2], Marcus Gallei[2], and Regine von Klitzing[1] — [1]TU Darmstadt, Condensed Matter Physics — [2]TU Darmstadt, Makromolekulare Chemie

For particle stabilized foams and emulsions the hydrophobicity of the used particles is an important parameter. For instance in case of Pickering emulsions(PE) the main effect of the particle hydrophobicity is the emulsion type (oil in water or water in oil). In an attempt to find a procedure determining the hydrophobicity of colloidal particles different types of silica-spheres were modified to achieve specific surface properties. Using silanization differently charged and hydrophobic groups were bound the surface. Contact angle measurements via sessile-drop are used to determine the surface energy of water on the coated wafer, which is a measure for the hydrophobicity of the surface. In the wetting case the contact angle depends on the roughness of the surface. Therefore, atomic-force-microscopy studies of the particle-layer were performed to determine the roughness and to ensure the comparability. It could be shown that the resulting emulsion type for prepared Pickering emulsions corresponds to the prediction (Bancroft rule) based on the measured particle-hydrophobicity.

CPP 50.52 Tue 14:00 P1C

Properties of droplets on (prestructured) switchable surfaces — •Leon Topp and Andreas Heuer — Westfälische Wilhelms-Universität, Institut für Physikalische Chemie, 48149 Münster, Germany

It is possible to switch the wettability of surfaces which consist for example of azobenzenes by external stimuli like light of a defined wavelength. When a droplet is placed on such a substrate and it is switched this leads to a relaxation of the droplet to the new surface properties and as a consequence to a change of the contact angle and shape.

To investigate this process theoretically we performed Molecular Dynamic Simulations of droplets placed on a fcc lattice consisting of Lennard-Jones particles. By changing the interaction strength between the liquid particles and the surface we can control the wetting properties and have the possibility to switch them. Thus, we considered different switching frequencies and study how the contact angle and the shape of the droplet evolves. Also we prestructured the surface and examine the influence of switching on droplets placed on such substrates.

CPP 51: Poster Session III-2

Topics: Active Matter (51.1-51.4), Glasses and Glas Transition (51.5-51.7), Hydrogels and Microgels (51.8-51.14).

Time: Tuesday 14:00–16:00 Location: P2/EG

CPP 51.1 Tue 14:00 P2/EG

Modeling the interaction of magnetically capped colloidal particles — •Maximilian Neumann[1], Artur Erbe[2], Sofia S. Kantorovich[3], Pedro A. Sánchez[3], Sibylle Gemming[1,2], and Gabi Steinbach[1,2] — [1]Institute of Physics, TU Chemnitz, D-09107 Chemnitz — [2]Helmholtz-Zentrum Dresden - Rossendorf, D-01328 Dresden — [3]Faculty of Physics, University of Vienna, A-1090 Vienna

Colloidal particles exhibiting spontaneous self-assembly are the precursors to bottom-up fabrication of advanced materials and micromechanical structures. There exists a comprehensive number of different particles with varying types of anisotropy with potential applications for controlled structure engineering. Here, we concentrate on particles that interact via polar fields, which are intrinsically anisotropic. More specifically, we focus on micron-sized silica spheres which are partly covered by a thin ferromagnetic layer with an out-of-plane magnetic anisotropy. With the goal of studying the assembly of such magnetic particles, we introduce a simple two-parameter model: A current-carrying coil enclosed inside a hard sphere is used to approximate an extended magnetization distribution. While the near field induced by the current reflects the extended magnetization, the far field mirrors the stray field of a point dipole. In this model the magnetization distribution is specified by the two coil parameters: The radius and the shift relative to the sphere's center. We present stable assemblies as a function of both parameters.

CPP 51.2 Tue 14:00 P2/EG

The effect of magnetic field and hydrogen peroxide on capped Janus particles — •Yara Alsaadawi[1], Anna Eichler-Volf[1], Michael Heigl[2], Manfred Albrecht[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute of Physics, University of Augsburg, Augsburg 86159, Germany

Janus particles are one type of artificial microswimmers consisting of two asymmetrically functionalized surfaces. With proper manipulation, one can control their displacement from one point to another at certain rate, as well as clustering, and orientation. In this work, we prepared Janus particles with caps consisting of Co/Pd, providing magnetic and H2O2-catalytic activity for particle propulsion, respectively. To employ both mechanisms, we conducted a systematic work that investigates propulsion under different combination of H2O2 concentrations and magnetic fields. Since the magnetic element in the cap plays a critical role in cap orientation and interaction with one another, we studied one particle system as well as two- and three-particle systems. Furthermore, as the swimming behavior is highly affected by the boundary conditions of its surrounding environment, varying surface properties were incorporated during experiments.

CPP 51.3 Tue 14:00 P2/EG

Analytical description of active polar filaments — •Christian Anton Philipps — Institute for Advanced Simulations, Forschungszentrum Jülich, 52428 Jülich, Germany

Nature provides a variety of active matter agents, which are self-propelled units consume either internal energy or extracting energy from their environment. A particular example on the cellular level are propelled polar semiflexible filaments, e.g., filamentous actin or microtubules in the cell cytoskeleton due to tread-milling and motor proteins [1]. Such active "polymers" exhibit interesting conformational and dynamical properties, even in dilute solution, which are absent in passive systems [2]. From a theoretical point of view, an analytical description of a polar active polymer is rather challenging, specifically due to the directed propulsion by the polar forces. We present an analytical solution of a polar filament with tangential driving forces, where the filament itself is described by the Gaussian semiflexible polymer model [3]. In particular, the inextensibility of the filament is taken into account. In detail, the polymer conformational and dynamical properties emerging by the active force will be discussed. [1] J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. 78, 056601 (2015); [2] R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, 101014 (2017); [3] A. Martin-Gomez, T. Eisenstecken, G. Gompper, R. G. Winkler, Soft Matter 15, 3957 (2019)

CPP 51.4 Tue 14:00 P2/EG

Interplay of surface forces for the directed transport of superparamagnetic beads above a thin film layer substrate — •Katharina Getfert, Rico Huhnstock, Dennis Holzinger, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

Directed transport of biofunctionalised magnetic particles over a substrate is a promising mechanism for sensitive analyte detection in lab-on-a-chip devices. Former publications present the realization of controllable superparamagnetic particle transport above a magnetically stripe patterned Exchange-Bias thin film layer substrate, revealing a complex interaction of surface forces between the particles and the substrate [1]. The interplay of these forces determines the steady state distance between both components, which is an important factor for the transport properties. In this work the influence of surface forces on the colloidal stability and, thus, on the particle transport is investigated. The impact on transport properties due to modifications in electrostatic and magnetic interactions between particle and substrate is analyzed by detecting the particle velocity. It can be shown, that the pH-value and thereby the ion-concentration of the surrounding medium plays an essential role in stabilization of the transport system due to its effects on the electrostatic interaction. Furthermore, the increase of the attractive magnetic interaction provides a higher sensitivity in measuring electrolyte dependent transport property changes.

[1] Ehresmann *et al.* (2015), Sensors, 15: 28854-28888.

CPP 51.5 Tue 14:00 P2/EG

Molecular dynamics and ionic conductivity of crown ether based discotics — Arda Yildirim[1], •Mohamed Aejaz Kolmangadi[1], Sabine Laschat[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und prüfung, Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut für Organische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

In present study, the molecular dynamics of asymmetric crown ether based discotics (KAL) bearing alkyl chains of different lengths were investigated by Broadband Dielectric Spectroscopy (BDS). Three dielectrically active relaxation processes were observed for both materials. At low temperatures, a γ-process in the Cry state was detected and is assigned to the localized fluctuations taking place in the alkyl chains. The $\alpha1$-process takes place at higher temperatures in the Cry phase. An $\alpha3$ process was found in the Colh mesophase. The temperature dependence of the relaxation rates of the $\alpha3$ process is a completely different than that of the $\alpha1$ relaxation. Molecular assignments of these different glassy dynamics are proposed. Tgthermal determined by DSC agrees with the dielectric data corresponding to the detected glassy dynamics. In addition, the conductivity contribution of both KAL compounds was analyzed. The conductivity contribution appears in both Cry and Colh phases at temperatures above 300 K.

CPP 51.6 Tue 14:00 P2/EG

Elektrische und mechanische Relaxationsspektroskopie von Säurehydraten — •Simon Ahlmann, Philipp Münzner, Roland Böhmer und Catalin Gainaru — Fakultät Physik, Technische Universität Dortmund, 44221 Dortmund

Phosphor- und Schwefelsäure besitzen für viele technische Anwendungen eine große Bedeutung. In wässrigen Lösungen sind diese Säuren durch eine anomal große Leitfähigkeit gekennzeichnet [1]. Es ist jedoch nicht abschließend geklärt, ob diese Leitfähigkeit vor allem auf einen schnellen Protonentransfer oder eher einen Vehikelmechanismus hindeutet, bei dem der Ladungstransport durch die molekulare Bewegung begrenzt wird.

Mittels Rheologie und dielektrischer Spektroskopie haben wir mechanische und elektrische Eigenschaften unterkühlter Phosphorsäure- und Schwefelsäure-Hydrate untersucht. Während die Form der mechanischen Relaxationsspektren des Schwefelsäure-Tetrahydrats temperaturunabhängig ist, gilt dies für Phosphorsäure-Monohydrat nicht. Dessen thermorheologische Komplexität deuten wir als Konsequenz der ausgeprägten temperaturabhängigen Trennung der mechanischen von den elektrischen Zeitskalen, die wir dielektrisch ermittelt haben [2]. Diese dynamische Entkopplung, die im Schwefelsäure-Hydrat deutlich geringer ausfällt, ist für Anwendungen interessant, die auf einer signifikanten Trennung von Masse- und Ladungstransport beruhen.

[1] M. Heres, Y. Wang, P. J. Griffin, C. Gainaru, A. P. Sokolov, Phys. Rev. Lett. 117, 156001 (2016) [2] M. Frey, H. Didzoleit, C. Gainaru, R. Böhmer, J. Phys. Chem. B 117, 12164 (2013)

CPP 51.7 Tue 14:00 P2/EG

How coupled elementary units determine heterogeneity in macroscopic glass-forming systems — •Lawrence Smith and Andreas Heuer — Westwälische Wilhelms-Universität, Münster, Germany

Elementary units of a binary Lennard-Jones glassformer can be identified through quantitative analysis of its underlying potential energy landscape. These units can be fully understood within the continuous time random walk formalism and are found to contain the complete information concerning thermodynamics and diffusivity, while displaying finite size effects with respect to relaxation times and spacial correlations [1]. Previous research has shown that it is possible to identify major contributions to the structural relaxation time τ_α and the non-Gaussian parameter as arising from the moments of the waitingtime distribution for jumps between metabasins of the potential energy landscape [2].

We investigate the impact of a coupling between elementary units on the non-Gaussian parameter (NGP) and τ_α to establish a relationship between this coupling and finite size effects that can be observed in molecular dynamic simulations. We extend this idea to gain insight into mechanisms underlying the emergence of dynamic heterogeneity as measured by four-point correlation functions in the stochastic model as well as in molecular dynamics simulations.

[1] C. Rehwald, A. Heuer, Phys. Rev. E 86, 051504 (2012)

[2] C. Schroer, A. Heuer, Phys. Rev. Lett. 110, 067801 (2013)

CPP 51.8 Tue 14:00 P2/EG

Co-nonsolvency transition of PNIPMAM-based block copolymer thin films in a series of binary mixtures — •Peixi Wang[1], Christina Geiger[1], Lucas P. Kreuzer[1], Tobias Widmann[1], Robert Cubitt[2], André Laschewsky[3], Christine M. Papadakis[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Institut Laue-Langevin, 38042 Grenoble, France — [3]Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany — [4]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

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(isopropylmethacrylamide) (PNIPMAM), which features a lower critical solution temperature (LCST) in aqueous solution, 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)*which exhibits an lower upper critical solution temperature (UCST) and shows a strong swelling transition in aqueous media, is newly studied. We focus on the co-nonsolvency behavior of PSBP-b-PNIPAM thin films in a series of deuterated binary mixtures by using time-of-flight neutron reflectometry (TOF-NR).

CPP 51.9 Tue 14:00 P2/EG

Hydrodynamics and Response of PNIPAM Microgel Aqueous Solution Subjected to Acoustic Waves — •Amin Rahimzadeh and Regine von Klitzing — Physics department, Technical University of Darmstadt, Germany

The poly(N-isopropylacrylamide)(PNIPAM) stimuli-responsive microgels were the subject of studies so far where their reaction to changes in temperature in aqueous solutions has been systematically investigated. Microgels shrink in the solution above their volume phase transition temperature(VPTT) due to the breaking of hydrogen bonds between PNIPAM and the solvent. Acoustic waves, on the other hand, can transfer a certain amount of energy by penetrating into a liquid solution. Depending on the wave frequency and amplitude, flow patterns inside of the liquid affected by the propagating waves can result in microstreaming to atomization and micro drop ejection. We transfer acoustic waves into a sessile water droplet containing PNIPAM microgels to study their response by carefully tuning the ultrasonic power. Therefore, the amount of energy enough for breaking the hydrogen bonds-that is not high to deteriorate the polymer chains-is a crucial parameter in this context. The shrinking/swelling behavior, dynamic stiffness, as well as streaming pattern of microgels, are subjected to analyze in this work.

CPP 51.10 Tue 14:00 P2/EG

PNIPAM microgels at the air-water interface - Influence of cross-linking concentration and distribution — •Franziska Jakob, Matthias Kühnhammer, and Regine von Klitzing — Technical University of Darmstadt, Department of Physics, Soft Matter at Interfaces, 64287 Darmstadt, Germany

Poly-N-isopropylacrylamide (PNIPAM) is a deformable and temperature-responsive polymer microgel, which can adsorb at liquid interfaces. It has been in the focus of multitudinous studies in the past years and is still being discussed very actively in the context of various possible applications, because of their ability to respond to external stimuli like temperature.

Spreading of microgels at the air-water interface depends considerably on various parameters. One important factor is the cross-linking density that has a strong influence on the microgel film formed at the air-water interface, and thus a significant impact on the compression isotherm[1].

In this contribution, films prepared from microgels with different cross-linking concentrations and different cross-linking distributions are studied. From this, conclusions regarding the degree of interdigitation (transition from core-core to shell-shell contact) of different microgels are drawn.

[1] C. Picard et al. Organization of Microgels at the Air-Water Interface under Compression: Role of Electrostatics and Cross-Linking Density. *Langmuir* **2017**, p.7973 f.

CPP 51.11 Tue 14:00 P2/EG

Magnetic nanogels in the flow — •Ivan Novikau[1], Ekaterina Novak[2], Pedro Sanchez[2], 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 dipole-dipole interaction (dipolar coupling parameter) between the MNPs [2].

Here, we investigate a suspension of magnetic NGs in a shear flow by means of molecular dynamics computer simulations coupled with Lattice-Boltzmann algorithm. Each NG is initially modeled as a system of bead-spring polymer chains randomly cross-linked into a polymer network. MNPs are randomly incorporated into this network [3].

Dipolar coupling, shear rate and viscosity of the carrier liquid are used as control parameters to alter both self-assembly of NGs and individual structural properties.

[1] Qing Wu et al., Nat. Commun., 10 (240), 2019.
[2] Novikau et al., JMMM, 2020.
https://doi.org/10.1016/j.jmmm.2019.166152
[3] Minina et al., J. Mol. Liq., 289, 2019.

CPP 51.12 Tue 14:00 P2/EG

Design and characterization of hydrogel bilayer strips with different crosslink densities — •Jonas Staudenmeir[1], Lukas Conrads[1], Sebastian Meyer[1], Niklas O. Junker[1], Dmitry N. Chigrin[1,2], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen, Germany — [2]DWI Leibniz Institute for Interactive Materials, Aachen, Germany

Hydrogels are three-dimensional structures made of cross-linked polymers that can absorb and store large amounts of solvents. By changing external parameters (temperature, pH, etc.) hydrogels react with large volume changes by ejecting or absorbing the solvent. Due to such volume changes, bilayers consisting of a hydrogel and a passive elastic material are known to show bending upon temperature changes. To develop a bistable system, which performs a snap-through transition between low- and high temperature states, hydrogel bilayer strips consisting of two poly(N-isopropylacrylamide) (PNIPAm) layers with different crosslinker density were designed and investigated in a water bath. Due to the different swelling properties of the layers, the strips showed a curvature that could be continuously changed by slow heating and cooling. By fixing the strip ends to a flexible polydimethylsiloxane (PDMS) frame, a sudden change in the direction of curvature was observed upon heating. Experimental and simulation results are compared.

CPP 51.13 Tue 14:00 P2/EG

Investigation of Non-Equilibrium Bending Dynamics of Microgel Disks — •Niklas O. Junker[1], Felix Jiang[1], Oliver Jung[2], Sebastian Meyer[1], Dmitry N. Chigrin[1,2], Ahmed Mourran[2], Martin Möller[2], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen, Germany — [2]DWI - Leibniz Institute for Interactive Materials, Aachen, Germany

Microgels are cross-linked polymer networks of micrometer or submicrometer dimensions which, in a solvent, can undergo large and fast volume changes in response to variations of external parameters (temperature, pH, etc.). Due to such volume changes, bilayers consisting of a hydrogel and a passive elastic material are known to show bending behavior. In the present work, bilayer disks of elliptical shape and consisting of a gold-nanorod-loaded, 5 micrometer thick poly(N-isopropylacrylamide) (PNIPAm) layer and a gold nanolayer are investigated in water. Non-equilibrium actuation dynamics triggered by conventional and photothermal heating is observed. The microgel structures are found to bend differently upon conventional temperature changes than upon photothermal heating. This behavior is systematically studied for different heating rates (up to 20°C/min for conventional heating and up to 1°C/ms for photothermal heating, in which the gold nanorods are used as photoabsorbers and local heaters).

CPP 51.14 Tue 14:00 P2/EG

Bending Simulations of Hydrogel Bi-layer Beams — •Sebastian Meyer[1], Lukas Conrads[1], Jonas Staudenmeir[1], Tobias Abel[1], Niklas Junker[1], Gero von Plessen[1], and Dmitry Chigrin[1,2] — [1]Institute of Physics (IA), RWTH Aachen, Germany — [2]DWI Leibniz Institute for Interactive Materials, Aachen, Germany

Hydrogels are cross-linked polymer networks that exhibit a great capacity to absorb and store large amounts of solvent. The amount of solvent in the hydrogel depends strongly on external parameters like the temperature, pH-value, etc., of the surroundings. Therefore, variations of these parameters can lead to large volume changes of the hydrogel. Two connected layers of differently cross-linked gels will start to bend, with the bending curvature depending on the temperature of the surroundings. Here, we present a theoretical description of such a bending for free and constrained hydrogel bi-layer beams using both classical beam theory and 3D finite volume simulations. Further, we compare the results to experimental observations.

CPP 52: Functional semiconductors for renewable energy solutions II (joint session HL/CPP)

Time: Tuesday 14:00–15:30 Location: POT 151

CPP 52.1 Tue 14:00 POT 151

Small-polaron transport and the role of defects in $BiVO_4$ photoanodes for solar water splitting — •Tim F. Rieth, Viktoria F. Kunzelmann, and Ian D. Sharp — Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Photoelectrodes can provide a route to a renewable energy supply by absorbing solar light and, thereby, drive an electrochemical reaction to produce chemical fuels. Bismuth vanadate ($BiVO_4$) exhibits the necessary properties for solar water splitting, namely visible light absorption, efficient charge carrier separation and well positioned band edges, and is the highest performing oxide photoanode to date [1]. Despite these advantages, the performance of $BiVO_4$ is inhibited by a low charge carrier mobility caused by small-polaron formation [2]. In our work, we investigate the limiting thermally activated hopping transport of small-polarons by the determination of the associated energy barrier E_h with temperature-dependent conductivity measurements on polycrystalline $BiVO_4$ thin films. Furthermore, we study how E_h is impacted by intentionally introduced defects such as vacancy defects and hydrogen impurities, which has been shown to greatly enhance the conductivity of $BiVO_4$ [3]. An improved understanding of charge carrier transport and its modification by defects can help to increase the performance of $BiVO_4$ and gives insights that aid in the development of new metal oxide photoelectrodes.

[1] I.D. Sharp et al., ACS Energy Lett. 2, 139 (2017)
[2] A.J.E. Rettie et al., Appl. Phys. lett. 106, 022106 (2015)
[3] J.K. Cooper et al., Chem. Mater. 28, 5761 (2016)

CPP 52.2 Tue 14:15 POT 151

InP(100) surfaces for efficient photoelectrochemical water splitting — •Olfa Dani[1], Mario Kurniawan[2], Agnieszka Paszuk[1], Manali Nandy[1], Andreas Bund[2], and Thomas Hannappel[1] — [1]Institute of Physics, Technische Universitaet Ilmenau, Germany — [2]Institute of Materials Science and Engineering, Technische Universitaet Ilmenau, Germany

To date, III-V semiconductor device structures enable the highest solar-to-hydrogen efficiencies. In this approach, a detailed understanding of the reactions at the semiconductor-electrolyte interface is essential to design the semiconductor surface for efficient charge transfer [1]. In this work, we studied the atomic structure of InP(100)-based photocathode surfaces before and after exposure to an aqueous electrolyte. The preparation of P- or In-rich surfaces on p-type InP(100) wafers with metal organic vapor phase epitaxy (MOVPE) was monitored in situ with reflection anisotropy spectroscopy (RAS). After contamination-free transfer from an MOVPE reactor to ultra-high vacuum, the surface structures were characterized by photoelectron spectroscopy (PES) and low-energy electron diffraction (LEED). Subsequently, the samples were transferred under nitrogen gas to a sealed photoelectrochemical cell for photocurrent density-potential measurements. In order to resolve changes in the surface chemistry and structure after exposure to the electrolyte, the samples were analyzed again by RAS, PES and LEED. For comparison, the same measurements were performed on InP(100) wafers with a native oxide layer. [1] M. M. May et al., J. Phys. Chem. C 118 (2014) 19032.

CPP 52.3 Tue 14:30 POT 151

Random structure search: Solving the kesterite-stannite puzzle in $(Cu,Ag)_2ZnSnSe_4$ solid solution — •Daniel Fritsch[1] and Susan Schorr[1,2] — [1]Department Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Department of Geosciences, Freie Universität Berlin, Malteserstr. 74−100, 12249 Berlin, Germany

$Cu_2ZnSnSe_4$ and $Ag_2ZnSnSe_4$ are both crystallising in the kesterite structure with the structurally similar stannite structure being energetically slightly less favourable. In the solid solution, however, there is experimental evidence that for some intermediate concentrations the stannite structure is energetically favoured. This behaviour is so far not understood.

Here, we're using density functional theory calculations to shed some light into the structure-property relations in $(Cu,Ag)_2ZnSnSe_4$. In order to simulate the different concentrations within the solid solution, we're employing the supercell approach based on the respective end members in the kesterite and stannite structure. The Ag and Cu cations are distributed randomly within the supercell, thereby creating several structure models for the solid solutions for further analysis. All random structure models are geometry optimised employing the recently developed SCAN functional. In order to obtain more reliable electronic and optical properties, selected optimised structures are subjected to single-shot calculations employing the more accurate hybrid functional HSE06.

CPP 52.4 Tue 14:45 POT 151

Photocatalytic performance of ALD-functionalized Nanoporous Anodic Alumina Photonic Crystals — •Carina Hedrich[1], Siew Yee Lim[2], Abel Santos[2], Robert H. Blick[1], and Robert Zierold[1] — [1]Center for Hybrid Nanostructures (CHyN), Universität Hamburg, 22761 Hamburg, Germany — [2]School of Chemical Engineering and Advanced Materials / Institute for Photonics and Advanced Sensing (IPAS) / ARC Centre of Excellence for Nanoscale BioPhotonics (CNBP), The University of Adelaide, South Australia 5005, Australia

Nanoporous anodic alumina (NAA) membranes feature self-organized, highly ordered pores with distinct geometrical characteristics. Modifying the electrochemical anodization parameters and applying pulse-like anodization profiles tailors the pore morphology from straight to modulated structures such as distributed Bragg reflectors or gradient index filters. The photocatalytic performances of these photonic crystals (PCs) can be enhanced by functionalizing the surface with photocatalytically active materials (e.g. TiO_2, ZnO, WO_3) or tuning the photonic stopband of the NAA by adapting the pore morphology. Herein, thickness-controlled surface modifications of NAA-PCs by atomic layer deposition (ALD) are conducted and the photocatalytic properties of these structures are investigated by studying the photodegradation of methylene blue. Optimizing and combining these different preparation strategies to further improve the photocatalytic efficiency and to tune the wavelength selectivity of NAA-PCs could expand their utilization as tailor-made photocatalysts.

CPP 52.5 Tue 15:00 POT 151

Thermoelectric transport properties of mesoporous silicon and mesoporous silicon - poly(3,4-ethylenedioxythiophene) hybrids — •Haider Haseeb[1,2], Danny Kojda[1], Klaus Habicht[1,2], and Tommy Hofmann[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie Gmbh, Hahn-Meitner-Platz 1, 14109 Berlin — [2]Universität Potsdam - Institut für Physik, Karl-Liebknecht-Straße 32, 14476 Potsdam

This presentation studies thermoelectric transport in mesoporous silicon (pSi) and mesoporous silicon-poly(3,4-ethylenedioxythiophene) (pSi-PEDOT) hybrids. We comprehensively explain electrochemical etching of pSi and infiltration of PEDOT based polymer blends (PEDOT:PSS, PEDOT:Tos) into pSi by dip- and drop-casting and vapor-phase polymerization. Surface sensitive SEM and volume sensitive nitrogen sorption isotherms probe morphological features such as pore size distributions, specific surfaces and porosities of as-etched pSi and pSi-PEDOT hybrids. Macroscopic transport measurements determine electrical and thermal conductivity, Hall mobility, charge carrier concentration and Seebeck coefficient of pSi, PEDOT, and pSi-PEDOT hybrids. We compare the temperature dependent thermoelectric performance of pSi-PEDOT hybrids with the properties of the corresponding inorganic and organic bulk systems. Our quantitative data analysis of charge and heat transport focuses on effective medium models.

CPP 52.6 Tue 15:15 POT 151

Impact of *p*-doping on the electronic and optical properties of copper iodide — •Michael Seifert, Claudia Rödl, and Silvana

Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The lack of viable p-type transparent conductors represents a critical bottleneck for future transparent electronics. CuI, with its direct band gap of 3.1 eV and its demonstrated p-type conductivity, is a promising candidate for such a material. Recently, it has raised significant renewed interest due to the production of transparent conducting bipolar CuI/ZnO heterostructure diodes, its applications as hole collection layer in organic electronics, or as promising candidate for a flexible, transparent thermoelectric material.

The possibility to enhance and tune key properties of the material is a major step towards potential technological applications. One ansatz to achieve this is substitutional doping. In a recent study by Graužinytė *et al.*, PCCP **21**, 18839 (2019), the chalcogen elements have been identified as promising candidates for p-type doping of CuI, due to thermodynamically accessible transition levels to a hole-generating charge state ($q = -1$). Here, the effect of such p-doping on the electronic structure and absorption spectrum is explored in the framework of density-functional theory and the properties of the doped material are compared to those of pristine CuI.

CPP 53: Perovskite and photovoltaics II (joint session HL/CPP)

Time: Tuesday 14:00–16:00 Location: POT 251

CPP 53.1 Tue 14:00 POT 251

Temperature-dependent exciton-phonon coupling in CsPbBr3 crystal using ultrafast two-dimensional electronic spectroscopy — •Xuan Trung Nguyen[1], Daniel Timmer[1], Yevgeny Rakita[2], David Cahen[2], Alexander Steinhoff[3], Frank Jahnke[3], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Institut für Physik, Carl von Ossietzky Universität, Germany — [2]Weizmann Institute of Science, Israel — [3]Institut für Theoretische Physik, Universität Bremen, Germany

Halide perovskites (HaPs) are promising semiconductor materials for developing efficient solar cells. It is, however, still debated how the unusual electron-lattice couplings in these materials affect their optical and electronic properties. Here, we investigate the temperature dependence of near band gap optical transitions in CsPbBr3 single crystals by 10fs-time-resolution two-dimensional electronic spectroscopy (2DES). At room temperature, the 2DES maps show rapid charge carrier relaxation within the continuum and the concurrent build-up of exciton screening by free carriers on a <30fs time scale [1]. At 70K, we detect large, persistent oscillations of both amplitude and resonance energy of the exciton peak with periods corresponding to the phonon modes of the lead-halide sublattice. Our results point to strong exciton-phonon couplings and to the importance of many-body interactions for the optical and transport properties in HaPs.

[1] Nguyen, X.T., et al., JPCL, 10, p. 5414-5421, 2019.

CPP 53.2 Tue 14:15 POT 251

Solution-Processed Two-Dimensional Materials for Perovskite Optoelectronics — •Antonio Gaetano Ricciardulli[1,2], Paul Blom[2], and Michael Saliba[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany

The efficiency of perovskite based perovskite solar cells and light-emitting diodes (PSCs and PLEDs, respectively) is limited by hole injection/transport and high leakage current, generated by a high hole injection barrier and poor perovskite morphology, respectively. Black phosphorus (BP), a newly emerged 2D layered semiconductor, is endowed with thickness-dependent bandgap, which spans from 0.3 eV (bulk) to 2.0 eV (monolayer). Hence, by carefully selecting the appropriate thickness, BP can be used as interlayer to enhance charge transport and injection in either PLEDs or PSCs. As a proof of concept, we reported a feasible strategy to reduce both hole injection barrier and defects at the perovskite interface by introducing 2D BP as hole injection layer in a PeLED stack. A continuous film composed of high*quality, ultrathin, and large BP sheets on top of PEDOT:PSS simultaneously improves the hole injection and morphology of the green*emitting CsPbBr3. Inclusion of BP enhances over 4 times efficiency of CsPbBr3 based PeLEDs. Incorporating BP to enhance the hole injection from PEDOT:PSS might also be of interest to increase the open*circuit voltage of PSCs of which the perovskite absorber has deeper valence band. Currently, we are developing novel PSCs based on 2D materials with specific functionalities.

CPP 53.3 Tue 14:30 POT 251

Ultrafast vibrational dynamics in lead halide perovskites — •Ajay Jha[1], Hong-Guang Duan[1], Vandana Tiwari[1], Golibjon Berdiyorov[2], Alexey Akimov[3], Pabitra Nayak[4], Zheng Li[1], Hernry Snaith[4], Michael Thorwart[5], Mohamed Madjet[2], and R. J. Dwayne Miller[1,6] — [1]MPSD, Hamburg — [2]Qatar Environment & Energy Research Institute, Doha — [3]Department of Chemistry, State University of New York — [4]Department of Physics, University of Oxford — [5]I. Institut für Theoretische Physik, University of Hamburg — [6]Departments of Chemistry and Physics, University of Tornoto

Hybrid organic-inorganic perovskites have gathered much attention owing to their unprecedented success in photovoltaics. To unravel the secrets to this success, we have studied the ultrafast dynamics of lead halide perovskites using heterodyne-detected transient grating and 2D spectroscopy in thin films for tetragonal (room temperature) and orthorhombic phases (T = 20 K). Our measurements capture the different ultrafast exciton dynamics in two phases of perovskite. In addition, we distinctly observe the ground and excited state vibrational modes corresponding to organic and inorganic sub-lattices in two phases. The interplay of strongly coupled dominant vibrational modes to ultrafast carrier generation process will be discussed. To rationalize our observations, we have employed density functional theory (DFT) predicting changes in the vibrational observations highlighting the importance of interaction between organic cation and inorganic sub-lattice in stabilization of charges upon photoexcitation.

CPP 53.4 Tue 14:45 POT 251

Lead-free co-evaporated perovskites for photovoltaic applications. — •Tim Schramm, Martin Kroll, Frederik Nehm, Zongbao Zhang, Karl Leo, and Yana Vaynzof — Dresden Integrated Center for Applied Physics and Photonic Materials(IAPP), Technische Universität Dresden

The performance of lead-based perovskites has dramatically increased over the past decade reaching power conversion efficiencies of over 25%. Despite these remarkable advances, lead-based perovskite suffer from serious challenges, most notably lead related toxicity and poor stability, which remain significant obstacles for their integration into industrial applications.

One promising route to circumvent these issues is by turning to novel absorber material systems such as the lead-free double perovskites. Herein, we present our recent results on the formation of $Cs_2AgBiBr_6$ perovskites by thermal evaporation. In particular, we employ a triple-source co-evaporation of the precursor materials, followed by thermal annealing and characterize their microstructure, crystallinity and optical properties. We identify processing conditions that lead to high quality crystalline films with large domains and investigate their performance in photovoltaic devices. Our results pave the route for further development of double perovskites for optoelectronic applications.

CPP 53.5 Tue 15:00 POT 251

Ion Migration Induced Modification of the Interfacial Energetics in Perovskite Solar Cells and its Effect on Device Performance — •Joshua Kress[1,3,4], Qingzhi An[1,3,4], Nir Tessler[2], and Yana Vayzof[1,3,4] — [1]TU Dresden — [2]Technion, Haifa — [3]Integrated Center for Applied Physics and Photonics — [4]Center for Advancing Electronics Dresden

The migration of ions in perovskite materials has been linked to many negative phenomena such as hysteresis and device degradation. Herein, we demonstrate that, under certain conditions, the migration of ions may also lead to an improvement in device performance. Specifically, by performing ultra-violet photoemission spectroscopy depth profiling experiments, we show that upon the application of an electric field during PV characterization of MAPbI3 inverted architecture solar cells, the migration of iodine ions to the interface between the perovskite active layer and electron extraction layer results in the modification of the electronic structure at that interface. The increase in the density of iodine ions leads to a band bending, resembling the electronic structure of iodine-rich overstoichiometric MAPbI3 films. This change in the interfacial electronic structure results in a significant enhancement of the built-in potential and open-circuit voltage of the photovoltaic cells in subsequent measurements, commonly observed by researchers in the field. Finally, our results are corroborated by numerical device simulations which include the presence and migration of ions.

CPP 53.6 Tue 15:15 POT 251

Reduction of s-shape formation induced by transparent top-contact sputter deposition in Perovskite solar cells — •Marlene Härtel[1,2], Ruslan Muydinov[1], Steve Albrecht[1,2], and Bernd Szyszka[1,2] — [1]Technische Universität, Berlin, Deutschland — [2]Helmholtz-Zentrum, Berlin, Deutschland

Depositing transparent top electrodes in Perovskite tandem solar cells without adequate buffer layers leads to damaging of the sensitive organic charge transport layers (CTL), due to harsh conditions during the sputter process. However, commonly used buffer layers utilize thermal atomic layer deposition, which is time consuming and could induce reactions with moisture. Therefore, direct sputter deposition is preferred, but sputter damage is mirrored in an s-shaped current-voltage characteristic, accompanied by a fill factor loss. In this contribution, the origin of the s-shape is analyzed by employing photoluminescence, and intensity and temperature dependent current-voltage measurement, and identified as an energetic barrier, which is formed at the CTL. The findings are supported by electrical simulations based on SCAPS. Moreover, two different sputter deposition techniques, namely radio-frequency magnetron and hollow cathode gas flow sputtering, are implemented and compared with regard to their application in damage-free sputter-deposition. By varying sputter process conditions, such as the power, or sample to target position, the s-shape in the solar cell devices can be reduced, thereby improving their electrical performance. Sputter damage-free TCO deposition allows for future enhancements in tandem device fabrication and their commercialization.

CPP 53.7 Tue 15:30 POT 251

Structural and optical properties of defect-engineered organic-inorganic halide perovskites — •Chang-Ming Jiang[1], Wen-Yu Cheng[1], Michael Ehrenreich[2], Gregor Kieslich[2], and Ian Sharp[1] — [1]Walter Schottky Institut, Technische Universität München — [2]Fakultät für Chemie, Technische Universität München

Incorporating large organic cations into the ABX3 hybrid perovskite is known to yield the so-called 'hollowed perovskite' structure. To accommodate the oversized cation onto the A-site, certain concentrations of B2+ cation and X- anion vacancies form. The presence of these point defects and associated dangling bonds are expected to affect the electronic properties, charge carrier dynamics, and phase stability. In the case of FASnI3, incorporation of ethylenediammonium (en2+) cations enlarges the optical bandgap and significantly improves the photovoltaic efficiency and stability. In this work, we aim at understanding the composition-dependent optical properties and relative phase stability in the defect-engineered (en)MAPbI3 system. Thin films with tunable bandgaps from 1.60-1.85 eV are fabricated, and the non-radiative recombination pathways associated with intentionally added point defects are studied by time-resolved PL techniques. Additionally, by measuring temperature dependence of PL, we find that both the orthorhombic-to-tetragonal and tetragonal-to-cubic phase transition temperatures are affected by the extent of large organic cation incorporation. This work sheds light on the interactions between organic cations and the inorganic lattice and provides insights into the defect tolerance in hybrid halide perovskite semiconductors.

CPP 53.8 Tue 15:45 POT 251

Band Gap Engineering of Double Perovskite Halides $Cs_2AgBiCl_6$ through Different Sites Alloying — •Dan Han, Masako Ogura, Andreas Held, and Hubert Ebert — Department of chemistry, Ludwig-Maximilians-Universität München, Munich, Germany

Recently, double perovskite halides have been proposed as potential Pb-free photovoltaic materials. However, many experimentally or theoretically reported double perovskite halides have indirect and large band gaps, hindering efficient sunlight absorbing. Thus, tuning the band gap of double perovskite halides is required for their future photovoltaic application. Forming alloys is a practical way for band gap engineering. Here, we presented a systematic study of alloying on different sites for a representative double perovskite halide $Cs_2B'B''X_6$(B'=Ag, B"=Bi, X=Cl) using the fully relativistic Korringa-Kohn-Rostoker (KKR) Green function in combination with the coherent potential approximation (CPA) method. $Cs_2Na_xAg_{1-x}BiCl_6$, $Cs_2AgSb_xBi_{1-x}Cl_6$ and $Cs_2AgBi(Br_xCl_{1-x})_6$ (x=0.25, 0.5, 0.75) all show a band gap bowing behavior, i.e., a nonlinear band gap dependence on the chemical composition. Additionally, we evaluated the mixing thermodynamical stability of $Cs_2AgSb_xBi_{1-x}Cl_6$ and show $Cs_2AgSb_xBi_{1-x}Cl_6$ alloy is thermodynamically stable at room temperature. Bloch spectral functions of alloys with different compositions exhibit broadening due to CPA technique. Alloys at B' and B" sites could tune the finite lifetime of carrier more effectively than alloys at X site.

CPP 54: Active Matter III (joint session DY/BP/CPP)

Time: Tuesday 14:00–16:00 Location: ZEU 160

CPP 54.1 Tue 14:00 ZEU 160

Uncovering novel phase transitions in dense dry polar active fluids using a lattice Boltzmann method — David Nesbitt, Gunnar Pruessner, and •Chiu Fan Lee — Imperial College, London, U.K.

The dynamics of dry active matter have implications for a diverse collection of biological phenomena spanning a range of length and time scales, such as animal flocking, cell tissue dynamics, and swarming of inserts and bacteria. Uniting these systems are a common set of symmetries and conservation laws, defining dry active fluids as a class of physical system. Many interesting behaviors have been observed at high densities, which remain difficult to simulate due to the computational demand. Here, we devise a new method to study dry active fluids in a dense regime using a simple modification of the lattice Boltzmann method. We apply our method to an active model with contact inhibition of locomotion, which has relevance to collective cell migration, and uncover multiple novel phase transitions: two first-order and one potentially critical. We further support our simulation results with an analytical treatment of the hydrodynamic equations.

Reference: D Nesbitt, G Pruessner, and CF Lee. Preprint: arXiv:1902.00530.

CPP 54.2 Tue 14:15 ZEU 160

Irreversibility in Active Matter Systems: Fluctuation Theorem and Mutual Information — Lennart Dabelow[2], •Stefano Bo[1], and Ralf Eichhorn[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Universität Bielefeld — [3]Nordita, Royal Institute of Technology and Stockholm University

We consider a Brownian particle, which, in addition to being in contact with a thermal bath, is driven by active fluctuations. These active fluctuations do not fulfill a fluctuation-dissipation relation and therefore play the role of a non-equilibrium environment. Using an Ornstein-Uhlenbeck process as a model for the active fluctuations, we derive the path probability of the Brownian particle subject to both, thermal and active noise. From the case of passive Brownian motion, it is well-known that the log-ratio of path probabilities for observing a certain particle trajectory forward in time versus observing its time-reserved twin trajectory quantifies the entropy production in the thermal environment. We calculate this path probability ratio for active Brownian motion and derive a generalized “entropy production”, 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.

CPP 54.3 Tue 14:30 ZEU 160

Rheotaxis of active drops in confinements — •Ranabir Dey[1], Carola M. Buness[1,2], Chenyu Jin[1], and Corinna C. Maass[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Goettingen — [2]Institute for the Dynamics of Complex Systems, Georg August Universitaet Goettingen

Biological microswimmers commonly navigate confinements having liquid flows, e.g. locomotions of spermatozoa through the reproductive tract and bacteria in the gut or in blood vessels. The directed motion of the microorganisms in response to the gradients in external flow velocity is classically called 'rheotaxis'. Recently, 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 drug 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 drops, in micro-confinements having Poiseuille flow. We experimentally quantify the rheotaxis of these droplet microswimmers, intrinsically undergoing Marangoni stress dominated 'self-propulsion', in response to velocity gradients of varying strength. We try to understand the observed rheotaxis of the active drops in confinements in the context of a hydrodynamic model– the active Jeffery-Bretherton model. We strongly feel that detailed understanding of artificial active matter rheotaxis will make significant contributions towards better design optimization for practical applications.

CPP 54.4 Tue 14:45 ZEU 160

Multiple Particle Correlation Analysis of Many-Particle Systems: Formalism and Application to Active Matter — •Rüdiger Kürsten[1], Sven Stroteich[1], Martín Zumaya Hérnandez[2], and Thomas Ihle[1] — [1]Universität Greifswald, Institut für Physik, Felix-Hausdorff-Str.6 — [2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Apartado Postal 48-3, Código Postal 62251, Cuernavaca, Morelos, México

We introduce a fast spatial point pattern analysis technique which is suitable for systems of many identical particles giving rise to multiparticle correlations up to arbitrary order. The obtained correlation parameters allow to quantify the quality of mean field assumptions or theories that incorporate correlations of limited order. We study the Vicsek model [1] of self-propelled particles and create a correlation map marking the required correlation order for each point in phase space incorporating up to ten-particle correlations. We find that multi-particle correlations are important even in a large part of the disordered phase. Furthermore, the two-particle correlation parameter serves as an excellent order parameter to locate both phase transitions of the system, whereas two different order parameters were required before [2].

[1] Phys. Rev. Lett. 75, 1226 (1995). [2] Phys. Rev. Lett. 92, 025702 (2004); Phys. Rev. E 77, 046113 (2008).

CPP 54.5 Tue 15:00 ZEU 160

Nonuniversality in scalar active matter with diffusivity edge under periodic confinement — •Benoît Mahault[1] and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Germany — [2]University of Oxford, United Kingdom

Scalar active matter is often described at the mean field level by nonlinear Fokker-Planck equations with density-dependent diffusion coefficients integrating fast degrees of freedom, as well as various equilibrium and/or nonequilibrium processes. A generic class, characterized by a diffusivity vanishing above some threshold density, was recently introduced [Golestanian, Phys. Rev. E 100, 010601(R)]. In presence of harmonic confinement, such 'diffusivity edge' was shown to lead to condensation in the ground state, with the associated transition exhibiting formal similarities with Bose-Einstein condensation (BEC).

Many active systems, such as self-propelled Janus particles, can however self-assemble into finite-size coexisting clusters. To account for such feature in the diffusivity edge framework, a periodic egg-crate confinement, that provides multiple sites for condensation, is considered in arbitrary dimensions. While for high barriers separating two minima the system essentially behaves as in the single harmonic trap case, for shallow potentials the transition is qualitatively different as the exponent associated to the scaling of the condensate fraction with an effective temperature is found to be nonuniversal. We nevertheless show from a generalized thermodynamic description that the overall phenomenology of BEC, such as the divergence of the isothermal compressibility at the transition, holds in both cases.

CPP 54.6 Tue 15:15 ZEU 160

Anomalous fluctuations accompany dynamical arrest in a cluster of chemically active colloids — •Suropriya Saha, Prathyusha K R, and Ramin Golestanian — Max Planck Institute for Dynamics and Self Organisation

Recent years have seen enormous scientific activity exploring the ability of catalytic colloids to collectively form patterns and clusters. However, fluctuations of individual colloids within a cluster remains unstudied, and is the focus of our work. Using the simplest example of active colloids, hard spheres that generate an isotropic chemical field, we find that an interplay of non-local interactions and finite system size results in the formation of a core and a surface layer in the cluster, both of which exhibit dynamics distinct from one another. The simplicity of our model suggests that aspects of the fluctuations revealed here are generic to matter driven phoretically, including enzymes.

CPP 54.7 Tue 15:30 ZEU 160

Transport coefficients of active particles: Reverse perturbations and response theory — •Thomas Ihle[1], Arash Nikoubashman[2], Alexander Unruh[1], Sven Stroteich[1], and Rüdiger Kürsten[1] — [1]Institute for Physics, Greifswald University — [2]Institute of Physics, Johannes-Gutenberg-University Mainz

Müller-Plathe's reverse perturbation method [Phys. Rev. E 59, 4894 (1999)] for shearing simple liquids is extended to the Vicsek model (VM) of self-propelled particles. It is shown how the shear viscosity ν and the momentum amplification coefficient λ, can be extracted from simulations by fitting to an analytical solution of the hydrodynamic equations for the VM. The viscosity consists of two parts, a kinetic and a collisional contribution. While analytical predictions already exist for the former [T. Ihle, J. Stat. Mech. 2016, 083205], a novel expression for the collisional part is derived by an Enskog-like kinetic theory [A. Nikoubahsman, T. Ihle, Phys. Rev. E 100, 042603 (2019)]. Using several methods to measure transport coefficients such as reverse perturbations, Green-Kubo relations and transverse current correlations, we find excellent agreement between the different methods and good agreement with theory. We introduce a novel kind of response theory that allows us to not only verify the analytical predictions of kinetic theory but also to efficiently obtain expressions for nonlocal (wavevector dependent) transport coefficients of active systems, avoiding tedious multiple-scale methods like the Chapman-Enskog expansion. The method is applied to the VM with metric and topological interactions as well as to a model with continuous time dynamics.

CPP 54.8 Tue 15:45 ZEU 160

Effect of Vicsek-like Activity on the collapse of a Flexible Polymer — •Subhajit Paul[1], Suman Majumder[1], Subir K Das[2], and Wolfhard Janke[1] — [1]Institüt für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]JNCASR, Jakkur P.O., Bangalore- 560064, India.

Dynamics of various biological filaments can be understood within the framework of active polymer models. In this context, we construct a bead-spring model for a flexible polymer chain in which the activity or self-propulsion of the beads has been defined in the Vicsek-like manner. Following a quench from a high-temperature coil phase to the low-temperature state we have studied the nonequilibrium dynamics of this model by solving the Langevin equation via molecular dynamics (MD) simulations. The low-T equilibrium state for the passive polymer in which the interaction among the beads modeled via standard LJ potential, is a compact globular one. Results from our MD simulations reveal that the globular state is also likely to be the final equilibrium in the active case also, the nonequilibrium dynamics is quite different than the passive case. We observe that the deviation from the intermediate 'pearl-necklace' arrangement and the formation of elongated structures for the polymer increases with activity. Also, it appears that whether smaller values of the activity makes the coarsening faster, activity beyond a certain value makes it slower. On this nonequilibrium front we also compare various results with that of the passive case, viz., scaling laws related to collapse time, cluster coarsening, etc.

CPP 55: Materials for Energy Storage and Conversion - Battery and Fuel Cell Materials (joint session MM/CPP)

Time: Tuesday 14:15–15:45 Location: IFW D

CPP 55.1 Tue 14:15 IFW D

Atomistic simulation of working interfaces: Towards understanding the role of complex multiphase grain boundaries in all-solid-state Li-ion batteries — •Sina Stegmaier[1], Roland Schierholz[2], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Theoretische Chemie, TU München — [2]IEK-9, Forschungszentrum Jülich

All-solid-state batteries (ASSBs) present a next-generation technology, promising increased operation safety and lifetime as compared to state-of-the-art Li-ion cells. The performance of solid-state electrolytes (SSEs) in ASSBs, though, is severely limited by poorly understood interfacial processes. Atomistic insight into the structure and transport processes at working SSE grain boundaries (GBs) [1] is required to enable rational progress.

To this end, we employ molecular dynamics (MD) simulations with a first-principles parametrized force field and study complex multiphase GBs in the SSE material LATP. An experimentally guided sinter protocol is established to model the formation of semi-amorphous domains at the interface of crystalline LATP grains. The resulting structural atomistic models enable the investigation of anisotropic lateral and transverse ion transport and the comparison to macroscopically accessible observables such as ion conductivity. Following this approach, we leverage experimental input for computational modeling and studying of more realistic solid-solid working interfaces.

[1] A. Mertens et al., Solid State Ionics 309, 180 (2017).

CPP 55.2 Tue 14:30 IFW D

Polaron Hopping Mechanism as a source for electronic conductivity in $Li_4Ti_5O_{12}$ (LTO) Batteries — •Matthias Kick[1], Cristina Grosu[1,2], Markus Schuderer[1], Christoph Scheurer[1], and Harald Oberhofer[1] — [1]Technische Universität München — [2]Forschungszentrum Jülich

State of the art lithium ion batteries rely on graphite as anode material due its remarkable lithium-intercalation properties. However due to the low intercalation potential of graphite, Li dendrite growth can occur during rapid charge processes, rendering a potential risk of having short-circuits in a battery cell. In addition, the large volume change during (dis)charging the battery results in unfavorable strain damaging the anode. Lithium titanium oxide $Li_4Ti_5O_{12}$ (LTO) shows the potential of being an excellent alternative to graphite anodes, as its volume stays stable during charge cycles and its high intercalation potential prevents Li dendrites to form. Unfortunately, the low conductivity of LTO still limits its use. To improve on this drawback, an elegant way is to introduce oxygen vacancies resulting in formation of Ti^{3+} centers. As a result, this blue colored LTO shows a lowering in its electronic resistance with improved electronic conductivity. By performing *Hubbard corrected density functional theory* (DFT+U) calculations we are able to show that in fact polaron formation and a possible polaron hopping mechanism can play a significant role in the experimental observed improved conductivities. Morevover we are able to gauge polaronic charge mobility by explicitly calculating polaron hopping barriers.

CPP 55.3 Tue 14:45 IFW D

Exploring defect structures in $Li_4Ti_5O_{12}$ (LTO): A combined theoretical and experimental approach — •Yute Chan[1], Cristina Grosu[1,2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]TU München — [2]IEK-9, FZ Jülich

Spinel $Li_4Ti_5O_{12}$ (LTO) is a fascinating anode material for next-generation all-solid-state Li-ion batteries (ASSB). Its "zero strain" charge/discharge behavior promises high safety and long cycling lifetimes. Nonetheless, pristine, white LTO possesses poor ionic and electronic conductivity. The latter can be increased by tailoring the sintering protocol to produce oxygen vacancies, resulting in a performant, blue LTO material. Heretofore, the detailed structure and distribution of the vacancies are unknown. Thus, powerful analytic techniques are needed to identify the defect structure inside the material. Positron lifetime spectroscopy (PALS) stands out from other experimental methods by the ability to sensitively collect positron lifetimes that correlate to different material defects. Data measured at the Garching positron source indicates that the positron lifetimes for LTO bulk and surface are distinguishable. To invert these lifetimes and gain information for the respective regions, we construct a series of LTO bulk and slab models and calculate theoretical lifetimes using two different self-consistent schemes within the framework of two-component density functional theory. We will discuss the relationship between experimental and theoretical lifetimes of LTO bulk and surface.

CPP 55.4 Tue 15:00 IFW D

A Neural Network Potential for Lithium Manganese Oxides — •Marco Eckhoff[1], Peter E. Blöchl[2], and Jörg Behler[1] — [1]Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany — [2]Technische Universität Clausthal, Institut für Theoretische Physik, Leibnizstraße 10, 38678 Clausthal-Zellerfeld, Germany

The lithium manganese oxide spinel $Li_xMn_2O_4$, with $0 < x < 2$, is an important cathode material in lithium ion batteries. The recently introduced local hybrid density functional PBE0r yields an accurate description of this material in good agreement with experiment. However, the accessible system size of molecular dynamics and Monte Carlo simulations is very limited when using density functional theory directly. Building on PBE0r data, we thus constructed a high-dimensional neural network potential, which provides a first-principles quality description of the potential energy surface at a fraction of the computational costs. This potential enables large-scale simulations of $Li_xMn_2O_4$ to study phase transitions and lithium diffusion.

CPP 55.5 Tue 15:15 IFW D

One parabola to fit them all: A response surface approach to computational catalyst screening — •Frederic Felsen, Christoph Scheurer, and Karsten Reuter — TUM, Munich, Germany

In the pursuit of sustainable power-to-fuel (P2X) technologies methanol fuel from renewable resources is one promising route towards reducing global carbon dioxide emissions. One of the many obstacles to overcome on the way to this ambitious goal is the efficient conversion of CO_2 rich syngas to methanol. Intricate interface structures are characteristic for all commonly employed catalyst materials for this process, like the state of the art $CuZnOAl_2O_3$ [1]. Understanding these surface effects is key for a rational improvement and design of future catalysts.

We present an approach to efficiently characterize solid-solid interface structures by a well defined set of single point DFT calculations. Exploiting ideas from response surface methodology [2], we actively distort interface structures to evaluate the response of the system on geometric changes. Resulting observables such as adsorption energies of reaction intermediates may directly provide insight into the catalytic activity of the respective interfaces. Furthermore, this novel interface characterization may enable computational screening for multi component catalyst materials. As a first test case metal thin films supported on transition metal oxides will be studied.

[1] M. Behrens et al., *Science*, 336, (2012).

[2] R. H. Myers et al., Response Surface Methodology, *Wiley*, (2009).

CPP 55.6 Tue 15:30 IFW D

Analysis of $Li_xMn_2O_4$ for catalysis of the oxygen-evolution-reaction (OER) using STEM-EELS — •Florian Schönewald[1], Max Baumung[1], Marcel Risch[1,2], and Cynthia Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Helmholtz-Zentrum Berlin für Materialien und Energie

Controlling the OER is an important step for achieving a sustainable renewable energy future. The process of generating molecular oxygen from water by chemical means is severely kinetically limited. Here $Li_xMn_2O_4$ is studied as a model electrocatalyst. To understand the role of manganese valence and covalency for the OER these are manipulated by electrochemical de-/lithiation. Characterisation of the particles is performed before and after OER, for different lithiation states. Specific attention is given to Mn at the surface since it is directly involved in electron transfer.

With EELS of the O K- and Mn L-edge a surface layer with strongly reduced Mn has been discovered and attributed to changes in Mn/O ratio. This state is also preserved under delithiation. In previous studies, this effect has been explained by tetragonal Mn_3O_4 forming at the surfaces [1]. However, no second phase matching Mn_3O_4 or related structures was identified by X-ray powder diffraction. According to the estimated surface volume share of about 10 %, Mn_3O_4 formation can be excluded. Instead, a combination of oxygen vacancies and additional manganese on tetrahedral sites as antisite defects is taken into account to explain the apparent Mn valence change at surfaces.

[1] Daichun Tang et al, Chem. Mater. 2014, 26, 11, 3535-3543

CPP 56: Focus: Exploitation of Anisotropy in Organic Semiconductors II (joint session CPP/HL)

Time: Wednesday 9:30–11:15 Location: ZEU 222

Invited Talk CPP 56.1 Wed 9:30 ZEU 222

Structural and photophysical properties of blends of weakly interacting organic semiconductors — •Katharina Broch[1], Clemens Zeiser[1], Giulio Cerullo[2], Roel Tempelaar[3], and Christopher Bardeen[4] — [1]Institute for Applied Physics, University of Tübingen, Germany — [2]Department of Physics, Polytechnic University of Milan, Italy — [3]Department of Chemistry, Northwestern University, USA — [4]Department of Chemistry, University of California at Riverside, USA

Blends of organic semiconductors are functional parts in many organic electronic devices and their structural, electronic and photophysical properties have been studied in great detail. So far, research focussed mainly on electron donating and accepting organic semiconductors due to their relevance for devices. However, also blends of weakly interacting compounds can be interesting from the viewpoint of a fundamental understanding of mixing behavior [1,2], or as tool to study the details of complex photophysical processes [3,4]. Anisotropies in structure formation and their impact on photophysical properties will be discussed using the example of acene blends.

[1] J.-O. Vogel et al., J. Mater. Chem. 20 (2010); [2] A. Aufderheide et al., Phys. Rev. Lett. 109 (2012); [3] D. Lubert-Perquel et al., Nat. Commun. 9, 4222 (2018); [4] K. Broch et al., Nat. Commun. 9, 954 (2018)

CPP 56.2 Wed 10:00 ZEU 222

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 56.3 Wed 10:15 ZEU 222

Favored face-on crystal orientation in poly(3-(6-bromohexyl)-thiophene) on graphene as a result of modified interfacial interactions — •Oleksandr Dolynchuk[1], Philip Schmode[2], Matthias Fischer[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

Directed crystallization on a substrate could be advantageous for inducing molecular orientation in semicrystalline conjugated polymers whose charge transport properties are anisotropic. Although a preferred face-one molecular orientation was shown in monolayers of poly(3-hexylthiophene) (P3HT) on graphite, a full face-one orientation in thicker P3HT films has not been realized so far. We assume that it is a result of two competing interfacial orientations initiated at the interfaces to vacuum and graphite. Here it is shown that modification of the chemical structure of P3HT side chains can alter the surface interactions and result in fully face-on oriented crystals. Specifically, we present a comparative study of the substrate induced orientation in thin films of poly(3-(6-bromohexyl)-thiophene) (P3BrHT) and P3HT on graphene. The crystal orientation in films of both polymers was explored by surface-sensitive grazing incidence XRD. The results indicated that P3BrHT on graphene had solely face-on oriented crystals in films up to 26 nm, whereas P3HT showed the mixed face-on and edge-on crystal orientation with edge-on crystals formed at the top surface that supports our assumption about competing interfacial orientations.

CPP 56.4 Wed 10:30 ZEU 222

Determining Anisotropic Effects in Strongly Coupled Metal Organic Hybrid Structures — •Maximilian Rödel[1], Thomas Stark[2], Markus Hecht[3], Jochen Manara[2], Matthias Stolte[3], Frank Würthner[3], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [3]Institut für Organische Chemie &Center for Nanosystems Chemistry (CNC), Julius Maximilian University of Würzburg, 97074 Würzburg

Coupling phenomena in metal organic hybrid structures enable unique possibilities to tune the properties of opto-electronic devices. Furthermore, the strong coupling between surface plasmons and excitons in organic semiconductors leads to novel hybrid states, which are termed plexcitons. By means of surface plasmon resonance spectroscopy we investigate these plexcitonic states in liquid-crystalline perylene bisimide (PBI) thin films exhibiting J-type coupling deposited on gold surfaces processed via doctor blading from solution. These new states show a characteristic coupling strength of ≈110 meV. Alignment of hydrogen-bonded PBI molecules and, thus, their transition dipoles results in long-range ordered films with a pronounced spatially anisotropy of structural and optical characteristics. A ratio of 2.78 can be evaluated between strongest and weakest coupling strength of the anisotropic system. Understanding the correlation between molecular order and optical properties will enable new device concepts utilizing the presented opto-electronic directionality in future applications.

CPP 56.5 Wed 10:45 ZEU 222

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 56.6 Wed 11:00 ZEU 222

On the Origin of Electronic Gap States in Molecular Semiconductor Thin Films — •Alexander Hinderhofer[1], Jan Hagenlocher[1], Satoshi Kera[2], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, 72076 Tübingen, Germany — [2]Institute for Molecular Science, Myodaiji, 444-8585, Japan

Electronic gap states within the HOMO-LUMO gap of molecular semiconductors play a key role in the energy level alignment of organic-organic and organic-inorganic interfaces and therefore are a defining parameter for device functionality and efficiency. The density of gap states originates from structural defects acting as dopants and it can be varied by different film preparation methods, e.g. by temperature variation during film deposition.

We present a systematic study of anisotropic structural parameters in thin films, including grain size, strain, dislocation density, mosaicity and coherently ordered domain size (in-plane and out-of-plane) studied by X-ray scattering and atomic force microscopy. The structural properties of several molecular semiconductors (Pentacene (PEN), Perfluoropentacene (PFP), 6-Phenacene (6Phen), etc.) are correlated with their electronic gap state density studied by ultra-low background ultraviolet photoelectron spectroscopy (UPS). We discuss which types of structural parameters have the strongest impact on the gap state density. Finally, we present examples of the energy level alignment in organic-organic heterojunctions controlled by their gap state density.

CPP 57: Hybrid Perovskite and Photovoltaics I (joint session CPP/HL)

Time: Wednesday 9:30–12:45 Location: ZEU 260

CPP 57.1 Wed 9:30 ZEU 260

Growth of High-quality (FAPbI$_3$)$_{0.9}$(MAPbBr$_3$)$_{0.1}$ Perovskite Single Crystals and their Optoelectronic Properties — •Julian Höcker[1], Mathias Fischer[1], Mehmet Özcan[2], Benedikt Bichler[2], Sebastian Hammer[1], Melina Armer[1], Volker Drach[1], Bert Nickel[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, JMU, 97074 Würzburg — [2]Soft Condensed Matter Group, LMU, 80539 München

Organo lead trihalide perovskites are potentially highly interesting class of semiconductors. Particularly the perovskite (FAPbI$_3$)$_{0.9}$(MAPbBr$_3$)$_{0.1}$ is one of the most important representatives of this material class. In order to further develop this complex perovskite system and thus foster its use, it is essential to investigate the chemical and physical properties of high-quality single crystals with the same stoichiometry. However, the liquid growth of perovskite crystals without seed crystals is usually challenging and becomes even more challenging with mixed cations/halides crystals, making it difficult to assess their properties. For this purpose, we have developed a new efficient re-fill crystallization method (RFCM) based on the Inverse Temperature Crystallization (ITC), which avoids seed crystals. We applied qualitative and quantitative analyses to identify the elemental composition and the exact stoichiometry of the grown crystals and studied their crystallographic properties, demonstrating a high single crystal quality. Optical and electrical measurements completed the structural and elemental analysis, and enabled us to derive relevant properties of this perovskite material.

CPP 57.2 Wed 9:45 ZEU 260

Revealing the Impact of Cesium/Rubidium Incorporation on the Photophysics of Multiple-Cation Lead Halide Perovskites — Yajun Gao, Kai Wang, Mingcong Wang, Jafar Khan, Ahmed Balawi, Stefaan De Wolf, and •Frédéric Laquai — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center, Thuwal, Saudi Arabia

The incorporation of cesium (Cs) and rubidium (Rb) ions in multiple-cation mixed lead halide perovskites increases their photovoltaic performance. Here, the reasons for the performance increase are investigated by steady-state and transient spectroscopy techniques. The band edge absorption shows that the Cs/Rb-ion incorporation increases the band gap, while exciton binding energies remain low, in the range of a few milli-electronvolts. Low Urbach energies determined by photothermal deflection spectroscopy suggest optimized microstructures upon Cs/Rb incorporation. The charge carrier recombination dynamics indicate that Cs/Rb-incorporation reduces not only the first-order (trap-assisted) recombination, but also the second-order recombination. Upon photoexcitation, carrier density-induced broadening of the photo-bleaching following the Burstein-Moss model is observed and effective carrier masses are determined to be in the range of a few tenths of the electron rest mass, explaining the excellent charge carrier mobilities of these perovskite films. Sub-picosecond hot carrier cooling is observed, indicating a strong charge-phonon coupling. Our results reveal the impact of cesium/rubidium incorporation on the photophysics of multiple-anion lead halide perovskites.

CPP 57.3 Wed 10:00 ZEU 260

Unraveling origin of performance instability in mixed perovskite solar cells — •Małgorzata Kot[1], Chittaranjan Das[2], Tim Hellmann[2], Carolin Wittich[2], Iwan Zimmermann[3], Mohammad Khaja Nazeeruddin[3], Wolfram Jaegermann[2], and Jan Ingo Flege[1] — [1]BTU Cottbus-Senftenberg, Germany — [2]TU Darmstadt, Germany — [3]EPFL Lausanne, Switzerland

A degradation mechanism of mixed perovskite solar cells is mostly attributed to the segregation of halide phases in the perovskite film. However, our studies have revealed, that the mixed perovskites degrade due to the migration of iodine and methylammonium ions across the solar cell. Nonetheless, an ultrathin RT-ALD-Al$_2$O$_3$ layer deposited on top of perovskite can very effectively limit this migration thanks to the reactive property of this interface.[1-3] Namely, there is a closed cycle of the charge transfer between ALD and perovskite films. Such ALD film doesn't cause any drastic changes in the perovskite morphology, chemical composition, optoelectronic properties or crystallinity. What more, it helps to preserve the initial properties of the film during exposure to the light and ambient air under real operating conditions and thus improves the stability of the solar cells. This ultra-thin Al$_2$O$_3$ layer prepared in an unusual RT process for ALD method significantly increases the lifetime of perovskite solar cells at a very low cost bringing thus the introduction of the perovskite solar cells into mass production. [1] M. Kot et al., ChemSusChem 11 (2018) 3640. [2] M. Kot et al., Energy Technol. 7 (2019) 1900975. [3] D. Schmeißer et al., J. Phys. Chem. C 123 (2019) 23352.

CPP 57.4 Wed 10:15 ZEU 260

Phase transitions of hybrid and inorganic perovskites simulated by machine-learning force fields — Ryosuke Jinnouchi[1,2], Jonathan Lahnsteiner[1], Ferenc Karsai[3], Georg Kresse[1], and •Menno Bokdam[1] — [1]University of Vienna, Vienna, Austria — [2]Toyota Central R&D Labs, Aichi, Japan — [3]VASP Software GmbH, Vienna, Austria

Finite-temperature simulations of complex dynamic solids are a formidable challenge for first-principles methods. Long simulation times and large length scales under isothermal-isobaric (NPT) conditions are required, demanding years of compute time. We applied the recently developed on-the-fly Machine-Learning Force Field (MLFF) scheme[1] to generate force fields for several hybrid and inorganic perovskites (APbX3, A={MA,Cs},X={I,Br,Cl}). The MLFFs open up the required time and length scales, while retaining the distinctive chemical precision of first principles methods. We study the entropy driven phase transitions of hybrid perovskites, which have never been accurately described in simulations. Simulations using machine learned potentials give direct insight into the underlying microscopic mechanisms. The ordering of the Methylammonium (MA) molecules as function of temperature is obtained. Furthermore, we relate the phase transition temperatures of different perovskites to the radii of the involved species, and we determine the order of the transitions in Landau theory.

[1] R. Jinnouchi et al., Phys. Rev. Lett. 122, 225701 (2019)

CPP 57.5 Wed 10:30 ZEU 260

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 57.6 Wed 10:45 ZEU 260

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 57.7 Wed 11:00 ZEU 260

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.

15 min. break

CPP 57.8 Wed 11:30 ZEU 260

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 57.9 Wed 11:45 ZEU 260

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 57.10 Wed 12:00 ZEU 260

Photodoping through local charge carrier accumulation in alloyed hybrid perovskites for highly efficient luminescence — •Sascha Feldmann, Stuart Macpherson, Satyaprasad Senanayak, Mojtaba Abdi-Jalebi, Jasmine Rivett, Guangjun Nan, Gregory Tainter, Tiarnan Doherty, Kyle Frohna, Emilie Ringe, Richard Friend, Henning Sirringhaus, Michael Saliba, David Beljonne, Samuel Stranks, and Felix Deschler — Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

Metal-halide perovskites have emerged as exceptional semiconductors for optoelectronic applications. Substitution of the monovalent cations has advanced luminescence yields and device efficiencies. Here, we control the cation alloying to enhance optoelectronic performance through alteration of the charge carrier dynamics in mixed-halide perovskites. In contrast to single-halide perovskites, we find high luminescence yields for photo-excited carrier densities far below solar illumination conditions. Using time-resolved spectroscopy we show that the charge-carrier recombination regime changes from second to first order within the first tens of nanoseconds after excitation. Supported by microscale-mapping of the optical bandgap, electrically-gated transport measurements and first-principles calculations, we demonstrate that spatially-varying energetic disorder in the electronic states causes local charge accumulation, creating p- and n-type photo-doped regions, which unearths a strategy for efficient light emission at low charge-injection in solar cells and LEDs.

CPP 57.11 Wed 12:15 ZEU 260

Perovskite solar cells from direct co-evaporation: Impact of hole transport materials on device performance — •Marcel Ross[1], Amran Al-Ashouri[1], Erica Magliano[1], Marko Jošt[1], and Steve Albrecht[1,2] — [1]Helmholtz-Zentrum Berlin, D-12489 — [2]Technical University Berlin, D-10587

Deposition of perovskite solar cell absorbers by co-evaporation offers a variety of advantages over solution based preparation such as homogeneous coating of large substrates and conformal coverage of different textures. Nevertheless, the majority of reported publications focusses on solution-based preparation of perovskite solar cells. This is likely due to the challenging evaporation characteristic of organic precursors and the limited understanding of the perovskite co-evaporation process itself. To achieve a better process control, we implement an evaporation setup with a thermal management system. This enables the deposition of high quality Methylammonium Lead Iodide perovskite films as confirmed by XRD, PL and optical measurements. To analyse the influence of substrate properties on film formation, perovskites are deposited on different hole transport materials (HTMs) such as PTAA and self-assembling monolayer (SAM) molecules. Furthermore, the impact of the substrate temperature during deposition of the perovskite is investigated. While the substrate temperature is mainly influencing the incorporation of methylammonium iodide into the film, the p-i-n solar cell performance is strongly affected by the used HTM. Finally, a stabilized efficiency over 20% is realized with the SAM hole transport layer and a proper substrate temperature.

CPP 57.12 Wed 12:30 ZEU 260

The impact of mobile ions on the open cicuit voltage decay of perovskite solar cells explained by time resolved drift-diffusion simulations. — •Mathias Fischer, David Kiermasch, Kristofer Tvingstedt, and Vladimir Dyakonov — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

The open circuit voltage decay (OCVD) is a characteristic transient response of an operating solar cell after the illumination is turned off. By analyzing such transients correctly, it is possible to obtain valuable information about charge carrier dynamics in a fully functional device. When additional charged species like mobile ions are present, extraordinary features can be observed during the OCVD. We use a self-programmed transient drift-diffusion simulator involving mobile ions with sub-nanoseconds time resolution, to show how quantitative information about the ionic species, such as concentration and diffusion coefficient can be obtained. The simulated transients showing characteristic ionic features are in excellent agreement with experimental data from methylammonium lead iodide ($CH_3NH_3PbI_3$) devices. Further, the ionic contributions to the OCVD are clearly visualized by specially resolved carrier profiles. This approach opens up new ways to interpret transient electrical measurements on perovskite based devices.

CPP 58: Modelling and Simulation of Soft Matter I (joint session CPP/DY)

Time: Wednesday 9:30–13:00 Location: ZEU 255

Invited Talk CPP 58.1 Wed 9:30 ZEU 255

Structure and dynamics of semiflexible polymers in bulk and confinement — •Arash Nikoubashman — Institut für Physik, Johannes Gutenberg Universität Mainz, Mainz, Deutschland

Semiflexible macromolecules are important constituents of living matter and also find various applications as versatile materials, in particular due to their possible liquid crystalline order. To better understand these systems, we employed coarse-grained molecular dynamics simulations to study lyotropic solutions of semiflexible polymers in the bulk as well as in confinement over a wide range of monomer densities, persistence lengths, and contour lengths. In bulk systems, we observed an isotropic-nematic transition and a nematic-smectic transition as the persistence length and monomer density were increased. Further, we found that semiflexible polymers exhibited a much lower diffusivity and higher shear viscosity compared to their flexible counterparts. Under spherical confinement, we discovered that densely packed semiflexible polymers could not anymore exhibit uniform nematic order when their contour length became of the same order as the sphere radius. Instead, confinement led to the emergence of topological defects on the sphere surface with competing ordering in the interior of the sphere. Each of the configuration variables including chain length, chain stiffness, packing density, and shell thickness uniquely affected the ordering, including the nature and relative orientation of the defects on the surface.

CPP 58.2 Wed 10:00 ZEU 255

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).

CPP 58.3 Wed 10:15 ZEU 255

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 58.4 Wed 10:30 ZEU 255

Morphology on Reaction Mechanism Dependency for Twin Polymerization — •Janett Prehl[1], Robin Masser[1], Peter Salamon[2], and Karl Heinz Hoffmann[1] — [1]Insitut für Physik, Technische Universität Chemnitz, Chemnitz, Germany — [2]Department of Mathematics and Statistics, San Diego State University, San Diego, USA

Within this presentation we will present our latest results [1] on the analysis of the structure formation process of twin polymerization via a previously introduced lattice-based Monte Carlo method, the reactive bond fluctuation model [2]. We analyze the effects of the model parameters, such as movability, attraction, or reaction probabilities on structural properties, like the specific surface area, the radial distribution function, the local porosity distribution, or the total fraction of percolating elements. From these examinations, we can identify key factors to adapt structural properties to fulfill desired requirements for possible applications. Hereby, we point out which implications theses parameter changes have on the underlying chemical structure.

[1] Hoffmann, K.H. and Prehl, J., *Reac. Kinet. Mech. Cat.* **123** (2018) 367-383; Huster, C., Nagel, K., Spange, S., and Prehl, J., *Chem. Phys. Lett.* **713** (2018) 145-148

[2] Prehl, J. and Huster, C., *polymers* **11** (2019) 878

CPP 58.5 Wed 10:45 ZEU 255

Effect of the Backbone Chemical Composition and Monomer Sequence on Phenylene Polymer Persistence Lengths — •Nancy C. Forero-Martinez[1], Björn Baumeier[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]University of Technology, P.O. BOX 513-5600 MB, Eindhoven, The Netherlands

The study of the physical properties of phenylene polymer precursors used in the fabrication of graphene nanoribbons poses open questions whose answers will contribute to the design of more efficient synthesis protocols. Particularly, size-exclusion chromatography combined with persistence length measurements assigns both, semiflexible to semi-rigid structures depending on the molecular weight of the precursor. Surprisingly, these results suggest an apparent structural change upon increasing the length of the polymer. In this work, we use a generic model to build phenylene polymer chains as random walks that take into consideration the nature of the arene substitutions along the backbone. In addition to conformational changes, this model allows one to study the backbone contribution to the persistence length by modifying a small set of parameters controlling chemical content and structure. We consider the flexibility of polyphenylene precursors in a theta-like solvent in terms of chain composition by building both, chains that are purely composed by meta or para connected repeat units, and randomly mixed chains with a given composition. We find that systems with apparently the same chemistry have different persistence length due to different monomer mixing ratios and sequence along the chain.

CPP 58.6 Wed 11:00 ZEU 255

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 analysis 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.

15 min. break

CPP 58.7 Wed 11:30 ZEU 255

Modeling Depletion Interactions in Blends of Branched and Linear Polymers — •Martin Wengenmayr[1,2], Ron Dockhorn[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]TU Dresden, Germany

Effective attractive interactions in colloidal systems are well understood and described by depletion potentials. Similar effective attractions have been found for a wide range of soft matter systems like brush coated particles and dendrimers as well. For colloidal particles the depletion potentials are deduced from volume exclusion layers around the hard particles, but this is not applicable for soft particles, which are interpenetrated by the depletant. In this work we present a mean field free energy approach modeling the origin of the soft matter depletion interactions by balancing the excess free energy between the soft particle and the depletant with the elastic repulsion between particles. This approach is adopted for a model system containing dendrimers as soft particles in the melt of linear polymer chains acting as depletant. From recent investigations [1] it is known that the dendrimers display so called crowded conformations that are compact but not fully collapsed and the dendrimers are strongly interpenetrated by linear chains. The mean field model is compared with coarse grained computer simulations applying the bond fluctuation model. This work contributes to the understanding of soft matter interactions and provides predictions for the occurrence of depletion interactions in experimental setups.

[1] Wengenmayr, Dockhorn, Sommer; *Macromolecules* **2019**, 52, 2616-2626

CPP 58.8 Wed 11:45 ZEU 255

Role of preferential adsorption in cononsolvency — •Swaminath Bharadwaj and Nico van der Vegt — Technische Universität Darmstadt, Germany

Cononsolvency is the phenomenon in which a polymer chain collapses in a mixture of good solvents. The solvation forces and interactions that drive this phenomenon however remain poorly understood. An important question which arises is whether the cononsolvency mechanism is generic. In this regard, studies have proposed simple and universal mechanisms depending on preferential cosolvent adsorption [1] and solvent-cosolvent clustering [2].

We demonstrate through computer simulations that cononsolvency is not a generic phenomenon driven by a universal interaction. We show that cononsolvency can occur with and without the preferential adsorption of the cosolvent and discuss the related experimental results [3]. We also discuss preliminary results on the role of attractive polymer-solvent/cosolvent interactions in cononsolvency. Our results highlight the need to understand the role of microscopic interactions in polymer solubility. The aforementioned generic models [1,2], though not universal, can still be employed on a case-by-case basis depending on the dominant underlying interactions.

[1]Mukherji, D., Marques, C. M. & Kremer, K. Nat. Commun. 5,4882 (2014).

[2]Zhang, G. & Wu, C. J. Am. Chem. Soc. 123, 1376 (2001)

[3]Bharadwaj, S. & van der Vegt, N. F. A. Macromolecules 52, 4131 (2019)

CPP 58.9 Wed 12:00 ZEU 255

Mesoscopic modeling of disordered morphologies of blends and block-copolymers for light-emitting diodes — •Jianrui Zhang, Kurt Kremer, Jasper Michels, and Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz, Germany

Experiments have demonstrated [1] that the luminous efficiency of polymer light emitting diodes can be significantly increased by blending the semiconducting polymer with an insulator. However, the limited thermodynamic stability of the disordered phase in polymer blends motivates the consideration of alternatives, e.g. block-copolymers (BCPs) comprising semiconducting and insulating blocks. We choose as model systems blends and BCPs of poly(p-phenylene vinylene) (PPV) and polyacrylates. Using a hybrid mesoscopic model, disordered morphologies of these blends and BCPs are obtained with Monte Carlo simulations. We study different compositions and vary the immiscibility to mimick annealing at different temperatures. We find that disordered blends and BCPs are heterogeneous because of fluctuations and local segregation. Local segregation is stronger in BCPs than in their equivalent blends, even though the strength of immiscibility, normalized by the mean-field spinodal, is the same. Using a qualitative charge-percolation model, we link the spatial distribution of PPV with electric conductance. We predict that the annealing temperature affects the electrical percolation in disordered BCPs much stronger than in blends. The observed differences between blends and BCPs are enhanced at high contents of insulator. [1] Abbaszadeh et al., Nature Materials 2016, 15, 628.

CPP 58.10 Wed 12:15 ZEU 255

Chemically-transferable structure-based coarse-grained models — •Kiran H. Kanekal and Tristan Bereau — Max Planck Institute for Polymer Physics, Mainz, Germany

An attractive feature of the popular Martini [1] coarse-grained force field is its chemical transferability. Multiple chemical fragments can be assigned to the same Martini representation based on their similar hydrophobicity, maintaining thermodynamic accuracy in the resulting simulations [2]. However, since the Martini force field was optimized in order to reproduce certain thermodynamic properties of various condensed phase systems in a top-down fashion, it does not accurately portray the internal structures of these systems when compared to results from corresponding simulations at atomistic resolutions. On the other hand, implementing bottom-up coarse-graining approaches results in highly accurate structural properties by construction, yet these methods are traditionally performed on a small set of compounds, limiting their chemical transferability. In this work, we establish a new technique for building chemically-transferable coarse-grained models with high structural accuracy by coupling bottom-up coarse-graining methods with unsupervised machine learning. We validate our results by comparing our new model to Martini and show how changing the resolution of our coarse-grained model affects these results. 1. Marrink, S. J. & Tieleman, D. P. Chem. Soc. Rev. 42, (2013). 2. Menichetti, R., Kanekal, K. H. & Bereau, T. ACS Cent. Sci. 5, (2019).

CPP 58.11 Wed 12:30 ZEU 255

Consistent representation of structural and dynamical properties from coarse-grained simulation models — •Joseph Rudzinski — Max Planck Institute for Polymer Research, Mainz, Germany

“Bottom-up” coarse-grained models retain chemical specificity by targeting the reproduction of properties from a higher-resolution reference model. These models are inherently limited by the molecular representation, set of interaction potentials, and parametrization method. These limitations often result in an inaccurate description of cross-correlations between coarse-grained degrees of freedom, complicating the stabilization of hierarchical structures in soft matter systems. Perhaps more troubling, reduced molecular friction and softer interaction potentials obscure the connection to the true dynamical properties of the system. In this talk, I will discuss the relationship between these two problems and introduce methodologies for characterizing and improving the dynamical properties generated by coarse-grained simulation models.

CPP 58.12 Wed 12:45 ZEU 255

Coarse graining of Bovine serum albumin (BSA) — •Frank Hirschmann[1], Hender López[2], and Martin Oettel[1] — [1]University of Tübingen — [2]Dublin Institute of Technology

The intercellular medium of living cells typically contains biomolecules (such as proteins) at high packing fractions, which directly affects diffusive and transport properties of the suspended components. Additionally, molecular shape plays a key role for interactions in crowded environments.

To treat these systems computationally, we present a coarse grained model of the globular antibody BSA, which neglects full atomistic details, but enables access to larger system sizes of hundreds to thousands of molecules. Using Brownian dynamics, we present static and dynamic properties of different implementations of our model. A particular emphasis is on the influence of molecule flexibility on diffusion coefficients. A comparison is made with an already existing coarse grained model of γ-Globulin (IgG), which is a significantly more flexible molecule.

CPP 59: Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Wednesday 9:30–12:30 Location: ZEU 114

CPP 59.1 Wed 9:30 ZEU 114

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 59.2 Wed 9:45 ZEU 114

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 59.3 Wed 10:00 ZEU 114

Construction of 1D hollow cube chains as a platform for synthesis of nanoscopic magnetic filaments. — •Deniz Mostarac[1], Yan Xiong[3], Pedro A. Sanchez[2], Oleg Gang[3,4], and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]Columbia University, New York, USA — [4]Brookhaven National Laboratories, New York, USA

Construction of smart materials with sophisticated magnetic response by incorporating magnetic nanoparticles (MNPs) within permanently cross-linked structures, opens up the possibility for synthesis of complex, highly magneto-responsive systems. Assembly using DNA origami frames where the structure building instructions are encoded via DNA sequencing, provides a new perspective on construction of filaments with MNPs. Using programable DNA origami assembly, one can create scaffolds that serve as a blueprints for chain-like conformations of MNPs. Challenge is to produce a DNA based backbone that can be populated with MNPs, which when not subjected to an external magnetic field would in its polymeric properties resemble a real polymer. We present synthesis approach and results of 1D hollow cube chain scaffolds, together with preliminary results of AFM, TEM and SAXS measurements. We present computational models with both explicit and implicit DNA linker modeling, demonstrating the utility of such systems and exploring the influence of the number of DNA linkers between the hollow cubes, and their length, on the polymeric properties of the chained assemblies.

CPP 59.4 Wed 10:15 ZEU 114

Dynamic Self-assembly of Magnetic Janus Particles — •Sofia Kantorovich[1,2], Pedro Sanchez[1,2], Maximilian Neumann[3], Sibylle Gemming[3,4], and Artur Erbe[3] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]Helmholtz-Zentrum Dresden-Rossendorf, Rosendorf, Germany — [4]Technische Universität Chemnitz, Chemnitz, Germany

In this contribution we explain how the interplay between hydrodynamics, magnetic interactions and the frequency of an applied magnetic field affect the structure and the size of clusters formed by magnetic Janus particles. We study silica particles (radius of 2.27μm) with a magnetic thin film coating (of a multilayer stack of Ta(3.0 nm)/Pd(3.0 nm)/[Co(0.28 nm)/Pd(0.9 nm)]8/Pd (1.1 nm)) on one hemisphere. Such a layer exhibits perpendicular magnetic anisotropy, i.e., the magnetic flux points out of the film plane [1]. Our previous combined experimental-simulation study showed that if the monolayer of such Janus particles is exposed to a low-frequency magnetic field, one can efficiently control self-assembly letting branched clusters of staggered chains, compact clusters, linear chains, and dispersed single particles to form and reconvert reversibly [2]. In the present contribution, we extend our investigation to high frequency out-of-equilibrium transformations.

[1] M. Albrecht et al., Nat. Mater. 4, 203 (2005). [2] Steinbach et al., PRE 100, 012608 (2019).

CPP 59.5 Wed 10:30 ZEU 114

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 59.6 Wed 10:45 ZEU 114

A biaxial nematic liquid crystal composed of matchbox-symmetric molecules — •Robert A. Skutnik[1], Immanuel S. Geier[1], and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische UniversitätBerlin, Straße des 17. Juni 115, 10623 Berlin, Germany — [2]Department of ChemicalEngineering, Imperial College London, South Kensington Campus, London SW7 2AZ,United Kingdom

By means of Monte Carlo simulations in the isothermal-isobaric ensemble we investigate the structure and phase behaviour of a thermotropic liquid crystal composed of matchbox-symmetric (or boardlike) molecules. Besides the isotropic phase the liquid crystal exhibits also uniaxial and biaxial nematic phases. We analyse the orientation distribution function which allows us to distinguish between intrinsic and extrinsic biaxiality. In addition, we study the orientation-dependent correlation functions. In the limit of large intermolecular separations the value of the orientation correlation function corresponds to the uniaxial and biaxial order parameters which are coupled in a complex fashion.

CPP 59.7 Wed 11:00 ZEU 114

Lyotropic liquid crystals in microfluidic environments — •Anshul Sharma and Anupam Sengupta — Physics of Living Matter Group, University of Luxembourg, Luxembourg City, Luxembourg

Recent progress in liquid crystal microfluidics has demonstrated how hydrodynamics, in combination with confinement and surface anchoring, can be harnessed to generate tunable flow and topological structures [1, 2]. Lyotropic liquid crystals (LLCs), solutions of disc-shaped amphiphilic mesogens with aromatic core, form linear stacks that aggregate to show nematic or columnar LC phases as a function of temperature or mesogen concentration. LLCs have long been studied for their role in drug and dye manufacturing, and more recently in rapid detection of pathogens. Yet, we lack a fundamental understanding of the response of LLC to micro-scale flows a universal parameter in medical, cellular and industrial settings. With aqueous solution of disodium cromoglycate as our model LLC, we study its behavior under different concentrations and micro-scale flow regimes. Static and flow-induced textures characterized using polarizing microscopy, conoscopy and particle tracking techniques, show emergence of distinctly oriented micro-domains in the flowing LLC. Our results indicate that, for a given surface anchoring, the domain size and lifetime vary with channel geometry and flow speed. Such spontaneous orientational domains could be harnessed to generate locally distinct transport properties within a globally advected material. [1] Sengupta et al., Liquid Crystals Reviews 2, 2014. [2] Giomi et al., PNAS 114, 2017. [3] Sharma et al. (in prep.)

15 min. break

CPP 59.8 Wed 11:30 ZEU 114

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., 6 (2016) 36443

CPP 59.9 Wed 11:45 ZEU 114

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 59.10 Wed 12:00 ZEU 114

Polymer Micelles with Crystalline Cores: self-assembly, molecular exchange kinetics and confinement effects — Nico König[1], Lutz Willner[2], and •Reidar Lund[1] — [1]Department of Chemistry, University of Oslo, Norway — [2]Institute for Complex Systems ICS, Forschungszentrum Jülich, Germany

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 . By using small-angle X-ray scattering (SAXS), densiometry and differential scanning calorimetry (DSC), we show that the n-alkane exhibit a first-order phase transition, but with reduced melting points compared to bulk. Correlating the structural and thermodynamic data, we found that the melting depression can be accurately described by the Gibbs-Thomson equation. The effect of core crystallinity on the molecular exchange kinetics is investigated using time-resolved small-angle neutron scattering (TR-SANS). We show that the melting transition is cooperative in the confined micellar core, whereas the exchange process is widely decoupled and unimeric in nature. Upon crossing the melting point, a discrete change in the activation energy is found. This suggests that a "local, single-chain melting process" preludes the molecular diffusion out of the micelle during chain exchange

CPP 59.11 Wed 12:15 ZEU 114

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 60: Focus: Fundamentals of molecular liquids, ionic liquids and mixtures I

Polyelectrolyte solutions and room temperature ionic liquids display remarkable physico-chemical properties that make them ideal candidates in view of renewable energy applications. The interplay of different intermolecular interactions provides an exceptional flexibility to fine-tune structural and thermodynamic properties of these systems. This also brings new challenges to current experimental and computational methods. The aim of this session is to invite scientists from both theoretical and experimental communities with the goal to discuss the fundamental concepts of charge solvation in complex fluids, which can be used for operational understanding and functional design. The session will emphasize ionic systems that are particularly interesting for environmentally friendly energy applications. Organized by: Debashish Mukherji (University of British Columbia, Canada), Robinson Cortes-Huerto (Max-Planck-Institut für Polymerforschung, Mainz) and Jörg Rottler (University of British Columbia, Canada).

Time: Wednesday 11:30–13:00 Location: ZEU 222

CPP 60.1 Wed 11:30 ZEU 222

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 $d/\lambda_{\mathrm{D}} \simeq 1$, 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 60.2 Wed 11:45 ZEU 222

Screening lengths in ionic fluids — Fabian Coupette[1], Alpha A. Lee[2], and •Andreas Härtel[1] — [1]Institut of Physics, University of Freiburg, Germany — [2]Cavendish Laboratory, Cambridge, United Kingdom

The decay of correlations in ionic fluids is a classical problem in soft matter physics that underpins applications ranging from controlling colloidal self-assembly to batteries and supercapacitors. The conventional wisdom, based on analyzing a solvent-free electrolyte model, suggests that all correlation functions between species decay with a common decay length in the asymptotic far field limit. Nonetheless, a solvent is present in many electrolyte systems. We show using an analytical theory and molecular dynamics simulations that multiple decay lengths can coexist in the asymptotic limit as well as at intermediate distances once a hard sphere solvent is considered. Our analysis provides an explanation for the recently observed discontinuous change in the structural force across a thin film of ionic liquid-solvent mixtures as the composition is varied, as well as reframes recent debates in the literature about the screening length in concentrated electrolytes.

Invited Talk CPP 60.3 Wed 12:00 ZEU 222

Operando Analysis of the Lithium/Sulfur Battery by Small-Angle Neutron and X-Ray Scattering — •Matthias Ballauff[1], Sebastian Risse[2], Eneli Härk[2], Günter Goerigk[2], Chanbum Park[2] und Joachim Dzubiella[3] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustrasse 3, 14195 Berlin, Germany — [2]Helmholtz-Zentrum Berlin fuer Materialien und Energie, Hahn Meitner Platz 1,14109 Berlin, Germany — [3]Applied Theoretical Physics and Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universitaet Freiburg, Hermann-Herder Strasse 3, D-79104 Freiburg, Germany

The lithium-sulfur battery is among the most promising candidates for future battery systems. Sulfur is an earth-abundant element and there are first applications of Li/S-batteries in aviation. In our presentation, we shall present our recent work on Li/S batteries in two parts: Part I is related to our recent studies of the carbonaceous materials used as cathodes in these systems. Here we improved the analysis by small-angle x-ray scattering in order to obtain reliable data on the internal surface and the average pore size. In a second part we shall discuss our operando-studies of the Li/S system by small-angle neutron scattering (SANS). SANS allows us to use contrast matching in order to see the precipitation and the dissolution of sulfur and lithium sulfide during the electrochemical cycling of the battery. The operando studies are combined with MD-simulations addressing the solvation of the soluble sulfur species during cycling of the Li/S-cell.

CPP 60.4 Wed 12:30 ZEU 222

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 60.5 Wed 12:45 ZEU 222

Emergence of molecular friction in liquids: bridging between the atomistic and hydrodynamic pictures — Arthur V. Straube[1,2], Bartosz G. Kowalik[3], Roland R. Netz[3], and •Felix Höfling[1,2] — [1]Department of Mathematics and Computer Science, Freie Universität Berlin — [2]Zuse Institute Berlin — [3]Department of Physics, Freie Universität Berlin

Friction in liquids arises from conservative forces between molecules and atoms. Although the hydrodynamics at the nanoscale is subject of intense research and despite the enormous interest in the non-Markovian dynamics of single molecules and solutes, the emergence of friction from the atomistic scale so far could not be demonstrated. Here, we fill this gap based on frequency-resolved friction data from high-precision simulations of three prototypical liquids, including water. Combining with rigorous theoretical arguments, we show that friction in liquids is non-local in time and emerges abruptly at a characteristic frequency, beyond which viscous liquids appear as non-dissipative, elastic solids [1]. At the same time, the molecules experience Brownian forces that display persistent correlations and long-lasting memory. A critical test of the generalised Stokes–Einstein relation, mapping the friction of single molecules to the viscoelastic response of the macroscopic sample, disproves the relation for Newtonian fluids, but substantiates it exemplarily for a supercooled liquid. The employed approach is suitable to yield novel insights into vitrification mechanisms and the intriguing mechanical properties of soft materials.

[1] Straube, Kowalik, Netz, and Höfling (submitted).

CPP 61: Perovskite and photovoltaics III (joint session HL/CPP)

Time: Wednesday 9:30–12:30 Location: POT 251

CPP 61.1 Wed 9:30 POT 251

Efficiency dependence on incident angle for CIGS solar cells — •Lilén Vöhringer[1], Janet Neerken[1], Hippolyte Hirwa[1], Jörg Ohland[1], Alfons Weber[2], Robert Lechner[2], Thomas Dalibor[2], Sascha Schäfer[1], and Stephan Heise[1] — [1]Ultrafast Nanoscale Dynamics, Institute of Physics, University of Oldenburg, D-26111 Oldenburg, Germany — [2]Avancis GmbH, Otto-Hahn-Ring 6, D-81739 München, Germany

Facing climate change, renewable energies are becoming more and more relevant. Hence, understanding their mechanisms in detail is important to improve their use. In photovoltaics, solar cells are used to convert solar energy into electrical energy. In general, the efficiency of a solar cell is measured and compared under standard test conditions, which may vary vastly from real conditions. Hence, it is important to investigate the dependence of the efficiency on different parameters, in order to find the best solar cell for each case of non-standard conditions. One of these parameters is the incident angle of light, which varies according to the suns position, but also depends on the orientation of the solar cell. Its influence on the efficiency is being tested in this study for Cu(In,Ga)(S,Se)$_2$ (CIGS) solar cells using IV-measurements. CIGS solar cells are thin-film solar cells which can reach efficiencies up to 23%. In particular, the role of the front glass for the angular-dependent efficiency is studied by investigating different front glass variations. The measurements show that the efficiency dependence on the incident angle cannot be explained by the reduced photon flux only.

CPP 61.2 Wed 9:45 POT 251

Reaching Efficiency Limts for Blue CsPbBr$_3$ based Light Emitting Diodes — •Tassilo Naujoks[1], Thomas Morgenstern[1], Carola Lampe[2], Alexander Urban[2], Matthew Jurow[3], Yi Liu[3], and Wolfgang Brütting[1] — [1]University of Augsburg, 86135 Augsburg, Germany — [2]Ludwig-Maximilians-Universität München, 80539 Munich, Germany — [3]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States of America

The unique optical properties of lead halide perovskites have drawn significant attention towards their application in light emitting devices. While quantum yield, emission wavelength and stability are already in the focus of many research groups, the orientation of the emissive transition dipoles is rarely investigated.

In this work, we investigate CsPbBr$_3$ nanoplatelets of variable thickness and determine the orientation of their transition dipole moments from thin film radiation patterns.

We use a thickness variation for nanoplatelets reaching from 2 to 6 monolayers to systematically study the tunability of the TDM orientation and the concomitant color shift, while the emission peak stays as narrow as it is for the green emitting nanocubes. Together with high photoluminescent quantum yields the efficiency limit of lead-halide perovskite based light emitting diodes can be re-estimated.

The present data reveal very promising new efficiency limits, for solution-processed light emitting diodes: A solution-processed, highly efficient blue emitter with strong horizontal orientation can be made of CsPbBr$_3$ nanoplatelets.

CPP 61.3 Wed 10:00 POT 251

Frenkel-Holstein Hamiltonian Applied to Quaterthiophene-based 2D Hybrid Organic-Inorganic Perovskites — •Svenja M. Janke[1], Mohammad B. Qarai[2], Volker Blum[1], and Frank C. Spano[2] — [1]Duke University, Durham, NC, USA — [2]Temple University, Philadelphia, PA, USA

In two-dimensional hybrid organic-inorganic perovskites (HOIPs), both the organic and inorganic components can contribute to the electronic properties at the electronic frontier levels and hence open up a wide area for design of new materials with high tunability. For development of new devices like solar cells or light emitting diodes, the understanding of electronic excitations and their photophysical signatures play a fundamental roll. Here, we show at the example of quaterthiophene-based lead-halide HOIPs that the organic contribution to 2D HOIP absorption and emission spectra can be theoretically investigated employing a Frenkel-Holstein Hamiltonian that treats electronic coupling and electron-phonon coupling on equal footing. We relate changes in the spectra to structural changes in the organic layer that in turn are caused by variation of the halide anion. Furthermore, we take first steps towards including the contribution of the Wannier exciton on the inorganic component into the framework of the Frenkel-Holstein Hamiltonian. Supported by the German Science Foundation (DFG), grant number 393196393.

CPP 61.4 Wed 10:15 POT 251

Environmental Stability of High Efficiency PbS Quantum Dot Solar Cells — •David Becker-Koch[1,2], Miguel Albaladejo-Siguan[1,2], Vincent Lami[3], Fabian Paulus[2], Hengyang Xiang[4], Zhuoying Chen[4], and Yana Vaynzof[1,2] — [1]IAPP, TU Dresden, Germany — [2]cfaed, TU Dresden, Germany — [3]KIP, Uni Heidelberg, Germany — [4]ESPCI, CNRS, Université Pierre et Marie Curie, Paris, France

Colloidal inorganic quantum dot (CQD) solar cells (SCs) are an emerging class of photovoltaics, which can be processed from solution at low temperature and their optoelectronic properties can easily be tuned by changing their size, shape and surface passivation. While power conversion efficiencies of ~12% have been demonstrated by employing lead sulphide (PbS) CQDs, their stability remains an unresolved issue preventing them from being integrated into industrial applications. In this work we focus on the influence of different atmospheres on the performance of high efficiency PbS CQDs SCs. We find that while N2 and humidity lead to a quick decline in performance, oxidation dominates the initial improvement and the subsequent deterioration of the device function. By applying a range of spectroscopic methods, we identify the pivotal layer for these processes and furthermore, we propose a model for the performance evolution. We conclude that the stability and performance can be improved by exchanging the extraction layer (EL) ubiquitously used in these devices. Finally, we present several promising organic, semiconducting replacement ELs and show preliminary results of their application as ELs in PbS CQDs solar cells.

CPP 61.5 Wed 10:30 POT 251

How does strain impact the solar cell performance at grain boundaries? — •Michael Stuckelberger[1], Irene Calvo-Almazán[2], Martin Holt[2], Megan Hill[3], Siddharth Maddali[2], Mariana Bertoni[4], Xiaojing Huang[5], Hanfei Yan[5], Evgeny Nazaretski[5], Yong Chu[5], Andrew Ulvestad[2], and Stephan Hruszkewycz[2] — [1]DESY, Hamburg, Germany — [2]ANL, Lemont IL, USA — [3]Northwestern University, Evanston IL, USA — [4]ASU, Tempe AZ, USA — [5]BNL, Upton NY, USA

Grain boundaries (GB) often limit the conversion efficiency of polycrystalline solar cells. Strain is particularly detrimental there, as it enhances the defect concentration and band fluctuations, leading to increased recombination rates. Unfortunately, standard methods cannot easily measure the strain distribution in working thin-film devices.

Based on nanodiffraction experiments, we demonstrate the assessment of the strain distribution at sub-100-nm resolution. In a multimodal detector design, we combined nanodiffraction with X-ray fluorescence (XRF) and X-ray beam induced current (XBIC) measurements. Mapping individual grains, this enabled us to correlate point-by-point the strain with composition and performance within grains and at GB.

In CIGS solar cells, we found that the strain increases towards GB, which is accompanied by an increase of the charge collection efficiency. In contrast, we found a decreasing lattice constant towards GB in CdTe solar cells. Similar correlative experiments are ongoing on perovskite solar cells, and we will present the latest results.

30 min. break

CPP 61.6 Wed 11:15 POT 251

Tuning Perovskite Halide Content to Engineer Environmental Stability — •Katelyn P. Goetz[1,2], Fabian Thome[1,2], Paul Fassl[1,2], Lukas M. Falk[1,2], Vincent Lami[1,2], Alexander D. Taylor[1,2], Qingzhi An[1,2], Fabian Paulus[1,2], and Yana Vaynzof[1,2] — [1]IAPP, Technical University of Dresden, Germany — [2]CFAED, Technical University of Dresden, Germany

The presence of surface defects in perovskite films has been linked to their stability; however, many questions remain regarding details of the degradation process. Here, we incrementally tune the iodine or bromide content in MAPbI3 or MAPbBr3 thin-films and examine the impact on optoelectronic properties. X-ray photoelectron spectroscopy is used to identify the density and type of surface defect. We examine the interaction of the defect with the environment by exposing the films to controlled levels of oxygen and humidity under light, and monitor changes to the films via photoluminescence (PL) spectroscopy. Here, we observe that, while halide-rich films exhibit lower PL quantum efficiency (PLQE) than halide-poor films, exposure to low levels of oxygen enhances the luminescence of all films. In solar cells, iodine-poor MAPbI3 samples show a tremendous drop in the short-circuit current after exposure to oxygen, while those with excess show no change. The MAPbBr3 solar cells show little dependence of the initial photovoltaic performance on the halide content, but upon exposure to air and light, bromide-deficient solar cells undergo a large Jsc boost, resulting in a near tripling of their initial PCE. These results highlight the strong role that chemical composition plays in stability.

CPP 61.7 Wed 11:30 POT 251

Enabling Versatile High-Efficiency Perovskite Photovoltaics by Charge-Selective Contact Design — •Amran Al-Ashouri[1], Artiom Magomedov[2], Marcel Ross[1], Marko Jošt[1], Martynas Talaikis[3], Ganna Christiakova[1], José M. Prieto[1], Eike Köhnen[1], Ernestas Kasparavičius[2], Bernd Rech[1], Tadas Malinauskas[2], Thomas Unold[1], Lars Korte[1], Gediminas Niaura[3], Vytautas Getautis[2], and Steve Albrecht[1] — [1]HZB, Berlin, Germany — [2]KTU, Kaunas, Lithuania — [3]FTMC, Vilnius, Lithuania

By establishing a simple, low-cost and robust perovskite solar cell device structure that employs self-assembled monolayers (SAMs) [1], we realized power conversion efficiencies of over 21 % for single junction cells, over 23 % for CIGSe/perovskite and well over 27 % for silicon/perovskite tandem solar cells. Using time-resolved and absolute photoluminescence spectroscopy together with an analysis of the energetic alignment between hole-selective contact and absorber, we identify design guidelines for an hole-selective interface without non-radiative recombination losses. A SAM model system further allows to study voltage and fill factor losses for an increased understanding of how to experimentally explore pathways towards theoretical efficiency limits.

[1] Al-Ashouri et al. *Energy Environ. Sci.* 2019, **12**, 3356

CPP 61.8 Wed 11:45 POT 251

Anharmonicity, short-range correlated disorder, and small Urbach energies in halide perovskites — •Christian Gehrmann and David A. Egger — Department of Physics, Technical University Munich, 85748 Garching, Germany.

Halide perovskites (HaPs) are known to show complex nuclear dynamics and structural effects. But seemingly in contrast to this effects, a low amount of disorder is implied by measurements of small Urbach energies and sharp optical absorption edges. Using density functional theory (DFT) and DFT-based molecular dynamics, we calculated spatial correlations in the disorder potential induced for electronic states due to nuclear dynamics in representative HaPs [1]. We find sizeable anharmonicity in the nuclear vibrations and a dynamic shortening of correlations in the disorder potential: the motion of especially A-site and X-site ions are found to have an important impact on the length of spatial correlations in the disorder potential, such that they become as short as atomic bonds in the material. We explicitly establish that these short-range correlated disorder potentials lead to narrow band-energy distributions, which imply small Urbach energies. We conclude that effective collection of sunlight in HaP based photovoltaic devices, as indicated by small Urbach energies and sharp optical absorption edges, is facilitated by this mechanism.

[1] C. Gehrmann & D. A. Egger, Nat. Commun. 10, 3141 (2019).

CPP 61.9 Wed 12:00 POT 251

Combined Multi-Photon-Excitation and Multi-Exciton-Generation Processes in $CsPbBr_3$ Supercrystals — •Anja Barfüsser[1], Alexander F. Richter[1], Aurora Manzi[1], Shixun Wang[2], He Huang[1], Andrey L. Rogach[2], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany — [2]Department of Materials Science and Engineering and Centre for Functional Photonics (CFP), City University of Hong Kong, Kowloon, Hong Kong

A fundamental problem limiting the power conversion efficiency of solar cells are photons with energies below the band gap, as they cannot be absorbed by linear processes, and above the band gap, as the excess energy typically is lost as heat. Multi-photon-excitation (MPE) and multi-exciton-generation (MEG) target this issue. Up to now, these processes have only been observed independently. Here, their combined effect is demonstrated for bulk-like $CsPbBr_3$ perovskite nanocubes forming a superlattice. For below-band-gap excitation energies (0.5-0.8 E_g) nonlinear absorption is observed. Interestingly, when the energy of multiple below-band-gap photons resonantly matches the energy of multiple excitons, a strong photoluminescence enhancement of up to 10^5 takes place. Excitation power dependent measurements reveal a high-order absorption process deviating from the typical two-photon absorption.

CPP 61.10 Wed 12:15 POT 251

The Versatility of Polyelemental Perovskite Compositions — •Michael Saliba — TU Darmstadt

Perovskites have emerged as low-cost, high efficiency photovoltaics with certified efficiencies of 22.1% approaching already established technologies. The perovskites used for solar cells have an ABX3 structure where the cation A is methylammonium (MA), formamidinium (FA), or cesium (Cs); the metal B is Pb or Sn; and the halide X is Cl, Br or I. Unfortunately, single-cation perovskites often suffer from phase, temperature or humidity instabilities. This is particularly noteworthy for CsPbX3 and FAPbX3 which are stable at room temperature as a photoinactive *yellow phase* instead of the more desired photoactive *black phase* that is only stable at higher temperatures. Moreover, apart from phase stability, operating perovskite solar cells (PSCs) at elevated temperatures (of 85 °C) is required for passing industrial norms.

CPP 62: Single Molecule Biophysics (joint session BP/CPP)

Time: Wednesday 9:30–13:00 Location: SCH A251

CPP 62.1 Wed 9:30 SCH A251

Magnetic tweezers reveal the mechanism of directional transcription termination in human mitochondria — Eugen Ostrofet[1], Flavia Stal Papini[1], Britney Johnson[2], Jamie Arnold[2], Craig Cameron[2], and •David Dulin[1] — [1]Junior Research Group 2, IZKF, FAU Erlangen-Nürnberg, Germany — [2]Department of Microbiology and Immunology, The University of North Carolina Chapel Hill, USA

Transcription termination is essential to synthesize functional RNA and to prevent transcription interference with downstream promoters. Therefor, it must be performed efficiently despite the stability of the elongating RNA polymerase (RNAP) on DNA. One approach adopted by eukaryotic cells is directional transcription termination upon collision of RNAP with a termination factor bound to DNA, as for human mitochondria RNAP (mtRNAP) and Pol I. How the termination factor senses the direction of transcribing RNAP remains to be found. We propose that the termination factor senses DNA unwinding, and consequently terminates transcription directionally. To interrogate this hypothesis, we employed a high throughput magnetic tweezers instrument and a hairpin-based force jump assay to mimic DNA unwinding and look into the human mitochondria transcription termination factor 1 (MTERF1). We found that MTERF1 blocks directionally hairpin opening, explaining directional transcription termination. Performing in situ force calibration, we determined accurately the energy landscape of MTERF1 bound to its termination site.

CPP 62.2 Wed 9:45 SCH A251

Magnetic Tweezers Protein Force Spectroscopy — •Jan Lipfert[1], Achim Löf[1], Philipp Walker[1], Steffen Sedlak[1], Sophia Gruber[1], Tobias Obser[2], Maria Brehm[2], and Martin Benoit[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 regulated by mechanical forces acting on them. Single-molecule manipulation techniques such as atomic force microscopy or optical tweezers have enabled unprecedented insights into the molecular mechanisms underlying such force regulation. However, these techniques have limited throughput and lack resolution at low forces. We have developed a versatile and modular approach for force measurements on proteins in magnetic tweezers [Löf et al. PNAS 2019] that enables ultra-stable (> days) and parallel measurements (> 50) of single molecules in a wide force range including very low forces (<1 pN). Leveraging our new assay, we directly probe regulatory low-force transitions within von Willebrand factor, a vascular protein that is activated for its critical role in hemostasis by hydrodynamic forces in the bloodstream. Or results reveal fast (~250 ms) opening and closing transitions in the dimeric VWF stem at a critical force of 1 pN, which like constitute the first steps in VWF mechano-activation.

CPP 62.3 Wed 10:00 SCH A251

Real-time imaging of DNA loop extrusion by condensin and their mutual interactions — •Eugene Kim[1], Jacob Kerssemakers[1], Indra Shaltiel[2], Christian Haering[2], and Cees Dekker[1] — [1]Department of Bionanoscience, Kavli Institute of Nanoscience Delft, Delft University of Technology, Delft, Netherlands. — [2]Cell Biology and Biophysics Unit, Structural and Computational Biology Unit, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany.

How is DNA spatially organized in our cells? By what mechanisms do chromosomes fold over long distances? In this talk, I will discuss our work on understanding the looping structures of DNA using fluorescence imaging assay at the single-molecule level. The major focus is on condensin, that is one of the SMC (Structural Maintenance of Chromosomes) complexes. This ring-shaped protein is the molecular motor that can extrude large loops of DNA, a mechanism thought to be the basis of the chromosome structures at various stages of the cell cycle. I will firstly show how a single condensin can extrude loops at a force-dependent speed of up to 2 kbp/s and it does so in a strictly asymmetric manner. I will then show how these individual condensins can form a dimeric structure by traversing one over the other, in turn forming a novel type of loop structure that we name as Z loop. This condensin dimer can extrude DNA in a symmetric fashion, thus may be able to contribute to chromosomal compaction in a more efficient way. We believe that our work will allow to disentangle the fundamental looping architecture of chromosomes, that is essential to all life.

CPP 62.4 Wed 10:15 SCH A251

Magnetic tweezers reveal two coexisting and interconverting bacterial RNA polymerase conformations with different open complex stability — •Subhas Chandra Bera[1], Mona Seifert[1], Santeri Maatsola[2], Eugen Ostrofet[1], Monika Spermann[1], Flavia Stal-Papini[1], Anssi M. Malinen[2], and David Dulin[1] — [1]Junior Research Group 2, Interdisciplinary Center for Clinical Research, Friedrich Alexander University Erlangen-Nürnberg (FAU), Cauerstr. 3, 91058 Erlangen, Germany — [2]Department of Biochemistry, University of Turku, Tykistökatu 6A, 6th floor, 20520 Turku, Finland

To start transcription, the RNA polymerase (RNAP) recognises the promoter, to form the closed complex (CC), and eventually unwinds the DNA to form the open complex (OC), and is then ready for RNA synthesis. OC stability decides the yield of expression in many genes, and is therefore of great importance to regulate expression of a given gene. Using high throughput magnetic tweezers, we investigated OC dynamics. Surprisingly, we observed two OC populations with nearly 10-fold difference in lifetime, where the stability of the OC varies as a function of the nature and the concentration of the anions, as well as the temperature. We further noticed that the RNAP completely dissociates upon return to CC and therefore the two OC populations do not originate from a single interconverting RNAP, but rather from two conformations of RNAP. Our study shows the power of single molecule techniques to resolve two interconverting populations of RNAP that have remained elusive to bulk assays so far.

CPP 62.5 Wed 10:30 SCH A251

Towards the Label-free Plasmonic Detection of Single Untethered Proteins — •Martin D. Baaske, Peter S. Neu, Nasrin Asgari, and Michel Orrit — Huygens-Kamerlingh Onnes Laboratory, Leiden University, Postbus 9504, 2300 RA Leiden, The Netherlands

Label-free optical detection schemes so far rely on specific chemical interactions between receptor and target molecules in order to facilitate analyte recognition. Here we present our first step towards the label-free recognition of untethered nanoscale analytes. We show that via a polarization selective technique and careful optimization of a confocal microscope, single gold nanorods, which are commonly used as labels, can be transformed into high-speed nanoscale sensors. We demonstrate the performance of our system by detecting microemulsion nanodroplets which mimic 250 kDA proteins as they diffuse through the near field of a single gold nanorod on nanosecond timescales.

CPP 62.6 Wed 10:45 SCH A251

How to gain reliable information from short trajectories — •Marie Schwebs[1], Torsten Paul[2], Marius Glogger[1], Philip Kollmannsberger[2], Markus Engstler[1], and Susanne Fenz[1] — [1]Department for Cell and Developmental Biology, Biocenter, University of Würzburg, Germany — [2]Center for Computational and Theoretical Biology, University of Würzburg, Germany

Trypanosoma brucei expresses a dense coat of GPI-anchored variant surface glycoproteins (VSGs). The fluidity of this coat is fundamental for the evasion of the host‘s immune system and thus for the survival of the parasite. So far, the VSG dynamics on living trypanosomes has been studied at the micron and second scale for the whole ensemble. In this project, we want to elucidate the dynamics of individual VSGs in relation to the flagellar pocket, the sole site for endo- and exocytosis, with single-molecule fluorescence microscopy. For this purpose, we have recently introduced super-resolution imaging of intrinsically fast-moving flagellates based on cyto-compatible hydrogel embedding. Building on this work, we are now able to track VSG dynamics on living trypanosomes at high spatial (localization precision ~30 nm) and temporal resolution (f = 100 Hz). The length of gained trajectories is mainly limited by the shape and size of trypanosomes (approx. 18 μm in length and 3 μm in width). Therefore, we use a self-written program based on an approach from Hoze and Holcman [Biophys. J., 2014] to make reliable statements about local forces and the diffusion tensor. The information is gained from a large number of short trajectories and will be presented in directed motion and diffusion maps.

30 min. coffee break

Invited Talk CPP 62.7 Wed 11:30 SCH A251

The mechanical stability of proteins regulates their translocation rate into the cell nucleus — •Sergi Garcia-Manyes — Department of Physics, Randall Centre for Cell and Molecular Biophysics King's College London

The translocation of mechanosensitive transcription factors (TFs) across the nuclear envelope is a crucial step in cellular mechanotransduction. Yet the molecular mechanisms by which mechanical cues control the nuclear shuttling dynamics of TFs through the nuclear pore complex (NPC) to activate gene expression are poorly understood. Here, we show that the nuclear import rate of myocardin-related transcription factor A (MRTFA) * a protein that regulates cytoskeletal dynamics via the activation of the TF serum response factor (SRF) * inversely correlates with the protein*s nanomechanical stability and does not relate to its thermodynamic stability. Tagging MRTFA with mechanically-stable proteins results in the downregulation of SRF-mediated gene expression and subsequent slowing down of cell migration. We conclude that the mechanical unfolding of proteins regulates their nuclear translocation rate through the NPC and highlight the role of the NPC as a selective mechanosensor able to discriminate forces as low as *10 pN. The modulation of the mechanical stability of TFs may represent a new, general strategy for the control of gene expression.

CPP 62.8 Wed 12:00 SCH A251

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, responsible for the green color of plants. Despite extensive research, the composition of its visible Q absorption band 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. Vis excitation was tuned to various wavelengths scanning 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. Tracing the relative angle Θ for different excitation wavelengths allows to determine the Qx contribution along the Q band region. In this way, Qx is found to contribute 40-60% to absorption of the lower energetic peak at 618 nm and to 75-100% 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. Further, we show that from our recent results the three-dimensional orientation of the Qx and Qy tdms can be resolved under guidance of quantum chemical calculations.

CPP 62.9 Wed 12:15 SCH A251

Power law decays of ligand concentrations in single-molecule kinetic experiments. — •Aykut Erbas[1], Monica Olvera de la Cruz[2], and John F. Marko[2] — [1]Bilkent University- UNAM, Ankara 06800, Turkey — [2]Northwestern University, Evanston 06202, USA

SPR (Surface Plasmon Resonance) or single-molecule kinetic methods rely on the relaxation of initially surface-bound ligands into a confined reservoir to measure the dissociation rates of the corresponding ligands. Similarly, biological processes such as exocytosis (emission of small molecules into the intracellular void for cellular communication) can be considered as a similar relaxation problem. Using molecular dynamics simulations and scaling arguments, we studied a model system closely related to the above cases. In our model, Brownian particles are released from their binding sites into a confined volume. Then, within this volume, we tracked how the concentration of particles throughout the volume changes as a function of time. Our results show that the dissociation process (more specifically rebinding rates of released particles) exhibits various power laws at times longer than the initial exponential decay. Interestingly, the cumulative rebinding number, which is robust against the concentration fluctuations, exhibits a distinct plateau regime as a result of the three-dimensional escape process of the particles from their initial binding sites. Overall our results can be used for new sensor applications to probe molecular kinetics at long tines.

CPP 62.10 Wed 12:30 SCH A251

Narrow escape: How long does it take for a camel to go through the eye of a needle? — •Elisabeth Meiser[1], Reza Mohammadi[2], Nicolas Vogel[2], and Susanne Fenz[1] — [1]University of Würzburg, Biocenter: Cell- and Developmental Biology, Würzburg, Germany — [2]Friedrich-Alexander University Erlangen-Nürnberg, Institute of Particle Technology, Erlangen, Germany

The narrow escape problem is a common problem in biology and biophysics. It deals with Brownian particles confined to a given domain with reflecting borders and only a small escape window where particles are absorbed. The mean first passage time (MFPT), the time it takes a set of particles to escape, can be analytically calculated in 2D and 3D for several geometries. It depends on the area of the domain, the size of the escape window and on the diffusion coefficient of the particle. We aim to systematically test the analytical solution of the NEP in 2D by variation of the relevant parameters. Experiments are being complemented by matching random walk simulations. For the experimental test, we prepared micro-patterned phospholipid bilayers from a combination of colloid lithography and vesicle fusion. We imaged fluorescently labeled lipids diffusing in circular membrane patches with diameters of 1-5 um using single-molecule microscopy at 100 Hz and a localization precision of 14 nm. While the area of the membrane was tuned during colloid lithography, the size of the escape window was adjusted in the course of the analysis. We will present our first results on membrane patterning as well as a comparison of our experimental and simulation results with the theoretical prediction for the MFPT.

CPP 62.11 Wed 12:45 SCH A251

Probing single molecular surface interactions on electroactive surfaces — •Julia Appenroth, Laura Mears, Pierluigi Bilotto, Alexander Imre, and Markus Valtiner — TU Wien, Applied Physics, Vienna, AT

Adhesive interactions between hydrophobic, charged and electroactive moieties steer ubiquitous processes in aqueous media, including the self-organization of biologic matter and adhesive interfaces in general. Recent decades have seen tremendous progress in understanding these interactions for macroscopic adhesive interfaces. Yet, it is still a challenge to experimentally measure interactions at the single-molecule scale and thus to compare with theory, especially on electroactive surfaces. Here, we directly measure and quantify the sequence dependence and additivity of charge-mediated and electroactive interactions at the single-molecule scale. We combined dynamic single-molecule force spectroscopy with MD simulations and show how electroactive surfaces can be probed with single molecules using force probe techniques.

CPP 63: Active Matter IV (joint session DY/CPP/BP)

Time: Wednesday 10:00–12:30 Location: ZEU 160

CPP 63.1 Wed 10:00 ZEU 160

Quantitative Assessment of the Toner and Tu Theory of Polar Flocks — •Benoît Mahault[1,2], Francesco Ginelli[3,4], and Hugues Chaté[1,5,6] — [1]Service de Physique de l'Etat Condensé, CEA, CNRS, Université Paris-Saclay, CEA-Saclay, France — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Germany — [3]University of Aberdeen, United Kingdom — [4]Università degli Studi dell'Insubria, Italy — [5]Beijing Computational Science Research Center, China — [6]LPTMC, CNRS UMR 7600, Université Pierre et Marie Curie, France

We present a quantitative assessment of the Toner and Tu theory describing the universal scaling of space-time correlations functions in polar phases of dry active matter. Using large-scale simulations of the Vicsek model in two and three dimensions, we find the overall phenomenology and generic algebraic scaling predicted by Toner and Tu, but our data on density correlations reveal some qualitative discrepancies. The values of the associated scaling exponents we estimate differ significantly from those conjectured in 1995. In particular, we identify a large crossover scale beyond which flocks are only weakly anisotropic. We discuss the meaning and consequences of these results.

CPP 63.2 Wed 10:15 ZEU 160

Swirl formation of active colloids near criticality — •Robert C. Löffler, Tobias Bäuerle, and Clemens Bechinger — Fachbereich Physik, Universität Konstanz, Konstanz D-78464, Germany

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. The propulsion applied to each ABP is thereby calculated based on information about its local neighbors. Through the variation of a single parameter in our interaction model, which is related to zonal models used in theoretical biology, 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 can also measure the susceptibility of the collective motion, peaking at a critical point within the transition. 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.

T. Bäuerle *et al., Nat. Comm.* **9**, 3232 (2018); F. A. Lavergne *et al., Science* **364**, 70-74 (2019).

CPP 63.3 Wed 10:30 ZEU 160

Probing mechanical properties of rod-shaped colloidal suspensions with active particles — •N Narinder and Clemens Bechinger — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Recently self-propelled colloidal particles have been shown to provide a novel tool to probe the mechanical properties of colloidal glassy states of spherical particles [1]. Unlike conventional micro-rheology, where one studies the coupling between the translational motion of a driven probe particle to a background, here the coupling of the host medium to the rotational dynamics of the self-propelled particle contains information about the mechanical properties of the host medium. Here, we apply this method to study the mechanical properties of assemblies of rod-shaped particles with a mean aspect ratio of 15. Such anisotropic colloidal suspensions exhibit a rather rich phase behavior including a two-step glass transition at the aspect ratio considered here [2]. Our first results demonstrate a strong variation of the rotational dynamics of the active particle with increasing area fraction of the rods.

[1] C. Lozano, J.R. Gomez-Solano, & C. Bechinger Nature Materials 18, 1118-1123 (2019).

[2] Z. Zheng, F. Wang, & Y. Han PRL 107, 065702 (2011).

CPP 63.4 Wed 10:45 ZEU 160

Statistical mechanical sum rules for active colloids at surfaces - a touch of equilibrium — •René Wittmann[1,2], Frank Smallenburg[3], and Joseph Brader[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Soft Matter Theory, Université de Fribourg, Switzerland — [3]Laboratoire de Physique des Solides, Université Paris Sud, France

We study the mechanical properties of active particles in the presence of curved walls by computer simulation of Active Brownian Particles (ABPs), Active Ornstein-Uhlenbeck Particles (AOUPs) and a passive system with effective interactions [R. Wittmann, F. Smallenburg and J. M. Brader, J. Chem. Phys. 150, 174908 (2019)]. The effective theory admits analytic results for pressure, surface tension and adsorption of an active ideal gas at a two-dimensional circular wall. It further predicts that an equilibrium sum rule also holds for active fluids, which we confirm numerically for both ABPs and AOUPs in the limit of small curvature.

More precisely, we find within each model that the slope of the pressure as a function of the curvature equals the surface tension and adsorption (up to an effective temperature scale) on a planar wall. Intriguingly, the explicit value of these coefficients is model-dependent, which can be explained by the different velocity distributions. We also discuss the influence of interactions and find that the effect of curvature on the wall pressure is reduced when increasing the density. Within numerical accuracy, the equality of the slope of the pressure and the planar surface tension appears to hold at finite density.

CPP 63.5 Wed 11:00 ZEU 160

Lorentz forces induce inhomogeneity and flux in active systems — •Hidde Vuijk[1], Jens-Uwe Sommer[1,2], Holger Merlitz[1], Joseph Brader[3], and Abhinav Sharma[1,2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Universite de Fribourg, Fribourg, Switzerland

We consider the dynamics of a charged active Brownian particle in three dimensions subjected to the Lorentz force due to an external magnetic field. We show that in the presence of a field gradient, a macroscopic flux emerges from a flux-free system and the density distribution becomes inhomogeneous. The flux is induced by the gradient of the magnetic field only and does not require additional symmetry breaking such as density or potential gradients, which stands in marked contrast to similar phenomena in condensed matter such as the classical Hall effect. We further demonstrate that passive tracer particles can be used to measure the essential effects caused by the Lorentz force on the active particle bath, and we discuss under which conditions this diffusive Hall-like effect might be observed experimentally. Lastly, we show that similar effects arise in case of inhomogeneous activity in combination with a constant magnetic field.

15 min. break.

CPP 63.6 Wed 11:30 ZEU 160

Interaction of Active Crystallites within the Active Phase-Field-Crystal Model — •Lukas Ophaus[1], Johannes Kirchner[2], and Uwe Thiele[1,2] — [1]Center for Nonlinear Science, Münster, Germany — [2]Institut für Theoretische Physik, Münster, Germany

We use the active phase-field-crystal (PFC) model, developed by Menzel and Löwen as a model for crystallizing self-propelled particles [1], to study the interaction of traveling crystalline patches. Within the active PFC model, these localized states exist besides periodic states, i.e., spatially extended crystals [2]. Due to the activity, crystalline states undergo a drift instability and start to travel while keeping their spatial structure. Using results for the parameter ranges where the individual states exist, we explore how two and more traveling localized states interact by performing numerical collision experiments. We show that a critical minimal free path is necessary to preserve the number of colliding localized states and that the active PFC model fails to exhibit dynamical clustering and motility induced phase separation.

[1] A.M. Menzel and H. Löwen, Phys. Rev. Lett. 110, 055702 (2013)

[2] L. Ophaus, S.V. Gurevich and U. Thiele, Phys. Rev. E 98, 022608 (2018)

CPP 63.7 Wed 11:45 ZEU 160

Continuum model for bacterial suspensions with density variations — •Vasco Marius Worlitzer[1], Avraham Be'er[2], Gil Ariel[3], Markus Bär[1], Holger Stark[4], and Sebastian Heidenreich[1] — [1]Physikalisch-Technische Bundesanstalt — [2]Ben-Gurion University — [3]Bar-Ilan University — [4]Technical University of Berlin

The various dynamical states found in bacterial suspensions are a fascinating illustration of the rich dynamics exhibited by active polar fluids. A recent study explored the phase space experimentally, identifying three major states: single-cell motion, collective swarming, biofilm formation and mixtures between them [1]. While a continuum model presented in [2] has been proven to describe the statistical features of the swarming phase quite successfully, it is not applicable outside this regime as a constant density is assumed. We show that new dynamical states are accessible by relaxing this assumption. In particular a regime similar to the mixed state of swarming and biofilm formation is covered, showing the same anomalous statistics as found experimentally. The new model is inspired by work on scalar active matter [3] and consist of a generic continuity equation for the density. The density is coupled to a local polar order parameter through a density dependent self-propulsion speed and an active pressure.

[1] H Jeckel et al., PNAS 116 (5) (2019) [2] J Dunkel et al., Phys.

Rev. Lett. 110 (2013) 228102. [3] J Bialké et al., EPL 103 (2013) 30008.

CPP 63.8 Wed 12:00 ZEU 160

A minimal model for dynamical symmetry breaking in active matter — Matt 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)

CPP 63.9 Wed 12:15 ZEU 160

Self-propelled thermophoretic colloidal swimmers — •Sergi Roca-Bonet and Marisol Ripoll — Theoretical Soft Matter and Biophysics, Institute of Complex Physics, Forschungszentrum Jülich, Germany

Self-propelled phoretic colloids have recently emerged as a promising avenue for the design of artificial microswimmers. We employ a hydrodynamic fluctuating mesoscale simulation approach to study both single and collective swimming. We investigate self-propelled colloidal multimers in which one monomer can eventually get higher temperature, and it is linked with one or more other monomers which induce the multimer motion. Single colloid swimming properties are varied by changing the number of the constituting monomers (here two or three), their spatial arrangement (rod-like or v-like) and the relative sizes of such monomers. We have investigated the effect of slid confinement in comparison to the 3d-bulk motion of these dimeric and trimeric colloids. The collective system properties are determined by the competition between hydrodynamic and phoretic interactions which vary as a function of the density, the colloid geometry, and the monomers phoretic affinity (philic or phobic). Examples of the resulting behaviour are clustering, swarming, or rotational motions.

CPP 64: Topical Session: Data Driven Materials Science - Materials Data Management (joint session MM/CPP)

Time: Wednesday 10:15–11:30 Location: BAR 205

Topical Talk CPP 64.1 Wed 10:15 BAR 205

Automated atomistic calculation of thermodynamic and thermophysical data — •Jan Janssen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

A major challenge in predicting the properties of materials at realistic conditions is the accurate inclusion of finite temperature effects. Doing this on an ab initio level often requires complex simulation protocols. These complex protocols, which often couple several specialized codes, make a quantitative description of error propagation and uncertainty quantification a critical issue.

To handle this high level of complexity we have developed an integrated development environment (IDE) called pyiron[1] - http://pyiron.org. pyiron has been specifically designed to scale simulation protocols from the interactive prototyping level up to the high throughput level, all within the same software framework.

We highlight two recent success stories towards automated calculation of phase diagrams: We first discuss with the automated convergence for all key parameters in DFT codes, followed by the calculation of melting points with a guaranteed precision of better than 1K. These fully automated high-precision tools allow us to study trends over the periodic table in an efficient and systematic way. Examples how such high-throughput screenings allow to develop new strategies in designing materials will be given.

[1]: J. Janssen, et al., Comp. Mat. Sci. 161 (2019)

CPP 64.2 Wed 10:45 BAR 205

Big data in materials science: Status of and needs for metadata and ontologies — •Maja-Olivia Lenz, Luca M. Ghiringelli, Carsten Baldauf, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In recent years, the amount of data in materials science has increased exponentially. Consequently, new ways to store and annotate data are necessary to ensure findability, accessibility, interoperability and re-usability, i.e. to fulfil the FAIR principles [1], and to do efficient, good and new science. Data describing and characterizing other data are called metadata. Often, the materials science community has no clear distinction between data and their metadata as it depends on the intended use of the data. In this talk, we present the NOMAD MetaInfo [2], a general descriptive and structured metadata scheme for materials simulations. Ontologies represent the next step on the semantic ladder, as they enrich pure (meta)data structures by relations and thereby enable semantic and syntactic interoperability between different software agents, people, and organizations. In fact, the NOMAD MetaInfo includes a number of relations between concepts and therefore goes beyond the simple metadata picture. It can be interpreted as a light-weight ontology and thus can easily be connected to other ontologies like the European Materials and Modeling Ontology, EMMO. We give an introduction to ontologies, explain why they are useful, and outline their role and current status in materials science.

[1] M. Wilkinson, *et al.*, Sci Data 3, **160018** (2016).

[2] L. M. Ghiringhelli *et al.*, npj Comput. Mater. 3, **46** (2017).

CPP 64.3 Wed 11:00 BAR 205

Benchmarking neural networks on sequence-determined polymer transport through lipid membranes — •Marco Werner[1], Yachong Guo[2], and Vladimir Baulin[3] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Germany — [2]National Laboratory of Solid State Microstructure, Department of Physics, Nanjing University, China — [3]Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona, Spain

We consider the transport of amphiphilic polymers through lipid membranes by passive diffusion as a function of the sequence of hydrophilic and hydrophobic building blocks. Massively parallel Rosenbluth sampling of polymer conformations is performed to estimate polymer translocation times through a membrane for all 2^N sequences and chain lengths $N \leq 16$. Our results confirm that smallest translocation times are found for polymers with balanced fraction of hydrophilic and hydrophobic units, and containing short blocks. Sequence-complete databases deliver an important ground truth for benchmarking machine-learning models against training data restrictions and biases. We demonstrate that multi-layer artificial neural networks show remarkable generalization performance when restricting the training data to relatively narrow windows of translocation times. The results indicate that relevant sequence patterns and their physical effect are approximated based on the restricted training set, however, accuracy drops towards unexplored corners in sequence space.

CPP 64.4 Wed 11:15 BAR 205

Analysis of Materials Structural Representations for Machine Learning Interatomic Potentials — •Berk Onat[1], Christoph Ortner[2], and James Kermode[1] — [1]School of Engineering, University of Warwick, Coventry, United Kingdom — [2]Mathematics Institute, University of Warwick, Coventry, United Kingdom

Representations of materials based on atomic structural environments have been used either in machine learning models to predict properties directly or as the core of machine learning interatomic potentials (MLIPs) to enable accurate simulations. Many MLIPs have been developed to translate atomic neighbourhood environments from atom positions to structural representations such as atom-centred symmetry functions, smooth overlap of atomic positions and atomic cluster expansion(ACE) with spherical harmonics. While use of these representations is becoming common practice for applications, the sensitivity of their structural mapping to the materials composition and whether their coverage of the hyper-dimensional space is over-determined or complete have not yet been fully analysed. In this presentation, we provide analysis of the invariance of the model transformation under translations and rotations as well as the sensitivity of descriptors to perturbations. A range of datasets extracted from the NOMAD Archive are used to assess the dimensionality of the representations. The outcomes of our analyses will be presented with discussions on the model sensitivities and their possible limitations. We further provide insights on our continuing affords to utilise structural representations in other models for data-driven materials modelling.

CPP 65: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)

Time: Wednesday 10:30–13:30 Location: GER 38

Invited Talk CPP 65.1 Wed 10:30 GER 38

Hybrid Perovskites: polarons, excitons and phase diagrams — •Georg Kresse, Menno Bokdam, and Ryosuke Jinnouchi — University of Vienna, Faculty of Physics and Center for Computational Materials Sciences

Halide perovskites are very promising solar cell materials. The first part of this presentation studies the formation of polarons and excitons in MAPbI3. We show that both, polarons and excitons, possess about similar binding energies. To obtain accurate results, the calculations have to be carefully converged with respect to the k-point sampling, something that has been often "overlooked" in the past [1].

The second part of the talk presents studies on the finite temperature behavior of MAPbI3. To achieve the required long simulation time and large length scales, an on-the-fly machine learning scheme that generates force fields automatically during first principles molecular dynamics simulations is used. This force field opens up the required time and length scales, while retaining the distinctive chemical precision of first principles methods [2]. Using machine learned potentials, isothermal-isobaric simulations give direct insight into the underlying microscopic mechanisms of the phase transitions. We observe that MAPbI3 is an very dynamic material even at room temperature, putting some question marks on the hereto considered static models.

[1] M. Bokdam, T. Sander, A. Stroppa, S. Picozzi, D. D. Sarma, C. Franchini, G. Kresse, Scientific Rep. 6, 28618 (2016); [2] R. Jinnouchi, J. Lahnsteiner, F. Karsai, G. Kresse, M. Bokdam, PRL 122, 225701 (2019).

CPP 65.2 Wed 11:00 GER 38

Assessing ab-initio methodology to compute electronic properties of organic-inorganic metal halide perovskites — •Cecilia Vona, Dmitrii Nabok, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Organic-inorganic metal halide perovskites (HaPs) are materials widely studied for their light-harvesting properties. Owing to the interplay between strong electron-electron interaction and spin-orbit coupling, their theoretical investigation is still a challenge. Here we evaluate the methodology to compute their electronic structure. To this extent, we explore several approaches, within density-functional theory and many body perturbation theory, to compute the electronic structure of PbI_2, which is the precursor of many HaPs. Spin-orbit coupling effects are taken into account, and the hybrid functionals PBE0 and HSE are at the center of the investigation. We first explore several methods to determine the mixing parameter α, which in PBE0 and HSE defines the amount of Hartree-Fock exchange mixed with the semi-local functional PBE. We then use the results obtained from HSE and PBE0 for different values of α as starting point of G_0W_0 calculations. All the calculations are performed with the full-potential all-electron computer package `exciting`, in which LAPW+lo bases are implemented. We observed that hybrid functionals with a proper α value are most suitable to compute the electronic structure of PbI_2. Moreover, we show that the methodology is transferable to $CsPbI_3$, and we expect the same behavior for the lead-iodine perovskites.

CPP 65.3 Wed 11:15 GER 38

Rashba-Dresselhaus Effect in Two Dimensional Layered Halide Perovskites — •Benedikt Maurer[1,2], Claudia Draxl[1,2], and Christian Vorwerk[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin — [2]European Theoretical Spectroscopy Facility

It has been shown that huge spin-orbit coupling in bulk hybride organic inorganic perovskites in combination with broken inversion symmetry leads to Rashba-Dresselhaus splitting, which influences the optoelectronic properties. This indicates that such effects also affect the optoelectronic properties of their two dimensional layered relatives, which are promising candidates as new light emitting materials. In this work, we aim at understanding which inversion symmetry breaking can lead to the Rashba-Dresselhaus effect in those materials. For this purpose, we develop model structures, where we replace the organic compounds by Cs atoms and disregard possible distortions in the inorganic layers, resulting in the structural composition $Cs_{n+1}Pb_nI_{3n+1}$. Using the all-electron full-potential density-functional-theory code `exciting`, we systematically study how atomic distortions impact the band structure for n=1, 2 and ∞. We identify displacement patterns that yield Rashba-Dresselhaus splitting, and determine the size of the splitting as a function of the displacement. Furthermore, we analyze the spin textures in electronic states around the band gap to differentiate between Rashba and Dresselhaus effect. Our study reveals in-plane lead displacements as the origin of the Rashba-Dresselhaus splitting.

CPP 65.4 Wed 11:30 GER 38

Intrinsic polarons on polar surfaces — •Michele Reticcioli[1,2], Zhichang Wang[2], Igor Sokolovic[2], Michael Schmid[2], Ulrike Diebold[2], Martin Setvin[2], and Cesare Franchini[2,3] — [1]University of Vienna, Center for Computational Materials Science, Vienna, Austria — [2]Institute of Applied Physics, Technische Universitaet Wien, Vienna, Austria — [3]University of Bologna, Department of Physics and Astronomy, Bologna, Italy

Uncompensated charge at the surface boundary of polar materials is conventionally expected to form a two dimensional electron gas (2DEG), as a result of the alternating charged-plane stacking in the ionic crystals, interrupted by the surface cut. By means of density-functional theory calculations and surface-sensitive experiments, we propose a different paradigm able to accommodate the uncompensated charge in a more effective way, establishing a more favorable ground state for the system, that is the polaron formation (local lattice distortions coupled with charge localization). In fact, the intrinsic uncompensated charge tends to spontaneously localize and form polarons, rather than a 2DEG. Only beyond the critical polaron density, excess charge arising from external doping or defects starts to build dispersed electronic states. Here, we show how polarons and 2DEG compete on the polar KTaO3(001) surface.

CPP 65.5 Wed 11:45 GER 38

Polarons in extended p-conjugated systems: the role of electron correlation. — •Daniele Fazzi[1], Klaus Meerholz[1], and Fabrizia Negri[2] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger str. 116, 50939 Köln, Germany — [2]Dipartimento di Chimica, Università di Bologna, via F. Selmi, 2, 40126 Bologna, Italy

Polarons play a crucial role in governing charge transfer in organic materials. An accurate description of their electronic structure and electron-phonon couplings is mandatory to understand their response and transport properties.

We report a comprehensive investigation of polarons in extended p-conjugated systems (ladder-type polymers, graphene nano-ribbons, and cyanine-based compounds [1-2]). We show how spin polarized DFT lead to solutions of the polarons wavefunction which are not the most stable ones. This aspect, can be traced back to the multireference character of polarons. Broken symmetry DFT can address the electronic and structural properties of polarons, providing a correct assessment of charge transport parameters, otherwise incorrectly computed [3]. Multi-reference wavefunction methods are also considered to take into account correlation effects in charged and excited states.

Our study calls for a careful assessment in the description of charged/excited states in conjugated materials.

[1] Wang, S., et al., Adv. Mater. 2018, 30, 1801898. [2] Medina, S. et al., Phys. Chem. Chem. Phys., 2019, 21, 7281-7288. [3] Fazzi, D. et al, J. Mat. Chem. C., 2019, 7, 12876-12885.

CPP 65.6 Wed 12:00 GER 38

Optical and x-ray absorption spectra of MgO from first-principles including many-body effects — •Vijaya Begum, Markus E Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany

We discuss the optical and x-ray absorption (XAS) spectra of MgO − a wide band gap oxide with versatile applications − in the framework of density functional theory (DFT) including many-body and excitonic corrections. The quasi-particle band gap improves over DFT with PBEsol as the starting exchange-correlation functional (4.58 → 7.52 eV) and is overcorrected with the hybrid functional HSE06 (6.58 → 8.53 eV) when compared to experiment (7.7 eV). Including excitonic effects by solving the Bethe-Salpeter equation (BSE) leads to excellent agreement with the experimental spectrum both for the real and imaginary part of the dielectric function, when starting with the HSE06 functional. Furthermore, the x-ray absorption spectra of the O and Mg K-edge calculated with the Exciting code exhibit good agreement with experiment regarding the positions of the prominent peaks, underlining the importance of including the core-hole and electron interactions within the G_0W_0+BSE. Projection of the electron-hole coupling coefficients from the BSE eigenvectors on the band structure allows to explore the origin of the peaks and identify the orbital character of the relevant contributions.

Funding by DFG CRC1242, project C02 is gratefully acknowledged.

CPP 65.7 Wed 12:15 GER 38

Strain effects on the lattice-dynamical properties of titanium dioxide — •Peter Weber, Sebastian Tillack, Pasquale Pavone, and Claudia Draxl — Humboldt-Univeristät zu Berlin, Physics Department and IRIS Adlershof, Germany

A fingerprint of temperature-related anharmonic effects in a crystal is the change of the phonon frequencies with the volume. For anisotropic crystals, this variation must be generalized by the introduction of the mode Grüneisen tensor, which expresses the change of the phonon frequencies with respect to any applied strain. In this work, we present the results of an *ab-initio* investigation of the strain effects on the lattice-dynamical properties of the rutile and anatase phases of TiO_2. In particular, we focus our attention to the determination of the generalized Grüneisen parameters at the Brillouin zone center. In order to obtain all independent components of the Grüneisen tensor for these phases, all polar and nonpolar phonon frequencies at the Γ point are calculated for several strained configurations. These calculations are performed using density-functional theory as implemented in the full-potential all-electron software package `exciting` [1]. The connection between the Grüneisen tensors of the acoustic branches and the elastic constants of these materials is analyzed and discussed. Our results are also compared with available Raman scattering data for strained TiO_2.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202

CPP 65.8 Wed 12:30 GER 38

Ab-initio phonon self-energies and fluctuation diagnostics of phonon anomalies: lattice instabilities from Dirac pseudospin physics in transition-metal dichalcogenides — •Jan Berges[1], Erik van Loon[1], Arne Schobert[1], Malte Rösner[2], and Tim Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands

We present an ab-initio approach for the calculation of phonon self-energies and their fluctuation diagnostics, which allows us to identify the electronic processes behind phonon anomalies. Application to the prototypical transition-metal dichalcogenide 1H-TaS_2 reveals that coupling between the longitudinal–acoustic phonons and the electrons from an isolated low-energy metallic band is entirely responsible for phonon anomalies like mode softening and associated charge-density waves observed in this material. Our analysis allows to distinguish between different mode-softening mechanisms including matrix-element effects, Fermi-surface nesting, and Van Hove scenarios. We find that matrix-element effects originating from a peculiar type of Dirac pseudospin textures control the charge-density-wave physics in 1H-TaS_2 and similar transition-metal dichalcogenides.

CPP 65.9 Wed 12:45 GER 38

Toward a general non-local polarizability density functional for van der Waals dispersion interactions — •Szabolcs Góger, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Density functional theory (DFT), while being a workhorse for electronic structure calculations, struggles with describing long-range electron correlations including van der Waals (vdW) dispersion interactions. Various promising approaches have been developed to include vdW interactions in DFT, but a broadly applicable method is yet to be found [1,2]. The first key issue is developing a general density functional for non-local polarizability in molecules and solids. In this work, we use different known properties of atomic and molecular polarizabilites including the direct relation between the dipole polarizability and vdW radius unveiled recently [3]. Diverse methods starting with the Slater-Kirkwood approach [4] are applied to simple quantum mechanical systems like the Drude oscillator and the hydrogen atom under the effect of various electric fields. Our model studies along with prior work on semi-local polarizability functionals [5] pave the way toward developing a unified non-local polarizability functional for molecules and materials.

[1] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[2] Stöhr *et al.*, Chem. Soc. Rev. **48**, 4118 (2019)
[3] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)
[4] Slater and Kirkwood, Phys. Rev. **37**, 682 (1931)
[5] Vydrov and Van Voorhis, Phys. Rev. Lett. **103**, 063004 (2009)

CPP 65.10 Wed 13:00 GER 38

Insights into van der Waals interactions from the quantum Drude oscillator model — •Dmitry Fedorov, Martin Stöhr, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

The quantum Drude oscillator (QDO) model [1] represents the response of all valence electrons in an atom by a single Drude particle with its charge, mass, and characteristic frequency. Due to the simple form, this model serves as an insightful approach for the description of atomic response properties and van der Waals (vdW) interactions [2]. Recently, the QDO model helped to unveil a non-trivial relation between the dipole polarizability and the atomic volume, $\alpha_{\text{dip}} \propto V^{4/3}$, [3] as well as the surprising direct relation between the multipole polarizabilities and the equilibrium distances in vdW-bonded atomic dimers [4]. Here, we provide a detailed insight into the physical background of the aforementioned findings. The connection between different striking scaling laws obtained by diverse ways shows the inner consistency and power of this simple but efficient model. We discuss the importance of the revealed quantum-mechanical relations between response and geometric properties of atoms for computational models like the Tkatchenko-Scheffler [5] and the many-body dispersion [2] methods.

[1] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[3] Kleshchonok and Tkatchenko, Nat. Commun. **9**, 3017 (2018)
[4] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)
[5] Tkatchenko and Scheffler, Phys. Rev. Lett. **102**, 073005 (2009)

CPP 65.11 Wed 13:15 GER 38

Conical intersections in molecular systems: 3D vs 2D models — •Erik Pillon, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg

The molecular Aharonov-Bohm effect [1], covering various phenomena caused by the Berry (geometric or topological) phase in molecular systems, is an important playground for understanding fundamental quantum physics as well as for building quantum electronic devices. The related non-adiabatic effects, stemming from the coupling between the electron and nuclear degrees of freedom, are especially pronounced in systems possessing conical intersections (CI) in potential energy surfaces, ubiquitous in condensed matter and molecular physics. Many toy models have been introduced to study the influence of CIs on the nuclear dynamics from a general point of view. However, most of them, including the linear vibronic coupling model [2, 3] widely used in literature, employ two-dimensional (2D) real Hamiltonians. In our work, we check whether such models capture all the important features of real molecular systems. To this end, we perform a comparison of the conventional approaches with the general treatment of a CI within the three-dimensional (3D) complex Hamiltonian possessing SU(2) symmetry [4]. The features present within the 3D model but missing in the 2D case are identified and discussed.

[1] Zygelman, J. Phys. B: At. Mol. Opt. Phys. **50**, 025102 (2017)
[2] Longuet-Higgins *et al.*, Proc. R. Soc. A **244**, 1 (1958)
[3] Jahn and Teller, Proc. R. Soc. A **161**, 220 (1937)
[4] Berry, Proc. R. Soc. A **392**, 45 (1984)

CPP 66: Focus Session: Big Data in Aquisition in ARPES (joint session O/CPP)

Due to the advancement of both electron detectors and light sources, ARPES data is increasing in volume and complexity. This applies to ARPES performed at 3rd and 4th generation light sources as well as lab-based sources. We have reached a point where data handling, workflow management, visualization and analysis is a severe challenge and potentially become the bottleneck in our workflows rather than data acquisition itself. Currently there exist mainly isolated, i.e. lab- or facility-specific, solutions for data acquisition and file formats, metadata definitions, data-processing workflows, and analysis approaches. A community-wide ARPES (meta)data schema in the quest for reproducible, scalable and transparent data analysis is not yet established. This focus session aims to reveal the great potential for speeding up our progress by attacking certain challenges in joint efforts.

Organized by: Ralph Ernstorfer (FHI Berlin), Michael Hartelt and Martin Aeschlimann (TU Kaiserslautern)

Time: Wednesday 10:30–13:15 Location: REC C 213

Invited Talk CPP 66.1 Wed 10:30 REC C 213
Towards FAIR experimental data — •Claudia Draxl — Humboldt-Universität zu Berlin — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Knowledge and understanding of materials is based on their characterization in terms of a variety of properties and functions. Surprisingly though, for only a very small number of materials this information exists. Making materials data available, opens avenues for data-driven research in terms of re-purposing (using materials for a different purpose than intended by the original work), detecting candidate materials for a given application, and finding descriptors by approaches of artificial intelligence. Prerequisite for all this is a FAIR (findable, accessible, interoperable, reusable) data infrastructure. In computational materials science, the NOMAD Laboratory (https://nomad-coe.eu) has set the stage for FAIR data [1], by offering services like free upload to the NOMAD Repository, the NOMAD Archive, the NOMAD Encyclopedia, and the NOMAD Analytics Toolkit. In this talk, I will address our concepts and first steps towards extension of this open-science platform towards experimental data and sample synthesis. Here, for instance, data volume and velocity are big issues for many measurement techniques, while large uncertainties may come from (often incompletely known) sample quality, instrumental resolution, or measurement conditions. These challenges are tackled within the non-profit association FAIR-DI (https://fairdi.eu) and FAIRmat (https://fairdi.eu/fairmat), a proposed consortium for the NFDI.

[1] C. Draxl and M. Scheffler, MRS Bulletin 43, 676 (2018).

CPP 66.2 Wed 11:00 REC C 213
NXarpes, the Data File Standard for ARPES in NeXus — •Moritz Hoesch[1], Pavel Dudin[2], and Tobias Richter[3] — [1]DESY Photon Science, Hamburg, Germany — [2]Synchrotron Soleil, Gif-sur-Yvette, France — [3]European Spallation Source, Lund, Sweden

NeXus is a common data format for neutron, x-ray, and muon science. It is being developed as an international standard by scientists and programmers representing major scientific facilities in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data (cited from [1]). Diamond Light Source has adopted the NeXus standard, including for the instruments HR-ARPES and nano-ARPES on beamline I05 [2]. The specific NXarpes format, deliberately focusing on the essentials and thus expandable without deviation from the standard is available to the community [3]. In this presentation I will show examples of NXarpes data files and discuss the reception of this format by the community of ARPES users.

[1] https://www.nexusformat.org; [2] https://www.diamond.ac.uk/I05 ; [3] http://download.nexusformat.org/sphinx/classes/applications/NXarpes.html

CPP 66.3 Wed 11:15 REC C 213
Handling Big Multidimensional Experimental Data on Small Desktop Computers — •Michael Hartelt, Benjamin Frisch, Tobias Eul, Eva Prinz, Marten Wiehn, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany

In the pursuit of discovering new phenomena, photoemission experiments have evolved to capture ever more information about the electronic properties of materials. Major progress was made in the parallel detection of more degrees of freedom, which can include real- or k-space, energies and spin states of the emitted electrons. Additional dimensions of the parameter space are opened up by state-of-the-art experimental techniques that vary the sample temperature, the photon energy of the light source, or the time-delay between ultrashort laser pulses. As a result, experimental datasets of a single experiment can nowadays be 4-dimensional or even more. This makes the analysis of experimental data a non-trivial task, both conceptually and computationally.

We present our approach for the easy handling of these multi-dimensional, bigger-than-memory datasets on a conventional office computer. Using the Python programming language gives us access to powerful open-source packages like h5py, opencv, numpy, pint, and pycuda. Taking advantage of these, we integrated them into a toolbox package, which manages storage of large datasets for optimized I/O performance. The user is provided with an interface based on physical context, to perform data evaluation procedures with high efficiency.

CPP 66.4 Wed 11:30 REC C 213
Data Acquisition and Treatment on a Scientific and Industrial Level — •Stefan Böttcher, Christian Fleischer, and Thorsten Kampen — SPECS Surface Nano Analysis GmbH, Voltastrasse 5, 13355 Berlin

The recent developments in angular resolved photoemission and momentum microscopy let arise scientific instruments which produce enormous amount of raw data, easily exceeding several Tb of file size. Solutions or attempts of standard data- or transfer-formats are present in many fields, such as XPS or SPM. Here we present our approach on the data acquisition and processing in the acquisition and analysis software. We show the classes of metadata available to the experiment and the routes to export the data into usable formats. The data handling and the storage of transformation is a critical aspect with the present discussion. Finally an outlook into possibilities for DIN/ISO standardization can be given.

CPP 66.5 Wed 11:45 REC C 213
Challenges in data collection at a modern cw laser-driven spin-ARPES system — Tristan Heider[1], Peter Baltzer[2], Claus M. Schneider[1], and •Lukasz Plucinski[1] — [1]FZ Jülich PGI-6, Jülich, Germany — [2]MBS AB, Uppsala, Sweden

At PGI-6 in Jülich we operate a laser-driven angle- and spin-resolved photoemission (spin-ARPES) system, based on the *A*1 hemispherical analyzer with the lens deflector (MBS AB) and a single *k*-point *Ferrum* spin detector (Focus GmbH). The details of the system are described in a separate talk [1].

The typical data sets at our laboratory are 3D k_x vs. k_y vs. E_{kin} spin-integrated ARPES and 2D k_x vs. k_y spin maps. The size of a typical 3D dataset is approx. 100 MB, and for a complete measurement with the 6eV *cw* laser we take 4 of such sets, two with linear and two with circular light polarizations. The angular range of a single set is approx. 35°, therefore often more than one sample position needs to be measured, and a daily dataset exceeds 1 GB.

We will discuss the data collecting techniques, the data format, the data plotting, and the data storage and backup. We typically use MATLAB for data evaluation, however, we will discuss other options that might be more efficient for quick scanning through the large 3D datasets. We will use datasets from Fe-based superconductor and from 3D topological insulator as examples, and discuss challenges in evaluation of such data.

[1] T. Heider et al. this conference.

CPP 66.6 Wed 12:00 REC C 213

Single event data processing for multidimensional photoemission spectroscopy — •Steinn Ymir Agustsson[1], Rui Patrick Xian[2], Yves Acremann[3], Maciej Dendzik[2], Kevin Bühlmann[3], Davide Curcio[4], Dmytro Kutnyakhov[5], Federico Pressacco[6], Michael Heber[5], Shuo Dong[2], Philip Hofmann[4], Martin Wolf[2], Wilfried Wurth[5], Jure Demsar[1], Laurenz Rettig[2], and Ralph Ernstorfer[2] — [1]JGU Mainz — [2]FHI Berlin — [3]ETH Zurich — [4]Aarhus University — [5]DESY Photon Science, Hamburg — [6]Uni-Hamburg

The advent of novel electron detectors has opened up the field of photoemission spectroscopy to the single event detection regime. This significantly extends the accessible multidimensional parameter space for data acquisition, but also drastically increases the output of data from such experiments to the tens of MB/s regime. Handling such data therefore requires new approaches for data treatment, but also presents the opportunity for more advanced post-processing and analysis techniques. We present a distributed workflow for processing multidimensional photoemission data into an open source unified data structure. This allows, when combined with open source analysis algorithms, to directly apply such routines on data sets obtained from different experimental setups, from large scale facilities to table-top systems.

Invited Talk CPP 66.7 Wed 12:15 REC C 213

Reproducible data analysis with Snakemake — •Johannes Köster — Algorithms for reproducible bioinformatics, Genome Informatics, Institute of Human Genetics, University of Duisburg-Essen, Hufelandstr. 55, 45147 Essen Germany

Data analyses usually entail the application of many command line tools or scripts to transform, filter, aggregate or plot data and results. With ever increasing amounts of data being collected in science, reproducible and scalable automatic workflow management becomes increasingly important. Snakemake is a workflow management system, consisting of a clean, human-readable, text-based workflow specification language and a scalable execution environment, that allows the parallelized execution of workflows on workstations, compute servers, clusters and the cloud without modification of the workflow definition. Snakemake is hugely popular and was used to build analysis workflows for numerous high impact publications. With about 350 citations in the last two years, it is one of the leading frameworks for reproducible data science. This talk will show how Snakemake can be used to easily document, execute, and reproduce data analyses.

CPP 66.8 Wed 12:45 REC C 213

Concept for Handling of Photoemission Data at European XFEL — •Markus Scholz[1], Dmytro Kutnyakhov[2], Michael Heber[2], Manuel Izquierdo[1], Hans Fangohr[1], Yves Acremann[4], Kai Rossnagel[3], Anders Madsen[1], and Serguei Molodtsov[1] — [1]European XFEL Facility, Holzkoppel 4, 22869 Schenefeld, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Ruprecht-Haensel-Labor, Christian-Albrechts-Universität zu Kiel and Deutsches Elektronen-Synchrotron DESY, 24098 Kiel and 22607 Hamburg, Germany — [4]Laboratorium für Festkörperphysik, ETH Zürich, 8093 Zürich, Switzerland

European X-ray Free Electron Laser (EuXFEL) is currently the world's biggest, brightest and highest repetition rate XFEL providing up to 27000 pulses/second. The planned open port named "Soft X-ray Port" (SXP), will allow time-resolved X-ray photoelectron spectroscopy (TR-XPES) experiments. In this contribution I will present how near-online analysis of photoemission data based on Jupyter notebooks could be realized and embedded in the EuXFEL software framework. For compute-intensive notebooks, it is possible to allocate dedicated nodes with user-specified hardware configuration from the Maxwell computer cluster to a running JupyterHub session. This is of particular value due to the size of data sets and the the remotely accessible analysis.

CPP 66.9 Wed 13:00 REC C 213

Processing workflow for band structure reconstruction from multidimensional photoemission data — R. Patrick Xian[1], Vincent Stimper[2], Shuo Dong[1], Maciej Dendzik[1], Samuel Beulieu[1], Bernhard Schölkopf[2], Martin Wolf[1], Stefan Bauer[2], Laurenz Rettig[1], and •Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

Recent advances in photoelectron detectors and light sources result in an increase of size and dimensionality of photoemission data, leading to new challenges in data preprocessing and analysis: the large number of adjustable parameters of modern electron optics require experiment-specific calibration and artifact correction [1]; visual inspection of multidimensional ARPES data may be hampered by the varying levels of contrast [2]. We discuss a workflow for conditioning volumetric three- and four-dimensional momentum microscopy data for band structure mapping from single-electron events to calibrated, reusable data [3].

[1] Xian et al., Ultramicroscopy 202, 133 (2019).
[2] Stimper et al., IEEE Access 7, 165437 (2019).
[3] Xian et al., arXiv 1909.07714.

CPP 67: 2D Materials IV: Interfacial Interactions (joint session O/HL/CPP)

Time: Wednesday 10:30–13:45 Location: WIL B321

CPP 67.1 Wed 10:30 WIL B321

Interplay between electronic instability and moiré structure of monolayer V_2S_3 on Au(111) — •Sahar Pakdel[1], Umut Kamber[2], Raluca-Maria Stan[1], Anand Kamlapure[2], Brian Kiraly[2], Fabian Arnold[1], Andreas Eich[2], Arlette S. Ngankeu[1], Marco Bianchi[1], Jill A. Miva[1], Charlotte Sanders[1], Philip Hofmann[1], Alexander A. Khajetoorians[2], and Nicola Lanata[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The formation of Moiré superstructures between 2D-materials and their substrates has attracted considerable attention, as it can influence their physical properties. Here we study monolayer V_2S_3 grown on an Au(111) substrate. Scanning tunneling microscopy experiments exhibit multiple domains with different Moiré structures. Comparing the calculated Fermi surfaces with angle resolved photo-emission spectroscopy data, we find that the substrate induces a substantial shift in the chemical potential. We show that the computed Lindhart function of V_2S_3 (at the measured chemical-potential) has a pronounced peak corresponding to a second-order reciprocal point of the prevalent Moiré structure. This suggests that the system tends to favor Moiré structures with modulations able to accommodate underlying electronic instabilities of V_2S_3. We speculate that this could be the manifestation of a more general mechanism and a promising route for tailoring the electronic structure of 2D-materials.

CPP 67.2 Wed 10:45 WIL B321

Probing the electronic structure of twisted transition metal dichalcogenide bilayers by photoemission — •bharti parashar[1], sven borghardt[2], kevin janssen[1], mateo jugovac[1], vitaliy feyer[1], dorota wilgocka slezak[3], józef korecki[3], lukasz plucinski[1], and claus m. schneider[1] — [1]PGI-6, FZ Jülich, Germany — [2]PGI-9, FZ Jülich, Germany — [3]Polish Academy of Sciences, Kraków, Poland

Moire bands in twisted transition metal dichalcogenide (TMDC) bilayers are predicted to host novel topological and correlated electronic phases [1]. We performed angle-resolved photoemission studies with few micrometer resolution (μ-ARPES) on several hetero- and homo-bilayers made from MoS_2 and WSe_2 by mechanical exfoliation and dry transfer technique. The twist angle between the layers was determined in a separate experiment by μ-LEED.

We determine the hybridization between the layers through monitoring the formation of new spectral features in normal emission spectra, that are not present in respected monolayers. The existence of hybridization indicates high quality of the interface that is critical to enable formation of interesting moire bands. Furthermore, our results allow to shed light on whether the valence band maximum is located at Γ or at K at various bilayers. This is improtant for predicted moire physics, since only at K the bands are spin-momentum locked.

[1] See e.g.: F. Wu, T. Lovorn, E. Tutuc, I. Martin, and A. H. MacDonald, Phys. Rev. Lett. 122, 086402 (2019), and refs. therein.

CPP 67.3 Wed 11:00 WIL B321

Electronic vs Structural Effects in the Moiré Pattern of MoS_2 on Au(111) — Caio C. Silva[1,2], Daniela Dombrowski[1,2], Nicolae Atodiresei[3], Wouter Jolie[2], Ferdinand Farwick zum Hagen[2], Jiaqi Cai[2], Paul T. P. Ryan[4], Pardeep Thakur[5], Vasile Caciuc[3], Stefan Blügel[3], David A. Duncan[5], Thomas Michely[2], Tien-Lin Lee[5], and •Carsten Busse[1,2,6] — [1]WWU Münster, Germany — [2]Universität zu Köln, Germany — [3]FZ Jülich and JARA, Germany — [4]Imperial College London, U. K. — [5]Diamond Light Source Ltd, U. K. — [6]Universität Siegen, Germany

The lattice mismatch between a monolayer of MoS_2 and its Au(111) substrate induces a moiré superstructure. The local variation of the registry between sulfur and gold atoms at the interface leads to a periodic pattern of strongly and weakly interacting regions. In consequence, also the electronic bands show a spatial variation.

We use scanning tunneling microscopy and spectroscopy (STM/STS), x-ray photoelectron spectroscopy (XPS) and x-ray standing wave (XSW) for a determination of the atomic structure and the resulting electronic properties. The experimental results are corroborated by density functional theory (DFT). We deduce the structure of the supercell with high precision, identify the fraction of interfacial atoms that are strongly interacting, and analyze the variation of the electronic structure in dependence of the location within the moiré cell and the nature of the band.

CPP 67.4 Wed 11:15 WIL B321

Complex moiré structures in rotated monolayer V_2S_3 on Au(111) — •Umut Kamber[1], Sahar Pakdel[2], Raluca-Maria Stan[2], Anand Kamlapure[1], Brian Kiraly[1], Fabian Arnold[2], Andreas Eich[1], Arlette S. Ngankeu[2], Marco Bianchi[2], Jill A. Miwa[2], Charlotte Sanders[2], Nicola Lanata[2], Philip Hofmann[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark

Moiré superlattices have led to the emergence of tunable many-body states of matter like superconductivity and Mott insulator states absent in the individual layers [1,2]. For transition metal dichalcogenides (TMDCs), there has been a strong interest in how electronic structure is modified near the single layer limit and potentially affected by the dielectric environment. Here, we show spatially periodic modifications to the electronic structure of single layer V_2S_3 grown on Au(111) varying with the underlying moiré pattern [3]. Similar modifications were observed in multiple moiré patterns, each arising from a different relative orientation between the monolayer and the Au(111) substrate. We characterize these spatial variations in electronic structure with respect to the atomic and moiré lattices via scanning tunneling microscopy and spectroscopy, with the help of ab initio calculations.

[1] Y. Cao et al., Nature, 556, 43 (2018).
[2] Y. Cao et al., Nature, 556, 80 (2018).
[3] F. Arnold et al., 2D Mater. 5, 045009 (2018).

CPP 67.5 Wed 11:30 WIL B321

Screening effects at the internal interfaces of bulk-like MoS_2 — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The two-dimensional nature of TMDCs is intrinsically linked to reduced screening. This renders the materials sensitive to their dielectric environment. Quasiparticle calculations of MoS_2 deposited on different substrates have shown the importance to account for environmental screening [1]. In this talk we discuss how screening effects modify the electronic structure across the internal interfaces of bulk-like MoS_2.

In a first step we use a tight-binding model to reproduce the band structure on a level of density functional theory. To include polarization effects, we extend the model by introducing a self-energy operator constructed from layer-resolved quasiparticle corrections calculated within the framework of GW. Using this GW-tight-binding approach, we show that environmental screening has strong impact on the formation of the subbands which originate from interlayer interactions. Most striking, at the K-point, the surface layer decouples from lower lying layers forming a direct gap which is distinctly different from that of the total system.

[1] M. Drüppel et al., Nat. Commun. **8**(1), 2117 (2017)

CPP 67.6 Wed 11:45 WIL B321

Charge density wave and superconductivity of single-layer NbSe2 on different screening environments — •Wen Wan, Paul Dreher, Marco Gobbi, and Miguel M. Ugeda — Donostia International Physics Center and Centro de Física de Materiales, San Sebastián-Donostia, Spain

Superconductivity and charge density wave order, typical collective electronic phases of transition metal chalcogenides (TMD), are highly sensitive to external perturbations. In the 2D limit, the properties, and even the mere existence, of these phases in monolayers of TMDs become mostly dependent on the supporting substrate due to charge doping/screening and hybridization effects [1,2]. Here, we carry out low-temperature STM/STS (350 mK) measurements to study the electronic structure of single-layer NbSe2 grown on different substrates by molecular beam epitaxy. In particular, we explore and compare the fate and fundamental properties of the superconducting and CDW states of single-layer NbSe2 on both highly metallic, semi-metallic and insulating TMD substrates [3].

[1] M. M. Ugeda, et al. Nature Physics 12, 92 (2016).
[2] Stan, et al. Phys. Rev. Mat. 3, 044003 (2019).
[3] W. Wan, et al., in preparation.

CPP 67.7 Wed 12:00 WIL B321

Incorporation of K and Cs into hBN/Ir(111) and hBN/Ru(0001) — •Jiaqi Cai[1,2,3], Caio Silva[2,3], Wouter Jolie[2], Thais Chagas[1], Kai Mehlich[1], David Duncan[4], Christoph Schlueter[4], Tien-Lin Lee[4], and Carsten Busse[1,2,3] — [1]Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [3]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [4]Diamond Light Source, Didcot OX11 0DE, Oxfordshire, United Kingdom

The bi-atomic unit cell of monolayer hexagonal boron nitride (hBN) makes its interaction with the substrate more complex in comparison with its famous cousin, graphene. To probe this interaction, we incorporate alkali metals into hBN/substrate systems. We choose alkali metals for two reasons: i) they tend to lose the electron in the out-most orbitals, thus introducing a strong electronic effect into the hBN/substrate system; ii) the alkali metal ions have full-shell structure, making them unlikely to chemically bond to hBN.

In this talk, we report our experimental results on K as well as Cs incorporation into epitaxial hBN on Ir(111) and Ru(0001). We rely on STM, LEED, XPS, and XSW for the determination of the atomic coordinates with high precision. We report a rich pool of structures (adsorption and/or intercalation of alkali metals), and find that the location of the alkali metal ions are determined by the hBN-substrate interaction strength, and the size of the alkali metal ions.

CPP 67.8 Wed 12:15 WIL B321

Control of interface alloying between silicene and a silver substrate — •Johannes Küchle[1], Aleksandr Baklanov[1], Felix Haag[1], David Duncan[2], Paul Ryan[2,3], Ari Seitsonen[4], Willi Auwärter[1], and Francesco Allegretti[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Diamond Light Source, Didcot, UK — [3]Imperial College London, UK — [4]Département de Chimie, École Normale Supérieure, Paris, France

Silicene, the silicon analogue of graphene, is a promising material with unique structural and electronic properties, which has been the focus of intense research in the past decade. The epitaxial growth *via* deposition of silicon on solid substrates is an established strategy for silicene preparation, however, strong interfacial interactions may modify the functional properties of the resulting layer. On metal substrates, interfacial alloying may occur, but surprisingly, its role is often underestimated. Here, we present our recent experiments with soft X-ray photoelectron spectroscopy (SXPS) at various Si coverages, indicating that during the growth of the most commonly studied (4×4) superstructure of silicene on Ag(111) a Si-Ag surface alloy is formed. Our scanning tunneling microscopy studies resolve a yet unreported phase, which we relate to the Si-Ag alloy. Notably, we show that the alloy related component in SXPS can be largely suppressed by growing silicene on a GeAg$_2$ surface alloy on Ag(111). In this case, a number of distinct structures are observed by low-energy electron diffraction, which differ significantly from all previously reported superstructures of silicene.

CPP 67.9 Wed 12:30 WIL B321

Curvature-Induced Charge Baskets in Two-Dimensional Semiconducting Monolayers — •bong gyu shin[1], jz-yuan juo[1], soon jung jung[1], and klaus kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569 Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The localized quantum states in two-dimensional (2D) materials are attractive for valley- and spin- related optoelectronics or other quantum applications. However, achieving these quantum states is still challenging due to technical difficulties. Here, we investigated strain-induced charge localization and quantum confinement in monolayer MoS$_2$ on a SiO$_2$/Si substrate using a gate-tunable home-built scanning tunneling microscope at $\sim$4.9K. Monolayer MoS$_2$ follows surface roughness of the substrate, which exhibits a bending strain with band gap reduction. This band gap reduction at a local regime acts like a potential well leading to charge localization. When the bending strain in MoS$_2$ is larger than 2% at a local region of $\sim$4 nm, quantum-confined energy levels are observed near the conduction or valence band edge due to the significant band gap reduction of $\sim$1 eV. Moreover, our theoretical results show that spatial flattening of the conduction (valence) band edge occurs by heavy electron- (hole-) doping of over $\sim 10^{13}$ cm^{-2}. The strain-induced quantum confinement in 2D materials can play an important role in the future development of quantum devices.

CPP 67.10 Wed 12:45 WIL B321

Long-range charge order induced by strain in layered IrTe$_2$ revealed by ARPES — •Chris W. Nicholson[1], Maxime Rumo[1], Geoffroy Kremer[1], Thomas Jaouen[1], Baptiste Hildebrand[1], Marie-Laure Mottas[1], Björn Salzmann[1], Aki Pulkinnen[2], Bernardo Barbiellini[2], Timur Kim[3], Saumya Mukherjee[3], Cephise Cacho[3], Matthias Muntwiler[4], Fabian von Rohr[5], Philipp Aebi[1], and Claude Monney[1] — [1]University of Fribourg, Switzerland — [2]LUT University, Finland — [3]Diamond Light Source, UK — [4]Swiss Light Source, Switzerland — [5]University of Zurich, Switzerland

Uniaxial strain combined with ARPES offers a relatively new route to studying the interplay between the lattice and electronic structure. The wide range of properties displayed by layered transition metal dichalcogenides makes them intriguing candidates for exploring this.

Here we present ARPES data revealing the influence of tensile strain on the electronic structure of IrTe$_2$, which exhibits a complicated mixture of one dimensional charge ordered phases at low temperatures but very broad electronic bands [1]. The application of strain induces a single, long-range ordered phase, with clear quasi-1D features at the Fermi level and sharp bands over a wide binding energy range. By comparison with electronic structure calculations, we will discuss the mechanism of this strain-induced stabilization with reference to the redistribution of charge between Ir and Te bonds [2].

[1] Ko et al, Nat. Comm 6, 7342 (2015)

[2] Nicholson et al, in preparation

CPP 67.11 Wed 13:00 WIL B321

Seeking 2D Ferromagnets among TMD materials — •Paul Dreher[1,2], Wen Wan[1,2], Adolfo O. Fumega[5], Md N. Huda[4], Shawulienu Kezilebieke[4], Santiago Blanco[2,3], Victor Prado[5], Hannu-Pekka Komsa[4], Marco Gobbi[2,3], Peter Liljeroth[4], and Miguel M. Ugeda[1,2] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Centro de Física de Materiales, San Sebastián, Spain — [3]CIC nanoGUNE, San Sebastián, Spain — [4]Department of Applied Physics, Aalto University School of Science, 00076 Aalto, Finland — [5]Departamento de Física Aplicada, Universidade de Santiago de Compostela, Campus Sur s/n, E-15782 Santiago de Compostela,Spain

We study the magnetic character of various monolayer TMD candidates (VSe2, CrSe2) grown by MBE on different substrates (NbSe2, graphene, graphite) by combining various characterization techniques. Our findings reveal that the substrate plays a crucial role on the magnetic order in the grown TMD monolayer. The CDW order in single-layer VSe2 causes a strong reduction in the DOS at EF incompatible with ferromagnetism. When grown on graphene substrates, the CDW persists VSe2 and it becomes paramagnetic [1]. Instead, the electronic structure of single-layer VSe2 on a superconducting substrate (NbSe2) shows features compatible with magnetism [2]. Finally, XMCD measurements on Cr-based TMD monolayers indicate the presence of an uncompensated spin in Cr, which retains a paramagnetic behavior even at low temperatures. [1] J.Phys.Chem.C, 123, 27802 (2019), [2] ArXiv:1909.10208 (2019).

CPP 67.12 Wed 13:15 WIL B321

Signatures of strong coupling between WS$_2$ excitons and surface plasmon polariton waves — Moritz Gittinger[1], Sven Stephan[1], Trung Nguyen[1], Antonietta deSio[1], •Martin Silies[1], Christoph Lienau[1], Alison Cadore[2], Ilya Goykhman[2], and Andrea Ferrari[2] — [1]Institute of Physics and Center of Interface Science, Carl von Ossietzky Universität Oldenburg — [2]Cambridge Graphene Centre, University of Cambridge, UK

All-solid-state strong coupling systems with large vacuum Rabi splitting energies are of great potential in future technologies such as quantum information processing. Here, atomically thin layers of transition metal dichalcogenides in close vicinity to metallic nanoparticles have recently been explored as excellent candidates for the observation of this coherent energy transfer from the exciton to its localized surface plasmon counterpart [1]. We here present first results of the interaction between surface plasmon polariton (SPP) waves induced in focused-ion beam written gratings in planar silver films with excitons from atomically-thin WS$_2$ flakes. By using confocal angle-resolved reflectance spectroscopy, the dispersion relation of the coupled system is mapped at room temperature. We observe a clear anti-crossing of the exciton and the SPP resonance with a normal mode splitting of up to 50meV. We take this splitting as a first signature for a strong coupling between the WS$_2$ exciton and the SPP wave in the silver grating [2].

[1] Schneider C. et al, Nature Comm. 9, 2695 (2018) [2] Vasa P, and C. Lienau, ACS Photonics 5, 2-23 (2018)

CPP 67.13 Wed 13:30 WIL B321

Substrate-dependent charge transfer mechanisms between monolayer MoS2 and molecular dopants — •Patrick Amsalem[1], Soohyung Park[1,2], Thorsten Schultz[1,3], Xiaomin Xu[1], Berthold Wegner[1,3], Areej Aljarb[4], Ali Han[4], Lain-Jong Li[4,5], Vincent C . Tung[4,6], and Norbert Koch[1,3] — [1]Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Berlin, Germany — [2]Korea Institute of Science and Technology (KIST), Seoul, South Korea — [3]Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin, Germany — [4]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia — [5]The University of New South Wales, Sydney, Australia — [6]Lawrence Berkeley National Lab, Berkeley, CA, USA

2D transition metal dichalcogenides monolayer films have recently gained enormous attention. Yet, to extend the range of applications of these emerging materials, tuning their Fermi level is of crucial importance. Here, we report on the adsorption of a strong p-type organic dopant, F6TCNNQ, as an efficient route for doping of MoS2 [1]. More specifically, we employ angle-resolved UV and X-ray photoelectron spectroscopy to reveal the charge transfer (CT) mechanisms taking place at a TMDC/organic interface as a function of the electrical properties of the employed supporting substrate, here sapphire, graphite and gold. The present findings can be exploited for the design of advanced hybrid heterostructures with tailored electronic properties. [1] S. Park et al., Communications Physics 2, 109 (2019).

CPP 68: Topical Session: Data Driven Materials Science - Descriptors (joint session MM/CPP)

Time: Wednesday 11:45–13:15 Location: BAR 205

CPP 68.1 Wed 11:45 BAR 205

Evaluating representations of atomistic systems for machine learning — •Marcel Langer[1] and Matthias Rupp[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Citrine Informatics, Redwood City, CA, USA

Interpolating between computationally expensive first-principles calculations with fast machine-learning surrogate models increases the feasible scope of exploration when a large space of potentially similar structures is sampled, for instance in the search for novel materials or the exploration of phase diagrams.

The choice of representation of the atomistic systems under consideration is important for the accuracy of such surrogate models. We present a rigorous empirical comparison of the Many-Body Tensor Representation [1], Smooth Overlaps of Atomic Positions [2], and Symmetry Functions [3] for energy predictions of molecules and materials. In this, we control for data distribution, hyper-parameter optimization, and regression method. We also investigate the relationship between predictive performance and computational cost, and discuss how to assess predictions beyond mean errors, which cannot fully describe model behaviour in practice. [4,5]

[1] H. Huo and M. Rupp, *arXiv*, 1704.06439 (2017)
[2] A. Bartók, R. Kondor., G. Csányi, *Phys. Rev. B* **87**, 184115 (2013)
[3] J. Behler, *J. Chem. Phys.* **134**, 074106 (2011)
[4] C. Sutton *et al.*, *ChemRxiv*, 9778670 (2019)
[5] Z. del Rosario *et al.*, *arXiv*, 1911.03224 (2019)

CPP 68.2 Wed 12:00 BAR 205

Information-theory-driven identification of compact descriptors for accurate machine-learning predictions — •Benjamin Regler, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Machine learning (ML) is useful for predicting materials behavior by relating physical and chemical properties (features) of known materials to the property of interest (target). Aiming at a rational, unbiased, and data-driven identification of relevant features, we use a combination of statistical and information-theoretical techniques to identify the subset of features that unequivocally represent each material in the data set and contribute most to predicting the target property. The novelty and power of our approach is that it does not assume any specific functional form of the “features → target” relationship. Based on the concept of cumulative mutual information, our framework assigns quantitative scores for the “strength” of the feature’s contributions, ranks the features by their scores, and selects the most contributing features to be relevant prior to ensuing data analysis. The scoring and selection algorithm is then supplemented by a purely ML procedure built on the selected and compact feature subset. We identify compact feature subsets for predicting (i) the ground-state crystal-structure of octet-binary compound semiconductors and (ii) elastic properties of inorganic crystalline compounds. In each case, we show that only a few features are actually required to obtain accurate predictions, thereby reducing the complexity of the ML model and sensitivity to the availability of materials data.

CPP 68.3 Wed 12:15 BAR 205

Size-Extensive Molecular Machine Learning with Global Descriptors — •Johannes Margraf[1], Hyunwook Jung[2], Sina Stocker[1], Christian Kunkel[1], and Karsten Reuter[1] — [1]Technical University Munich, Germany — [2]Yonsei University, South Korea

Machine learning (ML) models are increasingly used to predict molecular properties in a high-throughput setting at a much lower computational cost than conventional electronic structure calculations. Such ML models require descriptors that encode the molecular structure in a vector. These descriptors are generally designed to respect the symmetries and invariances of the target property. However, size-extensivity is usually not guaranteed for so-called global descriptors. In this contribution, we show how extensivity can be build into ML models with global descriptors such as the Many-Body Tensor Representation. Properties of extensive and non-extensive models for the atomization energy are systematically explored by training on small molecules and testing on small, medium and large molecules. Our results show that the non-extensive model is only useful in the size-range of its training set, whereas the extensive models provide reasonable predictions across large size differences. Remaining sources of error for the extensive models are discussed.

CPP 68.4 Wed 12:30 BAR 205

Hierarchical SISSO: predicting complex materials properties building on simpler ones — •Lucas Foppa[1], Sergey V. Levchenko[2,1], Matthias Scheffler[1], and Luca M. Ghiringhelli[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Skolkovo Institute of Science and Technology, Moscow, RU

Symbolic regression is a promising tool to identify analytical models (descriptors) for predicting materials properties that are otherwise accessed via rather expensive *ab initio* calculations. In this context, the sure-independence screening and sparsifying operator (SISSO),[1] which combines the systematic generation of large feature spaces with compressed sensing, has been successfully applied, e.g., to the prediction of the (meta)stability of binary systems and perovskites from atomic properties only. However, if the relationship between the features and the target property is too complex, the descriptor search can become very inefficient. Here, we tackle this issue via a hierarchical approach: features that are easily computed (e.g., atomic properties) are used for predicting simple properties (e.g., lattice constant) and the resulting descriptors are in turn used as candidate features for modeling more complex properties (e.g., bulk modulus, position of band centers or band gaps). We demonstrate the hierarchical approach by analyzing a dataset of >700 cubic simple (ABO_3) and double ($A_2BB'O_6$) perovskites for predicting mechanical and electronic properties. The learned models require only atomic features as inputs and are therefore suitable for high-throughput screening of such materials.

[1] R. Ouyang, *et al.*, *Phys. Rev. Mater.* **2**, 083802 (2018).

CPP 68.5 Wed 12:45 BAR 205

Similarity descriptors for data-driven materials science — •Martin Kuban, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Learning from materials data is a topic of increasing importance in materials science. This task is supported by the availability of data through large online databases, like NOMAD [1]. For the application of artificial-intelligence (AI) methodology, materials must be characterized by a set of features that together build up *descriptors*. The success of AI tasks depends heavily on the quality of these descriptors, since they must contain all relevant information to map the input data onto the target property. Recent advances in the development of high-quality descriptors have allowed for both accurate predictions of material properties as well as highly interpretable models [2]. In this work, we develop a new type of descriptors based on the similarity of materials. To achieve this goal, we use both existing and newly developed descriptors to establish metrics that serve as quantitative similarity measures. These measures are combined into "similarity descriptors", which are then used for the construction of AI models. The performance of these models is optimized with respect to their predictive power. We demonstrate the applicability of our approach by predicting target properties for different classes of materials, including oxides and 2D systems.

[1] C. Draxl and M. Scheffler, MRS Bulletin, 43, 676, (2018).
[2] L. Ghiringhelli *et al.*, PRL, 114, 105503, (2015).

CPP 68.6 Wed 13:00 BAR 205

Machine-learning descriptors with domain knowledge of the interatomic bond — •Thomas Hammerschmidt, Jan Jenke, Aparna P.A. Subramanyam, Jörg Kossmann, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The performance of machine-learning depends critically on the quality of the descriptors. In the case of learning atomic-scale properties, like formation energies obtained from density-functional theory (DFT) calculations, the descriptors typically measure the atomistic geometry and the distribution of chemical elements. Here, we construct descriptors that additionally include prior knowledge of the interatomic bond from a hierarchy of coarse-grained electronic-structure methods. In particular, we use tight-binding (TB) and analytic bond-order potentials (BOPs) that are derived from a second-order expansion of DFT. We demonstrate that a recursive solution of the TB problem and the closely related moments of the electronic density-of-states at the BOP level establish a smooth structure-energy relation. This first level of domain knowledge of the interatomic bond shows highly descriptive power in machine-learning applications already with simple, qualitative TB models. As second level of domain knowledge we include the bond chemistry in terms of bond-specific TB Hamiltonians that are obtained from downfolding the DFT eigenspectrum of molecular dimers. In the third level of domain knowledge we include the role of the valence electrons by determining non-selfconsistent bond energies with the bond-specific TB Hamiltonians.

CPP 69: Focus: Fundamentals of molecular liquids, ionic liquids and mixtures II

Time: Wednesday 15:00–18:45 Location: ZEU 222

Invited Talk CPP 69.1 Wed 15:00 ZEU 222
Modelling and Simulation of Organic Ionic Liquids — •Pietro Ballone — School of Physics, University Collge Dublin, Dublin 4, Ireland

Organic ionic compounds whose melting point falls below the conventional limit $T_M \leq 400$K, also known as room temperature ionic liquids (RTILs), represent a vast class of systems whose properties have been extensively investigated by experiments and simulations in view of applications as innovative solvents in industrial processes, as electrolytes, as lubricants and lubricant additives. Moreover, their selective interactions with biomolecules, providing further prospects for applications in pharmacholögy and biophysics.

I will briefly discuss the models used to describe these systems, and review selected simulation studies of RTILs in the electro-chemical context and in biophysics.

At the atomistic level, current models relies on either ab-initio (density functional) methods, or empirical force fields. I will briefly discuss the prospects and the challenges of polarisable force fields and especially of coarse grained models.

On the simulation side, I will present results on systems of interest as proton conductor electrolytes, covering in particular their water absorption and surface properties. Moreover, I will present simulation results relevant for biophysics, focusing on the effect of RTILs on biomembranes, of interest for pharmacology and toxicology, and analysing the ability of RTILs to either prevent or enhance the formation of amyloid fibrils.

CPP 69.2 Wed 15:30 ZEU 222
Dynamic Properties of Ion Jelly Studied by Dynamic Light Scattering and Dielectric Spectroscopy — •Jennifer Kraus, Florian Pabst, and Thomas Blochowicz — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Room temperature ionic liquids (RTILs) are molten salts liquid at room temperature, which are promising candidates for electrolytes in various electrochemical devices. For these electrolytes, however, a solid state would be desirable in terms of mechanical properties. Thus, the gelation of ionic liquids induced by polymers is one way to obtain a material with high conductivity despite a good mechanical strength, which is called ion jelly.

Mixing the ionic liquid 1-butyl-3-methylimmidazolium dicyanamide ($[\mathrm{BMIM}]^+$ $[\mathrm{DCA}]^-$) with gelatin and water, we study the dynamic properties of ion jelly by depolarized dynamic light scattering (DDLS) and broadband dielectric spectroscopy (BDS). While BDS is sensitive to ion conductive dynamics, DDLS measures the rotational dynamics of the optical anisotropic ions. By combining both methods we can disentangle the translational and rotational dynamics in neat [BMIM][DCA] and show that this dynamics is present nearly unchanged in the matrix of the ion jelly. However, DDLS measurements show that additional slow dynamic modes arise in the ion jelly which we tentatively ascribe to ions, which are slowed down in the proximity of the gelatin matrix.

CPP 69.3 Wed 15:45 ZEU 222
Molecular resolution force probe studies of confined molecular liquids — •Hsiu-Wei Cheng[1], Markus Mezger[2], and Markus Valtiner[1] — [1]TU Wien, Applied Physics, Vienna, AT — [2]MPI f. Polymer Research, Mainz, DE

Being able to probe structures and ion mobility of molecular liquids in nanometer confined cavities/pores is central for a fundamental understanding and steering of various processes. We will show how force probe experiments can be utilized for studying interfacial physics of molecular fluids confined at solid/liquid/solid interfaces. The talk will discuss recent technological achievements, and we will illustrate how micro-to-nano and ultimately subnanometer confinement can be achieved and probed using the Surface Forces Apparatus. Here, we will further discuss how high resolution AFM imaging and X-ray probes can complement the surface forces apparatus to reveal structural and dynamic information of ionic liquids and aqueous electrolytes, as well as their mixtures, at surfaces, and in confinement between two solid surfaces. We will also discuss how molecular interactions drive structural arrangement of liquids during electrochemical polarization of surfaces and interfaces.

CPP 69.4 Wed 16:00 ZEU 222
Role of Image Charges in Ionic Liquid Confined between Metallic Interfaces — •Samuel Ntim and Marialore Sulpizi — Johannes Gutenberg Universität, Institut für Physik, Staudingerweg 9, 55128 Mainz

The peculiar properties of ionic liquids in confinement have not only become essential for energy storage, catalysis and tribology, but still pose fundamental questions. Recently, an anomalous liquid-solid phase transition has been observed in atomic force microscopy experiments for 1-butyl-3-methylimidazolium tetrafluoroborate ([BMIM][BF4]), the transition being more pronounced for metallic surfaces. Image charges have been suggested as the key element driving the anomalous freezing. Using atomistic molecular dynamics simulations, we investigate the impact of image charges on structure, dynamics and thermodynamics of [BMIM][BF4] confined between gold electrodes. Our results not only unveil a minor role played by the metal polarisation, but also provide a novel description of the interfacial layer. Although no diffuse layer can be defined in terms of the electrostatic potential, long range effects are clearly visible in the dynamical properties up to 10 nanometers away from the surface, and are expected to influence viscous forces in the experiments.

CPP 69.5 Wed 16:15 ZEU 222
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 $\mathrm{C_{10}mim^+Cl^-}$ 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 69.6 Wed 16:30 ZEU 222
Solvent effect on electrical double layers (EDL) in ionic liquid (IL) solutions — •Takeshi Kobayashi[1], Maria Fyta[1], and Jens Smiatek[2] — [1]Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Boehringer Ingelheim Pharma GmbH & Co. KG, Development Biologicals, Biberach, Germany

The solvent effect on EDL in IL is studied through atomistic molecular dynamics (MD) simulations. Water and dimethyl sulfoxide (DMSO) in 1-Ethyl-3-methylimidazolium dicyanamide ([EMIM]+[DCA]-) in different concentrations show distinct features regarding the molecule accumulation near surfaces. A comparison between neutral [1] and charged surfaces clarifies the influence of the molecular size, molecule-molecule interactions, and surface-molecule interactions. Due to the large molecular size of DMSO, the accumulation of DMSO near the cathode is limited even at a high DMSO concentration. This indicates that DMSO hardly changes the EDL properties, while improving the conductivity of the solution. On the other hand, water accumulates near the surfaces regardless of the surface charge. This is not beneficial for practical applications due to the narrowing of the electrochemical window, though the total capacitance may increase. In order to further interpret the simulation results, we apply the lattice gas theory [2]. This allows us to understand the solvent effect for the prediction of better combinations of IL mixtures for EDL capacitors. [1] T. Kobayashi at al., J. Phys. Chem. C 2019, 123, 22, 13795-13803 [2] Alexei A. Kornyshev, J. Phys. Chem. B 2007, 111, 20, 5545-5557

15 min. break

Invited Talk CPP 69.7 Wed 17:00 ZEU 222

Charging Dynamics and Structure of Ionic Liquids in Nanoporous Supercapacitors — •Christian Holm[1], Konrad Breitsprecher[1], and Svyatoslav Kondrat[2] — [1]Universität Stuttgart, Institut für Computerphysik, Allmandring 3, 70569 Stuttgart — [2]Department of Complex Systems, Institute of Physical Chemistry, PAS, Kasprzaka 44/52, 01-224 Warsaw, Poland

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, M. Janssen, S. Kondrat, C. Holm, in preparation.

CPP 69.8 Wed 17:30 ZEU 222

Barrier-crossing infrared spectral signatures of proton-transfer dynamics in the $H_5O_2^+$ cation — •Florian N. Brünig and Roland R. Netz — Institut für theoretische Physik, Freie Universität Berlin

The direct intermediate of the excess-proton transfer in water is the $H_5O_2^+$ or Zundel cation, the simplest system for which the excess proton performs a barrier crossing, separating two meta-stable configurations, namely the association to either one of the two water molecules. Several recent 2D infrared spectroscopy studies identify a low-barrier double-well potential for this proton transfer between two water molecules in the bulk phase [1,2], which was confirmed in simulations and associated with continuum bands [3]. We now developed a general theory to predict the spectral signature of barrier-crossing processes and applied it to trajectories obtained from ab-initio molecular-dynamics simulations of the $H_5O_2^+$ cation thus capturing non-linearities and line shapes. We find three distinct contributions: the quasi-harmonic motion around the most probable configurations, which can be understood by normal-mode analysis, the fast transition-path contribution over the barrier and a low-frequency tail.

[1] Elsaesser, T. et. al. (2017) Science, 357, 491-495.

[2] Tokmakoff, A. et. al. (2018) Nature Chemistry, 10, 932-937

[3] Netz, R. R. et. al. (2018) Nature Communications, 9, 311

CPP 69.9 Wed 17:45 ZEU 222

Polysulfobetaines in aqueous solution — Bart-Jan Niebuur[1], Jonas Puchmayr[1], Viet Hildebrand[2], Peter Müller-Buschbaum[1,3], André Laschewsky[2,4], and •Christine M. Papadakis[1] — [1]TU München, Physik-Department, Fachgebiet Physik weicher Materie/Lehrstuhl für Funktionelle Materialien, 85748 Garching — [2]Institut für Chemie, Universität Potsdam, 14476 Potsdam-Golm — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching — [4]Fraunhofer Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm

Polysulfobetaines feature zwitterionic groups in their side groups. In aqueous solution, they show upper critical solution temperature (UCST) behavior. Their clearing point depends sensibly on the detailed molecular structure [1] and is very different in H_2O and D_2O. For some representatives of this class, the clearing point depends in a non-linear way on salt concentration [2]. Using dynamic light scattering, we investigate the temperature dependence of the diffusional behavior of poly(N,N-dimethyl-N-(3-(methacrylamido)propyl)ammoniopropane sulfonate) in dependence on molar mass and NaBr concentration in aqueous solution and find non-mean-field scaling behavior [3]. We discuss possible reasons for the peculiar behavior.

1. V. Hildebrand et al., *Polym. Chem.* **2016**, *7*, 731.
2. V. Hildebrand et al. *J. Biomater. Sci., Polym. Ed.* **2014**, *25*, 1602.
3. B.-J. Niebuur et al., *Materials* **2018**, *11*, 850.

CPP 69.10 Wed 18:00 ZEU 222

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 69.11 Wed 18:15 ZEU 222

Thermodynamics of NiPAM in Water: Insight from Experiments, Simulations and KB-Analysis — Jakub Polak, Daniel Ondo, and •Jan Heyda — University of Chemistry and Technology, Prague, Czechia

The behavior of thermoresponsive polymer PNiPAM in aqueous solutions attracted a lot of interest. Strikingly, the physico-chemical properties of aqueous NiPAM are similarly rich, but our knowledge is far from being complete. This stems from the lack of accurate thermodynamic data and quantitative model for atomistic simulations. In this joined study, we have probed the thermodynamic behavior of aqueous NiPAM by experimental methods, MD simulations, and Kirkwood-Buff (KB) analysis at ambient conditions.

From the partial molar volumes and simultaneously correlated osmotic coefficients, with excess partial molar enthalpies of NiPAM in water the concentration and temperature dependence of KB-integrals was determined. Microscopic insight in NiPAM-NiPAM, NiPAM-water, and water-water interactions is gathered from atomistic MD simulations, employing a novel NiPAM force-field, which reproduces KB-integrals and macroscopic thermodynamic quantities.

CPP 69.12 Wed 18:30 ZEU 222

Different solvation of elastin-like proteins in water-ethanol and -urea mixtures — •Yani Zhao[1], Manjesh K. Singh[1,2], Kurt Kremer[1], Robinson Cortes-Huerto[1], and Debashish Mukherji[3] — [1]Max-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Mechanical Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India — [3]Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver V6T 1Z4, Canada

Elastin-like polypeptides (ELPs), as recent experiments have confirmed, exhibit co-non-solvency behaviour in aqueous-ethanol mixtures. This phenomenon is typically associated with a wide range of synthetic (smart) polymers. Since ELPs are biopolymers, it is reasonable to use the available theoretical machinery to investigate their solvation effects. In this talk, we present the phase behaviour of peptides and ELPs in aqueous binary mixtures using molecular dynamics simulations. To this aim, we use all-atom and complementary explicit solvent generic models. The model parametrisation results from mapping the solvation free energy, obtained from the all-atom simulations, onto the generic interaction parameters. We derive segment-based generic parameters for four peptides: proline (P), valine (V), glycine (G) and alanine (A). Hence, we compare conformational behaviour of two ELP sequences, $(VPGGG)_{10}$ and $(VPGVG)_{10}$, in aqueous-ethanol and -urea mixtures.

CPP 70: Hybrid Perovskite and Photovoltaics II (joint session CPP/HL)

Time: Wednesday 15:00–16:15 Location: ZEU 260

CPP 70.1 Wed 15:00 ZEU 260

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.

CPP 70.2 Wed 15:15 ZEU 260

Shallow Nano-Textures for Light Management in Solution-Processed Perovskite Solar Cells — •Philipp Tockhorn[1], Johannes Sutter[1], Klaus Jäger[1], Amran Al-Ashouri[1], Christiane Becker[1], and Steve Albrecht[1,2] — [1]Helmholtz Zentrum Berlin - 12489 Berlin — [2]Technische Universität Berlin - 10623 Berlin

Metal halide perovskites have led to highly efficient thin-film solar cells in the past decade. Here, we report enhanced PCEs achieved by light management in spin-coated perovskite single junction solar cells on shallow nano-textures. For this, sinusoidal nano-textures with a period of 750 nm and a texture height of 380 nm are employed. In our p-i-n devices, the nano-textured substrate is coated with a bottom contact comprising ITO and a self-assembling monolayer as well as a spincoated perovskite, while the top contact is realised by evaporation. With this design, we obtain a PCE of 18.9%, which marks an increase of 3% with respect to its planar reference. This efficiency gain is mostly achieved by an increase in short circuit current density (Jsc), achieved through enhanced light scattering by the sinusoidal nano-textures. External quantum efficiency and reflectance measurements on these devices confirm the observed increase in Jsc of about +1 mA/cm2 promoted by the improved light in-coupling. Furthermore, we observe a systematic reduction of 10-20 mV in open-circuit voltage on the nano-textured devices. Therefore, we investigate the influence of the nano-textures on the electronic quality of the perovskite itself and its interfaces to charge selective contacts with absolute photoluminescence measurements as well as electrical simulations.

CPP 70.3 Wed 15:30 ZEU 260

Electronic structure nonionic surfactant-mixed PEDOT:PSS and its effects on perovskite solar cells — •Dongguen Shin[1,2,3], Donghee Kang[3], Na Eun Jung[3], and Yeonjin Yi[3] — [1]Institut für Physik & IRIS Adelershof, Humboldt-Universität zu Berlin, Brook-Taylor Straße 6, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]Institute of Physics and Applied Physics, Yonsei University, 50 Yonsei-ro, Seodaemoon-Gu, Seoul 03722, Republic of Korea

PEDOT:PSS, generally used hole transport layer, has the limitation of increasing the performance of perovskite solar cells (PSCs) due to its semi-metallic properties. One of the manners of tailoring the electronic properties of PEDOT:PSS is mixing of the nonionic surfactant (e.g. Triton X-100 (TX)) into PEDOT:PSS, which supposedly get the affirmative impact on the charge extraction and exciton quenching at the interface. In this work, we explore the electronic structure of PEDOT:PSS with nonionic surfactant TX mixture by using the X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) measurement, and investigate the power conversion efficiency (PCE) enhancement of perovskite solar cells (PSCs) by using the mixture of PEDOT:PSS and TX surfactant in PSCs. we reveal that it led to the prevention of interfacial recombination as the insulating tunneling layer without energetic junction loss at the interface MAPbI3 with PEDOT:PSS. Consequently, we establish an efficient charge extraction condition without the interfacial recombination on PSCs.

CPP 70.4 Wed 15:45 ZEU 260

In-situ study of slot-die printed titania films for up-scale fabrication of all-solid-state dye-sensitized solar cells — •Nian Li[1], Wei Chen[1], Manuel Scheel[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1,3] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany. — [2]Deutsches Elektronen-Synchrotron DESY Notkestrasse 85, D-22603 Hamburg, Germany. — [3]Heinz Maier-Leibnitz Zentrum (MLZ) Technische Universität München Lichtenbergstr. 1, D-85748 Garching, Germany.

Printing, a simple and low-cost technique, is employed to fabricate mesoporous titania films as electron-transporting layers for upscaling all-solid-state dye-sensitized solar cells (DSSCs). The deposition methods strongly affect the final titania morphology, and further solar cell efficiency. Therefore, a detailed understanding of structure formation is of crucial importance for optimizing the industrial coating films. In the present work, we provide insights into the structure evolution of slot-die printed films via in situ grazing-incidence small-angle X-ray scattering (GISAXS). The printing-solution synthesis is performed by sol-gel chemistry and a structure-directing template polystyrene-block-polyethylene oxide (PS-b-PEO) to achieve the structure tailoring. The evolution of nanostructure length scales of the titania/PS-b-PEO composite film is revealed in real-time and in situ during slot-die printing. The resulting mesoporous titania films with highly ordered structures serve as photoanodes of all-solid-state DSSCs.

CPP 70.5 Wed 16:00 ZEU 260

The role of anchors for the efficiency of p-type dye-sensitized solar cells — •Miftahussurur Hamidi Putra and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

In recent years, p-type dye-sensitized solar cells (pDSSC) have attracted a lot of attention as an alternative to conventional solar cells. However, the efficiency of this solar cell is still below 10% which hampers their utilization. One of the promising type of dyes for p-DSSC solar cells are ruthenium-based complexes $[Ru(bpy)_3]^{2+}$ [1]. The efficiency of p-DSSCs is critically influenced by the anchors through which they are bound to a semiconductor substrate such as NiO. First-principles electronic calculations based on time-dependent density functional theory (TDDFT) have been performed in order to evaluate the performance of various candidates for anchoring $[Ru(bpy)_3]^{2+}$ complexes. Results will be presented and discussed with respect to properties that are related to the efficiency of p-DSSC solar cells, such as injection free energy (ΔG_{inj}), light harvesting efficiency (LHE), hole injecting efficiency (HJE), regeneration free energy (ΔG_{reg}) and

the excited state lifetime (τ) [1,2].
[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. Photobiol. A: Chem. **219**, 235 (2011).
[2] A. Sen and A. Groß, Int. J. Quantum Chem. **119**, e25963 (2019).

CPP 71: Modelling and Simulation of Soft Matter II (joint session CPP/DY)

Time: Wednesday 15:00–16:45 Location: ZEU 255

CPP 71.1 Wed 15:00 ZEU 255

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.

CPP 71.2 Wed 15:15 ZEU 255

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 71.3 Wed 15:30 ZEU 255

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 71.4 Wed 15:45 ZEU 255

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 particle-based simulations. Albeit ECMC is a monte-carlo 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.

CPP 71.5 Wed 16:00 ZEU 255

Analytical and computational study of advection-diffusion-reaction processes in catalytic fibrous membranes — •Gabriel Sitaru and Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth

We investigate the efficiency of multi-step catalytic systems where a reactant species is flown through a set of fibrous catalytic membranes. The complexity of such systems arises from the interplay of three different time scales: advection, diffusion and reaction. A theory based on infinitely long cylindrical catalytic sites is developed for the steady-state of an advection-diffusion limited reaction. Additionally, the time-dependent concentration profiles are computed using a Lattice-Boltzmann based solver for both the advection-diffusion-reaction and the Navier-Stokes equations. The comparison shows a good agreement between the theory and the numerical results, our model breaking down only in the very low-Péclet regime (i.e. diffusive flow). Both methods can be easily used to predict the efficiency of a multi-step catalysis in fibrous membranes with various geometries.

CPP 71.6 Wed 16:15 ZEU 255

The stability field of the chiral CO2 water hydrate from molecular dynamics simulations — •Marcello Sega[1], Jakob Michl[2], and Christoph Dellago[2] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany — [2]Faculty of Physics, University of Vienna, Austria

Recent experimental evidence[1] shows that the water network characterizing the high-pressure CO2 hydrate[2] is, in fact, ice XVII, which possesses open helicoidal channels giving the structure a chiral nature. The question of the stability field boundaries of this hydrate is still open, and we report on recent molecular dynamics simulations[3] in which we found that the CO2-filled ice XVII is more stable than the sI clathrate and than the mixture of ice VI and dry ice at pressure values ranging from 6 to 18 kbar and in a wide temperature range. We propose a phenomenological correction to take into account the limitation of the model potentials, suggesting that the stability should more realistically range from 6.5 to 13.5 kbar. Our simulation results support the current hypothesis that the chiral CO2 hydrate is stable at temperatures above the melting curve of ice VI.

[1]L. Del Rosso, M. Celli, and L. Ulivi, Nat. Comm. 7, 13394 (2016)

[2]H. Hirai, K. Komatsu, M. Honda, T. Kawamura, Y. Yamamoto, and T. Yagi, The J. Chem. Phys. 133, 124511 (2010)

[3]J. Michl, M. Sega, and C. Dellago, J. Chem. Phys. 151, 104502 (2019)

CPP 71.7 Wed 16:30 ZEU 255

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 72: Polymer Networks and Elastomers

Time: Wednesday 15:00–17:30 Location: ZEU 114

Invited Talk CPP 72.1 Wed 15:00 ZEU 114

Physics of Fiberboids — •Igor Kulic — CNRS, Institut Charles Sadron, 23 rue du Loess BP 84047, 67034 STRASBOURG Cedex 2

Fiberboids are filaments trapped at the interface between two phases, able of harnessing energy and matter fluxes across the interface to produce a rolling-like self-propulsion. We experimentally demonstrate several common driving mechanisms and develop the physical framework for understanding the complex active dynamics of fiberboids. The phenomenon is highly generic and plays a role across scales, from the macroscopic realm down to the nanoscale, where it gives rise to chemical fuel-driven surface motility of various filamentous viruses.

[1] A. Baumann, A. Sánchez-Ferrer, L. Jacomine, P. Martinoty, V. Le Houerou, F. Ziebert & I. M. Kulić , Motorizing fibres with geometric zero-energy modes , Nature Materials, 17, 523 (2018) [2] F. Ziebert & I. M. Kulic, Frustriert in Bewegung, Physik Journal 11 (2018)

CPP 72.2 Wed 15:30 ZEU 114

Swelling of tendomer networks: a model system for topological gels — •Toni Müller[1,2], Michael Lang[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]TU Dresden, Germany

A polyrotaxane (PR) consists of many small cyclic molecules (”rings”) threaded onto a long polymer chain where stopper monomers at the chain ends prevent detachment of the rings. Polymer networks can be constructed by linking the rings in solution of PRs. We discuss the tendomer as a model system where only their very first rings of the PRs are connected while all remaining rings, m, form a one-dimensional repulsive gas along the PR. Pulling on pairs of chain ends next to the connected rings induces a compression of the sliding rings confined on the two chains. We investigate the force extension relation of the tendomers by computer simulations and compute numerically the exact solution of full partition function in the constant force ensemble. Our results show that tendomers are stiff for low applied forces and soften dramatically when reaching a stall force that is triggered by the density of non-crosslinked rings on the PRs. For large deformations, the finite extensibility of the chains results again in a lower susceptibiliy regarding an applied force [1]. These results are inserted into the Flory-Rehner model predicting the equilibrium degree of swelling, Q, of gels made by crosslinking tendomers. We find that Q scales with m by a power law of 3/4 and that entanglements are negligible.

[1] Müller, T., Sommer, J.-U., Lang, M. (2019) Soft Matter, 15(18), 3671-3679

CPP 72.3 Wed 15:45 ZEU 114

An Analysis of the Gel Point of Polymer Model Networks by Computer Simulations — •Michael Lang and Toni Müller — Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden

The gel point of end-linked model networks is determined from computer simulation data. It is shown that the difference between the true gel point conversion, p_c, and the ideal mean field prediction for the gel point, $p_{c,id}$, is a function of the average number of cross-links per pervaded volume of a network strand, P, and thus, contains an explicit dependence on junction functionality f for stoichiometric model networks. On the contrary, the amount of intramolecular reactions at the gel point is independent of f in first approximation and exhibits a different power-law dependence on the overlap number of elastic strands as compared to $p_c - p_{c,id}$. Therefore, the delay of the gel point, $p_c - p_{c,id}$, cannot be predicted from intramolecular reactions and vice versa in contrast to a long standing proposal in the literature about polymer networks.

CPP 72.4 Wed 16:00 ZEU 114

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]Institute 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 a thermodynamic 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 72.5 Wed 16:15 ZEU 114

Constitutive modelling of magneto-sensitive elastomers — •Sanket Chougale, Dirk Romeis, and Marina Saphiannikova — Institute Theory of Polymers, IPF, Dresden, Germany

One type of field-controllable materials are magneto-sensitive elastomers (MSEs) with magnetically switchable properties. They consist of magnetizable particles incorporated within an elastomer matrix. In the presence of an external magnetic field, the induced magnetic interactions and the corresponding particle rearrangements change the mechanical properties substantially. This leads to change in the macroscopic shape of MSE. The magnetic field also introduces a mechanical anisotropy with an axis of symmetry along the field. As a results, MSE can be studied phenomenologically as a transversely isotropic material. Our aim to derive an effective material model from the free energy of MSE in the dipole approximation. As a first step we consider uniaxial deformations parallel and perpendicular to the applied field direction. We compare the stresses derived from the physical model of MSE with the stresses derived from the phenomenological model and find a good agreement. This allows us to extract the coefficients of transversely isotropic material model. We thank the DFG for financial support through RTG-2430.

CPP 72.6 Wed 16:30 ZEU 114

Nonlinear mechanics of physically crosslinked elastomers: from molecular simulations to network models — •Joerg Rottler[1] and Amanda Parker[2] — [1]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada V6T 1Z1 — [2]Data 61, CSIRO, Melbourne, Australia

Thermoreversible (physical) crosslinking is a versatile strategy for improving the strength and toughness of elastomers that also permits self-healing upon thermal cycling. There is no universally applicable theory for predicting their mechanical response because the mechanical response is governed by the microscopic polymer chain conformations during deformation that cannot easily be measured experimentally. Here, we present a family of entropic network models that account for the stress contributions arising from chain crosslinks as well as entanglements by coupling analytical expressions for the strain energy density directly with chain deformations obtained through molecular dynamics simulations. Our theory quantitatively reproduces the macroscopic stress response of simulated linear and star block copolymer elastomers well into the nonlinear regime. The simulations reveal the evolution of entanglements and how the breakup of physical crosslinks contributes to additional strain hardening. Although developed for a classic sphere forming ABA block copolymer system, our approach can readily be applied to any (bio)macromolecular network in which a rigid phase anchors polymer chains otherwise forming a rubbery matrix.

15 min. break

CPP 72.7 Wed 17:00 ZEU 114

Morphology of adhesive creases — •Michiel van Limbeek[1], Martin Essink[2], Anupam Pandey[3], Jacco Snoeijer[2], and Stefan Karpitschka[1] — [1]Max Planck Institue for Dynamics and Selforgization, Göttingen, Germany — [2]University of Twente, Enschede, the Netherlands — [3]Cornell University, Ithaca, the Unitied States of America

The compression of an elastic material beyond a certain strain turns the free surface to become unstable. The material makes a sharp fold of the surface onto itself, releasing elastic energy in the bulk. The resulting morphologies are observed in growing tissues and swelling gels. Self adhesion within the folded region is known to affect nucleation and hysteresis: A uncreased sample requires a higher critical strain for creasing than a previously creased one. However, a detailed description of the crease phenomena has remained elusive. Here we resolve the geometry and mechanics of adhesive creases. We combine numerical simulations, analysis and experimental results, where we pay specific attention to the singular edge of the self-contact, which we managed to visualize using confocal microscopy. In the region of self contact, a competition emerges between elastic and surface energies. We compare the morphology for different gel-stiffnesses and it turns out that adhesive creases exhibit a universal shape after proper rescaling. We derive a scaling theory for the aforementioned bifurcation scenario of the hysteresis, explaining the nucleation of adhesive creases.

CPP 72.8 Wed 17:15 ZEU 114

Tough and Instantly Recoverable Hydrogels: Self-Reinforcement by Strain-Induced Crystallization — •koichi mayumi[1], chang liu[1], jiang lan[1], takamasa sakai[2], hideaki yokoyama[1], and kohzo ito[1] — [1]Graduate School of Frontier Sciences, The University of Tokyo, Chiba, Japan — [2]Graduate School of Engineering, The University of Tokyo, Tokyo, Japan

Most tough hydrogels are reinforced by introducing sacrificial structures that can dissipate input energy [1]. However, since the sacrificial damages cannot recover instantly, the toughness of these gels drops substantially during consecutive cyclic loadings. In this presentation, we will propose a new damageless reinforcement strategy for hydrogels utilizing strain-induced crystallization (SIC). In Slide-Ring (SR) gels where polyethylene glycol (PEG) chains are cross-linked by rings [2,3], crystalline of PEG repetitively forms and destructs with elongation and relaxation, resulting in both excellent toughness of 5.5 to 25.2 MJ/m^3 and 87% to 95% instant recovery of extension energy between two consecutive loading-unloading cycles. The instantly reversible tough hydrogels are promising candidates for applications in artificial connective tissues such as tendon and ligament.

[1] J. P. Gong, Soft Matter, 6, 2583 (2010). [2] K. Ito, Polymer Journal, 39, 489 (2007). [3] L. Jiang, C. Liu, K. Mayumi, K. Kato, H. Yokoyama, K. Ito, Chemistry of Materials, 30, 5013 (2018).

CPP 73: Organic Electronics and Photovoltaics II

Time: Wednesday 16:15–18:30 Location: ZEU 260

CPP 73.1 Wed 16:15 ZEU 260

Investigation of Sub-Molecular Parts in Blends for Organic Solar Cells — •Arthur Markus Anton[1,2], Shahidul Alam[3], Rico Meitzner[3], Martin Hager[3], Johannes Ahner[3], Ulrich S. Schubert[3], Wichard J. D. Beenken[5], Daniel Ayuk Mbi Egbe[6], Friedrich Kremer[2], and Harald Hoppe[3,4] — [1]The University of Sheffield, Department of Physics &Astronomy, Sheffield, UK — [2]Leipzig University, Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — [3]Center for Energy and Environmental Chemistry, Jena, Germany — [4]Friedrich Schiller University Jena, Institute for Organic Chemistry and Macromolecular Chemistry, Jena, Germany — [5]Technische Universität Ilmenau, Institute of Physics, Ilmenau, Germany — [6]Johannes Kepler University Linz, Institute of Polymeric Materials and Testing, Linz, Austria

It is believed that orientation and order of molecular units play an essential role for the performance of organic semiconductors. On the basis of infrared transition moment orientational analysis (IR-TMOA) [1] it is demonstrated how the orientation and order of sub-molecular parts in PBDB-T:ITIC and AnE-PVstat:ITIC polymer:acceptor blends can be analyzed. On the one hand, PBDB-T:ITIC is well suited for bulk heterojunction solar cells; on the other hand, AnE-PVstat:ITIC fall short, although photoluminescence indicates efficient quenching of donor emission [2]. A reason for this seemingly contradiction can be provided on the basis of molecular orientation. [1] A. M. Anton et. al., J. Am. Chem. Soc. 137 (2015) 6034 [2] S. Alam et. al., Chem. Pap. 72 (2018), 1769

CPP 73.2 Wed 16:30 ZEU 260

Simulation of active layer formation and stability in solution-processed organic solar cells — •Olivier Ronsin and Jens Harting — Helmholtz Institute Erlangen- Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Straße 248, 90429 Nürnberg, Germany

Solution-processed organic bulk-heterojunction active layers form sophisticated structures during the drying of the wet-deposited solution, because of complex physical processes such as crystallization and/or liquid-liquid phase separation. This structure highly impacts the photovoltaic performance and is usually far from equilibrium and hence unstable. In order to reach significant improvements, a better understanding of the physics driving the active layer formation and stability is strongly needed.

We propose a phase-field simulation framework to determine the dry film structure. To this end, evaporation, crystal nucleation and growth, liquid-liquid phase separation are taken into account. We show the impact of the thermodynamic (especially miscibility) and kinetic (evaporation, diffusion and crystal growth rate) parameters on the time-dependent morphology of the wet film during drying up to the dry state. We also investigate the structural evolution of the dry film.

15 min. break

CPP 73.3 Wed 17:00 ZEU 260

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 73.4 Wed 17:15 ZEU 260

Triplet Exciton Losses in Polymer:Non Fullerene Acceptor Blends — •Stefanie Dietz, Hannah Lindl, Jannis Klotz, Maria Kotova, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic bulk heterojunction solar cells utilizing non fullerene acceptors (NFA) received a lot of attention in the past few years as their power conversion efficiency exceeds 16%. This is achieved by a closer matching of donor and acceptor energy levels, but has unfortunately led to a new loss pathway via the now energetically lower lying triplet exciton. We build high performance bulk heterojunction solar cells using the polymer PM6 (a fluorine substituted PBDB-T, PBDB-T-2F) and the NFA Y6 (a fluorine-substituted BTP, BTP-4F). To probe potential losses due to triplet formation we use inherently spin-sensitive methods based on electrical and photoluminescence detected magnetic resonance (EDMR, PLDMR). By comparing pristine materials, blends and ultimately solar cells under realistic operating conditions conclusions can be drawn about potential radiative and non-radiative losses and the involvement of triplet excited states in these organic solar cells.

CPP 73.5 Wed 17:30 ZEU 260

Charge separation in non-fullerene acceptor solar cells — •Frédéric Laquai — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center, Thuwal, Saudi Arabia

In organic solar cells, the energetic landscape at the donor-acceptor interface provides the driving force for charge separation. The precise mechanism of and the prerequisites for efficient charge separation have been investigated intensively in fullerene-based systems. However, with the recent development of novel high-efficiency non-fullerene acceptors (NFAs), several of the findings previously obtained on fullerene-based systems are currently being revisited for NFA-based systems. In this contribution, I present our latest insight into the photophysical processes in NFA-based systems obtained by a combination of steady-state and transient (ultrafast) spectroscopy techniques. More precisely, I report on the driving force required for charge separation in a series of polymer and small molecular donor / NFA blends, including some of the current state-of-the-art material systems. Interestingly, we found that it is the ionization energy (IE) offset, which dominates the charge separation efficiency in many NFA-based systems, while the electron affinity (EA) offset seems to be of minor importance. The reasons for this striking observation and the implications for future donor / acceptor material design strategies are discussed.

CPP 73.6 Wed 17:45 ZEU 260

Effect of Solvent Additives on the Morphology and Device Performance of Printed Non-fullerene Acceptor Based Organic Solar Cells — •Kerstin S. Wienhold[1], Volker Körstgens[1], Sebastian Grott[1], Xinyu Jiang[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]1TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]2DESY, 22607 Hamburg — [3]3KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [4]4Heinz Maier-Leibnitz-Zentrum, Lichtenbergstr. 1, 85748 Garching, Germany

Printing of active layers of high efficiency organic solar cells with a meniscus-guided slot-die coater enables up-scaling of the solar cell production. However, an optimization of this thin film deposition is necessary as insights gained from spin-coating cannot simply be transferred to printed photovoltaics. In this work, active layers of the conjugated polymer PBDB-T-SF and the non fullerene small molecule acceptor IT 4F are slot die coated with different concentrations of 1,8 diiodoctane (DIO) and the effect on the inner nano structure and surface morphology of the material is studied with grazing incidence small angle X-ray scattering (GISAXS), grazing incidence wide angle X ray scattering (GIWAXS), scanning electron microscopy (SEM) and atomic force microscopy (AFM). The optical properties are studied with photoluminescence (PL), UV/Vis absorption spectroscopy and external quantum efficiency (EQE) measurements and correlated to the corresponding power conversion efficiencies.

CPP 73.7 Wed 18:00 ZEU 260

Barrierless free charge generation in the high-performance PM6:Y6 bulk heterojunction non-fullerene solar cell — •Lorena Perdigón-Toro[1], Huotian Zhang[2], Anastasia Markina[3], Feng Gao[2], Denis Andrienko[3], Safa Shoaee[1], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden — [3]Max Planck Institute for Polymer Research, Mainz, Germany

Organic solar cells are currently experiencing a second golden age thanks to the development of novel non-fullerene acceptors (NFAs). Surprisingly, some of these blends exhibit high efficiencies despite a low energy offset at the heterojunction. In this work, we investigate photocurrent generation in the high-performance blend of the donor polymer PM6 with the NFA Y6 as a function of internal field and excitation energy by means of time-delayed collection field (TDCF). Results show that generation is essentially barrierless with near-unity efficiency, regardless of excitation energy. Complementary temperature-dependent external quantum efficiency and open-circuit voltage measurements reveal that efficient generation is maintained over a wide temperature range, down to 100 K, despite the small driving force for charge generation. Studies on a blend with a low concentration of the NFA, measurements of the energetic disorder, and theoretical modelling suggest that charge generation is assisted by the electrostatic interfacial field which for Y6 is large enough to compensate the Coulomb dissociation barrier.

CPP 73.8 Wed 18:15 ZEU 260

Impact of Thermal Treatment and Humidity on Work Function of PEDOT:PSS Thin Films — •Aman Anand[1,2,3], Jose Prince Madalaimuthu[1,2,3], Rico Meitzner[1,2,3], Shahidul Alam[1,2,3], Ulrich S. Schubert[1,2,3], and Harald Hoppe[1,2,3] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany — [3]Jena Center for Soft Matter (JCSM), Friedrich Schiller University, Jena, Germany

Poly (3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is the most common and commercially, successful conductive polyelectrolyte in the field of optoelectronics. Its properties such as high transparency in the visible range, electrical conductivity, and work function enable multiple applications in the field of electronics. Properly tuning the work functions within semiconductor devices is very crucial in terms of performance and may be strongly influenced by unmonitored processing conditions. For example, PEDOT:PSS is highly hygroscopic in nature, which may impact on its functionality. 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. We find clear trends between the processing conditions and absolute work function as obtained with a carefully calibrated Kelvin Probe setup. As a conclusion, we can suggest suitable processing parameters for a wide range of formulations and targeted electronic properties.

CPP 74: Tribology: Surfaces and Nanostructures (joint session O/CPP)

Time: Wednesday 15:00–16:00 Location: GER 37

CPP 74.1 Wed 15:00 GER 37

Effect of Environment on Microstructure Evolution and Frictional Behavior of Au-Ni Multilayers — •Ebru Cihan[1,2], Heike Störmer[3], Katherine Jungjohann[4], Nicolas Argibay[5], Michael Chandross[5], and Martin Dienwiebel[1,6] — [1]Institute for Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany — [3]Laboratory for Electron Microscopy (LEM), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [4]Center for Integrated Nanotechnologies (CINT), Sandia National Laboratories, 87185 Albuquerque, NM, USA — [5]Material, Physical, and Chemical Sciences Center, Sandia National Laboratories, 87185 Albuquerque, NM, USA — [6]Fraunhofer Institute for Mechanics of Materials (IWM), MicroTribology Center μTC, 79108 Freiburg, Germany

We present results from a systematic investigation of environmental effects on microstructure and frictional behavior of Au-Ni multilayer films of varying interlayer spacing. Multilayer samples were initially analyzed under UHV and it was demonstrated that the interlayer spacing has a strong impact on friction due to the transition in the dominant deformation mechanism near the surface. A newly shear-induced phase, which can be interpreted as an AuNi alloy (60-65 at% Ni in Au) was observed in the tribolayer for thinner samples. Subsequently, experiments were performed in dry-nitrogen and higher friction forces were measured, leading to different microstructure evolution.

CPP 74.2 Wed 15:15 GER 37

Tuning the friction properties of reconstructed KBr on Ir(111) by intercalating a monolayer of graphene — Zhao Liu[1], Antoine Hinaut[1], Thilo Glatzel[1], Sebastian Scherb[1], Junyan Zhang[2], and •Ernst Meyer[1] — [1]Department of Physics, University of Basel, 4056 Basel, Switzerland — [2]State Key Laboratory of Solid Lubrication, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, 730000 Lanzhou, People's Republic of China

The intercalation of graphene and other 2D materials is an effective approach to alter the structures and properties of the top conductive or insulated layers on metal surface [1]. In this work, the growth of KBr islands on Ir(111) is characterized via non-contact atomic force microscopy and friction force microscopy measurement at room temperature in ultrahigh vacuum. We observed the formation of KBr monolayer with highly corrugated superstructure. These superstructures are due to the adaptation of the KBr atoms to the substrate lattice resulting from a tiny misfit of the KBr islands lattice. The superstructure presents a higher friction force of KBr/Ir(111) compared to the bulk KBr(001) as well [2]. We also show the possibility to tune the friction properties of KBr by intercalating a graphene monolayer. Obviously, the reduced friction force is accompanied by the vanishing of the KBr superstructure, with the observation of the common cubic configuration. It gives another view to increase the critical normal load to maintain the superlubric state at the nano scale.

[1] M. Andersen, et al, Phys. Rev. B, 90 (2014) 155428. [2] C. Wieferink, et al, Phys. Rev. B, 83 (2011) 235328.

CPP 74.3 Wed 15:30 GER 37

Stick-slip and surface rippling in plastic and abrasive wear on the nanoscale — •Enrico Gnecco[1], Jana Hennig[1], and Juan Mazo[2] — [1]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Germany — [2]Department of Condensed Matter Physics, University of Zaragoza, Zaragoza, Spain

The formation of regular surface structures as a result of plastic and abrasive wear processes is a general but scarcely understood phenomenon. Here we will discuss this topic with the examples of polymer [1] and silica glass surfaces [2] scratched by silicon and diamond nano- and microtips respectively. In spite of the different nature of the nanoscopic wear mechanisms, quasi-periodic ripple patterns are formed in both cases. The physical interpretation of the observed structures relies on the time evolution of the friction forces acting in the stick-slip motion of the tip, which is simultaneously indented and elastically pulled along the surfaces in order to scratch them. The geometric shapes of the surface structures as well as their dependence on the scan velocity are consequently reproduced by solving the corresponding equations of motion of the tips in an evolving energy landscape.

[1] J.J. Mazo et al., Phys. Rev. Lett. 122 (2019) 256101 [2] E. Gnecco et al., Phys. Rev. Materials 2 (2018) 115601

CPP 74.4 Wed 15:45 GER 37

Temperature Scaling of Contact Aging Rates on Amorphous Silica Surfaces — Matthias Vorholzer[1], J. Guilherme Vilhena[2], Ruben Perez[3], Enrico Gnecco[4], •Dirk Dietzel[1], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig-Universität Giessen, 35392 Giessen, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [4]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, 07742 Jena, Germany

Contact ageing is a fundamental aspect to understand dynamic sliding scenarios with alternating phases of halting and sliding. On the nanoscale, recent experiments showed, that ageing effects can be connected to the formation of interfacial bonds. In this work, we now analyze the temperature dependent bond formation dynamics of silica contacts by measuring the pre-rupture contact stiffness. Using this parameter instead of the seemingly more obvious choice of measuring static friction, we can eliminate all effects related to temperature dependent contact rupture. Our results show logarithmic contact ageing at all temperatures and reveal that the ageing can be described by a temperature dependent slope $\alpha(T) \propto T$, which is a characteristic fingerprint of thermal activation, anticipated both by analytical calculations and MD-simulation of the bond formation process.

CPP 75: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)

Time: Wednesday 15:00–17:30 Location: GER 38

Invited Talk CPP 75.1 Wed 15:00 GER 38

Electron-phonon interactions in realistic materials — •Fabio Caruso — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Functional materials used in actual devices are typically doped, they operate at finite temperature, and they may be subject to perturbations such as, *e.g.*, external fields and light pulses. These aspects may alter profoundly the electron-phonon interaction (EPI), its influence on the electronic properties of solids, and even lead to the manifestation of novel emergent phenomena absent in perfect crystals.

We conducted a first-principles investigation of the EPI in functional materials at realistic operational conditions based on many-body perturbation theory. Our work reveals that: (i) n-type doping of polar oxides, such as EuO and $\mathrm{TiO_2}$, allows one to trigger and control the formation of polarons (electrons dressed by a phonon cloud) [1]; (ii) in the record-breaking thermoelectric material SnSe, temperature may lead to a five-fold suppression of carrier lifetimes due to enhanced phonon emission [2]. Overall, the striking sensitivity to doping, temperature, and external fields, makes the EPI a powerful tool to tailor the opto-electronic properties of quantum materials. Possible strategies to extend the many-body theory of the EPI to the study of time-dependent phenomena will further be discussed [3].

[1] J. Riley, F. Caruso, C. Verdi, *et al.*, Nature Commun. **9** (1), 2305 (2018). [2] F. Caruso, M. Troppenz, S. Rigamonti, C. Draxl, Phys. Rev. B **99** (8), 081104 (2019). [3] F. Caruso, D. Novko, C. Draxl, arXiv:1909.06549v (2019).

CPP 75.2 Wed 15:30 GER 38

Fully Anharmonic, Non-Perturbative First-Principles Theory of Electronic-Vibrational Coupling in Solids — Marios Zacharias, Matthias Scheffler, and •Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The coupling between nuclear vibrations and the electronic structure plays a pivotal role for many material properties, including optical absorption and electronic transport. In this regard, however, today's state-of-the-art methodologies rely on two approximations [1]: the harmonic (phonon) approximation for the nuclear motion and the linear response description of the electronic structure with respect to harmonic displacements. In this work, we overcome ***both*** these approximations by performing fully anharmonic *ab initio* molecular dynamics (*ai*MD) calculations and by accounting for the non-perturbative, self-consistent response of the wave functions along the *ai*MD trajectory. By this means, we obtain fully anharmonic, vibronically renormalized spectral functions, from which macroscopic material properties like temperature-dependent band gaps and electronic transport coefficients are obtained. We validate our approach using silicon as an example, for which the traditional electron-phonon coupling formalism is recovered. Using cubic $SrTiO_3$ as example, we further demonstrate that anharmonic electronic-vibrational coupling effects are not captured in traditional formalisms, but they play a decisive role here and in other complex materials like perovskites.

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).

CPP 75.3 Wed 15:45 GER 38

Thermal conductivity of highly-doped Si: Role of electron-phonon and point-defect phonon scattering — •Bonny Dongre[1], Jesús Carrete[1], Shihao Wen[2], Jinlong Ma[2], Wu Li[2], Natalio Mingo[3], and Georg KH Madsen[1] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria. — [2]Institute for Advanced Study, Shenzhen University, Shenzhen 518060, China — [3]LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France.

Theoretical investigation of the thermal conductivity reduction in highly-doped Si is an area of active research. Recently, first-principles electron-phonon scattering was found to produce a significant reduction in the thermal conductivity of highly-doped Si. However, the study could not reproduce the experimental results.

In the present work, we calculate the first-principles phonon scattering rates by electrons and point defects, and use them to calculate the thermal conductivity of highly-P- and B-doped Si for a range of temperatures and concentrations. We find that the phonon scattering by electrons dominates at carrier concentrations below 10^{19} cm^{-3} and is enough to reproduce the experimental thermal conductivity reduction at all temperatures. However, at higher defect concentrations point-defect phonon scattering contributes substantially to the thermal conductivity reduction even at room temperature. With a combined treatment of the phonon scattering by electrons as well as phonons, an excellent agreement is obtained with the experimental values at all temperatures.

CPP 75.4 Wed 16:00 GER 38

Precise yet Fast High-Throughput Search for Thermal Insulators — •Florian Knoop, Thomas A.R. Purcell, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft

We present a systematic and numerically precise computational search for thermal insulators in material space performed with the *FHI-vibes* high-throughput framework [1]. *FHI-vibes* employs a robust metric that quantifies the degree of anharmonicity in the nuclear dynamics via the statistical comparison of first-principles forces with those forces that would act in the harmonic approximation. This enables us to efficiently scan over many materials, including complex oxides and chalcogenides as well as ternary structures like perovskites. By this means, we single out strongly anharmonic systems, for which we perform *ab initio* Green-Kubo simulations to assess their thermal conductivities, thereby naturally including all anharmonic effects [2]. Our strategy allows to avoid redundant calculations and to achieve a much higher quality of information than traditional high-thoughput studies. Besides validating the performed search and analyzing its results, we discuss how big-data analytics techniques can be utilized to further accelerate and guide this search.

[1] https://vibes.fhi-berlin.mpg.de

[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017)

CPP 75.5 Wed 16:15 GER 38

Ambivalent Impact of Electron-Phonon Interaction on Electronic and Transport Properties of Organic Semiconductors — •Frank Ortmann — Center for Advancing Electronics Dresden, Technische Universität Dresden, Germany

Vibrations are omnipresent in molecules and of great importance in Organic Semiconductors due to the softness of the materials and the strong electron-phonon coupling. One possibility to investigate this interaction is to study the low-energy edge of optical absorption spectra, which lacks an in-depth understanding for organic materials. We have recently observed a strong dependence of low-energy excitonic features on the molecular building blocks in organic films, which we associated to molecular flexibility and polaron deformation. We will discuss implications of low-frequency molecular vibrations on the polaronic and excitonic density of states in donor-acceptor mixtures featuring charge-transfer excitons. We will also discuss how a distinguished treatment of strong-coupling molecular vibrations of different energies leads to an improved description of charge carrier transport in organic materials.

CPP 75.6 Wed 16:30 GER 38

Quantum Nuclear Effects in Thermal Transport of Semiconductors and Insulators — •Hagen-Henrik Kowalski[1], Mariana Rossi[1,2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany

To date, the computation of thermal conductivities relies on either perturbation theory or (*ab initio*) molecular dynamics (MD) [1]. While perturbative approaches include quantum-nuclear effects (QNE), they typically neglect higher orders of anharmonicity. Conversely, classical MD includes all orders of anharmonicity, but neglects QNEs. To overcome these limitations, we have developed a formalism that accounts for ***both*** quantum-nuclear effects and all orders of anharmonicity. For this purpose, the nuclear dynamics are assessed via Thermostatted Ring Polymer MD (TRPMD) [2] and the thermal conductivity is obtained via the Green-Kubo formalism using a newly proposed TRPMD based heat-flux estimator. Using solid Argon and Silicon as model systems, we discuss the influence of QNEs on thermal transport by comparing velocity, energy, and heat-flux autocorrelation spectra. This allows to rationalize the impact of QNEs on vibrational frequencies, lifetimes, and on the thermal conductivity in different temperature regimes.

[1] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).

[2] M. Rossi, M. Ceriotti, D. Manolopoulos, *J. Chem. Phys.* **140**, 234116 (2014).

CPP 75.7 Wed 16:45 GER 38

Speeding-up *ab initio* molecular dynamics with hybrid functionals using adaptively compressed exchange operator based multiple time stepping — •Sagarmoy Mandal and Nisanth N. Nair — Department of Chemistry, Indian Institute of Technology Kanpur, India

Ab initio molecular dynamics (AIMD) with hybrid density functionals and a plane wave basis is known to predict the structural and dynamical properties of condensed matter systems accurately. However, such hybrid functional based AIMD simulations are not routinely used due to the high computational cost associated with the application of the Hartree-Fock exchange operator. We propose a strategy [1] to combine the Adaptively Compressed Exchange (ACE) operator formulation [2] and a multiple time step integration scheme to reduce the computational cost significantly. We also show that computing the ACE operator with localized orbitals can further improve the computational efficiency. Finally, we use this method in combination with the Well-Sliced Metadynamics approach to compute the free energy barrier of chemical reactions in systems containing hundreds of atoms.

[1] S. Mandal, N.N. Nair, J. Chem. Phys. **151** (2019) 151102.

[2] Lin Lin, J. Chem. Theory Comput. **12** (2016) 2242.

CPP 75.8 Wed 17:00 GER 38

Calculation of current-induced heating and vibrational instabilities in single molecule circuits — Giuseppe Foti and •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Current-induced heating in molecular wires arises from the interaction between tunneling electrons and localized vibrations. Vibrational instabilities occur when excitation of molecular vibrations is not balanced by dissipation mechanisms, and can lead to the breakdown of the junction. In this talk I will address predictions for vibrational instabilities in single molecule junctions with separated unoccupied resonances. We use DFT-NEGF to study the electronic structure of the junction under an applied bias, while rates of absorption and emission of vibrations are calculated using kinetic equations [1,2]. We find and characterize several unstable modes. These results are then generalized using model calculations to generate a stability diagram of the junction under bias [3]. The talk will discuss the effect of a self-consistent treatment of electron-vibration interaction, and highlight the role played by the structure of the electron-vibration coupling matrix. Our work reveals the interplay of electronic structure and electron-vibration coupling in a broad class of molecular wires.

[1] J-T Lü, P. Hedegaard and M. Brandbyge, Phys. Rev. Lett. 107, 046801 (2011).
[2] G. Foti and H. Vázquez, J. Phys. Chem. C 121, 1082 (2017).
[3] G. Foti and H. Vázquez, J. Phys. Chem. Lett. 9, 2791 (2018).

CPP 75.9 Wed 17:15 GER 38

***Ab Initio* Green-Kubo Approach of Charge Transport in Crystalline Solids** — •Zhen-Kun Yuan, Marios Zacharias, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

State-of-the-art approaches for calculating the charge transport coefficients in crystalline materials rely on a harmonic description of the lattice vibrations and a perturbative treatment of electron-phonon couplings (EPCs) [1]. For materials featuring sizable anharmonic lattice vibrations and/or strong EPCs, such approaches are, however, not applicable. Here, we present an *ab initio* approach based on the Green-Kubo theory of linear response [2] that does neither rely on the harmonic approximation nor on a perturbative treatment of EPCs, thus overcoming these issues. The electrical conductivity is obtained from the time correlations of the electric charge flux, which is computed along fully anharmonic *ab initio* molecular dynamics trajectories. We demonstrate our approach by calculating the electrical conductivity of the harmonic material Si and the anharmonic $SrTiO_3$. We carefully check the convergence behavior of the calculated results with respect to supercell size and examine possible strategies to overcome finite-size effects [3].

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
[2] R. Kubo, M. Yokota, and S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).
[3] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

CPP 76: Organic semiconductors II (joint session HL/CPP)

Time: Wednesday 15:00–17:30 Location: POT 112

Invited Talk CPP 76.1 Wed 15:00 POT 112

Ultrafast nonadiabatic dynamics and intermolecular conical intersections in organic photovoltaic materials — •Antonietta De Sio — Institut für Physik, Universität Oldenburg

Conjugated polymer and molecular aggregates, used as photoactive materials in organic optoelectronic devices, are large supramolecular assemblies which often present complex energy landscapes and many vibrational degrees of freedom. Coupling of electronic and nuclear motion in molecules may lead to special topologies of potential energy surfaces, such as conical intersections (CoIns). At CoIns, strong vibronic couplings drive ultrafast and efficient nonadiabatic transitions between electronic states and may thus profoundly influence the ultrafast pathways of energy flow and motion of charges. CoIns are of key importance in many photochemical and biological intramolecular processes. So far, however, not much is known about their possible occurrence and relevance for intermolecular excitations in functional condensed-phase assemblies. Here we discuss how ultrafast two-dimensional electronic spectroscopy (2DES) can provide detailed insight into vibronic couplings and nonadiabatic dynamics in technologically relevant organic materials. Specifically, high-time resolution 2DES allows us to experimentally reveal the ultrafast, sub-50-fs passage of a coherent vibrational wavepacket through an intermolecular CoIn in molecular aggregate thin films used in organic photovoltaics. Our results suggest that vibronic couplings and CoIns may help to efficiently steer the energy flow in functional nanostructures, thus opening up new opportunities for controlling transport in organic-based devices.

CPP 76.2 Wed 15:30 POT 112

Photoemission Spectroscopy of Organic Charge Transfer Interfaces — •Robert Kuhrt, Martin Hantusch, and Martin Knupfer — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

Understanding physical processes at interfaces involving organic semiconductors plays a key role in optimizing the performance of electronic devices such as solar cells, where absorber and transport layers form interfaces involving metals as well as organic semiconductors. Furthermore, charge transfer between organic molecules might result in interesting properties such as metallic conductivity or correlated electronic states like superconductivity.

In this contribution, we present photoemission spectroscopy studies of various interfaces involving the strong electron acceptor hexafluorotetracyanonaphthoquinodimethane (F6TCNNQ). We compare the electronic properties of organic based donor, acceptor systems. Significant changes are observed in both the core levels and the valence orbitals at the interface, indicating a charge transfer between the materials. Origin and character of the charge transfer as well as the influence of substrate and film structure are discussed.

Acknowledgement: Financial support by the DFG (KN393/25; KN393/26) is gratefully acknowledged.

CPP 76.3 Wed 15:45 POT 112

Vacuum processed single crystalline organic semiconductor thin films for high-performance electronic and optoelectronic device applications — •Shu-Jen Wang[1,2], Michael Sawatzski[1], Ilia Lashkov[1], Yulia Krupskaya[2], Hans Kleemann[1], Bernd Büchner[2], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research (IFW), Germany

Organic semiconductors enable many technologically important applications such as organic light emitting diodes, solar cells and flexible circuits due to their unique physical properties and chemical structure tunability. Conventional amorphous organic semiconductors show low carrier mobility as their charge transport is limited by their structural order. Therefore, charge transport in organic semiconductors can generally be improved by higher degree of structural order and crystallinity. In this presentation, we will show efficient conversion of vacuum processed amorphous thin films to single crystalline thin films through annealing with appropriate surface treatment. We will also show functional devices such as field-effect transistors and light emitting diodes built on the single crystalline thin films and discuss their potential for high performance circuit and optoelectronics applications.

30 min. break.

CPP 76.4 Wed 16:30 POT 112

Coherent Real-Space Charge Transport Across a Donor-Acceptor Interface Mediated by Vibronic Couplings — Ziyao Xu[1], Yi Zhou[1], Lynn Gross[2], Antonietta De Sio[3], ChiYung Yam[4], Thomas Frauenheim[2], GuanHua Chen[1], and •Christoph Lienau[3] — [1]Department of Chemistry, University of Hong Kong — [2]BCCMS, University of Bremen — [3]Institut für Physik, Universität Oldenburg — [4]Beijing Computational Science Research Center

Growing experimental and theoretical evidence suggests that vibronic couplings (VCs), couplings between electronic and nuclear degrees of freedom, play a fundamental role for the ultrafast excited-state dynamics in organic donor-acceptor materials. While VC has been shown to support charge separation at donor-acceptor interfaces, so far, little is known about its role for the real-space transport of charges in these systems. Here we theoretically study charge transport in thiophene-fullerene stacks using time-dependent density functional tight-binding theory combined with Ehrenfest molecular dynamics for open systems. Our results reveal coherent oscillations of the charge density between neighboring donor sites, persisting for ~200 fs and promoting charge transport within the polymer. At the donor-acceptor interface, vibronic wave packets are launched, propagating coherently over distances of >3 nm into the acceptor region. This supports previous experimental observations of long-range ballistic charge motion in organic photovoltaic systems and highlights the possibility of VC engineering as a concept for tailoring the functionality of organic devices

CPP 76.5 Wed 16:45 POT 112

Light-assisted charge propagation in organic semiconductor networks on hexagonal boron nitride — Matkovic Aleksandar[1], Genser Jakob[1], •Kratzer Markus[1], Lüftner Daniel[2], Chen Zhongrui[3], Siri Olivier[3], Puschnig Peter[2], Becker Conrad[3], and Teichert Christian[1] — [1]Institute of Physics Montanuniversität Leoben Franz Josef Strasse 18, Leoben 8700, Austria — [2]Institute of Physics Karl-Franzens-Universität Graz NAWI Graz Universitätsplatz 5, Graz 8010, Austria — [3]Aix Marseille University CNRS CINaM UMR 7325 Campus de Luminy 13288, Marseille cedex 09, France

Electrostatic force microscopy is utilized to track charge propagation in organic semiconductor nanoneedles. As model system, crystalline dihydrotetraazaheptacene needles epitaxially grown on ultrathin hexagonal boron nitride was investigated. Due to light exposure, the specific resistivity of the crystallites changed by two orders of magnitude. Exploiting the highly anisotropic optical properties of the organic nanoneedles, selective charge propagation along the crystallites was achieved by matching the incident light's polarization direction with the direction of the molecular backbones in the crystals. Thus, it was possible to guide charge propagation along desired paths in self-assembled crystallite networks. This way, polarized light can be used as a "light gate" to control charge propagation.

CPP 76.6 Wed 17:00 POT 112

Electron paramagnetic resonance in OLEDs based on dual-emitting host-guest systems — •Felix Braun[1], Tobias Grünbaum[1], Wolfram Ratzke[1], Sebastian Bange[1], Sigurd Höger[2], and John M. Lupton[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany — [2]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Straße 1, 53121 Bonn, Germany

OLEDs exhibit strong sensitivity to magnetic fields due to spin-dependent electron-hole recombination. Employing the dual-emitting host-guest system CBP:DB, we can optically assess the spin-permutation symmetry of charge-carrier pairs by their magnetic-field dependent electroluminescence.

We monitor the interconversion between singlet-like and triplet-like populations under electron paramagnetic resonance (EPR) conditions and observe the anticipated anticorrelation in the behaviour of singlet-like and triplet-like carrier pairs. Furthermore, using a deuterated counterpart of the dual-emitting system, we can verify the influence of the hyperfine fields on the linewidth of the EPR signal. We anticipate that altering the spatial distribution of hyperfine interactions between host and guest will allow us to pinpoint the molecular site on which a charge-carrier pair is formed by analysing the EPR linewidth. With the spin-sensitivity introduced by the dual emitter, we even hope to determine whether, e.g., a singlet-like carrier pair preferentially forms on the guest emitter or on the host matrix.

CPP 76.7 Wed 17:15 POT 112

Reverse Dark Current in Organic Photodetectors — •Jonas Kublitski[1], Andreas Hofacker[1], Christina Kaiser[2], Donato Spoltore[1], Hans Kleemann[1], Axel Fischer[1], Koen Vandewal[3], and Karl Leo[1] — [1]IAPP - TU Dresden, Germany — [2]Swansea University, UK — [3]IMO - Hasselt University, Belgium

Photodetectors (PDs) find broad applications in many fields of optics. While inorganic PDs are widely used, they lack in easy processability and narrow-band detection. Organic PDs can fulfill these demands, providing many further advantages in comparison to inorganic PDs. The limiting factor of OPDs is their low detectivity, mostly caused by high dark current (J_D) at reverse bias. Traps and sub-gap states are often observed in organic materials. Here, we investigate their effect on J_D. We observe that J_D follows a trend with the energies of the sub-gap CT states (E_CT). Furthermore, in specific donor:C_{60} blends, we find trap concentrations of around 10^{16} cm^{-3} with an energy of around 0.5 eV below the transport level of C_{60}. We intentionally vary the trap concentration in these blends and observe that*J_D scales accordingly. Dark current-voltage simulations show that the expected value of*J_D increases four orders of magnitude and rules the dark JV characteristics, when traps are included. The dependence of J_D on reverse bias can be understood as an enhanced detrapping by means of Poole-Frenkel effect. These results point out to a physical process that might be general in donor:acceptor structures, explaining the high*J_D commonly observed in OPDs. Moreover, optimized devices show J_D as low as 500 pA cm^{-2} at -1 V, and on/off ratio of 10^7.

CPP 77: Perovskite and photovoltaics IV (joint session HL/CPP)

Time: Wednesday 15:00–17:30 Location: POT 251

CPP 77.1 Wed 15:00 POT 251

Computational study of the effect of surfaces on the molecular orientation and optical properties of hybrid lead halogenide perovskites — •Gabriele Saleh, Giulia Biffi, and Sergey Artyukhin — Istituto Italiano di Tecnologia, Via Morego 30, Genova 16163 Italy

MAPbX3 perovskites (MA= CH3NH3+, X= Cl,Br,I) are attracting intense interest due to their outstanding performance in optoelectronic devices. The efficiency of MAPbX3 as photovoltaics is governed by the electronic excitation and de-excitation processes. It is widely recognized that MA molecules have an indirect yet strong influence on the band gap and on the optoelectronic properties in general. This effect is particularly intricate since it is depends on the mutual orientations of neighboring molecules (configurations), which is continuously changing at T>100 K [1]. Here we study the energetics of MA configurations near surfaces and the correlation between the dynamical behavior of MA molecules and the optical properties of MAPbX3. Force field molecular dynamics (MD) and electronic structure simulations are performed. We find a linear dependence of the band gap on the octahedral tilt angle of the PbX3 scaffold, which in turn is determined by the orientation of MA molecules. We show how the surface influences the dynamics of MA molecules, and how this affects the surface optical properties. Representative snapshots of MD simulations at different T are extracted and their electronic structure is analyzed in order to explain the measured MAPbBr3 photoluminescence spectra. [1] O. Selig et al. (2017) J. Am. Chem. Soc., 139, 4068

CPP 77.2 Wed 15:15 POT 251

New insights into emerging lead-free double perovskite materials for optoelectronics — •Fabian Schmitz[1], Jonas Horn[2], Teresa Gatti[1], and Derck Schlettwein[2] — [1]Justus Liebig University Gießen, Institute of Physical Chemistry — [2]Justus Liebig University Gießen, Institute of Applied Physics

Lead-halide perovskites have become top-notch photoactive materials for application in solar cells, photodetectors and LEDs, due to their ease of synthesis, low-costs and excellent solution processability. For photovoltaics particularly, an impressive growth in power conversion efficiency (PCE) has been realized in few years, with current certified record at 25.2 %. Nevertheless, the most efficient perovskite solar cells still suffer from poor environmental stability and contain toxic elements. In this regard, there have been attempts to substitute lead by other metals such as tin or germanium, but no significant improvement in stability has been achieved. Good perspectives are emerging from the use of an all inorganic double perovskite, namely $Cs_2AgBiBr_6$. In this species, divalent lead is replaced by equal molar amounts of monovalent silver and trivalent bismuth. The material is characterized by an excellent environmental stability, but PCE of solar cells containing it are never higher than 2.5 %. Here we report on an optimized preparation of $Cs_2AgBiBr_6$ films and on a method to estimate charge carrier diffusion lengths within them. We also provide insights into novel material design strategies for improving optoelectronic performance in this material, by resorting to 2D/3D engineering and doping/alloying.

CPP 77.3 Wed 15:30 POT 251

Costly efficient computational approach for calculating electronic structure of complex Organic/Inorganic Perovskites —

Mohammad Moaddeli, •Mansour Kanani, and Amir Tangestani — Department of Materials Science and Engineering, School of Engineering, Shiraz University

Predictive and costly efficient computational approaches are demanding for emerging perovskite structures including heavy elements. Despite large number of research productivity on this field, there is not a consensus of multiscale material design approach. One of the main bottlenecks comes from complexity of electronic interactions in such a structure which can only be analyzed using costly modified quantum mechanical methods. We introduce a hybrid quantum/molecular dynamics computational framework to deal with different diversities of synthesized perovskite layers. We use powerful reactive force field interatomic potentials for relaxing the organic part including the van der Waals effect and interactively get electronic structure using the DFT-1/2 approach. All the procedure is verified and may be modified by the accurate hybrid functional methods. Couple of potential inorganic cations with various combination of halides are considered via this approach. This let us to find best candidate among large number of combinations. Furthermore we could predict a modified fractional distribution and doping elements for some introduced mixed cation perovskites in the literature.

CPP 77.4 Wed 15:45 POT 251

Spatially elucidating the role of defects in the photophysics of mixed halide perovskites — •David O. Tiede[1], Juan F. Galisteo-López[2], Mauricio E. Calvo[2], and Hernán Míguez[2] — [1]University of Münster, Institute of Physics, Münster, Germany — [2]Instituto de Ciencia de Materiales de Sevilla (CSIC-US), Seville, Spain

Light-induced structural changes in mixed halide perovskites are among the most critical instabilities of this material that hamper their future commercialization. In particular, reversible light-induced phase segregation and its corresponding spectral cha ges in emission is a major drawback in precise bandgap tuning, which is crucial for both efficient light harvesting in tandem solar cells and modifying the spectral output of LEDs. Over the past years, various reports have pointed towards the critical role of defects in this process and a strong dependency on environmental effects. However, the exact mechanism of the migration of halides is still under debate.

In this work we have carried out a spectrally-resolved microphotoluminescence experiments, employing a confocal microscope, to study the formation of iodine-rich domains in CH3NH3PbBrxI3-x thin films. With macroscopic measurements we verify that defects account for a dominant role on phase segregation and cause the formation of iodine-rich domains in minor parts of the material. By modifying the atmospheric conditions and changing the stoichiometry of halide components during the synthesis, we clarify the impact of vacancies and interstitials on the photophysics of these materials.

30 min. break

CPP 77.5 Wed 16:30 POT 251

Study of photon recycling in perovskite optoelectronics — •Changsoon Cho[1,2,3,4], Baodan Zhao[1], Gregory Tainter[1], Frederik Nehm[2], Karl Leo[2], Jung-Yong Lee[3], Richard Friend[1], Dawei Di[1,4], Felix Deschler[1], and Neil Greenham[1] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, J.J. Thomson Avenue, Cambridge CB3 0HE, UK — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Dresden 01187, Germany — [3]School of Electrical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea — [4]State Key Laboratory of Morden Optical Instrumentation, College of Optical Science and Engineering, Zhejiang University, Hangzhou 310027, China

Photon recycling (PR), consisting of successive light re-absorption and re-emission processes, is a key mechanism to understand the distinct optical properties of perovskite light-emitting diodes (PeLEDs). Here we verify the existence of PR effect via the measurement of spatially-resolved photoluminescence (PL) and electroluminescence (EL). To quantify the PR effect in PeLEDs, we propose an optical modelling method taking photon re-absorption and re-emission into account. According to the optical analysis of currently reported state-of-the-art devices, PR is shown to be able to contribute to more than 70% of the EQEs. Finally, we introduce various optical designs of PeLEDs, to maximize PR effect and enhance the quantity and property of light emission.

CPP 77.6 Wed 16:45 POT 251

On the Radiative Recombination Efficiency and Carrier Lifetime in Halide Perovskite Solar Cell Materials — •Thomas Unold[1], Martin Stolterfoht[2], Jose Marquez-Prieto[1], Dieter Neher[2], and Thomas Kirchartz[3] — [1]Helmholtz-Zentrum Berlin — [2]Institute of Physics and Astronomy, Universität Potsdam — [3]Forschungszentrum Juelich GmbH

The open-circuit voltage, which is currently considered the main performance limitation of halide perovskite solar cells, is determined by bulk and interface recombination processes in the solar cell.[1] Under ideal conditions the open-circuit voltage approaches the internal quasi-Fermi level splitting (QFLS), which may be estimated by the measurement of the external photoluminescence quantum yield (PLQY) and the absorption properties.[2] The photoluminescence quantum yield and quasi-Fermi level splitting can also be estimated by measurement of the time-resolved photoluminescence (TRPL), if the radiative recombination constants and photon recycling are taking into account properly.[3] A survey of the literature shows that the reported PLQY for measured open-circuit voltages sometimes vary by orders of magnitude, which is difficult to understand from the point of theory. In this contribution we show that careful consideration of the above points leads to a consistent picture of the interrelation of the QFLS, PLQY and TRPL lifetime, and discusses possible sources of error in the analysis. [1] Stolterfoht et al., Nature Energy 3 (2018) 847 [2] Liu et al., ACS Energy Lett. 4 (2019) 110 [3] Staub et al., Phys. Rev. Appl. 6 (2016) 044017

CPP 77.7 Wed 17:00 POT 251

Carrier Diffusion in Bulk and Nanocrystalline Halide Perovskites — •Michael Lichtenegger and Alexander Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstr.10, 80539 Munich, Germany

Carrier injection, transport and extraction are crucial physical properties for optoelectronic applications such as solar cells and light-emitting diodes (LEDs). Depending on the magnitude of the exciton binding energy in a material, electron-hole pairs can exist as free carriers or can form a bound state, so-called excitons. Large binding energies appear especially for systems where at least one spatial dimension is confined, e.g. in nanocubes, 2D nanoplatelets 1D nanowires or 0D quantum dots. Consequently, carrier transport will be very different depending on the nature of the material.

Our goal is to investigate and understand carrier diffusion in large perovskite crystals and assemblies of nanocrystals. For this we have realized a contactless photoluminescence (PL) and confocal time-correlated single photon counting (TCSPC) setup. We use this to measure the diffusion length for bulk perovskite films, and thin films of nanocrystals. We modify the perovskite compositions, geometries and passivating ligands to investigate the nature of the transport processes and determine critical parameters such as diffusion lengths and diffusion coefficients.

CPP 77.8 Wed 17:15 POT 251

Temperature-dependent high spatial-resolution spectroscopy to investigate NCs in single micelles — •Markus Schoger, Carola Lampe, Moritz Gramlich, and Alexander Urban — Nanospectroscopy Group, Department of Physics, Ludwig-Maximilians-Universität, Munich, Germany

Halide perovskite nanocrystals (NCs) have shown outstanding potential for light-emitting applications with high quantum yields and an emission wavelength tunable throughout the visible spectrum. Despite these impressive advances, they still suffer from several issues, which currently impede widespread commercialization. To enhance their stability, we recently introduced a colloidal synthesis, wherein the NCs are grown inside diblock copolymer micelles.1 These nanoreactors additionally provide a protective shell, limiting degradation and ion migration. In order to maximize their potential and enable optoelectronic integration, an in-depth understanding of the nanostructure structure and resulting properties on a single micelle level is critical. Here, we present temperature-dependent high spatial-resolution spectroscopy to investigate single micelle-encapsulated perovskite NCs in temperature intervals from 4 K up to room temperature to gain insight into their fundamental properties.

1 V. A. Hintermayr, C. Lampe, M. Low, J. Roemer, W. Vanderlinden, M. Gramlich, A. X. Bohm, C. Sattler, B. Nickel, T. Lohmuller, and A. S. Urban, Nano Lett. 19 (8), 4928 (2019).

CPP 78: Scanning Probe Techniques I: Method development (joint session O/CPP)

Time: Wednesday 15:00–17:30 Location: TRE Ma

CPP 78.1 Wed 15:00 TRE Ma

Dynamics in spin excitation spectroscopy measurements — •Luigi Malavolti[1,2], Max Hänze[1,2], Gregory McMurtrie[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany. — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany.

Spin excitation spectroscopy has proven to be an essential tool for the investigation of magnetic phenomena at the atomic scale [1] forming the basis for RF-STM investigation of both electron spin resonance and spin dynamics [2]. However, certain spin dynamic phenomena can also be transduced directly via standard dIdV(V) measurements [3]. Here, the contribution of spin dynamic effects to static spectroscopy measurements is presented using a combined theoretical and experimental approach. Understanding these phenomena allows the behavior of spin systems with long-lived excitations to be anticipated, offering a fast and reliable way to access spin dynamics with standard STM techniques. [1] R. Wiesendanger, Rev. Mod. Phys. 81, 1495 (2009) [2] Loth S., Science, 329, 1628, (2010) [3] Rolf-Pissarczyk S., PRL, 119, 217201, (2017)

CPP 78.2 Wed 15:15 TRE Ma

Electron paramagnetic resonance of single Ti and Fe atoms with an out-of-plane magnetic field probed by STM — •Tom S. Seifert[1], Stepan Kovarik[1], Dominik Juraschek[1,2], Nicola A. Spaldin[1], Sebastian Stepanow[1], and Pietro Gambardella[1] — [1]ETH Zurich, Switzerland — [2]Harvard University, USA

Combining the sub-atomic resolution of scanning tunneling microscopy (STM) with the spectral resolution of electron-paramagnetic resonance (EPR) allows for sensitive probing magnetic interactions of single atoms on a surface [1]. However, the experimental requirements for driving the EPR transitions are still under debate [2,3]. In-depth understanding of what drives these spin rotations is mandatory to explore novel material systems and optimize the sensitivity of this technique. Here, we acquire EPR spectra of single Fe and hydrogenated Ti atoms on bilayer MgO on Ag using a radio frequency (RF) antenna close to the STM junction with a magnetic field applied perpendicular to the surface [4]. We investigate in a systematic way the impact of RF excitation strength and tunneling parameters on the EPR signal with emphasis on the electric and magnetic fields present at the tunnel junction. This analysis is supported by density functional calculations of the electronic and phononic density of states of the probed systems.

[1] S. Baumann et al., Science **350** (2015) [2] K. Yang, et al., PRL **122** (2019) [3] P. Willke et al., Nano Lett. **19** (2019) [4] T. S. Seifert et al., ArXiv 1908.03379 (2019)

CPP 78.3 Wed 15:30 TRE Ma

Electron spin resonance of an individual atom at mK temperature in a vector magnetic field — •Manuel Steinbrecher[1], Werner v. Weerdenburg[1], Jan W. Gerritsen[1], Niels v. Mullekom[1], Fabian D. Natterer[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands — [2]Department of Physics, University of Zurich, CH-8057 Zurich, Switzerland

It was recently shown that electron spin resonance (ESR) can be combined with spin-resolved scanning tunneling microscopy (STM) to quantify the resonant excitations of individual 3d transition metal atoms [1]. The combination of atomic-resolution and ultra-high energy resolution, compared to standard scanning tunneling spectroscopy, has e.g. enabled quantification of the hyperfine coupling of individual atoms at temperatures near 1K [2]. Nevertheless, probing small absolute energy scales down to MHz frequencies requires the implementation of this method at much lower temperature. We will present ESR performed in a home-made dilution refrigerator (T = 30mK) based spin-polarized STM including a vector magnet [3]. The ESR was recorded on individual atoms on a thin insulating film of MgO over a whole frequency range from several hundred MHz to tens of GHz. A vector magnetic field was applied and allowed ESR experiments in different crystallographic directions.

[1] S. Baumann *et al.*, Science **350**, 417 (2015)
[2] P. Willke *et al.*, Science **362**, 336 (2018)
[4] H. v. Allwörden *et al.*, RSI **89**, 033902 (2018)

CPP 78.4 Wed 15:45 TRE Ma

Electron spin resonance in scanning tunneling microscopy — •Andreas Heinrich — Center for Quantum Nanoscience, Seoul, Korea

The scanning tunneling microscope is an amazing tool because of its atomic-scale spatial resolution. This can be combined with the use of low temperatures, culminating in precise atom manipulation and spectroscopy with several microvolt energy resolution. In this talk we will apply these techniques to the investigation of the quantum spin properties of magnetic atoms sitting on thin insulating films. We will explore the superposition of quantum states which is inherent to spin resonance techniques. About 5 years ago it was demonstrated that electric field driven electron spin resonance (ESR) can be combined with STM on single Fe atoms on MgO (Science 2015). This technique combines the power of STM of atomic-scale spectroscopy with the unprecedented energy resolution of spin resonance techniques, which is about 10,000 times better than normal spectroscopy. We will give an update on recent advances in our team including pulsed ESR on Ti atoms on MgO (Science 2019).

CPP 78.5 Wed 16:00 TRE Ma

Transfer Function Compensation for High Frequency Radiation into an STM Tunnel Junction — •Maximilian Uhl, Piotr Kot, Robert Drost, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, Stuttgart

Creating constant amplitude radiation of varying frequencies in the tunnel junction of a scanning tunneling microscope is an important condition for probing the interaction of matter and electromagnetic waves at the nanoscale, such as for electron paramagnetic resonance [1]. The transfer function describes the transmission of an AC signal to the tunnel juntion and depends highly non-linearly on the frequency. A known transfer function can be compensated by a frequency dependent signal power. Reaching non-zero constant amplitudes at frequencies > 40 GHz has remained a challenge. Our setup makes this possible for frequencies up to 90 GHz. So far, transfer functions have been measured by plasmonic light emission [2] and rectification at current-voltage non-linearities [3]. Here, a new technique based on the Tien-Gordon equation [4] is demonstrated. It allows to probe even small AC voltages in the μV range, requiring only a single measurement point per frequency. For that, we use the coherence peak of a superconductor-insulator-superconductor junction. Generally, the technique can also be used with other peak types in the current-voltage derivative.

[1] S. Baumann et al.: Science **350** (6259), 417 (2015)
[2] C. Grosse et al.: Appl. Phys. Lett. **103**, 183108 (2013)
[3] W. Paul et al.: Rev. Sci. Instrum. **87**, 074703 (2016)
[4] G. Falci, V. Bubanja, G. Schön: Z. Phys. B **85**, 451 (1991)

CPP 78.6 Wed 16:15 TRE Ma

Hyperfine fields of magnetic adatoms on ultrathin insulating films — •Sufyan Shehada, Manuel dos Santos Dias, Filipe Souza Mendes Guimarães, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

Individual nuclear spin states can have a very long lifetime and could in principle be used as qubits. A promising step in this direction was the recent detection of the hyperfine interaction between the atomic nucleus and the surrounding electrons for single Fe and Ti adatoms on MgO/Ag(001) [1]. Here, we report on systematic first-principles calculations of the hyperfine fields of magnetic transition metal adatoms (from Ti to Cu) placed on different ultrathin insulators, such as MgO, NaCl, CuN and hBN. We analyze the trends and the dependence of the computed hyperfine fields on the filling of the magnetic d-orbitals of the adatom and on the type and strength of the bonding with the substrate, and what is the impact of an underlying metallic surface. We also identify promising candidates for future experimental investigation with scanning probe techniques.

This work was supported by the Palestinian-German Science Bridge BMBF program and the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] P. Willke *et al.*, Science **362**, 336–339 (2018)

CPP 78.7 Wed 16:30 TRE Ma

Mapping the perturbation potential of metallic and dipolar tips in tunneling spectroscopy on $\mathbf{MoS_2}$ — •Christian Lotze, Nils Krane, Gaël Reecht, Nils Bogdanoff, and Katharina J. Franke — Freie Universität Berlin, Germany

Single layer molybdenum disulfide (MoS_2) features a direct band gap and strong spin-splitting of the valence band at the K-point, which make it an interesting material for optoelectronic applications.

We grow a single layer of MoS_2 epitaxially on a Au(111) surface, adopting a recipe from [1], and employ its decoupling properties for high resolution scanning tunneling spectroscopy of single molecules [2]. Because of the band gap and small electron-phonon coupling strength of MoS_2, it is possible to resolve spectral features down to few meV. Differential conductance spectra of 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene (BTTT) molecules exhibit a multitude of sharp characteristic peaks, originating from vibronic states. Indeed, these allow even for an identification of different rotamers [2].

Here, we make use of these vibronic fingerprints to investigate the influence of the tip potential on the apparently shifted molecular states along the extended molecular backbone of BTTT. Our analysis further allows us to distinguish between the inhomogeneous shape of the bias potential in the junction and possible intrinsic tip dipoles [3].

[1] Sørensen, *et al.*, Langmuir, 31, 35, 9700 (2015)

[2] Krane, *et al.*, ACS Nano, 12, 11, 11698 (2018)

[3] Krane, *et al.*, Phys. Rev. B, 100, 035410 (2019)

CPP 78.8 Wed 16:45 TRE Ma

Fast quasiparticle interference mapping through traveling salesperson and sparse sampling optimization — •Jens Oppliger and Fabian D. Natterer — Department of Physics, University of Zurich, Switzerland

STM investigations are slow and render complex measurement tasks, such as QPI mapping, impractical. Conventionally, QPI patterns are composed from a Fourier-transform of hundreds of thousands of point-spectra that encode LDOS modulations from which the scattering space is inferred. Yet, despite this measurement complexity, we rely heavily on QPI since it provides insight into materials that are experimentally inaccessible to ARPES. Surprisingly, QPI patterns contain only little information, despite their origin from many data-points. Since sparsity is one key-ingredient for compressive sensing, we use it here to fundamentally speed-up QPI mapping [1]. In view of the incoherent measurements required for CS, we sparsely sample LDOS at randomly selected locations using constant and varying probability density. To that end, we move the STM-tip according to a traveling salesperson and ultimately achieve a 5-50 times faster QPI mapping. [1] J. Oppliger and F.D. Natterer, arXiv 1908.01903

CPP 78.9 Wed 17:00 TRE Ma

Development of a Variable-Temperature High-Speed Scanning Tunneling Microscope — •Zechao Yang, Leonard Gura, Jens Hartmann, Heinz Junkes, William Kirstädter, Patrik Marschalik, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Scanning probe microscopy allows for resolving the atomic structure of crystalline and vitreous thin oxide films on metal substrates. For understanding the structural transition of these films as a function of temperature in real space and at real time, we developed a variable-temperature high-speed scanning tunneling microscope (STM).

The experimental setup consists of a two-chamber ultra-high vaccum (UHV) system including a preparation and a main chamber. The preparation chamber is equipped with standard preparation tools for sample cleaning and film growth. The main chamber hosts the STM that is located within a continuous flow cryostat for counter-cooling during high-temperature measurements. The microscope body is compact, rigid, and highly symmetric to ensure vibrational stability and low thermal drift. We designed a scanner made of two independent tube piezos for slow and fast scanning, respectively. Here we have decided to implement non-conventional spiral geometries for high-speed scanning. A Versa Module Eurocard bus system enables the fast scan control and is implemented in the EPICS software framework.

With sprial scans, we atomically resolved diffusion processes within an O(2x2) coverage on Ru(0001) and achieved a time resolution of 25 milliseconds per frame.

CPP 78.10 Wed 17:15 TRE Ma

Integrated Electrodes in H:Si(001) for Scanning Gate Microscopy — •Matthias Koch, Alex Kölker, Leonid Shupletsov, Takashi Kumagai, and Martin Wolf — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Single atoms or molecules can not only be characterized but also manipulated by exploiting the incredible high spatial resolution of the scanning tunneling microscopy. However, often the electrical characterization is limited by the experimental setup which consists of only two electrodes (tip and sample). Although multi-tip setups or scanning gate microscopes exist their operation is often demanding [1].

Here, we demostrate a sample system, compatible to most commercial low-temperature SPMs, equipped with multiple integrated electrodes. These in-plane electrodes, which are in close proximity to the surface, act as drain or gate contacts. We realize the *m-large electrodes by ultra-shallow ion-implantation in an otherwise highly resistive silicon crystal [2]. Notably, even after high-temperature treatment to prepare atomically flat silicon, the electrodes behave ohmic. The optimal distance between two electrodes is determined by in-situ transport measurements. Furthermore, the applicability of our sample system is demonstrated by first gating experiments. In future it will be used to study lateral nano-circuits in-operando with the SPM tip as a mobile electrode.

[1] B. Voigtländer et. Al, Rev. Sci. Instrum. 89, 101101 (2018)

[2] A.N. Ramanayaka et. al Scientific Reports 8, 1 (2018)

CPP 79: Nanostructured Surfaces and Thin Films I: 1D and 2D Networks (joint session O/CPP)

Time: Wednesday 15:00–17:30 Location: WIL B321

CPP 79.1 Wed 15:00 WIL B321

Imaging the phase transition in thin film $\mathbf{VO_2}$ microstructures — •Jan O. Schunck[1,2], Florian Döring[3], Benedikt Rösner[3], Jens Buck[4], Sanjoy Mahatha[1], Moritz Hoesch[1], Christian Schüssler-Langeheine[5], Adrian Petraru[6], Hermann Kohlstedt[6], Kai Rossnagel[1,4], Christian David[3], and Martin Beye[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg — [2]Physics Department, Universität Hamburg — [3]Paul Scherrer Institut, Villigen-PSI, Switzerland — [4]Institut für Experimentelle und Angewandte Physik, CAU Kiel — [5]Helmholtz-Zentrum Berlin — [6]Nanoelektronik, Techn. Fakultät, CAU Kiel

Vanadium dioxide (VO_2) is an intruiging compound, since upon heating it exhibits an insulator-to-metal transition (IMT) at a critical temperature T_c of around 340 K, which is characterised by a decrease in resistivity of several orders of magnitude. On a microscopic level, the phase transition is accompanied by a rearrangement of the crystal structure as well as electronic bands around the Fermi level and proceeds in a percolative manner, meaning that both phases coexist over a temperature range of several K around T_c.

Here, we present results of an experiment which combines X-ray spectroscopic methods for electronic structure analysis with imaging capabilities of a few micrometers spatial resolution. Studying electronic structure changes during the thermally driven IMT in a pulsed laser deposition-grown and microstructured VO_2 thin film, shows that T_c differs by around 2 K between the edges and centres of VO_2 squares with an edge length of 30 μm.

CPP 79.2 Wed 15:15 WIL B321

investigation of Fe(CO)5 as precursor for gas-assisted electron beam lithography techniques on cobalt oxide surfaces — •Elif Bilgilisoy[1], Christian Preischl[1], Rachel Thorman[2], Howard Fairbrother[2], and Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany —

[2]Department of Chemistry, Johns Hopkins University, Baltimore, Maryland/USA.

Electron Beam Induced Deposition (EBID) is a gas-assisted direct write electron-lithography fabrication technique in which structures from certain precursor molecules are deposited. A second technique is Electron Beam Induced Surface Activation (EBISA). In EBISA, a focused electron beam is used to locally modify the substrate such that it becomes active towards the decomposition of subsequently dosed precursor molecules [1]. Both approaches were conducted with Fe(CO)5 on a Co3O4/Ir(100) surface. We will present first successful results on a clean Co3O4 surface with Fe(CO)5 for EBID and EBISA. To achieve a deeper understanding of the EBID process, corresponding surface science experiments were conducted, in which the dynamics and behavior upon low energetic electron[2] and ion beam irradiation of thin Fe(CO)5 layers at liquid nitrogen temperatures were investigated using x-ray photoelectron spectroscopy (XPS) under UHV. We will compare the corresponding results and discuss the reaction mechanisms of Fe(CO)5. [1] H. Marbach, Appl. Phys. A 117 (2014) 987 [2] S. G. Rosenberg, et al., J. Phys. Chem. C, 117 (2013)16053

CPP 79.3 Wed 15:30 WIL B321

Interaction of topological boundary states in graphene nanoribbon heterojunctions — •Qiang Sun[1], Oliver Gröning[1], Xuelin Yao[2], Akimitsu Narita[2], Klaus Müllen[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Labora-tory, 8600 Dübendorf, Switzerland — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Graphene nanoribbons (GNRs), narrow stripes of graphene, are promising candidates for future elec-tronic applications due to their widely adjustable electronic properties. The precise control of their atomic structure, including their termini, edges and width, allow for the realization of specific electronic quantum phases. For example, GNRs with chiral edges or cove edges have been predicted to host spin-polarized edge states. And recently, topological electronic quantum phases have been predicted and realized in the junctions between GNR segments belonging to different topological classes. Here, I will show the synthesis and characterization of width-modulated GNRs that host topological junction states. By investigating such GNRs as a function of the number of periodically aligned junction states along the GNR axis, we follow the evolution of the new electronic bands formed by the finite overlap between the junction states. Furthermore, we investigate the interaction between boundary states in topological heterojunctions, revealing an interaction-induced energy splitting that decays exponentially with their relative separation.

CPP 79.4 Wed 15:45 WIL B321

Determination of Carbon Nanomembrane Diffusion Coefficients via radioactive tracer experiments — Raphael Dalpke[1], Anna Dreyer[2], •Riko Korzetz[1], André Beyer[1], Karl-Josef Dietz[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University — [2]Faculty of Biology, Bielefeld University

In recent years, 2D materials have gained a lot of attention as highly efficient filter materials. One class of materials are carbon nanomembranes (CNM), which are fabricated by self-assembly of organic precursors onto metal substrates and subsequent cross-linking by electron irradiation. They can be released from their original substrate and transferred onto arbitrary supports. Specifically, CNMs made from terphenylthiol (TPT) exhibit a very high selectivity towards water in combination with an outstanding permeance [1].

Here, we present new permeation measurements of TPT-CNMs utilizing radioactively marked water as well as carbonate and phosphate ions. We show that water and carbonate can pass through while phosphate ions are completely blocked by the CNM. The resulting diffusion coefficients in combination with recent findings indicate that the permeation across the membrane primarily occurs by transport of neutral species. This implies a fast transport of CO_2 in aqueous solution, while dry TPT-CNMs are not permeable to CO_2, which suggests a facilitated transport in the presence of water.

[1] Yang *et.al., ACS Nano* **2018** 12(5), 4695-4701

CPP 79.5 Wed 16:00 WIL B321

The electronic structure of atomically-precise graphene nano-ribbons investigated by photoemission tomography — Lukas Reicht[1], Xiaosheng Yang[2,3], Larissa Egger[1], Philipp Hurdax[1], Francois C. Bocquet[2,3], Georg Koller[1], Petra Tegeder[4], Alexander Gottwald[5], Mathias Richter[5], Michael G. Ramsey[1], F. Stefan Tautz[2,3], Serguei Soubatch[2,3], and •Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany. — [3]Jülich Aachen Research Alliance (JARA), Germany — [4]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany. — [5]Physikalisch-Technische Bundesanstalt (PTB), Germany.

In this contribution we investigate the electronic structure of armchair graphene nanoribbons (AGNRs) by means of angle-resolved photoemission spectroscopy and density functional calculations. Specifically, using an orientated AGNRs with a width of 7 carbon atoms adsorbed on a stepped Au surface, we demonstrate how photoemission tomography can be used to shed light on the electronic structure of its frontier valence bands. We present a series of constant binding energy momentum maps which allow us to identify all relevant valence (sub)-bands of this graphene nanoribbon. By comparing theoretical results for free-standing and adsorbed ribbons, we investigate the degree of molecule-substrate hybridization and inter-ribbon interactions thereby demonstrating that photoemission tomography proves to be a powerful technique to study the electronic structure of such quantum confined 1D systems.

CPP 79.6 Wed 16:15 WIL B321

Tuning electronic transport of 1D coordination polymers by the choice of the transition metal: Fe, Co and Ni — •Aleš Cahlík[1], Christian Wäckerlin[1], Santhini Vijai Meena[1], Oleksander Stetsovych[1], Jesus Mendieta[1], Pingo Mutombo[1], Simon Pascal[2], Olivier Siri[2], and Pavel Jelínek[1] — [1]Institute of Physics, Czech Academy of Sciences, v.v.i., Czech Republic, — [2]Aix Marseille Université, CNRS, Marseille, France,

The choice of transition metal atom in organometallic complexes can significantly influence their electronic and spintronic properties. Here, we study the electronic transport through 1D coordination polymers contacted by the tip of a scanning probe microscope (SPM). The polymers are synthesized in-situ by co-deposition of Fe, Co or Ni atoms and the quinonediimine (2,5-diamino-1,4-benzoquinone-diimine) ligand onto Au(111). The combination of STM and nc-AFM allows for simultaneous measurement of the current, conductance and force gradient as a function of bias voltage and lifting height. We observe a distinct bandgap opening behavior depending on the incorporated metal element. In addition, we show the possibility to modulate the conductance of these wires between highly conductive and non-conductive by increased bias voltage or upon light illumination.

CPP 79.7 Wed 16:30 WIL B321

Nitrogen Doped Carbon Nanofiber Composites as Anode for Sodium-Ion Batteries — •Mo Sha, Long Liu, Huaping Zhao, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Recently, sodium-ion batteries (SIBs) have attracted increasing attention as an important supplement or alternative to lithium ion batteries (LIBs) due to the abundance of sodium resources and its much lower cost. A critical issue and great challenge in current battery research for the extensive application of SIBs is the development of earth-abundant and high-performance electrode materials. In various studies of these electrode materials, carbon nanofibers have been identified as promising anodes for SIBs, because of the low cost and environment friendly features. In this study, nitrogen-doped carbon nanofiber (NCNFs) have been synthesized by an electrostatic spinning technique and used as anodes for SIBs. The corresponding specific capacity can reach about 175 mA h g-1 at 0.1C after 100 cycles. The results demonstrate that this NCNFs composite is a promising anode material with good reversible capacity and cycling performance for SIBs.

CPP 79.8 Wed 16:45 WIL B321

Ultra Large Lifting Installations (ULLIS) on HOPG — •Tristan J. Keller, Georgiy Poluektov, Anna Jochemich, Anna Krönert, Stefan-Sven Jester, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie, Bonn, Deutschland

Self-assembled monolayers at the solid/liquid interface on graphite (HOPG) are investigated by scanning tunneling microscopy (STM). Recently, we reported *i*-gonal arylene-alkynylene macrocycles (i = 3,4,5,6) that form tiling patterns that correspond to the macrocycle shapes and the interdigitation of adjunct -$OC_{16}H_{33}$ side chains.[1]

Here, we present a novel approach for supramolecular surface patterning incorporating a tetraphenylmethane building block into a shape-persistent macrocycle in order to address the volume phase above the substrate. We observe monolayers with lattice constants in the range of 10 nm that are independent of the exact substitution of the pillar unit (e.g. propargylic alcohol, or fullerene). In addition, we present cocrystals of these triangular species and a molecular hexagon. The research aims at a detailed understanding on how functional groups that point into the third dimension can be incorporated in appropriate systems.

[1] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 29, 11062-11065.

CPP 79.9 Wed 17:00 WIL B321

Atomic-scale mechanical evidence of surface-catalyzed gold-carbon covalent bonding — •Benjamin Lowe, Jack Hellerstedt, Dhaneesh Kumar, and Agustin Schiffrin — School of Physics and Astronomy, Monash University, Clayton VIC 3800 Australia

Surface-confined self-assembly is a versatile method for creating and tuning the properties of low-dimensional nanostructures. Here we study the results of gold atoms and dicyanoanthracene (DCA) molecules deposited on Ag(111) in ultrahigh vacuum, characterized at 5K using combined scanning tunneling and non-contact atomic force microscopies (STM/nc-AFM). We found that the two-dimensional metal-organic self-assembly was composed of close-packed DCA-Au-DCA units, in which a single Au atom binds covalently to a carbon atom at the anthracene ends. This conclusion is based on submolecular resolution ncAFM imaging achieved with a CO-functionalized probe, as well as STM manipulation demonstrating the robustness of these DCA-Au-DCA units. Further experiments performed on an atomically thin insulator (hexagonal boron nitride) suggest the covalent DCA-Au-DCA bonding is catalyzed by the Ag surface. We expect these findings to inform the pursuit of metal-organic frameworks predicted to host topological electronic properties [1].

[1] Zhang, L. Z. et. al. Nano Letters (2016). 10.1021/acs.nanolett.6b00110.

CPP 79.10 Wed 17:15 WIL B321

Methyl and Vinyl Functional Groups in On-Surface Synthesis — •Marco Di Giovannantonio[1], José I. Urgel[1], Shantanu Mishra[1], Kristjan Eimre[1], Aliaksandr V. Yakutovich[1], Carlo A. Pignedoli[1], Pascal Ruffieux[1], Uliana Beser[2], Qiang Chen[2], Zijie Qiu[2], Akimitsu Narita[2], Klaus Müllen[2], and Roman Fasel[1,3] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland — [2]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [3]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland

On-surface synthesis has opened pathways to molecular nanostructures that have been inaccessible so far. Here, we demonstrate the successful use of methyl and vinyl groups to achieve one-dimensional (1D) polymers composed of repeat units with specific ring topologies.

Methyl groups are proven to undergo an oxidative cyclization to the neighboring phenyl, forming five-membered rings and affording unprotected indenofluorene isomers, some of which exhibit high radical character. Vinyl groups enable the formation of additional six-membered rings, affording benzo[k]tetraphene units after a stable intermediate with CH2 groups protruding out of five-membered rings.

The structure and electronic properties of the obtained polymers have been characterized by STM, nc-AFM, and STS, and supported by theoretical calculations. The observed reaction steps and products extend the knowledge of on-surface reactions to fine tune architectures and functionalities.

CPP 80: Droplets and Wetting (joint session DY/CPP)

Time: Wednesday 15:00–16:45 Location: ZEU 147

CPP 80.1 Wed 15:00 ZEU 147

Coalescence of liquid droplets in a quasi 2D liquid films — •Christoph Klopp, Ralf Stannarius, and Alexey Eremin — Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany

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] Paulsen et al., Coalescence of bubbles and drops in an outer fluid, Nat. Commun. 5, 3182 (2014)

[2] Aarts et al., Hydrodynamics of Droplet Coalescence, Phys. Rev. Lett. 95, 164503 (2005)

[3] Shuravin et al., Coalescence of viscous two-dimensional smectic islands, Phys. Rev. E 99, 062702 (2019)

CPP 80.2 Wed 15:15 ZEU 147

Surface wettability-induced magnitude change and sign inversion of the apparent line tension — •Binyu Zhao[1,4], Shuang Luo[2], Elmar Bonaccurso[3], Günter Auernhammer[4], Zhigang Li[2], and Longquan Chen[1] — [1]University of Electronic Science and Technology of China, Chengdu 610054, China — [2]The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong — [3]Airbus Central R & T, Materials X, Munich 81663, Germany — [4]Leibniz Institute of Polymer Research Dresden, Dresden 01069, Germany

Line tension is defined, thermodynamically, as the excess free energy per unit length of the contact line as postulated by Gibbs in 1878. Despite strenuous research efforts thence, the magnitude and sign of line tension remain in a hot debate. In this study, we determined the apparent line tension from the size-dependent contact angle of sessile nanodroplets on surfaces with different wettabilities via atomic force microscopy measurements. We showed that the apparent line tension changed its magnitude with the surface wettability and its sign changed from positive to negative for droplets on surfaces with an apparent contact angle higher than a critical value. Furthermore, using molecular dynamics simulations, we analysed the potential energy of liquid molecules within the nanodroplet and in the vicinity of the three-phase contact line. This allowed us to explain the surface wettability-induced magnitude change and sign inversion of the apparent line tension form the perspective of surface thermodynamics.

CPP 80.3 Wed 15:30 ZEU 147

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.

CPP 80.4 Wed 15:45 ZEU 147

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 80.5 Wed 16:00 ZEU 147

A bite of cotton candy physics — •Stephane Dorbolo[3], Floriane Weyer[1], Nicolas Vandewalle[1], and Alexandre Delory[2] — [1]GRASP, UR-CESAM, Departement de Physique, Universite de Liege, Belgium — [2]ESPCI, Paris, France — [3]FNRS, GRASP, UR-CESAM, Departement de Physique, Universite de Liege, Belgium

A cotton candy is made of kilometers of sugar fibers. These thin fibers are easily and quickly soluble into water. The system is generic and found applications in soldering and networks of nano-fibers. First, the wettability of the sugar is measured. The problem is complex since the sessile droplet modifies the substrate made of sugar. Second, the interactions of a sugar fiber with the humidity present in the air and with a single droplet are discussed through experimental investigations. Finally, a model is presented to describe the motion of a droplet along one single fiber.

CPP 80.6 Wed 16:15 ZEU 147

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 80.7 Wed 16:30 ZEU 147

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.

CPP 81: Plasmonics and Nanooptics V: Tunable Structures and Nanoparticles (joint session O/CPP)

Time: Wednesday 15:30–18:15 Location: WIL A317

CPP 81.1 Wed 15:30 WIL A317

Thermally regulated smart mid-infrared modulators enabled by phase-change materials and phase-transition materials — Xinrui Lyu[1], Andreas Hessler[1], Xiao Wang[2], Alfred Ludwig[2], Matthias Wuttig[1], and •Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen University — [2]Institute for Materials, Ruhr-University Bochum

Phase-change materials (PCMs) and phase-transition materials (PTMs) both show a large contrast in their optical properties upon switching, enabling compact optical components with diverse functionalities like sensing, thermal imaging and data recording. However, their switching properties differ significantly, i.e., non-volatile for PCMs while volatile for PTMs. For the first time, we combined PCMs, $Ge_3Sb_2Te_3$ (GST) or $In_3Sb_1Te_2$ (IST), with the PTM VO_2 as active layers in the design of the smart mid-infrared modulators with switchable absorption, reflection, and transmission. The VO_2 is employed as a dynamic mirror, switching between transmission (semiconducting VO_2) and absorption modes (metallic VO_2) with continuously tuned amplitudes up to 90%. Meanwhile, the PCMs on top of the VO_2 are used either for continuously shifting the absorption peak (up to 1.8 μm) by switching GST or for switching between reflection (R=0.85) and absorption modes (A=0.99) by switching IST. Merging the concepts of static (PCMs) and dynamic (PTMs) thermal modulation, the presented combination of non-volatile PCMs and volatile PTMs empowers new generation optical components like dynamic thermal imaging and optical switches.

CPP 81.2 Wed 15:45 WIL A317

Programmable Phase-Change Plasmonics with $In_3Sb_1Te_2$ — •Andreas Hessler[1], Sophia Wahl[1], Till Leuteritz[2], Matthias Wuttig[1], Stefan Linden[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen — [2]Physikalisches Institut, University of Bonn

The high optical contrast of non-volatile phase-change materials (PCMs) between their switchable amorphous and crystalline structural phases enables exciting nanophotonic functionalities [1,2]. So far, the employed PCMs mostly have dielectric optical properties in both phases. Now, we introduce the next-generation PCM $In_3Sb_1Te_2$ (IST) for reconfigurable nanophotonics. In contrast to the commonly used PCMs, its optical properties change from dielectric to metallic upon crystallization in the whole infrared spectral range. We show how resonant metallic nanostructures can be directly written and erased in an IST thin film by a pulsed switching laser, enabling direct and reconfigurable lithography. With this new technology, we demonstrate striking resonance shifts of plasmonic nanoantennas of more than 4 μm, a programmable mid-infrared perfect absorber with nearly 90% absorptance as well as screening and nanoscale "soldering" of metallic nanoantennas. Our novel concepts of programmable phase-change plasmonics could enable inexpensive fabrication and improved designs of programmable plasmonic devices for infrared optics, sensing and telecommunications.

[1] M. Wuttig et al., *Nature Photonics* **11**, 465-476 (2017)
[2] F. Ding et al., *Advanced Optical Materials* **7**, 1801709 (2019)

CPP 81.3 Wed 16:00 WIL A317

Tunable Heterostructure Polaritonic Cavity — •Mohsen Janipour[1], Matthias Hensen[2], and Walter Pfeiffer[3] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, Bielefeld 33615, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, Bielefeld 33615, Germany

Realizing and designing of tunable cavities at the infrared frequencies is crucial for achieving novel integrated photonic circuits. In the infrared regime, semiconductors like GaAs can support the excitation of surface phonon polaritons in the Reststrahlen band with the ability to tune through carrier concentration. In this study, we explore a novel heterostructure cavity composed of a hollow circular hole drilled in an Ag film which is stacked on a GaAs substrate. We show that this cavity can support two types of resonant modes consisting of circular cavity resonant modes and the surface modes due to the excitation of polaritonic modes in the Reststrahlen band. We indicate that the polaritonic modes can be tuned through controlling the distribution of the substrate*s carriers in the Reststrahlen band.

CPP 81.4 Wed 16:15 WIL A317

Silicon Metasurfaces for Nonlinear Holography and Wavefront Control — •Bernhard Reineke[1], Basudeb Sain[1], Ruizhe Zhao[2], Luca Carletti[3], Bingyi Liu[4], Lingling Huang[2], Costantino De Angelis[5], and Thomas Zentgraf[1] — [1]Department of Physics, Paderborn University, Warburger Straße 100, D-33098 Paderborn, Germany — [2]School of Optics and Photonics, Beijing Institute of Technology, Beijing 100081, China — [3]Department of Information Engineering, University of Padova, 35131 Padova, Italy — [4]Institute of Modern Optics, Department of Physics, Harbin Institute of Technology, Harbin 150001, China — [5]Department of Information Engineering, University of Brescia, 25123 Brescia, ItalyNational Institute of Optics (INO), CNR, 25123 Brescia, Italy

Metasurfaces based on dielectric nanostructures are an ideal platform for nonlinear optical experiments (such as third-harmonic generation). They provide high damage thresholds and strong nonlinear responses; Therefore, many works show progress dielectric metasurfaces with high nonlinear conversion efficiency. However, in achieving nonlinear wavefront control, less progress has been made. Therefore, we show the nonlinear wavefront control for the third-harmonic generation with a silicon metasurface. We choose a geometric phase approach to encode phase gradients and holographic images on a dielectric metasurface. In our experiment, we demonstrate the wavefront control and the multiplexed reconstruction of holograms at the third-harmonic wavelength. Our approach provides a simple principle for designing metasurfaces for nonlinear optical applications with dielectric building blocks.

CPP 81.5 Wed 16:30 WIL A317

Polarization-selective orbital angular momentum multiplexed meta-hologram — •Basudeb Sain[1], Hongqiang Zhou[2], Yongtian Wang[2], Christian Schlickriede[1], Lingling Huang[2], and Thomas Zentgraf[1] — [1]Department of Physics, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany — [2]School of Optics and Photonics, Beijing Institute of Technology, Beijing, 100081, China

Metasurface holography has the advantage of realizing complex wavefront modulation together with the progressive technique of computer-generated holographic imaging. Despite of having the well-known light parameters, like amplitude, phase, polarization and frequency, the orbital angular momentum (OAM) of a beam can be regarded as another important degree of freedom. Utilizing the orthogonality between different OAM modes and the OAM conservation law, here, we demonstrate orbital angular momentum multiplexed polarization-encrypted holography using a birefringent metasurface. The polarization selectivity of such metasurface relies on the birefringent response of the incident light. The holographic information can only be reconstructed with exact topological charge and a specific polarization state, providing an unprecedented advantage for holographic encryption. By using an incident beam with different topological charges as erasers, we mimic a super-resolution case for the reconstructed image, in analogy to the well-known stimulated emission depletion (STED) technique in microscopy. Such technique can open new avenues for beam shaping, optical camouflage, data storage, and dynamic displays.

CPP 81.6 Wed 16:45 WIL A317

Mode conversion in tilted plasmonic nanocones confirmed by second harmonic imaging — Christoph Dreser[1], Dominik A. Gollmer[1], Godofredo Bautista[2], Xiaorun Zang[2], Dieter P. Kern[1], Martti Kauranen[2], and •Monika Fleischer[1] — [1]Institute for Applied Physics and Center LISA+, Eberhard Karls University of Tübingen, Germany — [2]Laboratory of Photonics, Tampere University, Finland

Plasmonic nanocones offer strong, highly localized near-fields at the cone apex that can be utilized for applications in microscopy and sensing. However, for an efficient excitation of the tip mode the electric field vector of the exciting electromagnetic wave needs to have a significant component parallel to the vertical axis. To enable the excitation of the tip mode under vertical illumination, two processes for the nanofabrication of tilted gold nanocones with defined tip displacements are presented. The asymmetric geometry supports the transformation of an in-plane electric far-field to an out-of-plane plasmonic excitation. Extinction spectra and corresponding simulations will be shown, in which cones with different tilting angles are illuminated under various illumination angles. The tip excitation is confirmed by the nonlinear optical properties of the nanocones observed in second harmonic generation scanning microscopy with cylindrical vector beams.

[C. Dreser et al., Nanoscale 11, 5429 (2019)]

CPP 81.7 Wed 17:00 WIL A317

Hydrogen Sensing with Palladium-based Perfect Absorber under variable ambient pressures — •Ramon Walter[1], Florian Stern[1], Ediz Herkert[1,2], Tobias Pohl[1], and Harald Giessen[1] — [1]University of Stuttgart, Germany — [2]ICFO - The Institute of Photonic Sciences, Castelldefels (Barcelona), Spain

The increasing C02-content makes it necessary to replace the fossil energy carrier by alternative climate-neutral energy sources. Hydrogen has the potential to be one of this new energy sources. However, this gas has a high potential risk when mixed with oxygen. A reliable and sensitive sensor is needed to reduce this risk and safe lives.

Previous works showed that palladium is an ideal material for such a sensor. Nanoparticles made out of palladium will change under hydrogen pressure their lattice constant and consequently their dielectric properties. This will have a measurable influence of their optical properties depending on the hydrogen content in the lattice.

In this work, we investigate the potential of such palladium based perfect absorber devices as hydrogen sensor under different variable ambient pressures, which is required for a number of technically relevant applications. We believe that this should extend the range of possible applications without increasing a potential risk, as the sensor works pure optical and is completely separated by any kind of evaluation electronics. Furthermore, means to shield the sensor from contamination with other gases and the consequences for our sensing geometry are discussed.

CPP 81.8 Wed 17:15 WIL A317

Colloidal quantum dots coupled to electrically connected optical antennas — •Patrick Pertsch, René Kullock, Monika Emmerling, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Semiconductor quantum dots (QDs) attract a lot of interest due to their tunable light emission, high efficiency and single-photon characteristics. Combining them with optical antennas can not only lead to strong coupling [1] but also to enhanced and directional emission. To achieve that the QDs have to be positioned accurately within the antenna which, in the past, has been realized by complex and time consuming processes [2,3].

Here we report on a much simpler process, utilizing dielectrophoresis, to load the gap of electrically connected antennas with colloidal QDs. The QDs are positioned accurately inside the 30-nm gaps of the antennas, show strong photoluminescence and are promising for electro-optical applications. The reported method allows the preparation of QD-antenna systems within a few minutes.

[1] H. Groß et al., Science Advances 4, eaar4906 (2018)
[2] A. G. Curto et al., Science 329, 930-933 (2010)
[3] E. Tranvouez et al., Nanotechnology 20, 165304 (2009)

CPP 81.9 Wed 17:30 WIL A317

Plasmonic K-Au nanoparticles from helium droplet synthesis — •Roman Messner[1], Daniel Knez[2], Ferdinand Hofer[2], Wolfgang Ernst[1], and Florian Lackner[1] — [1]Technische Universität Graz, Institut für Experimentalphysik, 8010-A — [2]Technische Universität Graz, Institut für Elektronenmikroskopie und Nanoanalytik, 8010-A

We report on experiments on K-Au nanoparticles produced under UHV conditions by synthesis in helium nanodroplets. The particles are fabricated by coagulation of metal atoms after pickup by the cold droplets. The employed experimental techniques encompass in-situ spectroscopy as well as ex-situ investigations via transmission electron microscopy (TEM). Plain K clusters solvated in helium droplets exhibit a strong resonance at about 600 nm. The position of the resonance, thereby, depends on the K partial pressure in the pickup region, i.e. the size of the nanoparticles. After adding a gold shell-layer to the potassium particles, a blue shift of the resonance is observed, towards the well-known localized plasmon resonance of plain Au nanoparticles. An important aspect of our current research is to test the possibility of passivating the highly reactive K clusters with a Au shell, which would allow for the preparation of K-Au nanoparticle decorated substrates that can be investigated outside the UHV. First TEM investigations show promising results, opening up new perspectives for the production of novel material combinations for plasmonics with helium droplet based nanoparticle synthesis.

CPP 81.10 Wed 17:45 WIL A317

Synthesis of plasmonic Ag@ZnO core@shell nanoparticles inside superfluid helium droplets — •Alexander Schiffmann[1], Thomas Jauk[1], Daniel Knez[2], Harald Fitzek[2], Ferdinand Hofer[2], Florian Lackner[1], and Wolfgang E. Ernst[1] — [1]Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — [2]Institute of Electron Microscopy and Nanoanalysis & Graz Centre for Electron Microscopy, Graz University of Technology, Steyrergasse 17, A-8010 Graz, Austria

Plasmonic Ag@ZnO core@shell nanoparticles in the sub 10 nm size regime have been synthesized in a unique way by employing the helium nanodroplet approach. A peculiarity of this low temperature technique, where the particles are formed within a superfluid helium environment, is the complete absence of solvents and surfactants. Scanning transmission electron microscopy (STEM) and energy dispersive X-ray spectroscopy (EDS) give insight into the composition and structure of the particles, revealing a very uniform thickness and shape of the ZnO shells surrounding the Ag cores. The oxidation state of the shell was investigated by ultraviolet photoelectron spectroscopy (UPS). Photoelectron spectra of Ag@ZnO, ZnO, and Ag nanoparticles have been recorded by two-photon photoelectron (2PPE) spectroscopy. The employed laser with a photon energy of 3 eV is resonant to the localized surface plasmon in Ag. In the case of Ag and Ag@ZnO an excitation of this plasmon gives rise to an increased yield of electrons with high kinetic energy.

CPP 81.11 Wed 18:00 WIL A317

Helium Droplet Mediated Synthesis of Rhodamine B Functionalized Au Nanoparticles — Roman Messner[1], Harald Fitzek[2], Wolfgang E. Ernst[1], and •Florian Lackner[1] — [1]Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Institute of Electron Microscopy and Nanoanalysis & Graz Centre for Electron Microscopy, Graz University of Technology, Steyrergasse 17, 8010 Graz, Austria

Helium nanodroplets provide a new route for the synthesis of plasmonic nanoparticles. [1] Metal atoms are picked up by the droplets and agglomerate to particles, subsequent deposition on surfaces allows for the fabrication of plasmonic nanoparticle films without any solvents or surfactants. We show that the approach can also be used to produce complexes consisting of a plasmonic nanoparticle surrounded by a shell of molecules on the example of Au particles and rhodamine B. Surface enhanced Raman spectroscopy (SERS) indicates that the formed complexes stay intact after deposition. Our current efforts are geared towards the study of interactions between plasmon oscillations in the metal particles and the attached molecules. Therefore, experiments are carried out in-situ, while the particles are solvated in the helium droplets, employing laser induced fluorescence spectroscopy. The rhodamine B dye molecules are excited by a 532 nm laser, the detected fluorescence signal is found to be strongly quenched as soon as Au nanoparticles are added to the helium droplet.

[1]...Eur. Phys. J. D, 73 (5), 104 (2019)

CPP 82: Computational Materials Modelling - Solids and Molecules (joint session MM/CPP)

Time: Wednesday 15:45–17:00 Location: IFW B

CPP 82.1 Wed 15:45 IFW B

Molecular Adsorption Potential Energy Surfaces and their Reproducibility — •Lukas Hörmann, Andreas Jeindl, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Molecular adsorption on surfaces depends on a range of mechanisms: covalent bonds, charge transfer and van-der-Waals (vdW) interactions shape the potential energy surface (PES), making the PES key to understanding molecule-substrate interfaces. Describing these interfaces with density functional theory requires a wise selection of the exchange correlation functional and vdW correction scheme. To explore the robustness of the PES with respect to the choice of method, we present a benchmark of common local, semi-local and non-local functionals in combination with various vdW corrections. We investigate these methods using perylenetetracarboxylic dianhydride (PTCDA) on Ag(111), one of the most frequently studied systems.

We use an in-house developed Gaussian process regression algorithm, which requires only about 50 DFT calculations as input to generate a PES with DFT accuracy. This allows a detailed analysis of the PES's features, such as positions and energies of minima and saddle points. Comparing the results from different exchange correlation functionals enables us to identify trends and differences between the approaches. Finally, we compare key features, such as local minima, with experimental data to determine a "quality seal" for the different functionals and vdW corrections.

CPP 82.2 Wed 16:00 IFW B

The role of structural symmetry for proton tautomerization in aromatic molecules — •Antonios Raptakis[1,2], Alexander Croy[2], Rafael Gutierrez[2], Arezoo Dianat[2], and Gianaurelio Cuniberti[2] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

Proton tautomerization is a prototype reaction and controllable on a single molecule level. In particular, studies of aromatic molecules, such as porphyrins and phthalocyanines, show the potential of use in molecular electronics, sensor devices and solar cells. Here, we simulate the reaction paths using well-tempered Metadynamics simulations, in molecular dynamic engine of DFTB+. We study the influence of symmetric and asymmetric functionalization on the tautomerization rates and metastable states of porphyrin and porphyrazine cores.

CPP 82.3 Wed 16:15 IFW B

First-principles description of phase transitions in solids with rotating molecules and diffusing atoms — •Sergei Simak — IFM, Linköping University, Sweden

Solids with rotating molecules and diffusing atoms are examples of dynamically disordered phases of materials with great potential for applications, from fuel cells to optoelectronics. Description of thermodynamics of these materials is a challenge, as standard methods, like static phonon calculations fail due to the large displacements of atoms or the absence of well-defined equilibrium atomic positions. We briefly outline a method that offers a solution to the problem based on a stress-strain thermodynamic integration [1]. An example of lithium

carbide, a fascinating material that combines strong covalent and weak ionic bonding resulting in a wide range of unusual properties, is considered [2]. The mechanism of its phase transition from the ground-state orthorhombic to the high-temperature cubic crystal, which is subject to both rotations of C-C dumbbells and Li self-diffusion, is revealed, and the thermodynamics is described.
[1] J. Klarbring and S. I. Simak, Phys. Rev. Lett. 121, 225702 (2018).
[2] S. Filippov, J. Klarbring, U. Häussermann, and S. I. Simak, Phys. Rev. Materials 3, 023602 (2019).

CPP 82.4 Wed 16:30 IFW B

Development of a Neural Network Potential for Metal-Organic Frameworks — •Marius Herbold, Marco Eckhoff, and Jörg Behler — Georg-August Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

Metal-organic frameworks (MOFs) are crystalline porous materials with many applications in chemistry and materials science, from gas separation to heterogeneous catalysis. Computer simulations of chemical processes in MOFs are severely limited by the use of classical force fields (FFs), because most FFs are unable to describe bond formation and breaking. In principle, electronic structure methods, like density-functional theory (DFT), can overcome this problem, but often the required systems are too large for routine applications of DFT. Here a high-dimensional neural network potential (NNP) is presented for a series of MOFs, which combines the advantages of both worlds - the accuracy of first principle methods with the efficiency of simple empirical potentials. We demonstrate the possibility to obtain a reliable description of the potential-energy surface of bulk MOFs based on reference calculations of molecular fragments only.

CPP 82.5 Wed 16:45 IFW B

Analysis of organic-inorganic thermal interfaces in Metal-Organic Frameworks — •Sandro Wieser[1], Tomas Kamencek[1], Rochus Schmid[2], Johannes Peter Dürholt[2], Natalia Bedoya Martínez[3], and Egbert Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Chair of Inorganic Chemistry 2, CMC Group, Ruhr-Universität Bochum, Germany — [3]Materials Center Leoben, Austria

Metal-Organic Frameworks (MOFs) represent a type of porous materials that show promising properties for many applications including gas-storage and catalysis, which in most of the cases rely on the effectiveness of dissipating heat. Due to the complex structure of these materials, an in depth understanding of how the fundamental structural characteristics of individual building blocks, as well as their interconnection, impact the system's properties is necessary. To that aim, we investigate isoreticular and tetragonal MOFs utilizing classical non-equilibrium molecular dynamics simulations. The interatomic interactions are described by specifically tailored MOF-FF potentials fitted to density-functional-theory reference data. From the obtained temperature profiles one can conclude that the factor primarily limiting thermal transport is a weak thermal coupling across the interface between the inorganic nodes and the organic linkers combined with a poor conduction within the nodes. We additionally investigate, how the thermal coupling across the heterointerface is impacted by parameters like the mass and extent of the individual components and the docking chemistry.

CPP 83: Microfluidics (joint session DY/CPP)

Time: Wednesday 17:00–18:30 Location: ZEU 147

CPP 83.1 Wed 17:00 ZEU 147

Near-field acoustic manipulation in a confined evanescent Bessel beam — •Pierre-Yves Gires[1,2] and Cédric Poulain[1,3] — [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.

CPP 83.2 Wed 17:15 ZEU 147

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, see patent [1]. The flow is generated due to the periodic movement of liquid-vapor interfaces in a large number ($\approx 10^6$) of microcavities ($\Delta V \approx 1$ pl 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. They must be optimized to generate a reasonable valve action even at the small Reynolds numbers that are typical for micro pumps.
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. In each microcavity, the flow can be modelled as multiphase flow with time-dependent wetting properties as boundary conditions. It is implemented via a boundary element method. Additionally, an approximation is presented that allows the fast calculation of the stationary shape of liquid/vapor interfaces in electrical fields. Topological optimization methods for the optimization of the Tesla-Diodes are presented, in which the complete micro pump system is considered as well.
[1] Hoffmann, M., Dittrich, L., Bertko, M.; German patent DE11 2011 104 467 (2012)

CPP 83.3 Wed 17:30 ZEU 147

Digital magnetofluidics with planar Hall effect sensors — •Julian Schütt[1], Rico Illing[1], Oleksii Volkov[1], Tobias Kosub[1], Pablo 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., 01328 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.

CPP 83.4 Wed 17:45 ZEU 147

Positioning of Gold Nanoparticles by Thermo-Osmotic Flows

in Electrolytes — •Martin Fränzl and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

The application of gold nanoparticles as plasmonic sensors in fluidic applications requires exact positioning which is often only achieved by rigid templating using physical or chemical lithography. Here we investigate the control of single and multiple gold nanoparticles with the help of optically induced thermo-osmotic flows in electrolyte solution. Our control is using a thin gold film on substrates to allow for a local heating of an electrolyte solution in a liquid film. The local temperature rise at the gold induces thermo-osmotic flows at the gold electrolyte solution. By tuning the electrolyte concentration, we to confine the mobility of the gold-nanoparticles to a two-dimensional layer at a distance of a few 10 nanometers from the gold film in which a positioning with the help of thermo-osmotic flows is easily possible. The experimental results of the gold nanoparticle dynamics are compared the theoretical predictions.

CPP 83.5 Wed 18:00 ZEU 147

Flow in Responsive Porous Media — •Thomas Darwent[1], Enrico Segre[2], Ran Holtzman[3], and Lucas Goehring[1] — [1]Nottingham Trent University — [2]Weizmann Institute of Science — [3]Coventry University

Fluid flows in porous media, such as sand, rocks and biological tissues, are controlled by the geometry of that media and the properties of the fluids. Here, we explore the situation where the properties of the fluid and solid are coupled, such that an invading fluid modifies the structure of a porous medium around it. Specifically, we look at the case where the porous matrix is deformable, and we show that a new invasion pattern is seen: capillary fracturing. This results from the fluid pushing and pulling on individual grains making up the solid body, which changes the pressures required to flow past, or invade, those grains. This effect occurs in hydrocarbon recovery and CO2 sequestration where fluids are injected underground and deform the local structure. To study this problem, we use soft lithography and microfluidic techniques to produce PDMS micromodels, allowing us to tune the elasticity and disorder of a model porous medium. Along with numerical simulations, we show that deformation caused by the fluid leads to localised fingering patterns in more compliant materials, and that this effect is restricted by increasing the disorder in the system.

CPP 83.6 Wed 18:15 ZEU 147

Actuation of soft particles in oscillating Poiseuille flow — •Winfried Schmidt[1], Sebastian W. Krauss[2], Andre Förtsch[1], Matthias Laumann[1], and Walter Zimmermann[1] — [1]Theoretische Physik 1, Universität Bayreuth, 95447 Bayreuth, Germany — [2]Experimentalphysik 1, Universität Bayreuth, 95447 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.

CPP 84: Molecular Electronics and Photonics (joint session TT/CPP)

Time: Wednesday 18:00–19:00 Location: HSZ 304

CPP 84.1 Wed 18:00 HSZ 304

Efficient steady state solver for charge transport through single-molecule junctions — •Christoph Kaspar and Michael Thoss — Albert-Ludwigs-Universität, Freiburg, Germany

The steady state is a fundamental property used to describe the nonequilibrium transport of electrons through single-molecule devices. Its rigorous computation requires highly accurate methods such as the hierarchical quantum master equation approach [1,2]. This method gives access to the systematic inclusion of higher-order contributions resulting in the generalization of perturbative master equation approaches. The major disadvantage of calculating the steady state with this method is the excessive requirement of computational resources, e.g. needed for increasing strength of molecule-lead coupling or many molecular degrees of freedom [3,4]. In this contribution, we present an iterative approach enabling the efficient computation of the steady state for the transport through single-molecule junctions. Besides reducing the required computational time, the main benefit is a drastically decreased memory compared to conventional propagation schemes. We demonstrate the efficiency of our iterative approach on the scenario of a single-molecule junction with many system degrees of freedom.

[1] Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008)
[2] Schinabeck *et al.*, Phys. Rev. B **94**, 201407R (2016)
[3] Hou *et al.*, J. Chem. Phys. **142**, 104112 (2015)
[4] Zhang *et al.*, J. Chem. Phys. **147**, 044105 (2017)

CPP 84.2 Wed 18:15 HSZ 304

Low temperature single molecule transport measurements on fullerenes — •Alexander Strobel[1,2], Filip Kilibarda[1,2], Elke Scheer[2], and Artur Erbe[1,2] — [1]Helmhotz Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]University of Konstanz, Faculty of sciences, 78457 Konstanz, Germany

Molecular electronics offers a novel approach, for scaling traditional 3D electronics down to nanoscale dimensions in a quasi 1D system. This approach offers a deeper understanding of the electron transport behavior of molecules. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ) technique. Here we report electrical transport properties of fullerene molecules using a MCBJ setup. Fullerenes with their high stability and symmetry have become reference molecules for the development of measurement routines for molecular electronics applications. Our MCBJ setup enables us to evaporate C60 in situ and measure electrical characteristics under high vacuum conditions. Furthermore, low-temperature measurements down to 6 K are possible. Conductance histograms are recorded to measure the preferred conductance values of single C60 molecules. I-V curves, the differential conductance and inelastic electron tunneling spectra (IETS) are directly and simultaneously measured using lock-in measurement methods. IETS measurements are used to investigate electron-phonon Interactions. The experimental analysis of the charge transport by varying the electrode distance, the bias potential and the electrode metal at different conductance is presented.

CPP 84.3 Wed 18:30 HSZ 304

Ab initio study of current-induced forces in nanojunctions — •Susanne Leitherer[1], Nick Papior[2], Jing-Tao Lü[3], and Mads Brandbyge[1] — [1]Department of Physics, Technical University of Denmark — [2]Department of Applied Mathematics and Computer Science, Technical University of Denmark — [3]School of Physics, Huazhong University of Science and Technology, Wuhan, China

In ballistic nanoscale conductors the high current density can lead to substantial changes in the atomic structure, as seen in experiments [1]. We calculate the current-induced forces on the atoms of different models of nanojunctions under a high applied bias voltage, employing first principles electronic structure and transport calculations. Our findings show how the forces on the atoms are related to the chemical bonds, as evidenced in scanning probe experiments exploring currents and forces between two C_{60} molecules [2], as well as the electrostatic potential landscape in the junctions [3]. To study further the dynamical motion of atoms in nanojunctions including current-induced forces, we perform molecular dynamics simulations based on a semi-classical Langevin approach in combination with DFT calculations [4]. This allows us to study the influence of Joule heating, i.e. inelastic scattering by phonons, as well as other contributions to current-induced forces that do not conserve the energy of the atomic motion.

[1] C. Schirm et al., Nat. Nanotechnol. 8, 645-648 (2013)
[2] J. Brand et al., Nano Lett. 19, 7845-7851 (2019)
[3] S. Leitherer et al.,Phys. Rev. B 100, 035415 (2019)
[4] J.T. Lü et al., Manuscript in preparation

CPP 84.4 Wed 18:45 HSZ 304

Electrical transport through single polypeptides — •Diana Slawig[1], Nguyen Thi Ngoc Ha[2], Yossi Paltiel[3], Shira Yoshelis[3], and Christoph Tegenkamp[1,2] — [1]Leibniz Universität Hannover, Germany — [2]TU Chemnitz, Germany — [3]Hebrew University Jerusalem, Israel

The analysis of electrical transport through helical molecules gained a lot of interest within the last years, due to the unique spin filtering properties, named chiral induced spin selectivity (CISS) [1]. By utilizing this effect a proof of concept for a new type of chiral-based Si-compatible universal magnetic memory device was demonstrated [2]. Nevertheless, the electrical transport through helical peptides itself is not completely understood yet.

Our study focuses on transport through single lysine doped polyalanine (PA) molecules by means of mechanically controlled break junction. Molecular fragments containing different numbers of monomers were used to evaluate the length dependent transport behavior, leading to a strong indication for a tunneling dominated mechanism.

Based on the high number of observed stable conductance states in the statistical analysis, we propose a ratcheting model based on geometrical alignments of the molecules. This concept is closely related to the interdigitation effect observed by STM[3].

[1] R. Naaman et al., J. Phys. Chem. Lett., 3 (2012)
[2] O.Ben Dor et al., Nat. Commun. 4:2256 (2013)
[3] T. N.H. Nguyen et al., J. Phys. Chem. C 123, 612 (2019)

CPP 85: Focus: Polymers under confinement I

Polymers under confinement are ubiquitous in nature and technology, ranging from the crowded interior of biological cells to thin polymer coatings. Confinement can either be imposed externally or it can emerge spontaneously through the self-organization of the constituents. Confinement decreases substantially the available degrees of freedom, and can lead to a wealth of intriguing phenomena nonexistent in bulk systems. Important aspects include, e.g., the size, shape and rigidity of the bounding geometry, and the properties and packing fraction of the enclosed particles. In this focus session, we will explore the structure formation, dynamics, and other aspects of these systems. Organized by: Arash Nikoubashman (Johannes Gutenberg Universität Mainz).

Time: Thursday 9:30–12:45 Location: ZEU 222

Invited Talk CPP 85.1 Thu 9:30 ZEU 222

Molecular view on polymers adsorbed on nanoparticle surfaces — Mozhdeh Abbasi[1], Sol Mi Oh[2], So Youn Kim[2], and •Kay Saalwächter[1] — [1]Inst. f. Physik - NMR, Martin-Luther-Univ. Halle-Wittenberg, Halle (Saale), Germany — [2]School of Energy and Chemical Engineering, UNIST, Ulsan, Republic of Korea

The reinforcement effect of nanoparticles in a polymer matrix is related to an interphase with modified properties [1]. Previous results support a consensus picture of adsorbed components with locally increased Tg and gradient zone of a few nm [2]. This talk focuses on more recent results, mostly obtained by proton low-resolution NMR as a probe of the segmental dynamics, that challenge the generality of this picture. In the system poly(ethylene oxide)-silica, we do find strongly immobilized (yet intrinsically mobile) components forming a layer of up to 2 nm thickness around the particles [3], but the layer thickness is temperature-independent and is governed by a non-equilibrium process in dependence of end groups [3] and preparation conditions [4], and also of the curvature of the particles. Spin-diffusion NMR experiments, which probe the size of nanometric domains with distinct mobility, indicate that the smooth-mobility-gradient picture of the "glassy layer" must be replaced by a scenario ruled by dynamic heterogeneities associated with the increased glass transition [5].

[1] A. Mujtaba et al., ACS Macro Lett. 2014, 3, 481 [2] A. Papon et al., Phys. Rev. Lett. 2012, 108, 065702 [3] Y. Golitsyn et al., J. Chem. Phys. 2017, 146, 203303 [4] S. M. Oh et al., Phys. Rev. Lett. 2019, 123, 167801 [5] H. Schneider et al., Macromolecules 2017, 50, 8598

CPP 85.2 Thu 10:00 ZEU 222

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.

CPP 85.3 Thu 10:15 ZEU 222

The role of entanglements in non-equilibrium polymer films — •Hsiao-Ping Hsu and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

Equilibrating polymer melts containing highly entangled large polymer chains in confinement or with free surfaces is a challenge for computer simulations. We approach this problem by first studying polymer melts based on the soft-sphere coarse-grained model confined between two soft repulsive walls at a distance compatible with the simulation box of bulk melts in equilibrium and keeping the periodic boundary conditions in the directions parallel to the walls. Then we apply the backmapping methodology to reinsert the underlying microscopic details of the bead-spring model. Turning off the wall potential, the monomer density of confined polymer melts in equilibrium is kept at the bulk density even near the walls. By removing the walls we can study free standing, highly entangled polymer films. We start to stretch the initial films into two directions parallel to the free surfaces, and shrink the thickness of films, while keeping the surface pressure at zero. Finally, we quench the thin polymer films below the glass transition temperature to freeze the structure and analyze the local morphology.

CPP 85.4 Thu 10:30 ZEU 222

Growth Kinetics and Molecular Mobility of Irreversibly Adsorbed Layers in Thin Films of P2VP and PVME — •Marcel Gawek, Sherif Madkour, Andreas Hertwig, and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin

In well-annealed thin polymer films, with non-repulsive polymer/substrate interactions, an irreversibly adsorbed layer is formed. These adsorbed layers have shown enormous potential for technological applications. Due to the hard accessibility of these layers, their growth kinetics and molecular dynamics are still not fully understood. Here, the irreversibly adsorbed layers of Poly(2-vinylpyridine) (P2VP) and Poly(vinyl methyl ether) (PVME) thin films are revealed by solvent-leaching experiments. The growth kinetics of these layers is investigated as a function of original film thickness and annealing times. The thickness, topography and quality of the adsorbed layer is determined with Atomic Force Microscopy (AFM) and spectroscopic ellipsometry. Additionally, the molecular mobility of the adsorbed layer is investigated with Broadband Dielectric Spectroscopy (BDS). A recently developed nanostructured capacitor (NSC) is employed to measure the adsorbed layers with a free surface layer depending on annealing and solvent-leaching time. The results are quantitatively compared and discussed with respect to recently published work.

CPP 85.5 Thu 10:45 ZEU 222

Kinetically trapped chiral structures of diblock copolymers in cylindrical confinement — •Ludwig Schneider, Georg Lichtenberg, and Marcus Müller — Institut für Theoretische Physik, Georg-August Universität Göttingen

Reproducibly manufacturing morphologies of diblock copolymers inside cylindrical confinements is a long-standing question in directed self-assembly. It has been explored both in experiments and simulations. For non-neutral cylinder walls, it is expected that concentric lamellae are formed.

However, we discover interesting long-lived helical structures via large-scale Single-Chain-in-Mean-Field (SCMF) simulations. The requirements for these structures are neutral interactions between the confinement and the two polymer species and an incommensurable cylinder length with the natural lamellar spacing.

We believe the structures to be meta-stable but long-lived. The kinetic pathway after a spinodal decomposition consistently drives the morphology towards the helical structures. After the meta-stable structure is formed, it is long-lived because a transition towards equilibrium requires a global remodeling of the morphology – accompanied by a high free-energy barrier.

30 min. break

Invited Talk CPP 85.6 Thu 11:30 ZEU 222

Nonequilibrium Properties of Polymers in Confinement — •Roland G. Winkler — Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich

The interplay between polymer conformational degrees of freedom, confinement, and nonequilibrium forces results in intriguing structural and dynamical properties [1]. The out-of-equilibrium state can either be achieved by well established external fields, such as electric, magnetic, and flow fields, or by active forces, as for polar filaments of the cytoskeleton of a cell. Moreover, in living cells, nonthermal fluctuations (colored noise), induced by ATP-powered enzymes, are expected to play a major role in DNA organization and for the dynamics of the chromatin in the nucleus. The novel emerging phenomena of active soft matter render them a promising class of new materials [2]. We studied the properties of soft colloids, like linear polymers and star polymers under flow, specifically the interplay between flow, polymer conformations, and hydrodynamic interactions. In particular, we find that the latter strongly affect the properties of polymers in a channel [3]. For "active" polymers, we find that their internal degrees of freedom strongly affect the conformations, and in particular, the phase behavior. [1] R. G. Winkler, D. A. Fedosov, G. Gompper, Curr. Opin. Colloid Interface Sci. 19, 594 (2014) [2] R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, 101014 (2017) [3] R. Chelakkot, R. G. Winkler, G. Gompper, EPL 91, 14001 (2010)

CPP 85.7 Thu 12:00 ZEU 222

Confined polymer dynamics: an effective model for polymer transport in porous materials — •Paolo Malgaretti — Max Planck Institute for Intelligenst Systems

We study the translocation of polymers across varying-section channels. Using systematic approximations, we derive a simplified model that reduces the problem of polymer translocation through varying-section channels to that of a point-like particle under the action of an effective potential. Such a model allows us to identify the relevant parameters controlling the polymer dynamics and, in particular, their translocation time. By comparing our analytical results with numerical simulations we show that, under suitable conditions, our model provides reliable predictions of the dynamics of both Gaussian and self-avoiding polymers, in two- and three-dimensional confinements. Moreover, both theoretical predictions, as well as Brownian dynamic results, show a non-monotonous dependence of polymer translocation velocity as a function of polymer size, a feature that can be exploited for polymer separation.

[1] V.Bianco, P.Malgaretti JCP 145, 114904 (2016)

CPP 85.8 Thu 12:15 ZEU 222

Structure and Dynamics of Single-Chain Nanoparticles in Crowded Environments: A Combined SANS & NSE Study — •Timo Brändel[1], Paula Malo de Molina[2], Julian Oberdisse[3], Ingo Hoffmann[4], Lionel Porcar[4], Josetxo Pomposo[2], Arantxa Arbe[2], and Juan Colmenero[1,2] — [1]Donostia International Physics Center, San Sebastian, Spain — [2]Centro de Fisica de Materiales, San Sebastian, Spain — [3]Laboratoire Charles Coulomb, Montpellier, France — [4]Institut Laue-Langevin, Grenoble, France

Very recently, single-chain nanoparticles (SCNP) have been granted lots of attention in different fields of physical and chemical science. Due to their sparse-like structure, SCNP are often considered as versatile model-systems for a very interesting class of proteins, namely intrinsically disordered proteins (IDP). The synthesis of SCNP is carried out by intra-molecular crosslinking of single polymer chains by various cross-linking reactions. Therefore, SCNP are usually synthesized and investigated in strongly diluted solutions, but IDP exist rather under crowded conditions like most proteins. Hence, the effect of macromolecular crowding on SCNP is very important. Our study uses the outstanding possibilities of neutron scattering to investigate the effect of crowding on the structure and dynamics of SCNP. To address this issue, PS based SCNP are investigated in a completely contrast-matched matrix of deuterated linear PS chains by means of SANS and NSE. Important effects of the crowded environment on structural properties of the SCNP are observable and the internal dynamics are considerably slowed down compared to the dilute state.

CPP 85.9 Thu 12:30 ZEU 222

Glassy behavior of cyclic polymers in a confinement — •Stanard Mebwe Pachong[1], Jan Smrek[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Ackermanweg 55128, Germany — [2]Faculty of Physics, University of Vienna, Bolzmanngase 5, A-1090 Vienna, Austria

The behavior of a dense non-concatenated ring polymers within a confined spherical geometry is investigated. By increasing the temperature of a part of each chain, the activity based segregation is observed. We showed that introducing the activity in the system changes the topological state of the chains irrespective of the constraint imposed by the confinement. The dynamics and size analysis indicate that the chains swell when a part of it have its temperature increased. The swelling allow mutual threading of ring. We conclude that the enhance of mutual threading between chains due to thermal anisotropy, together with the chains' topological state drive the system into a kinetically arrested state.

CPP 86: Organic Electronics and Photovoltaics III

Time: Thursday 9:30–12:45 Location: ZEU 260

CPP 86.1 Thu 9:30 ZEU 260

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 86.2 Thu 9:45 ZEU 260

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 86.3 Thu 10:00 ZEU 260

Studying the dynamics of PTB7:PCBM blend films — •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, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active materials due to their superior performance compared to e.g. planar layered devices. In this optically active polymer layer, a photon is absorbed and an exciton created. After diffusion to a donor-acceptor interface, the exciton is dissipated and charge carriers can be extracted at the electrodes. A frequently applied and well-studied system is the combination of P3HT ((C10H14S)n) as electron donor and PCBM (C72H14O2) as electron acceptor. Previous studies have shown that internal dynamics and structural layout of the active layer influence its electronic properties and thus its performance in a device. A more modern, very promising low-band gap electron donor material is PTB7 ((C41H53FO4S4)n). We investigate films of PTB7, PCBM and a mixture of these two prepared out of chlorobenzene solutions. On these films we perform first quasielastic neutron scattering experiments. Hydrogen dynamics of pure compounds as well as blend films on a pico- to nanosecond timescale in a temperature range from 150 K to 400 K are investigated and compared with the established P3HT:PCBM system.

CPP 86.4 Thu 10:15 ZEU 260

Temperature dependence of the spectral linewidth of charge-transfer-state emission in organic solar cells; static vs. dynamic disorder contribution — •Kristofer Tvingstedt[1], Johannes Benduhn[2], and Koen Vandewal[3] — [1]Experimental Physics VI, Julius Maximillian University of Würzburg, 97074 Würzburg, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [3]Instituut voor Materiaalonderzoek (IMO), Hasselt University, Wetenschapspark 1, BE-3590 Diepenbeek, Belgium

The origin and impact of energetic disorder remains a topic of intense controversy in the research field of organic photovoltaics (OPV). As the amount of energetic disorder of the photovoltaic material have a pronounced impact on both the open circuit voltage and the effective drift mobility of operational devices, a proper account of its foundation is strongly desired. Currently, both Gaussian and exponential, as well as static and dynamic disorder models are interchangeably being employed. We herein aim to increase the understanding of disorder contribution in organic solar cells by evaluating the spectral width of charge-transfer-state emission as a function of both carrier injection conditions and temperature, with the primary objective to disentangle dynamic and static disorder contribution. Both photoluminescence (PL) and electroluminescence (EL) of a large set of complete devices made of both small molecules and polymers are evaluated under weak injection conditions to shed more light on this topic.

CPP 86.5 Thu 10:30 ZEU 260

Organic narrowband near-infrared photodetectors for industrial applications — •Johannes Benduhn[1], Rico Meerheim[1,2], David Wynands[1,2], Marcel Dahms[2], Paul Vincze[2], and Robert Brückner[1,2] — [1]Institut für Angewandte Physik, Technische Universität Dresden, Dresden, Germany — [2]Senorics GmbH, Dresden, Germany

Near-infrared (NIR) spectroscopy is a powerful method to analyse the composition of various analytes. Nowadays, this method is mainly used in well-equipped laboratories since todays spectrometers are very large and expensive. To overcome these limitations, we present organic photodetectors which enable narrowband detection of NIR photons with full width at half maximum down to 15 nm and can be produced easily and cost efficiently. These detectors are based on organic donor-acceptor blends forming an NIR-absorbing charge-transfer state which is massively enhanced by utilizing an optical micro-cavity. Tuning the cavity resonance, different wavelengths can be detected. Placing different of such detectors in an array results in a miniaturized lateral spectrometer which can be employed to measure for example moisture content of carton, using a reflection geometry. In the near future, such miniaturized spectrometers can be used to optimize the production of paper and carton by controlling the moisture content. Furthermore, various related applications and products can be addressed.

CPP 86.6 Thu 10:45 ZEU 260

Integrated All-Organic Oxygen Sensor — •Toni Bärschneider[1], Jakob Lindenthal[1], Simone Lenk[1,2], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden — [2]CeTI Cluster of Excellence, Centre for Tactile Internet with Human-in-the-Loop, Technische Universität Dresden

Organic electronics devices, such as light-emitting diodes (OLEDs) and photodetectors (OPDs) are cheap, easy-to-fabricate and very versatile. For these reasons, it is advantageous to use them for sensor applications. For instance in case of oxygen (O_2), which is the most abundant element on earth, there is a big need for cheap sensors. Especially industry and biological research require cheap trace oxygen sensors. Optical O_2 sensors represent a promissing type, since they offer fast response and no O_2 consumption. However, they suffer from photodegradation and a rather complex assembly. To overcome these drawbacks, organic electronics with their excellent adjustability can be used to realize a monolithic and therefore cheap implementation.

In this work, we developed a monolithic all-organic oxygen sensor which is composed of a biluminescent sensing layer, an ultraviolet OLED with a peak wavelength of 375 nm as an excitation source and a novel narrow bandwidth OPD. The biluminescent sensing layer shows fluorescence and phosphorescence at the same time which enables self referencing to avoid photodegradation caused distortion. Furthermore, the long lifetime phosphorescene allows sensing within the ultra-trace oxygen range.

CPP 86.7 Thu 11:00 ZEU 260

High-Speed and High-Current Vertical Organic Transistors — •Felix Dollinger[1], Kyung-Geun Lim[2], Axel Fischer[1], Petr Formánek[3], Hans Kleemann[1], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Dresden, Germany — [2]Korea Research Institution for Standard Science (KRISS), Daejeon, Korea — [3]Leibniz-Institut für Polymerforschung Dresden e. V. (IPF), Dresden, Germany

The Organic Permeable Base Transistor (OPBT) is a vertical organic transistor design allowing for very high current densities, and hence the fastest operating speed of all organic transistors with transit frequency reaching 40 MHz. The modulation of current in such a device is achieved by a thin aluminum base electrode, corresponding to the gate in a conventional field effect transistor. This base layer is located in the center of the vertical stack and is permeable for electrons.

Using an improved fabrication technique of the base layer, we show OPBTs with excellent properties. Specifically, the devices show very large current gain and reduced parasitic leakage currents. This has been achieved by applying electrochemical anodization to the base layer, which most interestingly, can be carried out atop of the organic semiconductor layer without compromising the transistor performance [Dollinger et al., **Advanced Materials, 2019**].

In addition, we investigate the behavior of OPBTs under electrical stress, which helps to understand the suitability of these transistors for long-time real-life applications [Dollinger et al., **Advanced Electronic Materials, 2019**].

15 min. break

CPP 86.8 Thu 11:30 ZEU 260

***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 University Gießen, Institute of Applied Physics

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 86.9 Thu 11:45 ZEU 260

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.

CPP 86.10 Thu 12:00 ZEU 260

Multifrequency Spin-Resonance Experiments on Organic LEDs based on Inter- and Intra-molecular Triplet-Singlet Conversion — •Sebastian Weissenseel, Rebecca Bönnighausen, Jeannine Grüne, Nikolai Bunzmann, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg

The world of organic light emitting diodes (OLEDs) regained a lot of attention with the publication of Goushi et al. in 2012 [1], where the thermal activation of non-radiative triplets via reverse intersystem crossing (RISC) was applied to enhance the fluorescence in OLEDs. This process can be investigated by spin sensitive techniques such as electroluminescence detected magnetic resonance (ELDMR). The idea behind these experiments is that the static magnetic field applied to devices under test modifies only the energy levels of triplet states due to the magnetic moment, resulting in Zeeman splitting, thus changing the emission rates. We observed that resonant microwave radiation, applied to OLEDs by a stripline, led to a change in electroluminescence [2]. Here, we show the difference between inter- and intra-molecular TADF systems by applying a broad range of resonance frequencies. With this method, we gain knowledge about the magnetic field dependence of the linewidth of the ELDMR signal.

[1] Goushi, et al., Nat. Photon. 6, 253 (2012)
[2] Bunzmann et al., arXiv:1906.06073. (2019)

CPP 86.11 Thu 12:15 ZEU 260

What is the effective electrical bandgap of an OLED? — •Axel Fischer, Jinhan Wu, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, TU Dresden

Organic light-emitting diodes (OLEDs) are used since several years in commercial products, such as displays. However, there are still open questions. For example, there is a lack of studies about the (effective) electrical bandgap of state-of-the-art OLEDs although it is quite important to know the energy that free charge carriers have to overcome before they can recombine. Here, we illuminate OLEDs with UV light which results in generation of free charge carriers that create an open-circuit voltage similar to what one typically observes for solar cells. A comprehensive analysis of temperature dependent measurements then allows to determine an effective electrical bandgap that will be compared to the energy levels of the molecules used in the investigated OLED [Wu et al., Adv. Opt. Mater. **2019**, 7, 1801426]. The future importance of the results relies in determining voltage losses, both, from internal non-radiative relaxation as well as from charge transport.

CPP 86.12 Thu 12:30 ZEU 260

Increasing the triplet-to-singlet ratio in photoluminescence of TADF emitters using phosphorescent sensitizers: a pathway to study non-linear effects — •Paulius Imbrasas, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, 01187 Dresden, Germany

Organic emitters based on thermally activated delayed fluorescence (TADF) have been extensively investigated in the past decade. The main appeal of TADF is that it allows excited triplet state upconversion to the singlet manifold, leading to increased light generation efficiencies. However, due to comparably long lifetimes of triplet states in TADF emitters, non-linear quenching mechanisms as triplet-triplet annihilation (TTA) or triplet-polaron quenching (TPQ) start playing a role. Adding to that, due to the nature of exciton generation in organic light-emitting diodes (OLEDs), 75% of created excitons are triplet states, which is different in the case of photophysical emitter studies. This typically leads to a high mismatch between triplet densities in photoluminescence (PL) and electroluminescence (EL). In this work, we introduce phosphorescent sensitizer molecules to TADF based emission layers to increase the triplet-to-singlet exciton density ratio under optical excitation to close the gap to EL exciton distributions. This allows us to investigate triplet-related detrimental effects under practical lab conditions. This simple and versatile approach represents a powerful toolbox to thoroughly probe unfavorable high brightness effects.

CPP 87: Wetting and Liquids at Interfaces and Surfaces I (joint session CPP/O/DY)

Time: Thursday 9:30–13:00 Location: ZEU 255

CPP 87.1 Thu 9:30 ZEU 255

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], Dmitrij Stehl[1], Anja Drews[2], Markus Gallei[3], and Regine von Klitzing[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]HTW Berlin, Berlin, Germany — [3]Universität des Saarlandes, Saarbrücken, Germany

Pickering Emulsions (PEs) describe emulsions stabilized by surface-active particles. The aim of the present work is to design PEs as a reaction environment for catalytic reactions. As a model reaction the hydroformylation of 1-dodecene is 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 dominated 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 prepared. 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.

CPP 87.2 Thu 9:45 ZEU 255

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 87.3 Thu 10:00 ZEU 255

Concentration measurements in binary liquids via Raman spectroscopy — •Alena K. Bell and Robert W. Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt, Deutschland

The optical measurement of concentration gradients in liquid mixtures plays a crucial role in understanding transport processes in various technical applications such as printing or medical technology. In particular Raman spectroscopy offers a direct approach to identify the substances and to quantify the concentration of the components in a binary liquid. In order to quantify concentration gradients confocal Raman spectroscopy can provide the necessary spatial and temporal resolution that is needed to monitor transport processes as they occur during the evaporation of binary droplets or during mixing processes in microchannels. To this end, chemically similar substances such as alcohols of different molecular weight need to be differentiated either through the analysis of the fingerprint region or through chemical labelling. However, using the weak Raman signals in fingerprint region reduces the temporal resolution drastically which makes chemical labelling much more convenient. We discuss the advantages and disadvantages of chemical labelling in order to discriminate spectroscopically between the components of a binary liquid. By using this approach concentration gradients can be calculated by comparing relative peak intensities and correlating these results with calibration curves. Thus, the temporal and spatial evolution of concentration gradients in binary mixtures of chemically similar fluids can be analysed.

CPP 87.4 Thu 10:15 ZEU 255

Hard sphere electrolyte solutions at heterogeneously charged substrates — •Maximilian Mussotter[1], Markus Bier[2], and S. Dietrich[1] — [1]Max-Planck Institut für Intelligente Systeme und Universität Stuttgart, 70569 Stuttgart, Germany — [2]University of Applied Sciences Würzburg-Schweinfurt, 97421 Schweinfurt, Germany

The structure of a dilute electrolyte solution close to a surface carrying a non-homogeneous surface charge distribution is investigated by means of classical density functional theory (DFT) within the approach of fundamental measure theory (FMT). In the case of electrolyte solutions, the effects of these inhomogeneities are particularly severe due to the corresponding length scale being the Debye length, which is large compared to molecular sizes. A fully three-dimensional investigation is performed, which accounts explicitly for the sol- vent particles, and thus provides insight in effects of ion-solvent coupling. The present work introduces a powerful framework to study a broad range of possible surface charge heterogeneities even beyond the linear response regime, showing a sensitive dependence of the density profiles of the fluid components and of the electrostatic potential on the magnitude of the charge as well as on the short ranged details of the surface charge pattern.

CPP 87.5 Thu 10:30 ZEU 255

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 87.6 Thu 10:45 ZEU 255

Depleting Hydrogels with Oil Flows — •Philipp Baumli[1], Emanuela Lorusso[2], Lukas Hauer[1], Azadeh Sharifi-Aghili[1], Katharina Hegner[1], Maria D'Acunzi[1], Burkhard Duenweg[1], Jochen Gutmann[2], Hans-Jürgen Butt[1], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Deutsches Textilforschungszentrum Nord-West ÖP GmbH, Adlerstraße 1, 47798 Krefeld, Germany.

Hydrogels are ubiquitous in our daily lives. Applications range from jelly pudding and diapers to scaffolds in tissue engineering. A hydrogel-coating is covalently attached to a micropillar array. Swelling the hydrogel-coating with water establishes a liquid-infused surface (LIS). On LIS, liquid-depletion is synonymous with loss of functionality.

We demonstrate that the hydrogel-based LIS can be kept lubricated upon a shear-flow of oil for a wide variety of flow conditions independent of the exact nature of the hydrogel-coating. Dehydration of the hydrogel-coating is followed by confocal laser scanning microscopy and progresses linearly independent of flow conditions and hydrogel. The mechanism is explained with the help of an extended diffusion model.

CPP 87.7 Thu 11:00 ZEU 255

Tracking nematic flows at microscales using small angle X-ray scattering — •Paul Steffen[1], Eric Stellamanns[2], Michael Sprung[2], Fabian Westermeier[2], and Anupam Sengupta[3] — [1]Göttingen — [2]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]Physics of Living Matter, Dept. of Physics and Materials Science, University of Luxembourg, Luxembourg

Liquid crystal microflows play a fundamental role in materials, modern display technologies, and biological systems. However, a quantitative, dynamic and spatially resolved measurement of the director field and surface anchoring remain a significant challenge. Here we present small angle X-ray measurements on stationary flows of 4-Cyano-4-pentylbiphenyl (5CB) in circular Kapton capillaries (under homeotropic and random planar anchoring) at temperatures between 280 and 310 K, and Ericksen numbers ranging from 0 to 200, with a spatial resolution of 1/1000 of the capillary dimension. The angular dependence of the scattering peaks from both periodic length scales was approximated by a double Gaussian fit with four parameters: amplitude, angle, width and background amplitude. The peak angles were found to be in good agreement with the director fields calculated using the Leslie-Ericksen theory. The width and the amplitude of the scattering patterns obtained from the larger length scale are less affected by the temperature than those from the smaller length scale.

15 min. break

CPP 87.8 Thu 11:30 ZEU 255

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 $Ca = \frac{\mu\phi v L}{K P_b}$ 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.

CPP 87.9 Thu 11:45 ZEU 255

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.

CPP 87.10 Thu 12:00 ZEU 255

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 87.11 Thu 12:15 ZEU 255

Simulations of Thermal Fluctuations with a Thin Film Lattice Boltzmann Model — •Stefan Zitz[1], Jens Harting[1,2], and Andrea Scagliarini[3] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nuremberg, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands — [3]Consiglio Nazionale delle Ricerche, Rome, Italy

The effect of thermal fluctuations on thin film flows is an interesting yet challenging phenomenon. Although in experiments their presence is undeniable thermal fluctuations are often neglected in the analysis of the results. Also in simulations their inclusion is far from being trivial due to the stochastic nature of the fluctuations.

Here we present a numerical approach to include the influence of thermal fluctuations. Based on our newly developed lattice Boltzmann method we show how to effectively match the thin film regime and further how to include thermal fluctuations in a self consistent matter [1].

One problem of deterministic thin film simulations is the discrepancy between experimental and simulated rupture times in dewetting experiments. It has been shown that the experimental rupture times are shorter than the ones predicted by deterministic simulations. We will show that adding fluctuations does reduce the rupture time to better match the experimental results. To this end we will also address the importance of the fluid substrate interaction, e.g. the equilibrium contact angle θ_{eq}.

S. Zitz, J. Harting et al., Phys. Rev. E 100:3, 033313, 2019

CPP 87.12 Thu 12:30 ZEU 255

Impact of submillimetre-sized droplets on freely suspended liquid membranes — •Florian von Rüling, Alexey Eremin, and Ralf Stannarius — Otto von Guericke University Magdeburg, Germany

Droplet impact and splashing phenomena at solid and fluid interfaces remain an exciting research topic with vast application possibilities [1]. Impact scenarios are primarily governed by capillary forces, inertia, oscillation dynamics of the droplets, and the dynamics of the thin air cushion entrapped between droplet and surface during impact [2,3]. We experimentally investigated the impact of large submillimetre- to millimetre-sized droplets on freely suspended smectic films. We were able to vary the droplet diameter from several hundred microns to one millimetre. Droplets can either be trapped or reflected by the film or tunnel through it, depending on geometrical and dynamical parameters. The film remains intact in all these scenarios. In addition to the drop size and impact velocity, material properties and the film thickness can affect the behaviour of both droplet and film.

[1] A. M. Worthington, The Splash of a Drop; Romance of Science. Society for the Promotion of Christian Knowledge, London, 1895.

[2] C. Antonini, A. Amirfazli, M. Marengo, Drop impact and wettability: From hydrophilic to superhydrophobic surfaces, Phys. Fluids 24 102104 (2012).

[3] S. Dölle, R. Stannarius, Microdroplets impinging on freely suspended smectic films: three impact regimes, Langmuir 31 6479 (2015).

CPP 87.13 Thu 12:45 ZEU 255

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 88: Responsive and Adaptive Systems

Time: Thursday 9:30–11:30 Location: ZEU 114

CPP 88.1 Thu 9:30 ZEU 114

Orientation approach to directional deformations in glassy azopolymers — •Bharti yadav, Jan Domurath, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V., PF 120411, 01069 Dresden

Glassy azopolymers deform in the presence of light even below the glass transition temperature , as the light induced stress is greater than the yield stress . The photodeformations are directional and depend on the polarization of light . For linearly polarized light the azopolymers elongate in the direction of polarization and for circularly polarized light in the plane perpendicular to the propagation vector. The cause of these directional deformations is the orientation potential which acts on each chromophore attached to the main chain and generates a light induced stress. We model the azopolymers as visco-plastic materials by implementing the stress in a finite element modelling software ANSYS. The true strains and elongations are calculated as a function of time for both linearly and circularly polarized light when the intensity of light is homogeneous [1]. Additionally, we implement the light induced stress corresponding to stripe-like Gaussian distributed light with polarization in the direction of intensity gradient to get the photodeformations and to compare with experimental results [2]. [1] B. Yadav, J. Domurath, K. Kim, S. Lee, M. Saphiannikova, J. Phys. Chem. B 122 (2019) 2001-2009 [2] A. Ambrosio , A. Camposeo, A. Carella,F. Borbone, D. Pisignano, A. Roviello, P. Maddalena, J. App. Phys. 107 (2010) 083110

CPP 88.2 Thu 9:45 ZEU 114

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, 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 1510/3-1.

[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 88.3 Thu 10:00 ZEU 114

Photo-switchable surfactants for responsive air-water interfaces: Azo vs AAP amphiphiles — •Marco Schnurbus[1], Richard Campbell[2], Jörn Droste[1], Christian Honnigfort[1], Philipp Gutfreund[3], Michael Hansen[1], and Björn Braunschweig[1] — [1]Institute of Physical Chemistry, WWU Münster — [2]Division of Pharmacy & Optometry, Manchester — [3]ILL, Grenoble

Two photo-switchable ammonium bromide surfactants (Azo-TB and AAP-TB) were compared with respect to their switching ability. Both surfactants were studied with UV/Vis and NMR spectroscopy in the bulk and with sum-frequency generation (SFG), neutron reflectometry (NR) and tensiometry at the air-water interface. The surfactants undergo photo-isomerization reactions from their Z and E conformation when irradiated with 365 nm UV and 520 nm green light. NMR spectroscopy showed a higher photostationary state (PSS) for the E-isomer under green light irradiation for the AAP-TB, whereas the Z-isomer under UV light had a higher PSS for the Azo-TB. Tensiometry demonstrates the surfactants ability to reversibly change the surface tension with light irradiation, which yields a maximum change in surface tension of 12 mN/m and 8 mN/m for AAP-TB and Azo-TB surfactants, respectively. Furthermore, the surface excess from NR as well as the aromatic C-H band and the nonresonant contribution to the SFG spectra demonstrate higher switching abilities for the AAP-TB surfactant. In addition, analysis of SFG spectra from O-H and C-H stretching bands of Azo-TB and AAP-TB surfactants indicate surfactant desorption from the air-water interface when irradiated with UV light.

CPP 88.4 Thu 10:15 ZEU 114

Polarization controlled fine structure of diffraction spots from optically induced azo-polymer surface relief grating: In-situ atomic force microscopy and diffraction efficiency measurements — •Joachim Jelken, Carsten Henkel, and Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Here we present an experimental and theoretical study of an observed fine structure in the diffraction spot of an azo-polymer surface relief grating. This is achieved utilizing a homemade setup [1] which consists of three parts: a two beam interference setup for topography structuring, an atomic force microscope (AFM) for in-situ recording of surface morphology, and a diffraction efficiency (DE) setup which enables to obtain information about the birefringence grating at the same time. Our findings show that the fine structure is a result of a gaussian intensity profile of the recording interference pattern [2], which will create a gaussian amplitude modulation (envelope) of the surface and birefringence grating. A wide probe beam will average across the grating which results in the observed fine structure of the diffraction spot. The spatial profile of the diffraction spot is thereby converting from a gaussian, to a *donut* (dark spot in the center) and finally to a *Saturn* (bright ring with bright center) structure with an increase in the SRG height. We will show that we can switch between the different spatial profiles by changing the polarization of the probe beam. [1]J. Jelken and S. Santer, RSC Advances, 2019, 9, 20295-20305 [2]J. Jelken, C. Henkel and S. Santer, Appl. Phys. B, 2019, 125, 218

CPP 88.5 Thu 10:30 ZEU 114

Unexpected Monolayer-to-Bilayer Transition of Arylazopyrazol Surfactants Facilitates Superior Photo-Control of Fluid Interfaces — •Christian Honnigfort[1], Richard A. Campbell[2], Dana Glikman[1], Marco Schnurbus[1], Philipp Gutfreund[3], Bart Jan Ravoo[1], and Björn Braunschweig[1] — [1]University of Münster, Germany — [2]University of Manchester, United Kingdom — [3]Institut Laue-Langevin, France

Interfaces that can change their chemistry on demand have huge potential for applications and are prerequisite for responsive or adaptive materials. We report on the performance of a newly designed n-butyl-arylazopyrazole butyl sulfonate (butyl-AAP-C_4S) surfactant that can change its structure at the air-water interface by E/Z photoisomerization in an unprecedented way. Large and reversible changes in surface tension ($\Delta\gamma \sim 27$ mN/m) and surface excess ($\Delta\Gamma > 2.9$ μmol/m^2) demonstrate superior performance of the butyl-AAP-C_4S amphiphile to that of existing ionic surfactants. Neutron reflectometry and sum-frequency generation spectroscopy reveal that these large changes are caused by an unexpected monolayer-to-bilayer transition. This exceptional behavior is further shown to have also dramatic consequences at larger length scales as highlighted by two application like the light-triggered collapse of aqueous foam which is tuned from high (>1h) to low (<10min) stabilities and light-actuated particle motion via Marangoni flows.

CPP 88.6 Thu 10:45 ZEU 114

Kinetics of phase separation in PNIPAM solutions after pressure jumps — Bart-Jan Niebuur[1], Leonardo Chiappisi[2,3],

Xiaohan Zhang[1], Florian A. Jung[1], Alfons Schulte[4], and •Christine M. Papadakis[1] — [1]TU München, Physik-Department, Fachgebiet Physik weicher Materie, 85748 Garching — [2]Institut Laue-Langevin, Large Scale Structures Group, 38042 Grenoble, France — [3]TU Berlin, Institut für Chemie, 10623 Berlin — [4]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, FL, U.S.A.

The thermoresponsive polymer PNIPAM in aqueous solution features lower critical solution behavior. Its cloud point depends on pressure with the coexistence line being an ellipse in the temperature-pressure frame. Performing fast pressure jumps from the one-phase to the two-phase region along with time-resolved small-angle neutron scattering, we can follow the pathway of phase separation with a time resolution of 50 ms and over a wide range of length scales [1]. Since the hydration state of PNIPAM depends on pressure, pressure jumps at low and at high pressures allow addressing the role of dehydration for the aggregate growth [2]. Varying the target pressure gives insight into the role of kinetic and thermodynamic factors.

1. B.-J. Niebuur et al., *ACS Macro Lett.* **7, 1155 (2018).**
2. **B.-J. Niebuur et al.,** *Macromolecules* **52, 6416 (2019).**

CPP 88.7 Thu 11:00 ZEU 114

Thermal behavior and co-nonsolvency of the amphiphilic diblock copolymers PMMA-*b*-PNIPAM in aqueous solution — •Chia-Hsin Ko[1], Cristiane Henschel[2], Geethu P. Meledam[1], Martin Schroer[3], Peter Müller-Buschbaum[1], André Laschewsky[2,4], and Christine M. Papadakis[1] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Institut für Chemie, University of Potsdam, Potsdam-Golm, Germany — [3]European Molecular Biology Laboratory, Hamburg, Germany — [4]Fraunhofer Institute for Applied Polymer Research IAP, Potsdam-Golm, Germany

Amphiphilic diblock copolymers having a hydrophobic poly(methyl methacrylate) (PMMA) block and a thermoresponsive poly(*N*-isopropylacrylamide) (PNIPAM) block form core-shell micelles in aqueous solution. The PNIPAM blocks are not only sensitive to temperature, but also to the solvent composition. Adding methanol as a cosolvent causes these blocks to collapse which reduces the transition temperature, i.e. co-nonsolvency is observed. We focus on investigating (i) the structure of the self-assembled micelles and the changes upon collapse and aggregation with increasing temperature, and (ii) the co-nonsolvency effect of PMMA-*b*-PNIPAM in pure D_2O and in different D_2O/CD_3OD mixtures using turbidimetry, differential scanning calorimetry (DSC), dynamic light scattering (DLS) and small-angle X-ray scattering (SAXS). The results reveal the role of the nature of the thermoresponsive block on the thermal behavior and the morphology changes upon temperature and solvent composition.

CPP 88.8 Thu 11:15 ZEU 114

Untethered and ultrafast soft-bodied robots — •xu wang[1], guoyong mao[2], jin ge[1], rico Illing[1], michae drack[2], gilbert santiago canon bermudez[1], jurgen fassbender[1], tobias kosub[1], martin kaltenbrunner[2], and denys makarov[1] — [1]Helmholtz-Zentrum Dresden - Rossendorf — [2]Johannes Kepler University Linz

Soft robots have been developed to fulfil demands of better deformability and adaptability to a changing environment.[1-4] The use of magnetic fields is appealing for diverse application scenarios (e.g. environmental, biological, medical), where the benefits stem from their long-range penetration, easy accessibility, and controllability.[1-4] There are numerous demonstrations of magnetically triggered miniatured soft robots performing multimodal locomotion[3] and complex 3D actuations.[4]

Here, we present ultrathin (7-100 μm) and lightweight (1.2-2.4 g/cm3) soft robots that can be actuated in a small magnetic field of 2 mT reaching full actuation amplitude in 10 ms only. By programming the foils into different geometries, these soft robots are readily used for multifunctional motions with a magnetic coil or a permanent magnet, such as a quick fly gripper, and a complex non-linear cross-clapping mimicked motion.

1. Z. Ren et al., Nat. Commun. 10, 2703 (2019). 2. Y. Kim et al., Science Robotics 4, eaax7329 (2019). 3. W. Hu et al., Nature, 554, 81(2018) 4. Kim. Y, et al., Nature, 558, 274 (2018)

CPP 89: Materials for Energy Storage (joint session KFM/CPP)

Time: Thursday 9:30–11:50 Location: HSZ 301

CPP 89.1 Thu 9:30 HSZ 301

Investigation of Li diffusion mechanisms in V_2O_5 — •Fabian Dietrich and Eduardo Cisternas Jara — Núcleo Milenio Multi-Mat & Departamento de Ciencias Físicas, Universidad de La Frontera, Temuco, Chile

Vanadium pentoxide (V_2O_5) is a promising candidate for the use as cathode material in lithium ion batteries (LiB) due to its layered structure. For the use as electrode material, it is necessary to understand fundamental aspects of its structure as well as mechanisms during the charging and discharging process. Hence, we investigate the diffusion of lithium ions in that material, paying attention to vanadium pentoxide species with different amount of inserted lithium.

The investigations are done by simulation of the processes using density functional theory (DFT) in the periodic boundary condition, also in combination with plane-wave basis sets and dispersion correction. Diffusion pathways are calculated using the nudged-elastic band (NEB) method. Resulting barrier heights are used for subsequent Monte-Carlo simulations. Frequency calculations are used to estimate the diffusion coefficients, which are also used in the MC simulations.

We assumed different diffusion mechanisms for the pure V_2O_5 and the lithiated species LiV_2O_5. While in V_2O_5 a quite free diffusion of Li ions is possible, the occupation of distinct lattice positions by Li ions leads to a blocking of certain pathways. Thus, the knock-off mechanism is proposed for LiV_2O_5. This assumption could be confirmed by the calculations, comparing different mechanisms for the diffusion in LiV_2O_5.

CPP 89.2 Thu 9:50 HSZ 301

Evaluation of the Applicability of the Brick Layer Model for Describing the Electrical Transport within Ceramic Materials — •Janis K. Eckhardt[1,2], Markus S. Friedrich[2,3], Matthias T. Elm[2,3,4], Peter J. Klar[2,3], and Christian Heiliger[1,2] — [1]Institute for Theoretical Physics, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [3]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [4]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany

In literature, the transport properties of ceramics such as the active cathode material within lithium ion batteries are commonly described by making use of the so called Brick Layer Model (BLM). The BLM cannot account for percolation effects. However, the microstructure of real devices, e.g. secondary materials of cathodes or thin films is such that disorder will lead to percolation effects. In order to account for these effects and to validate the applicability of the BLM an impedance network model based on Kirchhoff's current law has been developed. With its help it is possible to compute impedance spectra and current density distributions of defined or random structures that mimic the properties of the real microstructure. Comparing the computational result to the prediction of the BLM, it becomes obvious that an additional semicircle(s) and signal(s) respectively in the impedance and distribution of relaxation times spectra may occur. This effect can be attributed to the multidimensional transport mechanism within the structures which is not accounted for in the commonly used BLM.

CPP 89.3 Thu 10:10 HSZ 301

First principles calculation on intrinsic defects properties of Sodium Niobate — •Lorenzo Villa — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, TU Darmstadt, Otto-Berndt-Straße 3, D-64287 Darmstadt, Germany

In recent years extended research has been focusing on improving the properties of capacitors for energy storage applications. In this context, lead-free antiferroelectric materials (AFE) are excellent candidates due to their ability of displaying high energy density, high energy efficiency and low environmental impact. In this class of compounds, $NaNbO_3$ (NN) is amongst the most promising materials, due to the possibility to obtain double P-E loops at room temperature. One of the mostly used methods to obtain narrower antiferroelectric P-E loops is via doping. Intrinsic defects can interact with the dopants and therefore can have an impact on AFE properties. In order to investigate the interaction of intrinsic defects with dopants, we have studied the contribution of vacancies to intrinsic electron and hole conductivity and their interaction with different types of dopants (Sr, Ca, Mn). All calculations were performed in the framework of Density Functional Theory using Hybrid functionals. In particular, we have investigated the formation energies of all vacancy types considering all possible charge states in five different regions of the stability diagram.

20 min. break

CPP 89.4 Thu 10:50 HSZ 301

Glass ceramics with proton conducting crystalline phases — •Laura Weisshoff[1,2], Martin Letz[1,2], Martin Jourdan[1], and Martun Hovhannisyan[2] — [1]Johannes Gutenberg Universität Mainz — [2]Schott AG Mainz

Proton conducting crystal phases such as the perovskite type have their application in proton conducting fuel cells (PCFC), sensors and hydrogen separation. A reduction of the operating temperature due to highly efficient inorganic proton conducting materials is an important development target. For this, a proton-conducting electrolyte is a key component and an optimized material is required. Standard ceramic solutions show high sintering temperature and pores. A non-gas tight material can lead to a catastrophic failure of the PCFC. Therefore, we develop pore free glass ceramics with lower sintering temperature. The present talk reports the progress of glass ceramics with proton conducting crystalline phases.

CPP 89.5 Thu 11:10 HSZ 301

Rapid, clean and scalable synthesis of microporous functional MOFs and their non-conventional forms via mechanochemistry — •Krunoslav Užarević — Ruder Boskovic Institute, 10000 Zagreb, Croatia

Here we present the application of mechanochemical reactions,[1] i.e. reactions between solid reactants induced by mechanical force, for a rapid, green and room-temperature transformation of environmentally safe metal precursors, oxides or hydroxides into most relevant microporous MOFs, such as HKUST-1, MOF-74[5] or zirconium-based MOFs of UiO[3] and NU- families, and also their multi-metal or amorphous derivatives not accessible from solution. We show here how the milling produces high-quality MOFs quantitatively in multigram quantities by using only a catalytic amount of *green liquids, such as methanol or water.

In situ synchrotron X-ray powder diffraction monitoring[8] revealed that the mechanochemical formation of MOFs often proceeds through intermediate phases, most of which are inaccessible from solution procedures. It is possible to isolate and characterize these intermediates, and also use them for the controllable synthesis of multi-metal MOFs, such as various bimetal MOF-74 materials, with interesting magnetic properties and strong potential for new catalytic reactivity.

[3] James et al, Chem. Soc. Rev. 2012, 42, 7638. [2] Julien et al, J. Am. Chem. Soc., 2016, 138, 2929. [3] Užarević et al., Chem. Commun. 2016, 52, 2133. [8] a) Užarević et al., J. Phys. Chem. Lett, 2015, 6, 4129.

CPP 89.6 Thu 11:30 HSZ 301

Actuation and electrostriction of composite films with heteregenous filler clustering — •Elshad Allahyarov — Duisburg-Essen University, Theoretical Chemistry

Controlled actuation of electroactive polymers with embedded high dielectric nanoparticles is theoretically analyzed. If the inclusions are placed randomly in the elastomer body, the composite always contracts along the direction of the applied field. For a simple cubic distribution of inclusions, contraction occurs if the applied field is directed along the [001] direction of the lattice. For inclusions occupying the sites of other lattice structures such as body-centered or face-centered cubic crystals, the composite elongates along the field direction if it is applied along the [001] direction. The stability of the elongation against the imperfectness of the lattice site positions and the distortion ratio of the initial structures are examined. Finite elongation windows show up for the initially distorted body-centered cubic and face-centered cubic crystals as a function of the distortion ratio of the initial structure. The existence of these elongation windows are also predicted from the analysis of the electrostatic energy of the distorted body-centered cubic and face-centered cubic lattice structures. Our results indicate that the electrostriction effect, which is the main contribution to the actuation of low aspect-ratio composites, strongly depends on the geometry of the spatial distribution of nanoparticles, and can thereby largely be tuned.

CPP 90: Perovskite and photovoltaics V (joint session HL/CPP)

Time: Thursday 9:30–12:00 Location: POT 251

CPP 90.1 Thu 9:30 POT 251

Surface Properties of $FA_xCs_{1-x}Pb(I_yBr_{1-y})_3$ — •Julian Gebhardt[1], Daniel Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Wöhlerstraße 11, D-79108 Freiburg — [2]FMF Universität Freiburg, Stefan-Meier-Straße 21 D-79104 Freiburg

Since the rise of hybrid perovskites as promising material for photovoltaic applications inspired by $MAPbI_3$ (MA=$CH_3NH_3^+$), many research efforts have been directed towards overcoming practical issues of such light absorbing layers. Apart from replacing silicon as absorber in single-junction solar cells, a promising route is to combine perovskites with established materials in multi-junction tandem cells. For these applications, hybrid perovskite design, i.e., mixing inorganic and organic ions in order to balance stability and light absorbing properties, changes in terms of target properties. This search temporarily concluded in materials of the type $FA_xCs_{1-x}Pb(I_yBr_{1-y})_3$ (FA=$HC(NH_2)_2^+$), with $x \approx 0.8$ and $y \approx 0.7$. During the extensive search for perovskite based absorber materials, theoretical understanding has proven vital to navigate the huge combinatorial space. Naturally, such investigations focused on bulk properties. This neglects the important step from lab scale absorber materials design towards working devices that require contacting and possibly passivation.

We present an investigation of surface properties of the $FA_xCs_{1-x}Pb(I_yBr_{1-y})_3$ family by electronic-structure theory to guide future interface optimization for these and other absorber materials. Focusing on non-polar surfaces, we investigate the stability and effects on the electronic-structure.

CPP 90.2 Thu 9:45 POT 251

Theoretical analysis of ultrathin Cu(In,Ga)Se2 solar cells with Zn(O,S) buffer layer — •gabin landry mbopda tcheum[1,3], ariel teyou ngoupo[1], narngar guirdjebaye[1], soumaila ouedraogo[2], and jean-marie b. ndjaka[1] — [1]University of Yaounde I, Yaounde, Cameroon — [2]Université Joseph Ki-ZERBO, Ouagadougou, Burkina Faso — [3]Friedrich-Schiller-Universität, Jena, Germany

The optimisation of Cd-free buffer layer, for CIGS based solar cells, appears as an ingenious way to reduce the absorber thickness without compromising the solar cell*s performance. Therefore, we discuss and present simulated electrical properties of CIGS solar cells with Zn(O,S) buffer layers. We present the electrical performance of this type of thin films solar cells with ultra thin absorber and buffer layers. However, as ultra thin absorber leads to increasing recombinations at the back contact, we introduced SnSe and a highly doped CIGS layer (known as p+-CIGS layer) as back surface field between the Mo layer and CIGS absorber. Here, we discussed their impact on the cell*s efficiency and on the band alignment.

CPP 90.3 Thu 10:00 POT 251

A comprehensive argument for the defect tolerance of metal-halide perovskite solar absorbers — •Anoop Chandran, Irene Aguilera, Christoph Friedrich, Thomas Kirchartz, Uwe Rau, and Stefan Blügel — PGI-1, IAS-1 and IEK-5, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Charge transport and recombination probabilities are related to the defects in a semiconductor. Reduction of scattering centres is essential to preserve the optoelectronic properties of solar absorbers. The ability of semiconductors to retain its properties in the presence of defects or the elimination of defects by a self-reorganisation mechanism is collectively known as defect tolerance.

Defect states formation is dictated by the bonding behaviour of the band extremes. Compression or dilation of lattice from its equilibrium configuration results in the change of energy levels. Rate of this change can be used to measure the deformation potential and thereby defect tolerance of materials. We develop a turn-key solution for the automated computing of the deformation potential combining the FLEUR codes[1] with the open science platform AiiDA[2] to study metal-halide perovskites using density-functional-theory(DFT).

[1] www.flapw.de

[2] G. Pizzi et al. Comp. Mat. Sci. 111, 218-230 (2016)

We acknowledge the Center of Excellence MaX-Materials Science at the Exascale (EU H2020-INFRAEDI-2018) and the Jülich Supercomputing Center, (project CJPGI10) for support.

CPP 90.4 Thu 10:15 POT 251

Differences between vacuum deposition and solution processing of lead halide perovskites — •Martin Kroll, Ran Ji, Zongbao Zhang, Tim Schramm, Changsoon Cho, Frederik Nehm, Yana Vaynzof, and Karl Leo — TU Dresden, IAPP, Nöthnitzer Straße 61, 01187 Dresden

Vacuum deposition is the preparation technique of choice for large scale production of organic thin film solar cells, due to the superior control it offers over film formation and deposition of multilayers. It is also possible to deposit perovskite materials by thermal evaporation, however motivated by its simplicity and low associated costs, most research groups focus on solution processed perovskites. Nevertheless, recent reports show that power conversion efficiencies of vacuum deposited perovskite solar cells surpassed 20%, making them comparable to solution processed devices. The fabrication of perovskite thin films by thermal evaporation in vacuum faces different challenges that solution processing and often results in different film properties. We compare the properties and performance of perovskites fabricated by the two methods and report on the deviations we observe in morphology, stability and photovoltaic device performance. We discuss the influence of processing conditions during vacuum and solution processing on the properties of the perovskites films as well as their effect on the device performance, stability and reproducibility.

30 min. break

CPP 90.5 Thu 11:00 POT 251

Tuning the Grain Size and Porosity of MAPbI3 Perovskite films for High Efficiency Solar Cells — •Qingzhi An[1,2], Fabian Paulus[1,2], and Yana Vaynzof[1,2] — [1]Integrated Center for Applied Photophysics and Photonic Materials, TU Dresden, Germany — [2]Center For Advancing Electronics Dresden (cfaed), TU Dresden, Germany

In this work, a facile approach to control perovskite grain size and porosity is introduced. By slightly tuning the amount of H3PO2 (HPA) in the perovskite precursor solution, we demonstrate that the average perovskite grain size can be enlarged by one magnitude regardless of the underlying charge extraction layer. We correlate these microstructural changes to the photovoltaic performance of devices and demonstrate that optimal HPA concentration leads to open circuit voltages of 1.16 V and a power conversion efficiency of 19 %. We also demonstrate that further increase in the HPA amount in perovskite precursor solution results in the formation of a regular, porous perovskite networks with highly degree of crystalline orientation. Such porous structures can be of great interest to application in light-emitting diodes or semitransparent photovoltaic devices. This work demonstrates that tuning the fraction of HPA in perovskite precursor solution is an effective method to control the perovskite grain size and layer topology.

CPP 90.6 Thu 11:15 POT 251

Charge Carrier Transport in Halide Perovskites Investigated by Optical-Pump Terahertz-Probe Spectroscopy — Hannes Hempel[1], •Andrei Petsiuk[1], Martin Stolterfoht[2], Pascal Becker[1], Dieter Neher[2], Rainer Eichberger[1], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH — [2]Institute of Physics and Astronomy, Universität Potsdam

Metal-halide hybrid perovskites exhibit excellent optoelectronic properties except for their rather moderate charge carrier mobilities. The origin of these moderate mobilities has been attributed to several (contradicting) effects, such as the formation of large and small polarons, dynamic disorder due to the soft nature of these materials, slow rotational modes of the organic molecules, as well as to the confinement of charge carriers in grains, ferroelectric domains or nanostructures. To clarify the nature of the charge carrier transport, we probed different hybrid and inorganic halide perovskites thin films and nano-crystals by temperature dependent Optical-Pump Terahertz-Probe (OPTP) spectroscopy. We find a strongly increasing mobilities with lower temperature, thus excluding small polaron formation and hopping transport. Instead, this behavior can be modeled by conventional large polaron theory and Fröhlich-type electron-phonon scattering.

CPP 90.7 Thu 11:30 POT 251

Singlet Fission Processes in Hybrid Organo-Metal Halide Perovskites Semiconductors — •Karunanantharajah Prashanthan[1,2], Klaus Lips[1], Simone Raoux[1], and Rowan MacQueen[1] — [1]Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [2]Department of Physics, University of Jaffna, Jaffna, Sri Lanka

Solar cells made from Organo-Metal Halide Perovskites show power conversion efficiency very close to the record efficiency of commercially available thin film technologies. Looking to the future of these devices, there exists promising approaches to push the efficiency beyond the Shockley-Queisser single junction thermodynamic limit. Singlet fission is a quantum mechanical process which occurs in various organic molecules, whereby a photogenerated high-energy singlet exciton spontaneously splits into two lower-energy triplet excitons. In this work, we present the possible routes and challenges involved in combining singlet fission materials with low bandgap hybrid metal halide perovskite solar cells. Using time-resolved photoluminescence spectroscopy we investigate the dynamic processes involved in singlet fission and the subsequent injection of energy and charge into the perovskite layer. The objective is to form augmented photovoltaic devices which can efficiently harvest triplets from a singlet fission layer, substantially reducing the energy loss to carrier thermalization.

CPP 90.8 Thu 11:45 POT 251

Manganese Doping Induced Quantum Confinement in the Perovskite Nanocrystals via Ruddlesden-Popper Defects — •Kavya Reddy Dudipala, Sharmistha Paul, Tushar Debnath, Jochen Feldmann, and Lakshminarayana Polavarapu — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

The concept of doping manganese ions (Mn^{2+}) into II-VI semiconductor nanocrystals (NCs) has recently been extended to perovskite NCs. The transfer of the exciton energy from a semiconductor host to Mn^{2+} dopants leads to orange emission from a spin-forbidden 4T1-6A1 Mn d-d transition. To date, most studies on Mn^{2+} doped NCs focused on enhancing the emission related to the Mn^{2+} dopant via an energy transfer mechanism. Here, we show that the doping of Mn^{2+} ions into $CsPbCl_3$ NCs not only results in a Mn^{2+}-related orange emission, but also strongly influences the excitonic properties of the host NCs. We observe for the first time that Mn^{2+} doping leads to the formation of Ruddlesden-Popper defects and thus induces quantum confinement in host perovskite NCs. We find that a slight doping with Mn^{2+} ions improves the size distribution of the NCs, which results in a prominent excitonic peak. However, with increasing the Mn^{2+} concentration, the number of Ruddlesden-Popper planes increases leading to smaller single crystal domains. The enhanced confinement and crystal inhomogeneity cause a gradual blue shift and broadening of the excitonic transition.

CPP 91: Computational Biophysics (joint session BP/CPP)

Time: Thursday 9:30–13:00 Location: SCH A251

CPP 91.1 Thu 9:30 SCH A251

Effectiveness of Ca^{2+} clearance by PMCA pumps — •Barbara Schmidt[1], Cristina Constantin[2], Bernd Fakler[2], and Heiko Rieger[1] — [1]Center for Biophysics and Department of Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Institute of Physiology, University of Freiburg, 79104 Freiburg, Germany

Ca^{2+} influx through voltage-gated (Cav) channels leads to an increase in the intracellular Ca^{2+}-concentration ($[Ca^{2+}]_i$) that can be monitored by BK-type Ca^{2+}-activated K^+ channels. Due to their gating kinetics they may be used as sensors for $[Ca^{2+}]_i$ underneath the plasma membrane. Here, K^+ currents through BK channels were used to determine the Ca^{2+} transport activity of Ca^{2+}-ATPases of the plasma membrane (PMCA), the classical Ca^{2+} pumps. Experimentally we monitored PMCA-mediated Ca^{2+} clearance by the decay of BK-currents following their activation by a short (0.8 ms) period of Ca^{2+}-influx through Cav2.2 channels. Our theoretical model describes the Ca^{2+} diffusion within a spherical cell. Time- and Ca^{2+} concentration-dependent boundary conditions model the initial Ca^{2+} influx and the following outflow via the PMCA pumps. The time scale of this diffusion process is used to predict the strength of the PMCA pumps. Based on the experimentally determined density of Cav channels and PMCA pumps within the membrane we predict a PMCA pump strength that is at least 1.5 orders of magnitude larger than what has been assumed so far.

CPP 91.2 Thu 9:45 SCH A251

Talin impacts force-induced vinculin activation by 'loosening' the vinculin inactive state — Florian Franz[1,2] and •Frauke Gräter[1,2] — [1]HITS gGmbH, Schloß-Wolfsbrunnenweg 35, 69118 Heidelberg, Germany — [2]IWR - Interdisciplinary Center for Scientific Computing, Im Neuenheimer Feld 368, 69120, Heidelberg, Germany

Focal Adhesions (FA) are large, multi-protein complexes connecting the cytoskeleton to the extracellular matrix. Their adhesive functionality is tightly regulated by mechanical stress. A key component of FA-associated mechanosensing is vinculin, which can assume either a closed (”inactive”) or open (”active”) conformation. The underlying activation mechanism, however, remains yet to be fully understood.

Here, we employ molecular dynamics (MD) simulation to demonstrate that vinculin activation is greatly facilitated by the binding of vinculin on talin's vinculin binding site. Steered MD simulations reveal that the force required for activation is drastically reduced upon formation of the vinculin-talin complex. Using correlated motions and force distribution analysis, we illuminate how the force propagation through vinculin changes upon complex formation. Interestingly, after talin dissociation, vinculin returns to its native conformation on a submicrosecond time scale, with 60% of its native contacts restored.

Our results suggest a rapid dynamic equilibrium between 'tight' and 'loosened' inactive vinculin, which depends on talin and determines the level of mechanical stress required for activation. Our study has important implications for our understanding of mechano-sensing mechanisms at FAs.

CPP 91.3 Thu 10:00 SCH A251

Protein-ligand dynamics on multisecond timescales from submicrosecond atomistic simulations — •Steffen Wolf, Benjamin Lickert, Simon Bray, and Gerhard Stock — Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, 79104 Freiburg, Germany

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 rescaling" 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 milliseconds and 2-10 in the range of seconds.

CPP 91.4 Thu 10:15 SCH A251

Active processes in cellular networks and comparison with viscoelastic models — •Joris Paijmans[1], Mandar Inamdar[2], and Frank Jülicher[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Civil Engineering, Indian Institute of Technology Bombay, Mumbai, India — [3]Center for Systems Biology Dresden, Dresden, Germany

During morphogenesis, the collective behavior of many cells determines the emergence of tissue shape. How the mechanical properties and behavior of individual cells lead to a desired morphology is not well understood. Here we use a vertex model, modeling the cellular network, and a hydrodynamic theory, describing the tissue as a continuous viscoelastic material, to study this problem in epithelial tissues.

First, we consider different scenarios for how cells drive local stresses in cellular networks such as orientation dependent edge tensions and oriented cell divisions. Coarse-graining over the cellular dynamics, we find the large scale deformation of the tissue and how cells contributed to this deformation such as cell shape changes and rearrangements in the cell network. This allows us to compare the dynamics of the cellular network to a hydrodynamic model of a viscoelastic material with active and passive contributions to the stress and cell rearrangements in the tissue. We find that the large scale viscoelastic properties of the cellular network depend strongly on the details of how cells locally generate stress. We compare results with the developing wing blade in Drosophila, where phases of active and passive cell rearrangements are observed.

CPP 91.5 Thu 10:30 SCH A251

Morphology of spherical epithelial monolayers — •Aboutaleb Amiri[1], 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.

CPP 91.6 Thu 10:45 SCH A251

The role of thickness inhomogeneities in brain folding — •Lucas da Costa Campos[1,2], Svenja Caspers[2,3,4], Gerhard Gompper[1], and Jens Elgeti[1] — [1]Theoretical Soft Matter and Biophysics (ICS-2 / IAS-2), Research Centre Jülich, Jülich, Germany — [2]Institute of Neuroscience and Medicine (INM-1), Research Centre Jülich, Germany — [3]JARA-Brain, Jülich-Aachen Research Alliance, Jülich, Germany — [4]Institute for Anatomy I, Medical Faculty, Heinrich-Heine University, Düsseldorf, Germany

The morphology of the mammalian brain cortex is highly folded. Misfolds of the brain correlate with a long list of cognitive disabilities, such as schizophrenia and epilepsy. Having realistic models of gyrogenesis is the first step in the understanding of these issues. It has been hypothesized that mechanical instabilities play an essential role in gyrogenesis. However, the emergence of higher order folding, one of the main characteristics of the human brain, has not been fully tackled. We perform finite element simulations of rectangular slabs divided into two distinct regions. Differential growth is introduced by growing the top layer (gray matter) tangentially, while keeping the underlying layer (white matter) unchanged. The material is modelled as a Neohookean hyperelastic. Simulations are performed with system with either homogeneous or inhomogeneous cortical thickness. In early stages of development, we obtain structures reminiscent of the deep sulci in the brain, which can be mapped into the primary sulci.

As the cortex continues to develop, we obtain secondary undulations whose characteristics are consistent with those of higher order folding.

30 min. coffee break

Invited Talk CPP 91.7 Thu 11:30 SCH A251

Predicting Protein and RNA Structures via data inference: from Potts models 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. Going beyond anecdotal cases of a few protein families, systematic large-scale studies of >1000 protein families are now possible and other information, such as low-resolution experimental information (e.g. SAXS or FRET) can be used as further constraints in simulations.

CPP 91.8 Thu 12:00 SCH A251

A machine learning assessment of the two states model for lipid bilayer phase transitions — •Vivien Walter[1], Céline Ruscher[2], Olivier Benzerara[2], Carlos Marques[2], and Fabrice Thalmann[2] — [1]Department of Chemistry King's College London, London, UK — [2]Institut Charles Sadron, Strasbourg, France

We have adapted a set of classification algorithms, also known as Machine Learning, to the identification of fluid and gel domains close to the main transition of dipalmitoyl-phosphatidylcholine (DPPC) bilayers. Using atomistic molecular dynamics conformations in the low and high temperature phases as learning sets, the algorithm was trained to categorize individual lipid configurations as fluid or gel, in relation with the usual two-states phenomenological description of the lipid melting transition. We demonstrate that our machine can learn and sort lipids according to their most likely state without prior assumption regarding the nature of the order parameter of the transition. Results from our machine learning approach provides strong support in favor of a two-states model approach of membrane fluidity.

CPP 91.9 Thu 12:15 SCH A251

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.

CPP 91.10 Thu 12:30 SCH A251

Quantifying membrane curvature sensing — •Kai Steffen Stroh[1] and Herre Jelger Risselada[1,2] — [1]Institute for Theoretical Physics, Göttingen, Germany — [2]Leiden Institute of Chemistry, Leiden, The Netherlands

When considering the interplay of lipid membranes and proteins, membrane curvature is an important factor, as it can act as a control mechanism for protein function. Several proteins feature subunits that serve as membrane curvature sensors. This sensing ability together with the spatial information provided by membrane curvature allows for site specific binding, and thus regulation of, e.g., transport processes.

Naturally, the curvature-dependent binding free energy provides valuable quantitative information about a protein's curvature sensing abilities. Therefore, we present a novel molecular dynamics simulations protocol to obtain such free energy profiles.

CPP 91.11 Thu 12:45 SCH A251

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 musculoskeletal 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.

CPP 92: Focus: High-resolution Lithography and 3D Patterning II (joint session KFM/HL/CPP)

Chair: Robert Kirchner (TU Dresden)

Time: Thursday 9:30–12:20 Location: TOE 317

CPP 92.1 Thu 9:30 TOE 317

Curvilinear Magnetism: Fabrication and characterization — •Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Extending 2D structures into 3D space has become a general trend in multiple disciplines including electronics, photonics, and magnetics. This approach provides means to enrich conventional or to launch novel functionalities by tailoring curvature and 3D shape. We realize 3D curved magnetic thin films where new fundamental effects emerge from the interplay of the geometry of an object and topology of a magnetic sub-system [1]. The application potential of 3D magnetic architectures is explored for the realization of mechanically shapeable magnetoelectronics [2] for virtual and augmented reality appliances [3,4]. To advance in this research field, we develop novel theoretical methods [5-7], fabrication [1,8,9] and characterization techniques [8-11]. These topics will be addressed in the presentation.

[1] R. Streubel et al., J. Phys. D: Appl. Phys. 49, 363001 (2016). [2] D. Makarov et al., Appl. Phys. Rev. 3, 011101 (2016). [3] S. Cañón et al., Nature Electronics 1, 589 (2018) & Science Adv. 4, eaao2623 (2018). [4] J. Ge et al., Nature Comm. 10, 4405 (2019). [5] O. Volkov et al., PRL 123, 077201 (2019). [6] O. Volkov et al., Sci. Rep. 8, 866 (2018). [7] V. P. Kravchuk et al., PRL 120, 067201 (2018). [8] K. S. Das et al., Nano Let. 19, 6839 (2019). [9] M. Nord et al., Small 1904738 (2019). [10] R. Streubel et al., Nature Comm. 6, 7612 (2015). [11] T. Kosub et al., Nature Comm. 8, 13985 (2017).

CPP 92.2 Thu 9:50 TOE 317

3D printing of complex submillimeter-sized wide angle objectives — •Zhen Wang[1], Ksenia Weber[1], Simon Thiele[2], Alois Herkommer[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Institute of Technical Optics and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

Compact image sensors with a variety of focal lengths, fields of view, and other optical parameters, will be the enabling technology of integrated devices for industry 4.0. In order to miniaturize the imaging devices from currently several mm^3 to below 1 mm^3, and to achieve diameters of the optics below 1 mm, 3D printing with femtosecond laser pulses is the method of choice. Here, we present several multilens designs as well as printed objectives with fields of view that range from 60° to 95°, and focal lengths in the range of 200-300 μm, with diameters around 800 μm, which allow for wide-angle imaging. We characterize their performances and report how to overcome some issues when printing such challenging designs. In the future, those objectives can be directly printed onto CMOS imaging chips which will enable very compact image sensors.

CPP 92.3 Thu 10:10 TOE 317

Additive technology for X-ray optical applications — •Adam Kubec, Frieder Koch, and Christian David — Paul Scherrer Institut

X-ray optics are used in many setups connected to materials analysis. Due to very different properties of X-rays as compared to visible light different challenges, have to be tackled in order to manufacture optics. The refractive index has only a small difference to unity. This results in a relatively small optical power. This makes it challenging to manufacture refractive lenses. A successful concentration of X-ray using refractive lenses could only been shown in 1996 using a set of individual refractive lenses.

Today refractive lenses for X-rays are commercially available and are widely used in many synchrotron radiation sources. However, it is still challenging to manufacture aberration free lenses for X-rays. Therefore, custom-made radially symmetric corrector phase plates are used to reduce the aberrations. Spiral phase plates can generate X-ray beams carrying orbital angular momentum of various topological charges.

Additive technology can now also used in order to manufacture refractive lenses directly. Due to the versatility of 3D printed geometries, it is possible to manufacture lenses adapted specifically to improve measuring techniques, such as Ptychography.

We will also see further applications of 3D printing for X-ray applications such as 3D resolution pattern (Siemens Star). These can be can be used to quantify the quality of X-ray tomography setups.

CPP 92.4 Thu 10:30 TOE 317

Mass-producible microoptical elements by injection compression molding and focused ion beam structured titanium molding tools — •Simon Ristok[1], Marcel Röder[2], Simon Thiele[3], Mario Hentschel[1], Thomas Günther[2], André Zimmermann[2], Alois Herkommer[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Hahn-Schickard, Stuttgart, Germany — [3]Institute of Applied Optics and Research Center SCoPE, University of Stuttgart, Germany

Injection molded polymer is the material of choice for micro-optics used in mass producible devices such as smartphones or optical sensors. For feature sizes on the micrometer scale the molding tools are usually fabricated by nickel electroplating on a silicon master, which was previously structured by electron beam lithography and subsequent etching. In total, two inversion steps are necessary to transfer the structure from the silicon master to a plastic polymer part. Here, we introduce an alternative method that requires only a single inversion step. An extremely robust titanium molding tool is directly structured with high precision by focused ion beam milling. We demonstrate the fabrication of Fresnel lenses with 100 μm diameter and a maximum structure height of 1 μm. The inverse Fresnel lens structured into the titanium is transferred to polymer by injection compression molding, enabling rapid mass replication. We show that the optical performance of the molded Fresnel lenses is in good agreement with simulations, rendering our approach suitable for applications which require compact and high quality optical elements in large numbers.

20 min. break

Invited Talk CPP 92.5 Thu 11:10 TOE 317

3D Printing with Electrons - Advances and Opportunities — •Harald Plank — Institute of Electron Microscopy, Graz University of Technology, Graz, Austria

Since the advent of additive manufacturing, this technology class made tremendous progress. While achievable feature sizes continuously decreased from cm's over mm's towards the sub-micron range their 3D possibilities became increasingly powerful. Naturally, there is a strong interest to push 3D printing into the nano-scale, to take advantage of nanoscale effects. Within the small pool of relevant technologies at that scale, Focused Electron Beam Induced Deposition (FEBID) is a highly promising candidate, as it allows additive, direct-write manufacturing of even complex 3D architectures with feature sizes down to 20 nm on most materials and practically any given surface morphology. Together with an increasing availability of precursors with different functionalities, 3D-FEBID has advanced from a trial-and-error laboratory method to a predictable 3D nano-printing technology. In this talk, the audience is first introduced to the basic principles of 3D-FEBID, complemented by recent advances, which strongly increased precision, predictability and reliability. We then present software solutions for the comfortable upfront design of 3D objects and review several application examples, which strongly benefit from the here presented 3D nanofabrication appraoch. To highlight the industrial relevance of 3D-FEBID, we present concepts of advanced nano-probes for application in scanning probe microscopy. We close the talk with a view on current activities, remaining challenges and future opportunities.

CPP 92.6 Thu 11:40 TOE 317

Perfluorinated amidinate compounds for focused electron beam induced deposition (FEBID) — •Katarzyna Madajska and Iwona Szymańska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

FEBID is a direct maskless nanolithography technique, based on the local dissociation of adsorbates upon the irradiation with electrons.[1][2] Silver pentafluoropropionate was applied in the FEBID process yielding 2D and 3D deposits containing up to 70 at. % Ag. [3][4]

Here we report on our study of silver and copper complexes with perfluorinated amidines (CnF2n+1C(=NH)NH2), which are similar in structure to carboxylates but they differ in donor atoms (N,N-donor).

Thermal analysis, EI MS spectrometry, sublimation experiments and temperature variable infrared spectra analysis were carried out to determine the volatility of compounds and their thermal decomposition mechanism. The compounds selected, as based on the results of the volatility, were examined for their sensitivity to the electron beam, using an electron microscope (SEM, TEM).

[1] Utke and A. Gölzhäuser, Angewandte Chemie Int. Ed. 49 (2010) 9328-9330. [2] D. Belić, M. M. Shawrav, E. Bertagnolli, H. D. Wanzenboeck, Beilnstein J. Nanotechnol, 2017, 8, 2530-2543. [3] L. Berger, K. Madajska, I. B. Szymanska, K. Höflich, M. N. Polyakov, J. Jurczyk, C. Guerra-Nuñez, I. Utke, Beilstein J. Nanotechnol., 2018, 9, 224-232. [4] K. Höflich, J. M. Jurczyk, K. Madajska, M. Götz, L. Berger, C. Guerra-Nuñez, C. Haverkamp, I. Szymanska, I Utke, Beilstein J. Nanotechnol., 2018, 9, 842-849.

CPP 92.7 Thu 12:00 TOE 317

Synthetic strategies towards FEBID precursors — •Iwona Szymańska and Katarzyna Madajska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

The choice of the precursor is crucial for the success of focus electron beam induced deposition (FEBID) because its physicochemical features determine the composition of the deposit.[1] The applied compounds should effectively generate volatile metal carriers, which can be transport over a surface substrate. In the next stage adsorbed molecules should clearly decompose upon electron beam irradiation forming nanostructures. Additionally, the FEBID precursors should be air stable, easy handling, low cost, and safe. Research was focused on the coordination compounds of copper(II) and copper(I), silver(I) and rhenium(III) with N- and O-donor ligands, which seems to be promising for a FEBID process. The influence of structural features such as: 1) the kind of the central atom and its oxidation state; 2) the coordination sphere composition, 3) the modifications of the ligand substituents by fluorination or branching, were observed. [2,3]

Acknowledgements: Nicolaus Copernicus University in Toruń (Statute Research no.103) for the financial support.

References [1] I. Utke et al., J. Vac. Sci. Technol. B, 2008, 26, 1197. [2] L. Berger et al., Beilstein J. Nanotechnol., 2018, 9, 842. [3] K. Höflich et al., Beilstein J. Nanotechnol., 2018, 9, 842.

CPP 93: Scanning Probe Techniques II: Method development (joint session O/CPP)

Time: Thursday 10:30–12:45 Location: WIL C107

CPP 93.1 Thu 10:30 WIL C107

Identifying the atomic configuration of the tip apex using STM and FM-AFM with CO on Pt(111) — •Oliver Gretz, Alfred J. Weymouth, and Franz. J. Giessibl — Institute of Experimental and Applied Physics, Department of Physics, University of Regensburg, 93053 Regensburg

We investigated individual CO molecules adsorbed on Pt(111) with a metal tip using scanning tunneling microscopy (STM) and frequency-modulation atomic force microscopy (FM-AFM). When tips terminate in multiple atoms, the individual atoms are visible not only in the FM-AFM image but also in the raw STM image. This is in contrast to CO on Cu(111), where individual atoms cannot be identified in the raw STM image [J. Welker and F. J. Giessibl, Science 336, 444 (2012)]. We consider the mechanisms behind the higher spatial resolution on Pt, and rule out the increase stiffness of the adsorbed CO, concluding that CO bending does not strongly affect the STM image on either Cu or Pt.

CPP 93.2 Thu 10:45 WIL C107

Atomic Force Microscopy study of the complex surface unit cell of CaF_2(111) with a CO-terminated tip — •Alexander Liebig[1], Prokop Hapala[2], Alfred J. Weymouth[1], and Franz J. Giessibl[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, D-93053 Regensburg, Germany — [2]Department of Applied Physics, Aalto University, 00076 Aalto, Espoo, Finland

A chemically inert tip apex of an atomic force microscope (AFM), such as a carbon-monoxide (CO) molecule, allows to enter the repulsive interaction regime without destroying tip or sample. Imaging in a gentle repulsive regime has led to unprecedented spatial resolution of organic molecules [1] and opened the way for numerous results on different sample systems [2,3]. Here, we probe the ionic CaF_2 (111) surface with a CO-terminated tip over a range of distances, starting from a regime, where short-range electrostatics dominate the AFM contrast, down to distances, where Pauli repulsion and CO bending lead to a complete reversal of the atomic-scale contrast. By comparing the data to simulations, we demonstrate that a mechanical model using the overlap of electron densities [4] as well as the Lennard-Jones potential [5] is reproducing experimental AFM images even at tip-sample distances, where strong lateral forces cause strong lateral deflection of the CO molecule at the tip apex. [1] L. Gross et al., Science 325, 1110 (2009). [2] P. Jelínek, J. Phys.: Condens. Matter 29, 343002 (2017). [3] F. Huber et al., Science 366, 235 (2019). [4] M. Ellner et al., ACS Nano 13, 786 (2019). [5] P. Hapala et al., PRB 90, 085421 (2014).

CPP 93.3 Thu 11:00 WIL C107

Tip induced configuration change of a CO molecule on a copper surface — •Norio Okabayashi[1], Thomas Frederiksen[2,3], and Franz J. Giessibl[4] — [1]Kanazawa University — [2]Donostia International Physics Center — [3]Basque Foundation for Science — [4]University of Regensburg

Live coverage of a reaction process between the two atomic scale objects is one of the central goals in nanoscience. This can be achieved by combining atomic force microscopy to measure the potential energy between the tip apex and a molecule on a surface and inelastic electron tunneling spectroscopy (IETS) to measure the vibrational state of the molecule in the force field [1,2]. Here we demonstrate that the configuration change of a CO molecule in the force field produced by the tip can be traced with unprecedented quality by combining these two techniques and density functional theory (DFT). We found that when the tip is located laterally just above the CO molecule with upright configuration on a copper surface and approaches to the molecule, the CO molecule keeps the upright configuration from the attractive force regime to the beginning of the repulsive force regime; with further approaching the tip, the CO molecule suddenly changes its configuration from upright to tilted with the angle of 20 degree from the surface normal. This scenario is confirmed by IETS with adopting isotope 13C16O and 12C18O molecules. [1] N. Okabayashi, A. Peronio, M. Paulsson, T. Arai, and F. J. Giessibl, PNAS 115, 4571 (2018). [2] A. Peronio, N. Okabayashi, F. Griesbeck, and F. J. Giessibl, Rev. Sci. Instrum. (in press)

CPP 93.4 Thu 11:15 WIL C107

Nonequilibrium Bond Forces in Single-Molecule Junctions — Jonathan Brand[1], Susanne Leitherer[2], Nick R. Papior[3], •Nicolas Néel[1], Yong Lei[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Center for Nanostructured Graphene, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [3]Department of Applied Mathematics and Computer Science, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Passing a current across two touching C_{60} molecules imposes a nonequilibrium population of bonding and antibonding molecular orbitals, which changes the equilibrium bond character and strength. A current-induced bond force therefore contributes to the total force at chemical-bond distances. First-principles calculations and scanning probe experiments exploring currents and forces in a wide C_{60}–C_{60} distance range consistently evidences the presence of current-induced attraction that occurs when the two molecules are on the verge of forming a chemical bond. The unique opportunity to arrange matter at the atomic scale with the atomic force and scanning tunneling microscope tip has enabled closely matching molecular junctions in theory and experiment. The findings consequently represent the first report of current-induced bond forces at the single-molecule level and further elucidate the intimate relation between charge transport and force.

CPP 93.5 Thu 11:30 WIL C107

Electrostatic Force Separation in Electrochemical Strain Microscopy — •Sebastian Badur[1], Diemo Renz[2], Thomas Göddenhenrich[1], Bernhard Roling[2], and André Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Gießen, Germany — [2]Philipps-University Marburg, Germany

In electrochemical strain microscopy an AC voltage is applied to a conductive SPM tip in contact to a mixed conductor. Detection of a few picometer of Vegard-strain allows characterization of electrochemical processes on the nanoscale. However, electrostatic contributions conceal the small displacements and thus are the major challenge to be overcome. Here, we present a novel compensation method, where the frequency dependence of Vegard-strain is utilized in a low and a high frequency regime in order to separate the electrostatic contribution and quantify electrochemical strain on mixed conducting $Cu_2Mo_6S_8$ under ultra high vacuum conditions.

CPP 93.6 Thu 11:45 WIL C107

Sensing with an ultra-sensitive cantilever — •Marc-Dominik Krass, Urs Grob, Raphael Pachlatko, Alexander Eichler, and Christian Degen — ETH Zürich, Solid State Physics, Switzerland

Magnetic resonance force microscopy (*MRFM*) is a scanning probe technique capable of detecting nuclear magnetic resonance (*NMR*) signals from nanoscale sample volumes. The sample is attached to the cantilever tip and is brought in close proximity to a sub-micrometer sized magnet which provides a magnetic field gradient. Periodic spin inversions synchronized with the cantilever frequency generate an oscillatory force at the tip apex.

The forces generated by nuclear spins in a nanometer-sized volume are on the order of 10 aN and detection requires very compliant cantilevers (spring constant below 10^{-4} N/m). Though mounted in pendulum geometry, strong interactions between the magnet and the cantilever lead to snap-in distances of tens of nanometers, resonance frequency shifts over one order of magnitude, and significant changes of the effective spring constant even for small scan ranges.

We present our latest setup improvements in order to obtain an artifact-free 3D magnetic resonance image on nanometer scale. This includes the correction of static cantilever deflections as well as the determination of the instantaneous dynamic spring constant, and real-time adjustments of feedback damping parameters.

CPP 93.7 Thu 12:00 WIL C107

Coupling broadband single-cycle THz pulses from a spintronic emitter to an STM junction — •Melanie Müller[1], Natalia Martín Sabanés[1,2], Sarojini Mahajan[1], and Martin Wolf[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

THz-gated Scanning Tunneling Microscopy (THz-STM) combines submolecular spatial with femtosecond temporal resolution, as first impressively demonstrated in 2016 [1]. Combined with plasmonic enhanced optical excitation THz-STM provides a powerful platform to study the atomically-resolved dynamics of photoexcited surfaces. We have developed an ultrahigh-vacuum STM for broadband excitation from the VIS through the THz spectral range. In particular, we employ an ultra-broadband (1-30 THz) spintronic THz emitter (STE) as source of single-cycle THz pulses to modulate the junction bias. To characterize the bandwidth, phase and voltage amplitude of the THz near-field, we sample the tip-enhanced THz waveform via THz-induced modulation of photocurrents [2]. Careful comparison to the far-field waveform allows us to investigate the antenna properties of the STM tip. Considering strong tip-induced low pass filtering, frequencies up to 10 THz can be detected in the near-field. We further demonstrate versatile phase and polarity control of the THz waveform via the STE excitation conditions, and show that THz transients with a half-cycle period of 115 fs and several Volts amplitude can be achieved in the current setup. References: [1] Cocker T., el at, Nature 539, 263-267 (2016); [2] Yoshida S., et al, ACS Phot. 6, 1356-1364 (2019)

CPP 93.8 Thu 12:15 WIL C107

Single Asperity Sliding Friction across the Superconducting Phase Transition — Wen Wang, •Dirk Dietzel, and Andre Schirmeisen — Insititute of Applied Physics, Justus Libieg Universtity Giessen, 35392 Giessen, Germany

In sliding friction, different energy dissipation channels have been proposed, including phonon and electron systems, plastic deformation, and crack formation. However, the details of how energy is coupled into these channels is heavily debated, and especially the relevance of the electron system for energy dissipation often remains elusive. Here, we present contact mode AFM friction experiments of a single asperity sliding on a high T_c BSCCO-superconductor in a wide temperature range from 40 K to 300 K. Overall, friction decreases with temperature as expected based on thermally activated friction models, but we find an unexpected large peak around T_c of 95 K. We model these results by a superposition of different energy dissipation channels, where the influence of electronic contributions vanishes when cool- ing below the superconducting phase transition T_c. Our experiments thereby unambiguously link electronic friction effects to the number of normal state electrons in the superconducting phase below T_c, allowing us to quantify the relative importance of the electron system to overall friction.

CPP 93.9 Thu 12:30 WIL C107

Non-contact heat transfer between metallic surfaces — •Paul Philip Schmidt and Carsten Henkel — Universität Potsdam, Institut für Physik und Astronomie

The heat transfer at distances beyond contact can be described by fluctuating electrodynamics developed by Rytov [1]. Recent experiments provide deviations from the theoretical predictions. In the measurements, a flat gold surface was approached by a gold-coated probe tip, the distance between the two being less than 10nm [2,3]. In this work we model the measured data in a phenomenological way. The basic assumption is that at a critical distance, the heat flow between flat surface elements saturates, proportional to the number of transport channels. When combined with the proximity force (Deryagin) approximation, this "snap-in model" is in good agreement with the experimental data [4].

[1] D.V.H.M. Polder and M. Van Hove, PRB **4** (1971) 3303.

[2] K. Kloppstech, N. Könne, S.-A. Biehs, A. W. Rodriguez, L. Worbes, D. Hellmann, and A. Kittel, Nature Commun. **8** (2017) 14457.

[3] L. Cui, W. Jeong, V. Fernández-Hurtado, J. Feist, F. J. García-Vidal, J. C. Cuevas, E. Meyhofer, and P. Reddy, Nature Commun. **8** (2017) 14479.

[4] C. Henkel and P. P. Schmidt, JOSA B **36** (2019) C10.

CPP 94: TEM-based Nanoanalysis and Microstructure of thin films (joint session KFM/CPP)

Chair: Bernd Rellinghaus (Dresden Center for Nanoanalysis, TU Dresden)

Time: Thursday 14:10–16:20 Location: HSZ 301

CPP 94.1 Thu 14:10 HSZ 301

The effect of dynamical scattering in ferroelectrics on the measurements of internal electric fields by momentum-resolvedSTEM — •Achim Strauch[1,2], Andreas Rosenauer[3], Andrei Sokolov[4], Evgeny Tsymbal[4], and Knut Müller-Caspary[1,2] — [1]Forschungszentrum Jülich — [2]RWTH Aachen University — [3]IFP Universität Bremen — [4]University of Nebraska-Lincoln

Ferroelectric tunnel junctions (FTJs) are one focus of next-generation memories. With these non-volatile memories, the energy consumption can be reduced. Devices with $BaTiO_3$ tunnel junctions cannot be reversibly polarised at ferroelectric thickness below approximately 3 nm [1]. For investigations, a STEM method would be desirable to map the ferroelectric domain structure in ferroelectric nanofilms exploiting the recently accessible four-dimensional data sets from momentum-resolved STEM [2]. In this contribution, we address the impact of systematic errors arising from dynamical scattering, violated inversion symmetry, sample tilt, and redistributions of electrons due to chemical bonding in a simulation study accompanied by experiments on $BaTiO_3$ and $PbZr_xTi_{1-x}O_3$. The effects of dynamical scattering can lead, depending on thickness, to a systematic error [3] in the order of the expected unit-cell averaged electric fields. Finally the influence of surfaces charges will be discussed.

[1] Garcia et al., Nature Comm. 5, 4289 (2014)
[2] K. Müller et al., Nature Commun. 5, 5653 (2014)
[3] K. Müller et al., Phys. Rev. Lett. 122 (2019)

CPP 94.2 Thu 14:30 HSZ 301

A Novel High-Pressure Tin Oxynitride Sn_2N_2O — •Philipp Gollé-Leidreiter[1], Shrikant Bhat[2], Leonore Wiehl[1], Ute Kolb[1], and Ralf Riedel[1] — [1]Technische Universität Darmstadt — [2]Photon Science DESY

The crystal structure of a novel high pressure high temperature tin oxynitride phase (Sn_2N_2O) was solved via Automated electron Diffraction Tomography (ADT) [1]. The new phase was synthesized from a Sn-N-O precursor at 20 GPa and 1200-1500°C. Due to strong overlaps of symmetrically non-equivalent reflections, the unknown structure could not be solved based on X-ray powder diffraction data. Using the ADT method three dimensional electron diffraction data from a single nanocrystal can be collected in a TEM [2]. The crystal is tilted in 1° steps and diffraction patterns are measured sequentially. Thereby, the reconstructed reciprocal space delivers the unit cell as well as the space group. The intensities of the reflections can be extracted and used to solve the crystal structure via approaches like *direct methods*. The new phase crystallizes in space group Pbcn with the unit cell parameters: a=7.8Å, b=5.53Å, c=5.54Å. The crystal structure could be solved and refined applying kinematic and dynamic theory. It is a Rh_2S_3 type structure where the Sn atoms are sixfold coordinated by O and N atoms. The refined structure compares very well with DFT calculations. This shows the value ADT can provide for the structure solution of high pressure and high temperature materials.

[1]Bhat S, et al. (2019) Chem. Eur. J. 10.1002/chem.201904529

[2]Kolb U, et al. (2019) doi.org/10.1107/S2052520619006711

CPP 94.3 Thu 14:50 HSZ 301

The role of spatial coherence for the creation of and imaging with atom size electron vortex beams — •Darius Pohl[1,2], Stefan Löffler[4], Sebastian Schneider[2,3], Peter Tiemeijer[5], Sorin Lazar[5], Kornelius Nielsch[2], and Bernd Rellinghaus[1,2] — [1]Dresden Center for Nanoanalysis, TU Dresden, D-01062 Dresden, Germany. — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany. — [3]Institute for Solid State Physics, TU Dresden, D-01062 Dresden, Germany. — [4]University Service Centre for Transmission Electron Microscopy, TU Wien, 1040 Wien, Austria. — [5]Thermo Fisher Scientific, PO Box 8066, 5600 KA Eindhoven, The Netherlands.

Recently discovered electron vortex beams (EVBs), which carry quantized orbital angular momenta (OAM), are envisioned to be used in combination with measurements of the electron magnetic circular dichroism (EMCD) to determine the magnetic properties of a material in transmission electron microscopes. Since EVBs can be easily focused down to sub-nanometer diameters, this novel technique bears enormous potential for the quantification of spin and orbital magnetic moments with unrivalled lateral resolution. We use specially designed condenser apertures to generate isolated atom size EVBs with user-selectable OAM. Since the "purity" of the beam regarding the chosen OAM depends on the coherence of the electron source, we have used the monochromator in a double aberration corrected FEI Titan^3 80-300 microscope to control the degree of this coherence. It will be presented, how a likewise improved coherence will affect the quality of the EMCD measurements.

10 min. break

CPP 94.4 Thu 15:20 HSZ 301

Ferroelectric and structural properties of epitaxial NaxBi1-xTiO3 and BaxSr1-xTiO3 based thin films for electrocaloric studies — •Bruno Magalhaes[1,2], Stefan Engelhardt[1,2], Christian Molin[3], Sylvia Gebhardt[3], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [2]Institute of Material Science, TU Dresden, Dresden, Germany — [3]Fraunhofer IKTS, Fraunhofer Institute for Ceramic Technologies and Systems, Winterbergstraße 28, D-01277 Dresden, Germany

The purpose of our study is to investigate the electrocaloric effect in lead-free epitaxial NaxBi1-xTiO3 (NBT) and BaxSr1-xTiO3 (BST) based thin films. We are focusing on microstructural changes to identify the basic mechanisms of the caloric effects, which might enable a further optimization. Our aim is to investigate the influence of the deposition parameters as well as the functional properties in these material systems. Therefore, NBT and BST based thin films were grown on different single crystalline substrates by pulsed laser deposition. The structural characterization verifies an epitaxial growth of both materials with an additional tetragonal distortion. Temperature and frequency dependent measurements of the dielectric properties as well as polarization were used to determine the temperature of maximum permittivity and the ferroelectric properties, respectively. Finally, we will discuss the impact of the deposition parameters on the structural and functional properties of the grown films. This work is supported by the DFG priority program 1599 Ferroic cooling.

CPP 94.5 Thu 15:40 HSZ 301

Uncloaking structural information of ultra-thin oxide films by surface enhanced Raman spectroscopy — •Mads C. Weber[1], Sebastian Heeg[2], Roman Wyss[3], Martin Sarott[1], Morgan Trassin[1], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Department of Information Technology and Electrical Engineering, ETH Zurich — [3]Department of Mechanical and Process Engineering, ETH Zurich

Strained oxide thin films are a source for properties nonexistent in bulk form such as ferrelectricity in $SrTiO_3$ or altered conductivity in nickelates. These physical properties result commonly from subtle structural distortions. Unfortunately, subtle distortions and specifically oxygen displacements are chronically difficult to probe hindering an in-depth understanding of the phenomena. Here, we introduce surface enhanced Raman spectroscopy (SERS) – a technique so far restricted to molecules and carbon-nanostructures – to scrutinize the structure of oxide thin films. A porous gold membrane deposited on the sample acts as antenna and amplifies the Raman signal of the outer layers only. Using this method, we set the Raman spectra of our model thin film $LaNiO_3$ apart from the substrate giving the important structural insight. Beside information on the strain state of $LaNiO_3$, we identify an ultra-thin surface layer structurally different from the rest of the film. Such a surface layer was so far only theoretically predicted, however, never observed. In general, we anticipate that the introduction of SERS to reign of complex oxides films will help to understand the link between novel physical phenomena and structural distortions.

CPP 94.6 Thu 16:00 HSZ 301

Characterizing self-assembled nanostructures in a hierarchical-structured film by coherent two-dimensional microscopy — •Donghai Li[1], Evgenii Titov[1], Maximilian Roedel[2], Verena Kolb[2], Sebastian Goetz[1], Roland Mitric[1], Jens Pflaum[2,3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Lehrstuhl für Experimentelle Physik VI, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), Magdalene-Schoch-Str. 3, 97074 Würzburg, Germany

Self-assembled nanostructures facilitate the development of functional materials with widely tunable properties. Hierarchical architectures consist of nanoscale building blocks spatially modulated by microscale patterns. Despite its relevance for applications and devices, characterization is demanding with existing methods because typically the local molecular-scale assembly pattern within the nanostructure cannot be resolved. Here, we determine nanostructure morphology in a hierarchically structured organic film using coherent two-dimensional (2D) micro-spectroscopy in combination with theoretical modelling of excitonic spectra. We obtain local 2D spectra with diffraction-limited spatial resolution of 260 nm. Using first principles calculations of exciton spectra for model aggregates we connect the experimentally observed signal to the characteristic lengthscale of the nanocrystallites. Thus we obtain a spatial map of nanoscale self-assembly size and confirm it to be correlated with the local slope of the microstructured film surface.

CPP 95: Focus: Polymers under confinement II

Time: Thursday 15:00–16:15 Location: ZEU 222

CPP 95.1 Thu 15:00 ZEU 222

Confined Glassy Dynamics in a Star-Shaped Polymer Induced by Crystallization: Case study of Polyhedral Oligomeric Polysilesquioxane - Isotactic Polystyrene (POSS-iPS) — •Martin Tress[1], Arthur Markus Anton[1], Maximilian Vielhauer[2], Pierre Lutz[3], Rolf Mülhaupt[2], and Friedrich Kremer[1] — [1]Universität Leipzig — [2]Universität Freiburg — [3]University Strasbourgh, France

In semi-crystalline polymers, segmental motion is often constrained. While segments far away from the crystallites have unperturbed dynamics (mobile amorphous fraction), the segments in their proximity move significantly slower (rigid amorphous fraction). Here, we present a study combining broadband dielectric spectroscopy (BDS) and Fourier transform infrared spectroscopy (FTIR) which reveals the opposite effect in a star-shaped polymer, namely a faster mean relaxation time of the amorphous part in the semi-crystalline state [1]. A decomposition of the respective relaxation time distributions yields three fractions of different dynamics. These are assigned to a rigid amorphous fraction around the crystallites, a mobile amorphous fraction, and a confined amorphous fraction of enhanced dynamics presumably located around the POSS centers. Complementary FTIR measurements can address crystalline and amorphous moieties and trace their temperature dependence. These data sets give insight into the mechanism how the combination of crystallites and a star-like architecture constrains the dynamics in a way resembling spatial confinement.

[1] Tress et al. Macromolecules 51 (2018) 501-511

CPP 95.2 Thu 15:15 ZEU 222

Polymer diffusion across lipidic nanochannels — •Reza Ghanbari[1,3] and Raffaele Mezzenga[1,2] — [1]ETH Zurich, Department of Health Sciences and Technology, Schmelzbergstrasse 9, CH-8092 Zurich, Switzerland; — [2]ETH Zurich, Department of Materials, Wolfgang-Pauli-Strasse 10, 8093 Zurich, Switzerland — [3]Present: Adolphe Merkle Institute, University of Fribourg, Chemin des Verdiers, CH-1700 Fribourg, Switzerland

We present an experimental investigation on the diffusion of unfolded polymers in the triply-periodic water-channel network of inverse bicontinuous cubic phases. Depending on the chain size, our results indicate the presence of two different dynamical regimes corresponding to Zimm and Rouse diffusion. We support our findings by scaling arguments based on a combination of blob and effective-medium theories and suggest the presence of a third regime where dynamics is driven by reptation. Our experimental results also show an increasing behavior of the partition coefficient as a function of polymer molecular weight, indicative of a reduction of the conformational degrees of freedom induced by the confinement. Further, the molecular diffusion is discussed across different symmetries, that is, double diamond (Pn3m) symmetry and the double primitive (Im3m) cubic phase.

CPP 95.3 Thu 15:30 ZEU 222

Physics of driven DNA polymers in confinement — •Ulrich Keyser — Cavendish Laboratory, University of Cambridge, JJ Thomse Ave, Cambridge, CB3 0HE, UK

Nanopore sensing has emerged as one of the most promising means for the analysis of single molecules. For DNA sequencing as well as molecule identification the physics governing molecular shape, velocity and fluctuations have to be understood and controlled. Here we show that we can design DNA molecules to measure velocity fluctuations during individual single molecule events [1]. The measurements reveal that friction between molecule, fluid and nanopore plays a crucial role. Based on these results we use electro-osmotic flow to force DNA to go through nanopores unfolded - facilitating molecular sensing [2]. Finally we investigated the details of polymer fluctuations and find that velocity and correlations crucially depend on the configurations of the molecules before initiation of translocation [3]. Our results guide efforts in developing DNA storage systems using nanopores [4].

[1] N. A. W. Bell, et al. Asymmetric dynamics of DNA entering and exiting a strongly confining nanopore. Nature Communications, 8:380, 2017. [2] N. Ermann, et al. Promoting single-file DNA translocations through nanopores using electroosmotic flow. The Journal of Chemical Physics, 149:163311, 2018. [3] K. Chen, et al. In preparation. [4] K. Chen, et al. Digital Data Storage Using DNA Nanostructures and Solid-State Nanopores. Nano Letters, 19:1210, 2019.

Invited Talk CPP 95.4 Thu 15:45 ZEU 222

Active Polymeric Liquid Crystals Under Confinement — •Juan de Pablo — University of Chicago, Chicago, USA

Polymeric materials that comprise mechano-chemically active components are able to undergo spontaneous structural rearrangements that generate internal stresses and motion. These stresses can be particularly large in the case of liquid crystalline polymers, where elasticity becomes important. When confined, at intermediate to high concentrations such materials form nematic phases that are riddled with defects that serve as attractors for solutes or colloidal particles, and can be used for directed transport. Going beyond passive nematic systems, introducing internal activity in the form of molecular motors leads to the emergence of new structural and dynamical features that are not found in materials at rest. This lecture will focus on the relationship between structure, activity, and motion in confined lyotropic liquid crystalline polymeric systems that include colloidal particles. More specifically, results will be presented for actin and tubulin suspensions, where activity is generated by kinesin or myosin motors. A distinctive feature of these biopolymers is that characteristic contour lengths can range from hundreds of nanometers to tens of microns, thereby making them amenable for study by optical microscopy. By relying on molecular and meso-scale models, it is possible to arrive at a comprehensive description of these suspensions that helps explain the connections between molecular structure, the formation and shape of distinct topological defects, the localization of particles in such defects, activity, and defect dynamics.

CPP 96: Organic Electronics and Photovoltaics IV

Time: Thursday 15:00–18:00 Location: ZEU 260

CPP 96.1 Thu 15:00 ZEU 260

Single particle spectral functions of the Holstein model for organic crystals — •Michel Panhans and Frank Ortmann — Center for Advancing Electronics Dresden, Technische Universität Dresden, 01069 Dresden

Despite multifaceted theoretical efforts to understand the effect of electron-phonon interaction on electrons and holes in organic semiconductors, there is no unbiased approach to justify or falsify typical approximations in the existing theories. One of the central questions is under which conditions a classical or a quantum treatment of the vibrations is appropriate. We present a numerical method to study the role of electron-phonon coupling in the Holstein model for single-particle spectral functions of polarons. We compare the spectral functions of an exact treatment of electron-phonon coupling with the static approximation where the modes are decoupled. We find parameter regions where such a treatment of the modes is or is not justified. We therefore are able to separate modes that may be treated quasi-classically or quantum mechanically. The results can be used to predict single-particle spectral functions for organic model crystals such as rubrene.

CPP 96.2 Thu 15:15 ZEU 260

Strongly anisotropic charge transport in crystalline polymer-based materials — •Petros Skopelitis, Michel Panhans, Sebastian Hutsch, Thorsten Arnold, and Frank Ortmann — Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden

The description of charge transport in polymer materials is complicated by the effect of electron-phonon coupling, electronic anisotropy and uncertain transport mechanism. Here we focus on the relation between intrachain and interchain transport of polymer materials and study crystalline PBTTT-C14 as a model system. We derived an expression for the Kubo formalism that combines coherent and incoherent transport in different directions. The validity of the traditional hopping formula for the mobility is studied and compared to the formula we derived from the Kubo formalism. Various intrinsic aspects of the PBTTT-C14 system are studied and analysed, such as phase coherence, diffusivity and mobility edges. The insights we acquired from the analysis made it possible for us to calculate, within the assumptions of our framework, the transfer integrals in the direction of the alkyl chains in PBTTT-C14, using experimental measurements for conductivity and mobile carrier density as input.

CPP 96.3 Thu 15:30 ZEU 260

Why is electronic transport in conjugated organic materials rather inefficient? From organic semiconductors to covalent organic frameworks. — •Christian Winkler, Oliver T. Hofmann, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz

In a recent work [1] we demonstrated for organic semiconductors using dispersion-corrected density-functional theory that molecular arrangements with high inter-molecular electronic couplings are typically energetically unfavorable, which can be traced back to Pauli exchange repulsion of neighboring π-systems. This correlation is not only of importance for charge transport in organic semiconductors but also plays a crucial role in electrically conductive covalent organic frameworks (COFs). COFs are crystalline structures, where the molecular building blocks are covalently bonded within a 2D plane and these planes are then π-stacked. We will show that also in these systems, Pauli exchange repulsion prevents a perfectly coplanar stacking of consecutive layers. Instead, one has to expect small shifts between consecutive layers, where these shifts have only a very minor impact on the powder x-ray diffractograms of the studied COFs. In spite of this small impact on structural parameters, the slip can change the electronic coupling between consecutive COF sheets by orders of magnitude. This suggests that for optimizing charge transport in organic materials, one cannot rely on the (self) assembly of the π-systems but needs to include additional chemical functionalities that modify the packing motif. [1] C. Winkler et al., Chem. Mater. 2019, 31, 17, 7054-7069

CPP 96.4 Thu 15:45 ZEU 260

Explaining Charge Mobility Regimes in Amorphous Materials: The correction energy concept — Markus Krammer[1], Chris Groves[2], and •Karin Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Department of Engineering, Durham University, United Kingdom

Charge transport in amorphous materials like organic semiconductors happens via hopping between localized states of profound energetic disorder. The charge mobility reflects how swiftly charges are transported through such an energy landscape. Evidently, it is desirable to predict mobility-limiting bottlenecks and roadblocks directly from analyzing the energy landscape. However, external electric fields and interactions with other charges are as relevant for transport as the landscape, so that mobility-limiting features can be quantified only after having fully simulated entire charge trajectories respecting those influences. We developed a new simulation technique to calculate the mobility, which further permits to predict and interpret the dependence of the mobility on the external electric field and the charge density based on the energy landscape. The key idea is to modify the energy landscape by local correction energies that account for the ability of the charges to explore the underlying local landscape in the presence of all other charges, external electric fields, and temperature. To demonstrate the appealing ease of interpreting our simulations, we will explain the reasons for the field and the charge carrier-density dependence of the mobility.

CPP 96.5 Thu 16:00 ZEU 260

Ordered phases of (A1-D-A2)n polymers: What can we learn from simulations? — Deyan Raychev[1,2], Gotthard Seifert[2,3], Jens-Uwe Sommer[1,2,4], and •Olga Guskova[1,2] — [1]IPF Dresden — [2]DCMS, TU Dresden — [3]Theoretische Chemie, TU Dresden — [4]Institut für Theoretische Physik, TU Dresden

The lamellar morphologies of (A1-D-A2)n polymers consisting of diketopyrrolopyrrole (A1 with linear or branched alkyls) and benzothiadiazole (A2) acceptor units linked together via aromatic donor (D, thiophene or furan) are studied using a combination of DFT and MD simulations [1]. We show that the morphology of the macromolecular arrays is very sensitive to the branching of the alkyl substituents of DPP cores and to D type. They affect not only the planarity of the conjugated macromolecules but also cause various π-π stacking distances and lamellar intervals in the ordered phases of polymers. The next results are related to the stacking motifs of the conjugated copolymers. We conclude that the samples with linear side chains have segregated stacking motif, in which acceptor units and donors build their own columns. On the contrary, branched alkyls lead often to defective structures and irregular stacking.

This work is funded by the European Regional Development Fund and the Free State of Saxony via the European Social Fund project 100231947 (Young Investigators Group - Computer Simulations for Materials Design "CoSiMa").

[1] D. Raychev, et al. Macromolecules, 2019, 52 (3) 904.

CPP 96.6 Thu 16:15 ZEU 260

Predicting the reorganization energies of organic semiconductors via machine learning — •Ke Chen, Christian Kunkel, Johannes Margraf, and Karsten Reuter — Technical University of Munich, Garching, Germany

The chemical space of possible organic semiconductors is enormous, and only few of them have been experimentally tested so far. It is therefore likely that many high performance organic semiconductors are still unknown. High-throughput computational screening can help accelerate their discovery, in particular when combined with highly efficient machine learning (ML) models. In this contribution, we focus on the so-called reorganization energy, which is one of the most critical molecular properties correlated with high charge carriers mobility in organic semiconductors.

The ML models presented herein use the smooth overlap of atomic positions (SOAP) for a local representation of atomic environments [1]. Based on this, two different global representations are studied to represent the molecular structures, namely the average global kernel and the 'auto-bag' method of Hammer et al. [2]. These representations are combined with linear and kernel ridge regression.

We find that these ML models can reliably identify the best candidates in a large chemical space of organic molecules. Furthermore, data-efficiency, prediction cost and the reliability of uncertainty estimates are compared.

[1] A. P. Bartók et al., Phys. Rev. B 87, 184115 (2013). [2] S. A. Meldgaard et al., J. Chem. Phys. 149, 134104 (2018).

CPP 96.7 Thu 16:30 ZEU 260

Assessing Crystal Structure Prediction Based on Density Functional Tight Binding and Evolutionary Algorithms — •Sebastian Hutsch and Frank Ortmann — Center for Advancing Electronics Dresden, Technische Universität Dresden, Germany

The prediction of crystal structures for organic molecules is a computationally expensive task due to the large number of atoms in the unit cell and the associated number of possible configurations. The computational load can be compensated by the use of classical force fields, which however lack transferability to new molecules and necessitate an extensive training for complex molecules. Here, we study an approach to crystal structure prediction based on evolutionary algorithms and a combination of Density Functional Tight Binding (DFTB) and Density Functional Theory (DFT). This combination allows us to cost efficiently compute crystal structures for new materials on a high level of accuracy. A comparison of the calculated crystal structures with experimentally known structures will be made.

CPP 96.8 Thu 16:45 ZEU 260

Accurate Phonon Calculations in Molecular Crystals: The Instructive Case of Naphthalene — •Tomas Kamencek[1,2], Sandro Wieser[1], Natalia Bedoya-Martínez[3], Johannes P. Dürholt[4], Rochus Schmid[4], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Physical and Theoretical Chemistry, Graz University of Technology, Austria — [3]Materials Center Leoben, Austria — [4]Chair of Inorganic Chemistry 2, Ruhr University Bochum, Germany

Over the past decades the properties of molecular crystals have been studied extensively to improve the performance of organic electronic devices. Many of the materials properties relevant in this context are crucially affected by phonons. For example, strong electron-phonon coupling is a limiting factor for charge transport in molecular crystals, and entropic contributions from phonons play a decisive role for the relative stability of polymorphs. The simulation of phonon band structures with ab initio methods like dispersion-corrected density-functional theory, however, poses a sizable challenge for all but the simplest systems. Therefore, here we test the suitability of more approximate methods, which can be applied not only to simple systems, but also to practically relevant materials. These methods comprise density-functional tight binding and various classical force fields (FFs). Besides transferable FFs of varying sophistication (GAFF and COMPASS) we tested MOF-FF which was specifically parametrized for our benchmark system. As the latter we chose deuterated naphthalene, for which phonon band structures have also been studied experimentally.

15 min. break

CPP 96.9 Thu 17:15 ZEU 260

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 96.10 Thu 17:30 ZEU 260

Theoretical study of ferroelectricity in tetramethylbenzidine-tetracyanoquinodimethane (TMB-TCNQ) — •Shoji Ishibashi, Sachio Horiuchi, and Kiyoyuki Terakura — National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

Some of mixed-stack organic charge transfer complexes show ferroelectricity. Tetrathiafulvalene-*p*-chloranil (TTF-CA) is a typical example. Kobayashi et al. successfully obtained a polarization value of 6.3 μC cm^{-2} in TTF-CA [1]. This value is more than 20 times larger than that of the point charge model and their directions are opposite. We made theoretical analyses of this exotic ferroelectricity in TTF-CA in terms of Born effective charges as well as maximally-localized Wannier orbitals [2,3]. We have shown that only 2 bands below the band gap are responsible for the emergence of polarization and also that the electron flow from cell to cell on these electronic states is the origin of the exotic polarization in TTF-CA. Recently, Mezzadri et al. have reported the mixed-stack crystal structure of the low-temperature phase of tetramethylbenzidine-tetracyanoquinodimethane (TMB-TCNQ) and pointed out that this phase is potentially ferroelectric [4]. In the present study, we have applied the above-mentioned theoretical methods to investigate the ferroelectricity in TMB-TCNQ and report similarities and dissimilarities to that of TTF-CA.

[1] K. Kobayashi et al., Phys. Rev. Lett. **108**, 237601 (2012). [2] S. Ishibashi and K. Terakura, J. Phys. Soc. Jpn. **83**, 073702 (2014). [3] K. Terakura and S. Ishibashi, Phys. Rev. B **91**, 195120 (2015). [4] F. Mezzadri et al., Cryst. Growth Des. **18**, 5592 (2018).

CPP 96.11 Thu 17:45 ZEU 260

Theoretical Characterization and Design of Organic Open-Shell Materials: From Bi- to Tetraradicals — •Sebastian Schellhammer and Frank Ortmann — Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden

In recent years, organic molecules with stable open-shell ground states have attracted growing interest due to their outstanding properties, i.e. responsive spin structures, singlet fission or non-linear optical properties. Although the number of interesting material classes is growing, the molecules often have low thermal stability, hindering their use in electronic devices.

In this presentation, we will highlight routes but also dead ends in the quest for high-spin configurations in hydrocarbons. By using a computational approach based on density functional theory (DFT) and CASSCF, different structure-property relationships are discussed. We demonstrate that optimization of material properties can be achieved by manipulating the wavefunctions of the unpaired electrons. Here, well known chemical functionalization strategies such as benzannulation, push-pull design, or tuning of intramolecular interactions can be combined to create molecules with well-defined properties.

CPP 97: Nanostructures, Nanostructuring and Nanosized Soft Matter

Time: Thursday 15:00–17:00 Location: ZEU 255

Invited Talk CPP 97.1 Thu 15:00 ZEU 255

Grain coarsening dynamics in cylinder-forming block copolymer thin films — •Michele Perego — CNR-IMM, Unit of Agrate Brianza, Italy

The all-organic polystyrene-block-poly (methyl methacrylate) (PS-b-PMMA) block-copolymer (BCP) thin films have been widely investigated for advanced lithographic applications, due to the possibility to promote perpendicular orientation of the nanodomains by easy neutralization of the surface with the appropriate random copolymer. In this BCP system, the Flory-Huggins parameter X is weakly dependent on T and, consequently, the segregation strength XN can be modulated by simply changing the degree of polymerization N. In this respect, thin films of cylinder forming PS-b-PMMA represent a perfect test system for fundamental investigations on the evolution of ordering in two-dimensional hexagonal lattices. In this talk, we will revise our experimental studies about the grain coarsening process in PS-b-PMMA thin films with different N. The evolution of the correlation length as a function of time follows a power law with a specific growth exponent for each value of N. The exponential decay of the growth exponent as a function of N is perfectly consistent with a diffusion limited mechanism of the grain coarsening process. Interestingly for very small N, growth exponent value 1/2 suggests that the lateral ordering process is guided by a curvature limited mechanism.

CPP 97.2 Thu 15:30 ZEU 255

Gold cluster growth/formation on zwitterionic thin block copolymer coatings — •Apostolos Vagias[1], Simon J. Schaper[2], Christina Geiger[2], Lucas P. Kreuzer[2], Wei Chen[2], Suzhe Liang[2], Marc Gensch[2,3], Pallavi Pandit[3], Matthias Schwartzkopf[3], Stephan V. Roth[3], Jonas Drewes[4], Niko Carstens[4], Thomas Strunskus[4], Franz Faupel[4], Andre Laschewsky[5,6], and Peter Müller-Buschbaum[1,2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenberstr.1, 85748 Garching, Germany — [2]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22607 Hamburg — [4]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, Kaiserstr. 2, 24143 Kiel — [5]Institut für Chemie, Universität Potsdam, Karl-Liebknechtstr. 24-25, 14476 Potsdam-Golm, Germany — [6]Fraunhofer Institute for Applied Polymer Research IAP, Geiselbergstr. 69, 14476 Potsdam-Golm, Germany

Zwitterionic polymer (e.g. polysulfobetaines) films, serve as excellent antifouling coatings. Polymer-metal nanocomposites hold tremendous potential for plasmonics and organic catalysis. Sputtered gold can exhibit wetting selectivity with different affinities for each constituent of block copolymer films. Correlating gold growth and affinity to given polymer constituent remains elusive. By in-situ microfocus GISAXS (μGISAXS) we present the evolution of nanostructural gold growth on thin (<100 nm) films of zwitterionic copolymers and respective homopolymer films, commenting on metal selectivities during sputtering.

CPP 97.3 Thu 15:45 ZEU 255

A new polymorph in triglyceride nanoparticles prepared by antisolvent precipitation — •Isabel Schuldes[1], Dennis M. Noll[1], Klaus Götz[1,2], and Tobias Unruh[1,2] — [1]Institute for Crystallography and Structural Physics, Universitaet Erlangen-Nuernberg, Erlangen, Germany — [2]Interdisciplinary Center for Nanostructured Films, Universitaet Erlangen-Nuernberg, Erlangen, Germany

Antisolvent precipitation (AP) is a low-cost bottom-up method for the preparation of nanoparticles, e.g. for pharmaceutical applications. We report small (˜ 25 nm in diameter) triglyceride (tripalmitin, trimyristin) nanoparticle dispersions prepared by AP, which exhibit unexpected structural characteristics: differential scanning calorimetry (DSC) and wide-angle X-ray scattering (WAXS) measurements show an uncommon melting behaviour and an untypical crystalline phase. The presence of said untypical phase has been reported in triglyceride nanosuspensions previously, but has not been studied as it represented only a minor fraction of the dispersion [1]. In contrast, we have observed that in dispersions prepared by AP this phase is predominant. Small-angle X-ray and neutron scattering (SAXS, SANS) measurements further revealed an interfacial structure of the liquid triglyceride nanoparticles. Such structure was recently suggested to be a general feature among small nanoparticles prepared by AP [2] and might play a role in the formation of the observed untypical phase. Our findings may help to tailor triglyceride nanoparticles for application as drug delivery systems. [1] H. Bunjes et al., Langmuir, 2000, 16, 5234. [2] I. Schuldes et al., Langmuir, 2019, 35 (42), 13578.

CPP 97.4 Thu 16:00 ZEU 255

Sputter deposition of Ag on nanostructured PMMA-b-P3HT copolymer thin films — •Marc Gensch[1,2], Matthias Schwartzkopf[1], Simon J. Schaper[2], Lucas P. Kreuzer[2], Nian Li[2], Jonas Drewes[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Peter Müller-Buschbaum[2,4], and Stephan V. Roth[1,5] — [1]DESY, Photon Science, Notkestr. 85, D-22607 Hamburg, Germany — [2]TUM, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, D-85748 Garching, Germany — [3]MaWi, Christian Albrechts-Universität zu Kiel, Kaiserstr.2, D-24143 Kiel, Germany — [4]Heinz Maier-Leibniz Zentrum (MLZ), TUM, Lichtenbergstraße 1, D-85748 Garching, Germany — [5]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Nanostructured polymer-metal-composite films demonstrate great perspectives for optoelectronic applications, e.g. as sensors or photovoltaics. To enhance properties of such devices the metal cluster self-assembly process needs to be understood. We studied the silver cluster morphology during the growth on PMMA-b-P3HT by grazing incidence small-angle X-ray scattering (GISAXS), as well as the crystallinity of the metal film formation with grazing incidence wide-angle X-ray scattering (GIWAXS) in situ during sputter deposition. The scattering experiments were combined with surface differential reflectance spectroscopy (SDRS). Our study reveals the selective wetting of silver on the polymer blocks and the influence of the template on the percolation behavior of the silver layer, which was measured by resistivity measurements during the sputter deposition.

CPP 97.5 Thu 16:15 ZEU 255

Colloidal self-assembly route towards efficient designing of nanophotonic architectures — •Swagato Sarkar[1,2], Joby Joseph[1], and Tobias A.F. König[2,3] — [1]Dept. of Physics, Indian Institute of Technology Delhi, New Delhi-110016, India — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden, Germany — [3]Technical University of Dresden, Physical Chemistry, 01062 Dresden, Germany

For many photonic applications, it is important to confine light of a specific wavelength at a certain volume of interest at low losses. So far, it is only possible to use the polarized light perpendicular to the solid grid lines to excite waveguide plasmon polaritons in a waveguide supported hybrid structure. In this contribution, we use a plasmonic grating fabricated by colloidal self-assembly [König, Fery et al. Adv. Optical Mater. 2018, 1800564] and an ultrathin injection layer to guide the resonant modes selectively.[Sarkar, Joseph, König ACS Appl. Mater. Interfaces 2019, 11, 14, 13752-13760] We use gold nanoparticles self-assembled in a linear template on a titanium dioxide (TiO2) layer to study the dispersion relation with conventional UV-vis-NIR spectroscopic methods. Compared to metallic grids, the experimentally observed (supported by simulation) range of hybridized guided-modes can now be extended to modes along the nanoparticle chain lines. With future applications in energy conversion and optical filters employing these cost-efficient and up-scalable directed self-assembly methods, we discuss its direct application in refractive index sensing.

CPP 97.6 Thu 16:30 ZEU 255

Surface Lattice Resonances in the Visible Optical Range by Soft Lithography Templates and Directed Self-Assembly. — •Vaibhav Gupta[1], Andreas Fery[1,2], and Tobias a.f. König[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Straße 6, D-01069 Dresden, Germany — [2]Physical Chemistry, Technical University of Dresden, 01062 Dresden, Germany

We demonstrate a novel approach towards mechanically tunable, cost-efficient and low-loss plasmonic nanostructures, whose pronounced optical anisotropy upon mechanical deformation can be detected by naked eye.1 Soft interference lithography and template-assisted colloidal self-assembly are used to fabricate a stretchable macroscopic periodic square lattice of gold nanoparticles. Surface scanning methods reveal a full coverage of the array. The high structural quality results in a narrow bandwidth surface lattice resonance with a line width of 25. Stretching of the system results in reversible transition from the square lattice to a rectangular symmetry and corresponds to pronounced changes in the optical properties of the ensemble. We show the hybrid nature of the optical response using angle dependent UV-vis spectroscopy and numerical simulations. Based on these findings and our colloidal metasurface concept.2 We discuss potential applications as strain sensor and mechanically tunable filters.

CPP 97.7 Thu 16:45 ZEU 255

Nanoparticle Contaminations on the Skin - Can They be Removed? — •Jonas Schubert[1,2] and Max Schnepf[1,2] — [1]Functional Colloidal Materials, Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Germany — [2]Physical Chemistry of Polymer Materials, Technische Universität Dresden, D-01062 Dresden, Germany

Nanoparticles (NPs) are used now for centuries and more and more they find their way into applications and products on the market. As the usage of nanoparticles is increasing, also accidental release of NPs is now an important issue for a safe work environment. We found that after a skin contact with quantum dot particles, these NPs are barely to remove by applying soap or other typical decontamination agents. From literature we know that some of the NPs can penetrate the skin and are then potentially be harmful for human health.[1] In this contribution, we present a gel that allows a complete removal of NPs from the skin. This marks a first step towards safe handling of nanomaterials, especially since this point is not yet covered by up-to-date occupational safety guidelines. The presented gel displays therefore an important step for the sustainable and safe use of nanomaterials.

[1] Nafisi, S.; Maibach, H. I., Chapter 3 - Skin penetration of nanoparticles. In Emerging Nanotechnologies in Immunology, Shegokar, R.; Souto, E. B., Eds. Elsevier: Boston, 2018; pp 47-88.

CPP 98: Composites and Functional Polymer Hybrids

Time: Thursday 15:00–17:00 Location: ZEU 114

CPP 98.1 Thu 15:00 ZEU 114

A mesoscopic approach to magnetostriction of magnetic gels and elastomers — Lukas Fischer and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, 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]. 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, which can play a qualitative role [2].

We assume identical, well-separated particles, all identically magnetized from outside [1]. Depending on the discrete particle arrangement and the compressibility of the elastic material, overall contraction or elongation along the magnetization axis results. For randomized particle arrangements, a trend of elongation along the magnetization axis is found, in line with previous experiments [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] G. Pessot et al., *J. Chem. Phys.* **141**, 124904 (2014).
[3] C. Gollwitzer et al., *J. Chem. Phys.* **128**, 164709 (2008).

CPP 98.2 Thu 15:15 ZEU 114

Self-Structuring formation of filler particles in low concentration magnetoactive polymers — •Dirk Sindersberger, Nina Prem, and Gareth Monkman — OTH Regensburg, Regensburg, Deutschland

The formation of micro-structures in magnetoactive polymers (MAP) is a recently discovered phenomenon found only with very low filler particle concentrations (less than 3 wt%). Due to the degassing process, filler particles collect around an ascending bubble, which dissolves at a certain point leaving particulate rings within the matrix. The formation of toroidal micro-structures commences as filler concentration approaches 1wt%. The development of coherent parallel aligned rings with a compact order continues as particle concentrations increase toward 2 wt%. Between 2 and 3 wt% capillary doublets develop, while mass percentages higher than 3 wt% results in increasing entropy as the random order of particle agglomeration found in higher concentration MAP dominates. Self-structured samples of different filler material and concentrations between 1 and 3 wt% have been investigated using X-Ray tomography, where the emerging structures can be observed and visualized. Additionally, this work utilizes a range of spectroscopic analysis methods (UV/VIS and FTIR) and their applicability to MAP characterization at wavelengths ranging from 200 nm to 25 μm.

CPP 98.3 Thu 15:30 ZEU 114

Magneto-sensitive elastomer beyond the linear magnetization regime — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

Magneto-Sensitive Elastomer (MSE) describes a composite material of a soft-elastic polymer network with embedded micron-sized magnetizable particles. Upon applying an external magnetic field, it can undergo large deformations. Due to the long-range nature of the magnetic interactions, the pronounced sensitivity to preparation conditions and a complex interplay of different mechanisms, such as deformation- and field-induced particle rearrangements, the theoretical description of MSE represents a challenging task. Accordingly, various simplifying assumptions are introduced. A very prominent simplification is the restriction to an exclusive linear magnetization behavior. Often in experiments, and in order to yield pronounced effects, rather large magnetic fields are applied where the linear approximation regime is no longer justified. We will present a generalized theoretical approach which correctly describes the low and the large field limit, and also provides a reasonable approximation for intermediate field strengths. Furthermore, we show how this formalism can be adopted to account additionally for different MSE sample forms.

CPP 98.4 Thu 15:45 ZEU 114

Molecular dynamics simulations of magnetoactive elastomers — •Alla Dobroserdova[1], Malte Schümann[2], Dmitry Borin[2], Pedro Sanchez[1,3], Stefan Odenbach[2], and Sofia Kantorovich[1,4] — [1]Ural Federal University, Ekaterinburg, Russia — [2]Technische Universität Dresden, Dresden, Germany — [3]Helmholz-Zentrum Dresden-Rosendorf, Dresden, Germany — [4]University of Vienna, Vienna, Austria

Magnetic elastomers are the systems consisting of magnetic particles distributed in a nonmagnetic elastic matrix. We perform Molecular Dynamics Simulations to investigate the influence of particle shape, their magnetic interactions, their coupling with polymer matrix and external magnetic field on the structural and magnetic properties of these systems. In order for the results to be predictive for a realistic class of magnetic elastomers, we match simulation parameters to those obtained from theological, tomographic and magnetic measurements. Based on the qualitative agreement between simulations and experiment, we can explain asymmetry of magnetic hysteresis loops, particle orientational ordering in field and shift of the FORC diagram maxima.

CPP 98.5 Thu 16:00 ZEU 114

Simulations of complex nanoparticles in block copolymer ultrathin films: colloidal anisotropy and inhomogeneity — •Javier Diaz[1], Marco Pinna[2], Andrei V. Zvelindovsky[2], and Ignacio Pagonabarraga[1] — [1]École polytechnique fédérale de Lausanne, Switzerland — [2]School of Maths and Physics, University of Lincoln,UK

Block copolymers (BCPs) are perfect candidates to control the position (and orientation, for anisotropic colloids) of nanoparticles (NPs) due to the microphase separation in several ordered morphologies: lamellar, cylinders, etc. Moreover, the presence of nanoparticles can modify the properties of the hosting BCP, including its morphology [1] and result in ordered co-assembled structures.

Anisotropic nanoparticles can display a high ordering within block copolymer ultrathin films, with a rich phase behaviour both in terms of NP position and orientation, depending on relative lengths and interactions with the BCP. We present a computational model [2] that allows to study anisotropic NPs with different shapes (rectangles, ellipsoids and rhomboids), comparing with recent experiments on nanorods and nanoplates.

Chemically inhomogeneous Janus NPs(JNPs) possess an additional orientational degree of freedom that can lead to ordered co-assembled phases with JNPs forming lamellar-like structures within the BCP [3].

[1] Diaz, J., Pinna, M., Zvelindovsky, A. and Pagonabarraga, I., 2019 Soft Matter, 15, 9325-9335 [2] Diaz, J., et al, 2019. Macromolecules 52, 21, 8285-8294 [3] Diaz, J., et al, 2019 Soft matter, 15(31), 6400-6410

CPP 98.6 Thu 16:15 ZEU 114

Dipolar Molecular Rotors in Surface-Anchored Metal Organic Frameworks — •Xianghui Zhang[1], Sebastian Hamer[2], Ritesh Haldar[3], Daniel Reuter[4], Florian Paneff[1], Dirk Volkmer[4], Peter Lunkenheimer[4], Ian Howard[3], Rainer Herges[2], and André Beyer[1] — [1]Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany — [2]Otto-Diels-Institute for Organic Chemistry, Christian-Albrechts-University of Kiel, 24098 Kiel, Germany — [3]Karlsruhe Institute of Technology (KIT) Institute of Functional Interfaces (IFG) and Light Technology Institute (LTI), 76344 Karlsruhe, Germany — [4]Experimental Physics V, University of Augsburg, 86135 Augsburg, Germany

Molecular rotors arranged in ordered two- and three-dimensional lattices are an emergent quantum mechanical system. We use dipolar molecular rotors as building blocks to synthesize surface-anchored metal-organic framework (MOF), which serves as a structural architecture to arrange the molecular rotors precisely in ordered arrays. The torsional barrier of single rotors was computed by ab initio DFT calculations, while dipole-dipole interactions were estimated from classical calculations. Dielectric spectroscopy was used to investigate the rotation dynamics of molecular rotors, where thermally activated reorientations of the dipolar rotors lead to an enhanced dissipation when the driving frequency is close to the natural fluctuation rate of the dipolar rotors. Both the activation energy and relaxation rates were determined experimentally and compared with theoretical calculations.

CPP 98.7 Thu 16:30 ZEU 114

Model cement systems studied by Colloidal-Probe AFM (CP-AFM) — •Simon Becker and Regine von Klitzing — Soft Matter at Interfaces, Institut für Festkörperphysik, TU Darmstadt, Germany

In nowadays construction industry due to ecological and financial reasons the tailored rheology of building materials such as concrete and therefore cement is of great importance. Especially the rheology of cement pastes in the early stage can be influenced by additives such as polycarboxylate ether (PCE) type super plasticizers in a viscosity reducing manner. For tuning the system a better understanding of the interplay between the nanoscopic forces on cement particles and the macroscopic rheology is of essential importance.

In the present study the interaction between model particles is investigated with colloidal-probe atomic force microscopy (CP-AFM). Thereby micrometer scaled spherical silica beads are used as model cement grains to imitate the silicate phases of cement clinker. Furthermore spray dried clinker particles are used for a more application-related approach. The latter ones are restricted to measurements in non-aqueous solutions to prevent hydration. The influence of the interaction forces in presence of different pH and different ionic strength and ion types such as KCl and $CaCl_2$ is investigated for these model systems.

CPP 98.8 Thu 16:45 ZEU 114

Calorimetric study on the vitrification kinetics, molecular mobility and rigid amorphous fraction in epoxy-based nanocomposites — •Paulina Szymoniak, Xintong Qu, and Andreas Schönhals — Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany

It was found for inorganic/polymer nanocomposites that a so-called rigid amorphous phase (RAF) is formed in the interfacial region by adsorption of polymer segments onto the nanoparticles. The segmental dynamics of RAF is expected to be altered, as compared to the pure matrix, which might percolate into the entire system, affecting the overall PNC properties. Here, the structure and molecular mobility of epoxy-based PNCs with different nanofillers (layered double hydroxide and boehmite) was studied by a combination of calorimetric and X-Ray scattering techniques. Temperature modulated DSC (TMDSC) showed that depending on the nanofiller, RAF can reach up to 40 wt % of the system or, on the contrary, the overall mobility of the matrix might increase due to the presence of particles. Such contrasting results, including the high amount of RAF, which was never shown before for epoxy-based PNCs, emphasize the importance of interfaces. Additionally, glass transition and glassy dynamics were investigated by a novel technique, Flash DSC (heating rates up to 10 kK/s) employed for the first time to a thermosetting system. It was used to study both the vitrification kinetics and glassy dynamics of the PNCs, for instance further confirming the presence of RAF and its impact on the overall material properties.

CPP 99: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)

Time: Thursday 15:00–17:30 Location: GER 38

Invited Talk CPP 99.1 Thu 15:00 GER 38

Huge quantum effects on the 250 K superconducting lanthanum hydride — •Ion Errea — University of the Basque Country, Donostia/San Sebastián, Spain

The discovery of superconductivity at 200 K in the hydrogen sulfide system at large pressures was a clear demonstration that hydrogen-rich materials can be high-temperature superconductors. The recent synthesis of LaH10 with a superconducting critical temperature (Tc) of 250 K place these materials at the verge of reaching the long-dreamed room-temperature superconductivity. Here we show that quantum atomic fluctuations stabilize in the superconducting pressure range a high-symmetry Fm-3m crystal structure consistent with experiments, which has a colossal electron-phonon coupling of 3.5. Even if ab initio classical calculations predict this structure to distort below 230 GPa yielding a complex energy landscape, the inclusion of quantum effects evidences the Fm-3m as the true ground state. The agreement between the calculated and experimental Tc values further supports this phase as responsible for the 250 K superconductivity. The relevance of quantum fluctuations questions many of the crystal structure predictions made for hydrides within a classical approach that at the moment guide the experimental quest for room-temperature superconductivity. Furthermore, quantum effects are revealed to be crucial to stabilize solids with extraordinary electron-phonon coupling, which may otherwise be destabilized by the large electron-phonon interaction, reducing the pressures needed for their synthesis.

CPP 99.2 Thu 15:30 GER 38

Self-Interaction Corrected SCAN for Solids: All-Electron Implementation with Numeric Atom-Centered Basis Functions — •Sheng Bi[1], Igor Ying Zhang[2], Christian Carbogno[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Fudan University, Shanghai, China

For all semi-local density-functional approximations (DFAs), electronic self-interaction errors lead to an erroneous description of charge-transfer processes, a systematic underestimation of band gaps in semiconductors, and incorrect total energies [1]. These errors can be alleviated via localized-orbital scaling corrections [2] or via self-interaction corrections (SIC) [3]. In this work, we have implemented a reciprocal-space formulation of self-consistent SIC in the all-electron, numeric atomic-orbitals code *FHI-aims*, which is applicable for all semi-local DFAs, including the promising meta-GGA “strongly constrained and appropriately normed” (SCAN) functional [4]. We validate our implementation by inspecting charge transfer, cohesive energies, and band gaps for a test set of molecules and solids, showing that SIC considerably improves SCAN calculations and yields results on par with standard *GW* calculations at a fraction of the computational cost. This allows us to use SCAN-SIC for studying the adsorption of organic molecules on the H-Si(111) surface.

[1] A. J. Cohen *et al.*, *Chem. Rev.* **112**, 289 (2011).
[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).
[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).
[4] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).

CPP 99.3 Thu 15:45 GER 38

Understanding the lattice dynamics of 3D hexagonal boron nitride (h-BN): beyond the LDA approach — •Luigi Cigarini, Michal Novotný, and František Karlický — Department of Physics, Faculty of Science, University of Ostrava, Czech Republic

It is fundamental to achieve a clear depiction of the lattice dynamics of 3D h-BN in order to understand the experimental outcomes. Five different stacking conformations are possible for 3D h-BN and at least two or three of them are systematically present in samples in variable amounts [1-2], resulting as a source of irreproducibility for experiments, such as the infrared optical response [3-4].

The lattice dynamics of h-BN is particularly tough to describe, stated the different nature of the forces participating in it: covalent bonds and Van der Waals interactions. The LDA approach seemed to be the most effective compromise, at the DFT level [1,5-6].

In this work we explain the surprisingly good performance of LDA. We also show that it is possible to achieve better results, in comparison with experimental IR spectra, by using, instead, the GGA approach to DFT and treating separately the two parts of the dynamical matrix. Besides, we found that IR spectroscopy is able to give some information about stacking composition. [1]. Liu, L. et al., Phys. Rev. B, 68(10), 104102 (2003). [2]. Constantinescu, G. et al., Phys. Rev. Lett., 111(3), 036104 (2013). [3]. Çamurlu, H.E. et al., Ceram. Int., 42(5), 6312-6318 (2016). [4]. Mukheem, A. et al., Nanomaterials, 9(4), 645 (2019). [5]. Cuscó, R. et al., Phys. Rev. B, 97(15), 155435 (2018). [6]. Serrano, J. et al., Phys. rev. lett., 98(9), 095503 (2007).

CPP 99.4 Thu 16:00 GER 38

Error Estimation of Energy-per-Atom of Semiconductor Compounds Using Statistical Learning — •Daniel T. Speckhard[1,2], Sven Lubeck[2], Christian Carbogno[1], Luca Ghiringhelli[1], Claudia Draxl[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

Material databases such as NOMAD give researchers the ability to work with millions of material simulation results [1]. However, it is typically unclear to which extent calculations performed with different numerical settings and computer codes can be trusted and related to each other. This project presents statistical learning strategies to model errors in energies for two all-electron DFT codes, *FHI-aims* and `exciting`, for different basis-set sizes and **k**-point densities. Specifically, we use mutual information scores to select features that are able to capture the energy-per-atom errors. With respect to several metrics, random forest regression on the selected features shows the most promising results. This work lays the foundation for estimating errors in DFT data in NOMAD and helps to save computing resources by *a priori* predicting the DFT simulation settings required to achieve a desired level of precision. This also enables us to estimate the basis-set and **k**-point converged results of not fully converged calculations.

[1] C. Draxl and M. Scheffler, *J. Phys. Mat.*, **2** 036001 (2019). https://nomad-coe.eu

CPP 99.5 Thu 16:15 GER 38

Force balance approach for advanced approximations in density functional theories — •Mary Leena Tchenkoue[1], Markus Penz[1], Iris Theophilou[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York NY 10010, USA

We propose a systematic and constructive way to determine the exchange-correlation potentials of density-functional theories including vector potentials. The approach does not rely on energy or action functionals. Instead it is based on equations of motion of current quantities (force balance equations) and is feasible both in the ground-state and the time-dependent setting. This avoids, besides differentiability and causality issues, the optimized-effective-potential procedure of orbital-dependent functionals. We provide straightforward exchange-type approximations for different density functional theories that for a homogeneous system and no external vector potential reduce to the exchange-only local-density and Slater Xα approximations.

CPP 99.6 Thu 16:30 GER 38

Combining embedded mean field theory with linear-scaling density functional theory — •Joseph Prentice[1,2], Robert Charlton[2], Arash Mostofi[2], and Peter Haynes[2] — [1]St Edmund Hall and Department of Materials, University of Oxford, Oxford, UK — [2]Department of Materials, Department of Physics and the Thomas Young Centre, Imperial College London, London, UK

We demonstrate the capability of embedded mean field theory (EMFT) within the linear-scaling density-functional theory code ONETEP, which enables DFT-in-DFT quantum embedding calculations on systems containing thousands of atoms at a fraction of the cost of a full calculation. We perform simulations on a wide range of systems from molecules to complex nanostructures to demonstrate the performance of our implementation with respect to accuracy and efficiency. This work paves the way for the application of this class of quantum embedding method to large-scale systems that are beyond the reach of existing implementations.

CPP 99.7 Thu 16:45 GER 38

Topological semimetallic phase in PbO$_2$ promoted by temperature — •Bo Peng[1], Ivona Bravić[1], Judith L. MacManus-Driscoll[2], and Bartomeu Monserrat[1] — [1]Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom

Materials exhibiting topological order host exotic phenomena that could form the basis for novel developments in areas ranging from low-power electronics to quantum computers. The past decade has witnessed multiple experimental realization and thousands of predictions of topological materials. However, it has been determined that increasing temperature destroys topological order, restricting many topological materials to very low temperatures and thus hampering practical applications. Here, we propose the first material realization of temperature promoted topological order. We show that a semiconducting oxide that has been widely used in lead-acid batteries, β-PbO$_2$, hosts a topological semimetallic phase driven by both thermal expansion and electron-phonon coupling upon increasing temperature. We identify the interplay between the quasi-two-dimensional nature of the charge distribution of the valence band with the three-dimensional nature of the charge distribution of the conduction band as the microscopic mechanism driving this unconventional temperature dependence. Thus, we propose a general principle to search for and design novel topological materials whose topological order is stabilized by increasing temperature. This provides a clear roadmap for taking topological materials from the laboratory to technological devices.

CPP 99.8 Thu 17:00 GER 38

How Electric Fields Affect Intermolecular van der Waals Interactions — •Mohammad Reza Karimpour, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

van der Waals (vdW) dispersion interactions between atoms or molecules originate from electromagnetic forces caused by the zero-point quantum-mechanical fluctuations of electronic charge densities. They are ubiquitous in nature and present in many areas of physics, chemistry, biology, and nanotechnology. Recently, it has been shown that the strength of vdW interactions can be controlled and tailored by external electric charges [1]. In addition, an external field strongly modifies the dispersion interaction between two hydrogen atoms and can change both its spatial dependence and its attractive or repulsive character [2]. To describe such important phenomena in large molecular systems, we employ the Many-Body Dispersion (MBD) method [3] based on the quantum Drude oscillator model. Since the conventional MBD method includes only dipole-dipole coupling, it does not capture the effects of external fields on vdW interactions. Therefore, we first extend the approach to dipole-quadrupole and quadrupole-quadrupole couplings. Then, the developed formalism is applied to calculate the MBD energy in the presence of an external electric field for low-dimensional systems including bilayer graphene.

[1] Kleshchonok and Tkatchenko, Nat. Commun. **9**, 3017 (2018)
[2] Fiscelli *et al.* arXiv:1909.03517 (2019)
[3] Tkatchenko *et al.* Phys. Rev. Lett. **108**, 236402 (2012)

CPP 99.9 Thu 17:15 GER 38

Electronic structure of β-SiAlON: effect of Al/O doping and of finite temperature — •Saleem Ayaz Khan[1], Ondrej Šipr[2], Jiří Vackář[2], Robin Niklaus[3], Wolfgang Schnick[3], and Jan Minár[1] — [1]University of West Bohemia, Plzen, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]LMU Munich, Germany

Electronic structure of a series of ordered and disordered β-Si_{6-z}Al_{z}O_{z}N_{8-z} systems is investigated by means of ab initio calculations, using the FLAPW method as implemented in the wien2k code and Green function KKR method as implemented in the SPR-KKR code. Finite temperature effects are included within the alloy analogy model. We found that the trends with the Al/O doping are similar for ordered and disordered structures. The electronic band gap decreases with increasing z by about 1 eV when going from z=0 to z=2. The optical gap decreases analogously as the electronic band gap. The changes in the density of states (DOS) at Si and N atoms introduced by doping β-Si_{3}N_{4} with Al and O are comparable to the DOS at Al and O atoms themselves. The bottom of the conduction band in β-Si_{6-z}Al_{z}O_{z}N_{8-z} is formed by extended states residing on all atomic types. Increasing the temperature leads to a shift of the bottom of the conduction band to lower energies. The amount of this shift increases with increasing doping z.

CPP 100: Focus: In-situ probes toward better understanding of hybrid halide perovskites (PhD symposium) I (joint session CPP/AKjDPG)

Metal-halide perovskites have attracted tremendous attention as absorber material in solar cells due to their rapid increase in power conversion efficiency. However, results within the field suffer from a range of variation and a lack of reproducibility. Thus detailed understanding of the highly dynamic material need correlation with the measurement conditions. To this end in-situ, operando and multimodal measurements are being developed. In this symposium, we want to bring together this in-situ expertise from various techniques which help to unravel material responses in hybrid perovskites. Organized by: Shambhavi Pratap (TU München), Hannah Funk (Helmholtz-Zentrum Berlin für Materialien und Energie) and Klara Suchan (Lund University, Sweden).

Time: Thursday 17:15–18:30 Location: ZEU 222

Invited Talk CPP 100.1 Thu 17:15 ZEU 222

Real-time Investigation of Crystallization Pathways of Organo-Metal-Halide Perovskites Solar — •Michael F Toney — SLAC National Accelerator Laboratory, Menlo Park, Ca, USA

Perovskite solar cells (PSCs) have gained tremendous attention as materials for photovoltaics due to their high efficiencies and their compatibility with low-cost low-temperature fabrication methods (such as solution processing). Perovskite film formation is complex, involving the formation of intermediates and/or metastable phases that strongly affect the final perovskite film microstructure. Therefore, understanding the mechanism of perovskite formation and the crystallization pathways is key for facile control of perovskite formation. We are using time-resolved x-ray scattering to investigate the perovskite formation of MAPbI3-based perovskites and mixed cation (Cs, FA)PbI3 perovskites in-situ during spin coating and the subsequent post-deposition treatments. Our work highlights the importance of real-time investigation of perovskite film formation which can aid in establishing processing-microstructure-functionality relationships and help to provide a fundamental understanding of the mechanisms of perovskite formation.

CPP 100.2 Thu 17:45 ZEU 222

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.

CPP 100.3 Thu 18:00 ZEU 222

Small-Footprint Optical Monitoring to Study Perovskite Thin Film Formation — Aboma Merdasa[1,2], Rahim Munir[1], Carolin Rehermann[1], Katrin Hirselandt[1], Janardan Dagar[1], Klara Suchan[2], and •Eva Unger[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Lund University, Sweden

Record performance of Metal-Halide Perovskite (MHP) based solar cells have been achieved for small area devices based on spin-coating. Developing this device technology towards larger area prototypes will require the utilisation of scalable process technology. Processing strategies developed for spin-coating have been developed by incremental modifications of MHP ink and process conditions. Translating these processing strategies to scalable process technology requires a fundamental understanding of the formation mechanism. We recently developed a small-footprint spectroscopy setup based on fibre-optics enabling the monitoring of thin film formation processes. The setup can be easily integrated in process equipment such as spin-coater or slot-die coaters. UV-Vis measurements in reflectance mode enable us to describe the thinning of precursor solution during initial stages of MHP deposition as well as the onset of MHP crystallisation. As examples, the role of the anti-solvent drip in thin film formation, inhomogeneous crystallisation of MHP materials from mixed bromide/iodide precursors, crystallisation of reduced dimensional 2D/3D materials and effect of spin-coating and annealing time on MHP device performance will be discussed.

CPP 100.4 Thu 18:15 ZEU 222

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 101: Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)

Time: Thursday 18:45–19:45 Location: ZEU 260

Duration 60 min.

CPP 102: Nanostructured Surfaces and Thin Films II: 1D and 2D Networks (joint session O/CPP)

Time: Thursday 15:00–17:15 Location: WIL B321

CPP 102.1 Thu 15:00 WIL B321

Edges in group-IV monochalcogenides: stability and electronic properties — •Mahdi Ghorbani-Asl and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

The group-IV monochalcogenides including tin sulfide (SnS) and germanium sulfide (GeS) are layered semiconductors with an anisotropic crystal structure giving rise to several unusual physical properties. In this study, based on density functional theory combined with different dispersion corrections, we systematically investigated the structure, stability and electronic properties of monolayer and multilayer SnS and GeS with various possible stoichiometric and nonstoichiometric terminations of the edges. It was found that the (110) facet has the lowest energy and it is thus expected to be the most stable edge. We further demonstrated that nonstoichiometric edges can exist as they provide reconstructed structure or covalent interlayer coupling between layers, which lowers the formation energies of the edges. The results indicate that the stability of the edges generally decreases for higher facet indices. The electronic structure calculations showed that most of the studied compounds are semiconductors with a band gap in the range of 0.2 - 1.6 eV, depending on the crystallographic direction of the edge and its chemical termination. For both GeS and SnS nanoribbons, the band gap is smallest in the case of the (010) edge and largest for the (110) edge. The edge states are more pronounced in multilayer than monolayer nanoribbons.

CPP 102.2 Thu 15:15 WIL B321

MoS2 monolayers under cluster ion irradiation: a molecular dynamics study — •Sadegh Ghaderzadeh, Vladimir Ladygin, Mahdi Ghorbani-Asl, and Arkady V. Krasheninnikov — Institue of Ion beam Physics and Materials Research Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

Ion irradiation is a powerful method to tailor the properties of low-dimensional materials, and is thought to be particularly promissing for patterning two-dimensional (2D) materials through tuning the energy, type, charge state of the incident particles and the supporting substrate. This tool is recently employed to tackle the important issue of controlled pore creation in 2D materials to be performed as filters for water desalination, gas sensing, etc. This aim requires a clear insight into the microscopic process which is yet to be fully understood. In this work, we use classical Molecular Dynamics (MD) simulations to shed light on the behavior of 2D materials under cluster ion irradiation, and specifically focous on the production and characterization of defects. To a great extent, the properties of the induced defects depend on the size and energy of the clusters, which has not been studied beyond graphene so far. In particular, we are focused on the response of MoS2 monolayers, which have shown various exciting properties complementary to graphene, under cluster irradiation. Furthermore, we show that depending on the incident angle and energy of the clusters, sulfur atoms can be sputtered mainly from the top layer, creating unique opportunities for patterning MoS2 monolayers.

CPP 102.3 Thu 15:30 WIL B321

One-dimensional molecular chains of Quinacridone on Ag(100) and Cu(111): STM- and SPA-LEED-investigations — •Niklas Humberg[1], Rémi Bretel[2], Alexander Eslam[1], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany — [2]University of Paris-Saclay, Institut des Sciences Moléculaires D'Orsay, France

One-dimensional molecular aggregates are of high interest because they often show specific and pronounced coupling effects for electronic excitations, e.g. in optical spectra. Here, we report a structural analysis of two such systems, quinacridone (QA) on Ag(100) and Cu(111), by STM and SPA-LEED.

On Ag(100) QA grows in homochiral domains of parallel one-dimensional chains at room temperature (RT), forming a metastable structure. Within these chains the molecules are parallel and linked pairwise via two hydrogen bonds. The distance between chains varies with coverage. After annealing at 500 K, a 2D commensurate heterochiral structure is formed. It consists of homochiral dimers forming periodically indented and closely packed chains. On Cu(111), QA grows in similar fashion at RT, but compared to QA/Ag(100) the structure shows stronger disorder in form of kink-like defects in the chains. Annealing at different temperatures between RT and 600 K leads to different chain-like structures, that are stable at RT. The comparison to the similar system QA/Ag(111) [1] indicates that the structures of QA/Cu(111) at RT are determined by kinetic limitations.

[1] Wagner et al, J. Phys. Chem. C 2014, 118, 20, 10911-10920.

CPP 102.4 Thu 15:45 WIL B321

Fabrication of highly regular Moth-Eye inspired Nanostructures to generate Anti-Reflective Surfaces — •Louise Kaeswurm, Zhaolu Diao, Johannes Hirte, Klaus Weishaupt, and Joachim Spatz — Max-Planck-Institute for Medical Research, Jahnstr. 29, 69120 Heidelberg, Germany

We developed a possibility to create highly regular moth-eye inspired anti-reflective (AR) nanostructures on different substrates such as silica glass, sapphire, diamond and silicon. Although thin-film technology can solve reflection related problems to a certain extent, AR moth-eye nanostructures have many advantages.

The method proposed is based on block copolymer micellar lithography to apply an etching mask and reactive ion etching to nanostructure the surface. Compared to other fabrication methods, this approach is fast and easily scalable. The method is based on the principle of index matching: the generated nanostructures lead to the reported reduction of the reflectivity. For transparent substrates the transmission is severely increased, for non-transparent the absorption. Since nanopillars and bulk are the same material, mechanical stress is reduced enabling applications in the high-energy regime. I.e. laser systems and EUV technology can profit from such an AR treatment. Additionally, AR sapphire windows for endoscopes can improve the imaging quality and AR silicon enhances the efficiency of different electronic devices. Further developing the processes will enable the use of the full potential of such AR surfaces for a variety of applications ranging from electronics to medical and optical applications.

CPP 102.5 Thu 16:00 WIL B321

Length dependent symmetry in narrow chevron-like graphene nanoribbons — •Koen Houtsma[1], Mihaela Enache[1], Remco Havenith[1,2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands — [2]Stratingh Institute for Chemistry, University of Groningen, Groningen, the Netherlands

Graphene nanoribbons (GNRs) are an exciting material that has aroused much interest due to their excellent and tunable electronic properties. Using on-surface synthesis, narrow chevron-like GNRs, which host a mixture of armchair and zigzag edge terminations, were synthesized from the prochiral molecular building block 6,12-dibromochrysene on a Au(111) substrate [1]. An interesting property of these ribbons is the changing structural symmetry depending on the number of monomer units incorporated in the ribbon, where ribbons consisting of an odd and even number of monomers are point and mirror symmetric, respectively. In our research, we characterized the electronic properties of these GNRs using scanning tunneling spectroscopy, also in dependence of their length and parity.

[1] T.A. Pham et al., Small 13 (2017) 1603675.

CPP 102.6 Thu 16:15 WIL B321

Chirality transfer to supported metal particles and within organic dye films — •Natalie Fehn, Alexander von Weber, Matthias Jakob, Philip Stanley, Aras Kartouzian, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry and Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Chirality - the absence of improper rotation axes within a structure or molecule - is a phenomenon known since the early 19th century and leads to optical activity of the substance such as optical rotatory dispersion and circular dichroism. The phenomenon plays an important role in medication, biochemistry, and fine chemicals and still opens many questions such as the origin of life. We are especially interested in the transfer of chirality from chiral surfaces to small metal particles and adsorbates, which is addressed via circular dichroism spectroscopy and second harmonic generation-circular dichroism spectroscopy. We already observed induced circular dichroism in silver nanoparticles [1] and organic dye thin films [2]. Now, the question arises whether chirality can be introduced into metal clusters which may serve as catalysts in asymmetric heterogeneous catalysis [3].

[1] M. Jakob, A. von Weber, A. Kartouzian, U. Heiz *PCCP* **31** (2018), 20347-20351, DOI: 10.1039/c8cp02970a. [2] A. von Weber, P. Stanley, M., Jakob, A. Kartouzian, U. Heiz *J. Phys. Chem. C* **14** (2019), 9255-9261, DOI: 10.1021/acs.jpcc.9b01323. [3] A. Kartouzian *Chirality* **31** (2019), 641-657, DOI: 10.1002/chir.23113.

CPP 102.7 Thu 16:30 WIL B321

Enhanced efficiency of graphene-silicon Schottky junction solar cell through inverted pyramid arrays texturation — •Jiajia Qiu[1], Huaping Zhao[1], Long Liu[1], Wenhui Ma[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany — [2]State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology, Kunming 650093, China

Nanostructures of silicon are gradually becoming hot candidate due to outstanding capability for trapping light and improving conversion efficiency of solar cell. In this paper, silicon nanowires (SiNWs) and silicon inverted pyramid arrays (SiIPs) were introduced on surface of Gr-Si solar cell through silver and copper-catalyzed chemical etching, respectively. The effects of SiNWs and SiIPs on carrier lifetime, optical properties and efficiency of Gr-SiNWs and Gr-SiIPs solar cells were systematically analyzed. The results show that the inverted pyramid arrays have more excellent ability for balancing antireflectance loss and surface area enlargement. The power conversion efficiency (PCE) and carrier lifetime of Gr-SiIPs devices respectively increase by 62% and 34% by comparing with that of Gr-SiNWs solar cells. Finally, the Gr-SiIPs cell with PCE of 5.63% was successfully achieved through nitric acid doping. This work proposes a new strategy to introduce the inverted pyramid arrays for improving the performance of Gr-Si solar cells.

CPP 102.8 Thu 16:45 WIL B321

Spatial Extent of Surface Photovoltage in the Vicinity of Individual Plasmon Excited Nanoparticles — •Katharina Engster, Kevin Oldenburg, Karl-Heinz Meiwes-Broer, Sylvia Speller, and Ingo Barke — Institute of Physics, University of Rostock

The investigation of photophysical processes of heterogeneous systems largely relies on local probing techniques [1]. For plasmon assisted electron-hole generation a key property is the size of the region that is affected by enhanced charge carrier density which is accessible via the local surface photovoltage (SPV). Here we present SPV studies of single resonantly excited Ag clusters [2] on Si(100)-(2x1) measured by energy-resolved two-photon photoemission electron microscopy (2PP-PEEM). Analysis of the distance dependence from the particles reveals an enhanced plasmon induced charge carrier density which decays on the scale of 1 μm. This observation is corroborated by comparing spatially averaged SPV for different particle densities. We envision opportunities in the context of plasmon enhanced solar cells, particularly regarding the choice of optimal particle concentrations.

[1] K. Sell *et al.*, Phys. Stat. Sol. (b) **247**, 1087 (2010).

[2] K. Oldenburg *et al.*, J. Phys. Chem. C **123**, 1379 (2019).

CPP 102.9 Thu 17:00 WIL B321

Supramolecular nanopatterns of arylenes and arylene-alkynylenes: Addressing the third dimension — Georgiy Poluektov, Tristan J. Keller, Joshua Bahr, David A. Hofmeister, Anna Krönert, Anna Jochemich, Dirk Laux, Daniel Kalle, Sebastian Henzel, Steven Becker, •Stefan-Sven Jester, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie der Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Arylenes and arylene-alkynylenes that carry long alkoxy side chains physisorb at the solid/liquid interface on graphite (HOPG). The resulting two-dimensional (2D) supramolecular nanopatterns have periodicities in the order of 3 nm to 10 nm and are *in situ* imaged by scanning tunneling microscopy (STM) with submolecular resolution. The electronic and mechanic decoupling of the active units in such systems from (i) the substrate surface and (ii) adjacent species within the nanopatterns is essential for a single-molecule functionality similar to systems in a solution. Here, we report on bicyclophanes as well as shape-persistent stars and macrocycles, all carrying anchor groups that point along the surface normal.

CPP 103: Topical Session: Data Driven Materials Science - Machine Learning for Materials Characterization (joint session MM/CPP)

Time: Thursday 15:45–17:15 Location: BAR 205

Topical Talk CPP 103.1 Thu 15:45 BAR 205
Machine learning tools in analyticat transmission electron microscopy — •Cécile Hébert and Hui Chen — LSME, Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Analytical scanning transmission electron microscopy probes the chemistry of the investigated sample by recording spectral information as a function of electron probe position. The acquired spectra can consist of X-Ray photons emitted by the sample after the incoming electron probe has excited it (EDX) and/or an analysis of the energy lost by the incoming electron when it excites the sample (EELS). Both EELS and EDX spectra can be recorded on a scanned area consisting of 1000x1000 pixels of even more, leading to a so called *hyperspectral datacube* of up to several 10^6 spectra. Such a vast amount of data calls for machine learning tools belonging to the family of multivariate statistical analysis (MSA). Such methods have been implemented and used since the mid-ninties, however, there are still many challenges related to their application. MSA methods are very sensitive to detector artifacts, they deliver components, which do not necessarily bear a physical meaning, they might discard small and very localized signal, etc. In this presentation, I will review the use of unsupervised machine learning in analytical TEM, and present some new results based on a dictionary learning approach where we implement knowledge we have about the shape of the spectral components.

CPP 103.2 Thu 16:15 BAR 205
Automatic semantic segmentation of Scanning Transmission Electron Microscopy (STEM) images using an unsupervised machine learning approach — •Ning Wang, Christoph Freysoldt, Christian Liebscher, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

The recent substantial advance of machine learning provides us with a rich toolbox to successfully address problems in materials science. Here we present an unsupervised machine learning approach for automatic semantic segmentation of STEM images. We propose a robust descriptor, the local correlation map, for characterization of the local periodicity, which is then fed into an unsupervised clustering algorithm in order to segment the STEM images into different crystalline regions. The semantic segmentation works as an initial step for further data analysis, such as image denoising, extraction of lattice vectors and so on. As a proof of concept, we apply our approach to STEM images of Cu grain boundaries, Ni stacking faults and twin boundaries, and Fe2Nb phase boundaries, and observe very good robustness and resolution.

CPP 103.3 Thu 16:30 BAR 205
Bayesian models and machine-learning for NMR crystal structure determinations — •Edgar Albert Engel[1], Andrea Anelli[2], Albert Hofstetter[3], Federico Maria Paruzzo[3], Lyndon Emsley[3], and Michele Ceriotti[2] — [1]TCM, University of Cambridge, United Kingdom — [2]COSMO, Ecole Polytechnique Federale de Lausanne, Switzerland — [3]LRM, Ecole Polytechnique Federale de Lausanne, Switzerland

NMR spectroscopy is a key tool for determining the atomic structure of powdered and amorphous solids, which usually proceeds by finding the best match between experimentally observed NMR chemical shifts and those of candidate structures. However, the reliability of structure determinations depends on the errors in the predicted shifts. I will demonstrate how a Bayesian approach based on knowledge of the typical errors, coupled to visualisations of the similarity of the candidate structures, allows to quantify and understand the resultant confidence in the identifications of the experimental structure [1]. The applications highlight that using self-consistently determined uncertainties instead of commonly used global estimates make it possible to use 13C shifts to improve the accuracy of structure determinations. I will further outline how a machine-learning approach including uncertainty estimation [1,2] ties in with the above structure determination framework and that it can provide a surrogate for costly or even outright unfeasible first-principles predictions of NMR shifts.

[1] E. A. Engel et al., Phys. Chem. Chem. Phys., 21, 23385 (2019) [2] F. M. Paruzzo et al., Nature Comm., 9, 4501 (2018)

CPP 103.4 Thu 16:45 BAR 205
Teaching machines to learn dynamics in NMR observables — •Arobendo Mondal, Karsten Reuter, and Christoph Scheurer — Chair for Theoretical Chemistry, TU Munich, Germany

NMR is a powerful tool for studying the structural and electronic properties of molecules and solids. However, the interpretation of NMR spectra for large systems is often challenging as a result of the free or constrained dynamics of the ligands attached to the NMR active nucleus. Computed NMR parameters can aid in the interpretation. Their accuracy depends on the level of method used, with the high computational cost of highly accurate first-principles calculations quickly limiting the tractable system sizes and number of such computations.

In this respect, emerging machine learning approaches are an appealing option. The key challenge here is an efficient data representation, as NMR parameters depend strongly on their local chemical environment with often non-negligible effects of the second and third coordination sphere. To this end, we use a combination of multiple SOAP descriptors[1] to learn NMR parameters for the Antamanide peptide molecule from quantum chemical data computed on a small subset of a long 90 ns molecular dynamics trajectory. The trained model is found to predict NMR parameters within DFT accuracy for 90,000 snapshots from this trajectory that were not contained in the training data.

[1] Phy. Rev. B, **2013**, *87*, 184115

CPP 103.5 Thu 17:00 BAR 205
Automatic Identification of Crystallographic Interfaces from Scanning Transmission Electron Microscopy Data by Artificial Intelligence — •Byung Chul Yeo[1], Christian H. Liebscher[2], Matthias Scheffler[1], and Luca Ghiringhelli[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Characterizing crystallographic interfaces in synthetic nanomaterials is an important step for the design of novel materials, e.g., catalysts, gas sensors, etc. In principle, trained materials scientists can assign interface structures of materials by looking at high-resolution imaging and diffraction data obtained by aberration-corrected scanning transmission electron microscopy (STEM). However, the high-acquisition rates in STEM pose a challenge to a purely human-based identification of interfaces or defects. As of today, STEM datasets are being massively accumulated, but they cannot be fully exploited due to the lack of automatic analysis tools. Here, we present a newly developed artificial-intelligence tool for accurately extracting the key features of (poly)crystalline materials, i.e., crystal-structure prototype, lattice constant, and (relative) orientation from atomic-resolution STEM images. The tool is based on a convolutional neural network and operates on both high-angle annular dark-field (HAADF) and convergent beam electron diffraction (CBED) images. The network is trained on 13 200 simulated STEM images, including structures distorted by thermal noise, and our model achieves excellent predictive performance for automatically identifying crystal structure and lattice misorientations.

CPP 104: Topical Session: Data Driven Materials Science - Machine Learning Applications (joint session MM/CPP)

Time: Thursday 17:30–19:00 Location: BAR 205

CPP 104.1 Thu 17:30 BAR 205

How polymorphism of adsorbate molecules determines the physical properties of metal/organic interfaces: a large scale study — •Johannes J. Cartus, Andreas Jeindl, Lukas Hörmann, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria

The work function of metallic surfaces can be readily tuned via the interface dipole that emerges when adsorbing organic electron-donor or -acceptor molecules. Despite extensive research in the field and a wealth of experimental data available, it is presently still not possible to predict the magnitude of the dipole based on the choice of the interface materials alone. This is because molecular properties and the structure of adsorbate layers are rarely considered simultaneously, even though both are known to have great impact.

In this work, we present a systematic study of selected substrate/adsorbate combinations, for which we computationally determine the electronic structure of various surface polymorphs. This allows us to explore which kind of structures preferentially form for different molecule classes and directly relate them to the interface work function and other system properties.

CPP 104.2 Thu 17:45 BAR 205

Investigation of short-range order in multicomponent alloys with the use of machine-learning interatomic potentials — •Tatiana Kostiuchenko[1], Alexander Shapeev[1], Fritz Körmann[2,3], and Andrey Ruban[4,5] — [1]Skolkovo Institute of Science and Technology, Moscow, Russia — [2]Delft University of Technology, Delft, The Netherlands — [3]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [4]KTH Royal Institute of Technology, Stockholm, Sweden — [5]Materials Center Leoben Forschung GmbH, Leoben, Austria

Multicomponent alloys, such as high-entropy alloys or multi-principal element alloys, are promising structural materials. However, the vast range of chemical compositions and long annealing times offer an opportunity for their study with ab initio methods. The drawback of ab initio methods is their huge computational costs. We address this drawback by developing efficient data-driven interaction models with accuracy close to those of ab initio methods, namely the low-rank interatomic potential (LRP) [Shapeev A., 2017]. They are used in a Canonical Monte Carlo algorithm as an “on-lattice” model that can take into account local lattice distortions. In this work, we investigate the equiatomic VCoNi system. It represents a medium-entropy alloy with a distorted fcc lattice which leads to an outstanding strength-ductility relationship as reported in [Sohn S. et al., 2019]. We simulate this system by including, implicitly, magnetism into LRP by fitting on spin-polarized DFT calculation. The LRP has the error of about 1-3 meV/atom and is used to study the formation of the short-range order.

CPP 104.3 Thu 18:00 BAR 205

An equation for membrane permeability: Insight from compressed sensing — •Arghya Dutta and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Using a material’s structure and readily available properties to predict a difficult-to-measure but important property is crucial in natural sciences and engineering. Data mining—the process of discovering associations, correlations, and anomalies in data—can significantly facilitate the search for these generalized structure-property relationships by providing relevant descriptors. To give an example, the efficacy of a targeted drug depends on whether or not it can go through a cell membrane. This capacity is quantified by permeability which measures the drug’s flux across the membrane. However, calculating permeability is computationally expensive. In this presentation, I will discuss results from our ongoing search for a simple and interpretable equation, which is a function of key physical descriptors, for permeability using compressed sensing methods. This simplified description of permeability will allow simulation-free prediction, and, potentially, assist in rapid screening of candidate drug molecules.

CPP 104.4 Thu 18:15 BAR 205

Transferable Gaussian Process Regression for prediction of molecular crystals harmonic free energy. — •Marcin Krynski[1] and Mariana Rossi[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany

Organic molecular crystals are a large group of compounds with properties tied strongly to the crystallographic structure of their numerous polymorphs. While thermodynamic free energies are necessary for obtaining a reliable polymorph energy ranking[1,2], their inclusion in large-scale simulations for polymorph screening is challenging, because dispersion-corrected DFT accuracy is needed in order to capture the complex charge rearrangement and bond-softening. Therefore, to predict harmonic Helmholtz free energies, we devised a framework that employs the transferable Gaussian Process Regression model with Smooth Overlap of Atomic Positions[3] descriptors representing local atomic environments. We developed strategies based on farthest point sampling to minimize the size of the training set and to ensure statistical diversity. We benchmark our framework on a set of 444 hydrocarbon crystal polymorphs. Superior performance and high prediction accuracy, with mean absolute deviation below 0.1 meV/atom is achieved by a hyperparameter optimisation performed on empirical-potential models, ensuring sensitivity to longer-range structural patterns.
[1] J. Nyman and G. Day, *CrystEngComm* **17**, 5154 (2015);
[2] M. Rossi, P. Gasparotto, M. Ceriotti, *PRL* **117**, 115702 (2016);
[3] A. P. Bartók, R. Kondor, G. Csányi, *PRB* **87**, 184115 (2013).

CPP 104.5 Thu 18:30 BAR 205

Bayesian modeling for potential energy surface minimization — •Estefania Garijo del Rio, Sami Juhani Kaapa, and Karsten Wedel Jacobsen — CAMD, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Computational simulations using electronic structure methods of materials and molecules require the (meta-)stable structure of the system under investigation to be known. In the absence of experimental structural data, the usual procedure is to use quantum chemistry codes together with some optimization algorithm to find successive approximations of a (local) minimum of the potential energy surface under the Born-Oppenheimer approximation. In this context, methods that incorporate machine learning surrogate models that are built on the fly to reduce the number of evaluations have recently gained popularity. Here, we explore and compare how different choices for the kernels can affect the performance of the optimization when Gaussian process regression is used to fit energies and forces.

CPP 104.6 Thu 18:45 BAR 205

A computational route between band mapping and band structure — R. Patrick Xian[1], •Vincent Stimper[2], Marios Zacharias[1], Shuo Dong[1], Maciej Dendzik[1], Samuel Beaulieu[1], Matthias Scheffler[1], Bernhard Schölkopf[2], Martin Wolf[1], Laurenz Rettig[1], Christian Carbogno[1], Stefan Bauer[2], and Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

In solid state physics, the electronic band structure imprints the multidimensional relations between energy and momentum of periodically confined electrons. Photoemission spectroscopy has provided a reliable source of experimental validation for electronic structure theory and the understanding of electronic properties. Recent advancements in UV sources and detector technology leads to the growth of band mapping data in resolution, size and scale. This offers fresh opportunities for high-throughput material characterization. Here, we present an efficient probabilistic machine learning framework to connect photoemission band mapping with band structure calculations by reconstructing the full 3D valence band structure of tungsten diselenide within its first Brillouin zone. We then digitize the empirical shape of the reconstructed bands using orthonormal bases for multiscale sampling and comparison with theory. Our approaches open up avenues for the precise quantification of band structures and realize a viable path integrating band mapping data with computational materials science databases.

CPP 105: Focus: In-situ probes toward better understanding of hybrid halide perovskites (PhD symposium) II (joint session CPP/AKjDPG)

Time: Friday 9:30–12:15 Location: ZEU 222

Invited Talk CPP 105.1 Fri 9:30 ZEU 222

Time-resolved X-ray scattering to understand perovskite materials — Oliver Filonik[1], Christopher Greve[2], Meike Kuhn[2], Michael Buchhorn[2], Adrian Ebert[2], Richard Kellnberger[2], and •Eva M. Herzig[1] — [1]MSE - Herzig Group, TU München, Lichtenbergstr. 4a, 85748 Garching — [2]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

The formation of perovskite thin films is of interest since this process determines the final material quality. In-situ X-ray scattering can help to learn more about the formation of perovskite crystals and how the crystallization is altered by the use of additives or other parameters. The film formation mechanism directly influences the performance of, for example, solar cells. We apply different techniques to extract time-resolved information and will show the opportunities and limitations of these in the quest for understanding formation-function relationships in perovskites.

CPP 105.2 Fri 10:00 ZEU 222

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 105.3 Fri 10:15 ZEU 222

The zero step for degrading perovskite solar cells: what atmosphere should we choose? — •Renjun Guo[1], Wei Chen[1], Lennart K. Reb[1], Manuel A. Scheel[1], Stephan Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607 Hamburg, Germany

The power conversion efficiency (PCE) of perovskite solar cells (PSCs) reached the champion value of 25.2 percent, making this technique competitive with commercial silicon solar cells. Despite such advantages, the application of PSCs is currently limited by combining high performance and operational stability because PCE of PSCs can degrade due to the presence of temperature, light, humidity, and oxygen. Besides, current degradation research on PSCs is carried out without standard protocol. Therefore, it is necessary to make the standard protocol for the long term degradation of PSCs. We investigated degradation processes of PSCs under both AM 1.5G and different atmosphere conditions with in-situ grazing incidence wide-angle X-ray scattering (GIWAXS) and grazing incidence small-angle X-ray scattering (GISAXS). With these approaches, we can follow the evolution of characteristic structures and of the inner morphology under the operational condition. After understanding the degradation mechanisms upon different atmosphere (nitrogen and vacuum), we can choose a reasonable atmosphere which allows for the standard aging routine to guide industrial development.

CPP 105.4 Fri 10:30 ZEU 222

Growth of Methylammonium and Formamidinium Lead Halides by Co-Evaporation Analyzed with in situ X-ray Diffraction — •Karl Heinze, Thomas Burwig, Roland Scheer, and Paul Pistor — Martin-Luther-Universität Halle-Wittenberg, Halle an der Saale, Germany

Crystalline lead halide perovskite (e.g. Methyl Ammonium (MA) PbI$_3$), thin-film solar cells reach efficiencies far over 20%. These films are commonly prepared by solvent-based methods such as spin-coating, with limited scalability. An industrially attractive technique for the deposition of thin films is co-evaporation. Using a vacuum chamber with a built-in in-situ X-ray diffraction system, we are able to investigate the influence of varying processing conditions during the co-evaporation of MA lead halides (MAPbX$_3$, with X=I,Br,Cl) and formamidinium lead halides (FAPbX$_3$) on the film formation process and can cross-relate our findings to opto-electronic properties and solar cell performance. More specifically, we analyze the effect of different precursors flux rate ratios and substrate temperatures on the crystal growth and compare sequential to simultaneous co-evaporation. We find a strong impact of the processing temperature on crystal size and morphology and determine suitable process windows for optimal absorber compositions with small amounts of PbI$_2$ secondary phases. We note that processing conditions have also a strong impact on the crystal orientation of the films. This is especially pronounced for FAPbBr$_3$, where we were able to grow films with nearly complete orientation in either (100) or (111) direction.

Invited Talk CPP 105.5 Fri 10:45 ZEU 222

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 microscopy is a powerful tool to investigate dynamic transformations in materials. To observe such transformations the focused electron probe in scanning transmission electron microscope (STEM) can be used to both stimulate and image the movement of atoms [1]. Here we apply such dynamic STEM to directly observe ion migration in hybrid and inorganic halide perovskites.

Direct in-situ heating of samples can also be used inside electron microscopes to provoke phase changes with special heating holders [2]. We use in-situ heating in STEM to track the phase transitions in inorganic CsPbI3 perovskites from an orthorhombic δ- phase to a cubic α-phase. An intermediate phase with layered configuration was observed during the transition.

[1] C. Li, Y. Y. Zhang, T. J. Pennycook, Y. L. Wu, A. R. Lupini, N. R. Paudel, S. T. Pantelides, Y. Yan and S. J. Pennycook, Column-by-column observation of dislocation motion in CdTe: dynamic scanning transmission electron microscopy, Appl. Phys. Lett. 2016, 109, 143107

[2] C. Li, E. S. Sanli, H. Strange, M. D. Heinemann, D. Greiner, R. Mainz, W. Sigle, D. Abou-Ras and P. A. v. Aken, Diffusion-assisted grain boundary migration in CuInSe2. under review

15 min. break

CPP 105.6 Fri 11:30 ZEU 222

Band structure and electronic properties of lead halide perovskites from photoemission studies — •Fengshuo Zu[1,2], Patrick Amsalem[1], David Egger[3], Christian Wolff[4], Rongbin Wang[1,7], Maryline Ralaiarisoa[1], Honghua Fang[5], Maria Antonietta[5], Dieter Neher[4], Leeor Kronik[6], Steffen Duhm[7], and Norbert Koch[1,2] — [1]HU Berlin — [2]HZB Berlin — [3]TU Munich — [4]Universität Potsdam — [5]University of Groningen, Netherland — [6]Weizmann Institute of Science, Israel — [7]Soochow University,China

Photovoltaic devices based on halide perovskites with outstanding optoelectronic properties have exhibited tremendous progress in performance. To understand the origin of these properties comprehensively, detailed knowledge on the underlying electronic band structure is required. Here, we present complementary results from low-energy electron diffraction, angle-resolved photoelectron spectroscopy, and density functional theory calculations for CH3NH3PbBr3 and CH3NH3PbI3 single crystals. For both, sharp LEED patterns corresponding to the (001) surfaces of CH3NH3PbBr3 and CH3NH3PbI3 were observed together with well-resolved, dispersive valence band features. Furthermore, the fundamental differences between linear and logarithmic methods in determining the VB onset are discussed and addressed.[1] In addition, surface photovoltage effect, which has so far hardly been discussed in this context, is found to play significant effect in photoemission studies.[2] [1] Zu et al., J. Phys. Chem. Lett. 2019, 10, 601,[2] Zu et al., ACS Appl. Mater. Interfaces, 10.1021/acsami.9b05293.

CPP 105.7 Fri 11:45 ZEU 222

Energy-Level Alignment of Formamidinium Tin Iodide with Organic Contact Materials — •Jonas Horn, Pascal Schweitzer, and Derck Schlettwein — Justus Liebig University Gießen, Institute of Applied Physics

The alignment of energy levels at the interfaces of a perovskite absorber with adjacent hole- and electron-transporting materials affects the formation of space-charge regions and interfacial recombination. These have consequences for charge transport in the layers and for the efficiency of devices. To analyze such alignment we used Kelvin-probe force microscopy (KPFM). This study is focused on formamidinium tin iodide (FASnI$_3$) as perovskite absorber, which avoids the toxicity problems of lead and is known to yield the highest power conversion efficiencies amongst all lead-free perovskite absorbers. The most common solar cell geometry for FASnI$_3$ implements C$_{60}$ as electron-transporting material, which is prepared onto the perovskite by physical vapor deposition (PVD). Intermittently to PVD, we used KPFM to simultaneously monitor morphology and work function of C$_{60}$ during its growth on FASnI$_3$. We show that a sufficiently high deposition rate is needed to avoid island formation of C$_{60}$ and obtain a homogeneously covering film with constant work function. We further show that the width of the space charge layer in C$_{60}$ is larger than the film thickness often implemented in perovskite solar cells. A band bending in the range of 300 meV is observed and consequences for prospective device operation are discussed.

CPP 105.8 Fri 12:00 ZEU 222

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.

CPP 106: Wetting and Liquids at Interfaces and Surfaces II (joint session CPP/DY/O)

Time: Friday 9:30–12:15 Location: ZEU 260

Invited Talk CPP 106.1 Fri 9:30 ZEU 260

Slide electrification: charging of surfaces by moving water drops — •Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

Water drops sliding over insulating surfaces can lead to surface charging. In contrast to charging caused by friction between two solids, drop slide electrification is largely unexplored. Slide electrification has been consistently reported, but results are difficult to reproduce. One reason for the lack of quantitative understanding is that the deposition of charge is a non-equilibrium effect and depends essentially on microscopic processes at the contact line. We address both the experimental and theoretical sides of this problem. We reproducibly measure the charge gained by water drops sliding down hydrophobic surfaces. To explain these results, we theorize that some fraction of the charge in the Debye layer is transferred to the surface rather than being neutralized as the drop passes. Given that nearly every surface in our lives comes in contact with water, this water-dependent surface charging may be a ubiquitous process that we are only beginning to understand.

CPP 106.2 Fri 10:00 ZEU 260

Spreading on viscoelastic solids: Are contact angles selected by Neumann's law? — Mathijs van Gorcum[1], •Stefan Karpitschka[2], Bruno Andreotti[3], and Jacco H. Snoeijer[1] — [1]Physics of Fluid Group, University of Twente, Enschede, Netherlands — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]Laboratoire de Physique Statistique, Univ. Paris-Diderot, Paris, France

The spreading of liquid drops on soft substrates is extremely slow, owing to strong viscoelastic dissipation inside the solid. A detailed understanding of the spreading dynamics has remained elusive, partly owing to the difficulty in quantifying the strong viscoelastic deformations below the contact line that determine the shape of moving wetting ridges. Here we present direct experimental visualizations of the dynamic wetting ridge, complemented with measurements of the liquid contact angle. It is observed that the wetting ridge exhibits a rotation that follows exactly the liquid angle, as was previously hypothesized [Karpitschka et al., Nat. Commun. (2015)]. This experimentally proves that, despite the contact line motion, the wetting ridge is still governed by Neumann's law. Furthermore, our experiments suggest that moving contact lines lead to a variable surface tension of the substrate. We set up a new theory that incorporates the influence of surface strain, the so-called Shuttleworth effect, for soft wetting. It includes a detailed analysis of the boundary conditions at the contact line, complemented by a dissipation analysis, which shows, again, the validity of Neumann's balance.

CPP 106.3 Fri 10:15 ZEU 260

Formation of a thin film during drop merging leads to fingering instability — •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

The coalescence and interaction between two drops have been the subject of intensive studies in recent years [1], due to its wide range of application and the presence in the nature.

Here, we study the merging of partially miscible drop. We deposit drops of different liquids on a substrate. Under appropriate conditions, the merging process generates an instability which resembles the Rayleigh-Plateau instability. If the liquid with higher surface activity is deposited as a second droplet. Its vapor can diffuse through the air and induce a Marangoni flow inside the already deposited droplet. This induced flow can pull a thin liquid layer over the surface , which decays into drops by a Rayleigh-Plateau instability.

We present a detailed study of this instability analyzing the onset of the instability and its characteristic length scales. Finally, a model is presented to explain the Marangoni flow induced by the gas phase. This model is validated by particle tracking.

References [1] S. Karpitschka, C. Hanske, A. Fery, and H. Riegler, Langmuir, vol. 30, no. 23, pp. 6826*6830, 2014.

CPP 106.4 Fri 10:30 ZEU 260

Condensation frosting on lubricant impregnated surfaces — •Lukas Hauer[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 icing on surfaces. Understanding the nature of frosting and icing is indispensable to this effort. While icing on surfaces is commonly studied by localized nucleation mechanisms, the formation of frost is comparable more complicated. Condensation frost is characterized by multi-step and multi-physical phenomenon. The formation of condensate droplets, percolation, and frost front propagation is an inherently stochastic process. Despite its ubiquitous nature, a quantitative model for frost growth on surfaces remains elusive. Lubricant impregnated surfaces are known for improved anti-icing properties. They experience lower ice drop adhesion and allegedly delayed surface frosting. 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 enabled us to monitor the dynamic lubricant migration during condensation frosting on micro-structured surfaces. We present a model of the lubricant migration, utilizing lubrication theory. This work serves to improve understanding of lubricant dynamic during condensation frosting, providing future roadmaps towards the future design of anti-icing surfaces.

CPP 106.5 Fri 10:45 ZEU 260

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 106.6 Fri 11:00 ZEU 260

Liquid-liquid phase separation in contact with deformable surfaces — •Hansol Jeon[1,2] and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-Universität Göttingen

The capillary forces of droplets on top of soft solids deform the solid surface into sharp wetting ridges. The amplitude of the wetting ridge is governed by elasto-capillary length, the ratio of liquid surface tension to the solid's shear modulus. Previous experiments on soft wetting used large liquid-vapour surface tensions and thus were in a highly nonlinear regime regarding the response of the solid. This led to debates in the literature regarding the effects of strain dependent solid surface tensions or the dynamics of soft wetting. Liquid interfaces with small surface tensions could instead probe the linear regime of soft wetting and shed new light onto the static and dynamic behaviours of solid surface tension. Thus we investigate the liquid-immersed case of soft wetting, aiming for a control of the liquid and solid surface tensions. We tested various liquid combinations and explored a wide range of surface tensions and substrate shear moduli, finding valid Neumann constructions in all cases.

15 min. break

CPP 106.7 Fri 11:30 ZEU 260

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 perspective 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 106.8 Fri 11:45 ZEU 260

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 106.9 Fri 12:00 ZEU 260

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.

CPP 107: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Friday 9:45–12:15 Location: ZEU 255

CPP 107.1 Fri 9:45 ZEU 255

Machine-Learned Polarizabilities: from Molecules to Bulk Raman Spectra — •David Wilkins, Andrea Grisafi, and Michele Ceriotti — Laboratory of Computational Science and Modelling, Institute of Materials, EPFL, Switzerland

The polarizability α of a chemical system is key in theoretically determining the results of spectroscopic experiments. However, α requires a high level of theory as well as extra computational effort on top of the ground-state electronic structure, meaning that to calculate an accurate polarizability can take several days for even a modest-sized molecule. Since an evaluation of spectra requires α to be known for an entire molecular simulation, the expense required would seem to stymie efforts to calculate an accurate spectrum.

The recently developed symmetry-adapted Gaussian process regression (SA-GPR) approach allows the prediction of tensor properties for general systems. I begin by showing that a model based on SA-GPR predicts the molecular α with the accuracy of coupled-cluster calculations, in a matter of seconds. This model can be applied to complex molecules with very high accuracy, suggesting that machine-learning should be the method of first resort for α predictions, rather than density functional theory, which is generally less accurate.

I finally show that SA-GPR is applicable also to the condensed phase, facilitating a prediction of spectroscopic experiments. In particular, I develop a model that allows a fast and accurate calculation of Raman spectra of bulk aqueous systems, as well as paving the way for the simulation of more complex nonlinear spectra.

CPP 107.2 Fri 10:00 ZEU 255

Machine learning the molecular dipole moment with atomic partial charges and atomic dipoles — •Max Veit[1], David Wilkins[1], Yang Yang[2], Robert DiStasio Jr[2], and Michele Ceriotti[1] — [1]Laboratory of Computational Science and Modeling, IMX, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853, USA

The gas-phase molecular dipole moment is a central quantity in chemistry. It is essential in predicting molecular infrared and sum-frequency-generation spectra, as well as in describing long-range molecular interactions. Furthermore, it can be extracted directly from expensive, but highly accurate, quantum mechanical calculations, making it an ideal target for machine learning. We choose to represent this quantity with a physically-inspired machine learning model that captures the two distinct physical effects contributing to molecular polarization: Local atomic polarization is captured within the symmetry-adapted Gaussian process regression (SA-GPR) framework, which assigns a dipole moment to each atom, while movement of charge across the entire molecule is captured by assigning a partial (scalar) charge to each atom. These models are fitted together to reproduce the quantum mechanical molecular dipole moment, achieving better results than either model alone. The results show how transparency and physical interpretability can aid not only the understanding of a machine learning model, but allow it to achieve higher accuracy as well, regardless of which physical property is being modelled.

CPP 107.3 Fri 10:15 ZEU 255

Combining experimental and quantum mechanical descriptors to understand chemical bonding in solids — •Stefan Maier[1], Simon Steinberg[2], Michael Schumacher[3], Pavlo Golub[4], Jean-Yves Raty[5,6], Ryky Nelson[2], Oana Cojocaru-Miredin[1], Richard Dronskowski[2], and Matthias Wuttig[1] — [1]Institute of Physics IA, RWTH Aachen University, 52074 Aachen — [2]Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, — [3]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen — [4]National University of Singapore, Department of Mechanical Engineering, 9 Engineering Drive 1, Singa-pore 117575 — [5]CESAM and Physics of Solids, Interfaces and Nanostructures, Université de Liège, B4000 Sart-Tilman — [6]UGA, CEA-LETI, MINATEC campus, 17 rue des Martyrs, F 38054 Grenoble

How are atoms held together? This question stood at the very beginning of the natural sciences and has played (and still plays) a central role in solid state physics, chemistry and materials science. Exactly eight decades after Linus Pauling published his famous book: The Nature of the Chemical Bond in 1939, we look at this fundamental question again in a different light. In the meantime, the quantum mechanical methods and experimental techniques available to study chemical bonding have improved tremendously, which allows studying chemical bonding by using new experimental methods combined with advanced quantum-mechanical methods.

CPP 107.4 Fri 10:30 ZEU 255

Operando observation of reaction intermediates above one atmosphere under Fischer-Tropsch conditions — •Patrick Lömker[1], Kevin Ploner[3], Mikhail Shipilin[2], Jörgen Gladh[2], Norbert Köpfle[3], Thomas Götsch[4], Heshmat Noei[1], Christoph Schlueter[1], Anders Nielsson[2], and Peter Amann[2] — [1]Photon Science, DESY, 22607 Hamburg — [2]Department of Physics, Stockholm University, 10691 Stockholm — [3]Institute of Physical Chemistry, University of Innsbruck, 6020 Innsbruck — [4]Fritz Haber Institute, Inorganic Chemistry, 14195 Berlin

The quest for a sustainable future poses challenges, especially with regard to the storage and distribution of fuels. The Fischer-Tropsch synthesis and can be part of a sensible production for these fuels. Yet literature detailing the reaction mechanisms is lacking.

As seen by many publications XPS can address the reaction mechanisms in question. However, combining ultra-high vacuum, required for XPS and high pressures above atmosphere have posed significant technical challenges.

We use an instrument designed at Stockholm University utilizing a virtual cell concept, directing a gas flow on the surface to increases the pressure, while minimizing the electron scattering in gas. This instrument is now in operation at the new HAXPES beamline P22 at PETRA III. We present data of CO:H2 with pressure up to 1025 mbar on a Co(0001) crystal. Intermediates and adsorbed species were identified under the reaction. We clearly observe a transition in the adsorbed species between 500-1000mbar – in line with recent literature.

CPP 107.5 Fri 10:45 ZEU 255

Modulating Selectivity of Nitrites Reduction by Leveraging Polymer-Induced Solvation Effects — •Pengcheng Huang, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98693, Ilmenau, Germany.

Closing the nitrogen cycle is essential for mitigating the negative environmental impact of fertilizers run-offs from intensive -crops production and -farming.1 The key in these processes is to activate nitrogen-containing species (e.g. nitrites, nitrates, and nitro-organic molecules) in heavily diluted aqueous environments into inert products (e.g. nitrogen) in the presence of reducing agents using supported metal catalysts. The modification of the metal and/or support chemistry, nanoarchitecture, and topology can lead to changes in the transport and binding of the reactive species, which can be leveraged to favor a specific pathway of the reaction.2 In this contribution, we propose a strategy to modulate the selectivity of N-O bond activation reactions by tailoring the solvation-microenvironment around the metal cluster. To demonstrate this concept we have developed polymer over-coatings on metal-catalysts that can act as *co-solvents* to simultaneously; 1) control the selectivity and activity of the catalyst towards the desired product to maximize atom-efficiency of the process, and 2) prevent catalyst deactivation by preventing the sintering, lixiviation, and poisoning. In this contribution, we will show the effects of the polymer brushes chemistry (poly(N-isopropylacrylamide) on the molecular transport, catalyst selectivity and activity of Pd-supported on nonporous SiO2 colloidal particles as model catalysts.

CPP 107.6 Fri 11:00 ZEU 255

The new Small Angle X-ray Scattering Beamline for Materials Research (SAXSMAT) at PETRA III — •Sylvio Haas, André Conceicao, Xiao Sun, and Saskia Pfeffer — Deutsches Elektronen Synchrotron (DESY), Photon Science Division, Hamburg, Germany

Modern applications and basic research in catalysis, biotechnology and materials are often concerned with hybrid and synergetic systems. In other words, systems that brings enhanced properties and performances due to their internal complexity. The challenge is now in understanding the interactions leading to their assembly and operation. Due to their inherent chemical and structural complexities, a combination of several techniques simultaneously and/or an advanced method is mandatory to determine structural and chemical information of materials.

Small-Angle X-ray scattering (SAXS) is a well-established method to investigate nanostructured materials. Information about particle size distribution, particle shapes, and inter-particle interaction potentials can be determined. Currently, DESY is commissioning a new beamline (P62; SAXSMAT) dedicated to this technique that will be open for user operation in the near future. The X-ray energy can be tuned between 3.5 keV to 35.0 keV. In this presentation the SAXSMAT beamline will be presented including the key features of the beamline:

I.) anomalous SAXS/WAXS: adding element sensitivity II.) SAXS/WAXS computed tomography: adding 3D spatial resolution III.) In situ and In operando SAXS/WAXS: adding time resolution

15 min. break

CPP 107.7 Fri 11:30 ZEU 255

Improved virtual orbitals for the calculation of X-ray absorption spectra for organic molecules — •Rolf Würdemann[1] and Michael Walter[2,3] — [1]reiburger Materialforschungszentrum, Freiburg, Germany — [2]Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany — [3]Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany

X-ray absorption spectroscopy (XAS) is an element specific local probe used for the analysis of materials. One way to compare and interpret experimentally measured spectra is to perform ab initio calculations of XAS spectra for molecules in given geometries. By this different isomers can be distinguished and a deeper understanding of the bonding situation can be gained.

Common ways to calculate XAS spectra by density functional theory (DFT) either utilize fractional charges in the frozen cores or restrict the state-space of linear time-dependent DFT. In our contribution we examine the possibility to utilize the combination of range-separated functionals (RSF) with Huzingas improved virtual orbitals to calculate XAS spectra. This combination has been successful in the calculation of charge transfer excitations[1].

[1] Würdemann, R. and Walter, M., J. Chem. Theory Comput. 2018, 14, 7, 3667-3676

CPP 107.8 Fri 11:45 ZEU 255

Quantum tunnelling in the Marcus inverted regime — •Eric R. Heller and Jeremy O. Richardson — ETH Zürich, 8093 Zürich, Switzerland

Electron transfer rates between weakly coupled states are predominantly calculated using Marcus theory. Due to its inherent classical character, however, experimental reaction rates can deviate from the Marcus result by several orders of magnitude due to the influence of quantum tunnelling and zero-point energy. These effects prove to be of particular importance in the so called "inverted" regime, where reaction rates become smaller with increasing thermodynamic driving force.

In principle the correct quantum mechanical rate can be obtained by applying Fermi's golden rule. This, in turn, requires knowledge of the nuclear wavefunctions of the two reactive wells, which are not accessible for all but very small systems.

Semiclassical instanton theory is able to capture nuclear quantum effects in a numerically efficient way allowing application to complex, anharmonic systems. Recently this method has been extended to describe the inverted regime by locating an optimal tunnelling pathway formed by two trajectories, one of which travels in negative imaginary time giving a picture reminiscent of the scattering of particles and antiparticles.

The method thus constitutes a semiclassical path-integral version of Fermi's golden rule applicable not only to electron-transfer reactions but also light-matter interactions, electrochemistry and many more.

CPP 107.9 Fri 12:00 ZEU 255

3D-printed humidity chamber for neutron scattering on thin films — •Tobias Widmann, Lucas P. Kreuzer, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

The investigation of thin soft matter films with neutrons allows a non-destructive probe with good scattering statistics. It entertains a broad field of scientific interest that studies structures and performance of various soft matter systems such as hydrogels or organic solar cells. However, soft matter samples are very sensitive to humidity and temperature and require well-defined ambient conditions. As such, specialized sample environments are needed which provide stable control over the hydrodynamic parameters at the sample position. In the framework of the FlexiProb project, a quickly interchangeable sample environment for experiments at the European spallation source (ESS) is designed. We focus on the design and fabrication of a specialized sample environment for the investigation of thin film samples with grazing incidence small angle scattering (GISANS). At its core stands a 3D-printed humidity chamber that offers the necessary control. The spherical chamber design has well distributed fluidic channels inside its walls which provide a stable and rapidly adjustable temperature. The control over the atmospheric composition around the sample is realized by a remote-controlled gas-flow array that mixes up to three different humidified or dry air streams. The novel chamber design provides a first step into a 3D-printed sample environment for neutron experimentation.

CPP 108: Closing Talk: Frank Jülicher (joint session BP/DY/CPP)

Time: Friday 12:30–13:15 Location: HSZ 02

Invited Talk CPP 108.1 Fri 12:30 HSZ 02

Physics of active droplets — •Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, Dresden

Phase separation provides a general physical mechanism for the spatial organization of cells and for the compartmentalization of chemical processes. Proteins together with other molecules can condense to form liquid-like droplets that provide localized chemical environments and that can serve as micro-reactors for biochemical reactions without an enclosing membrane. The cell cytoplasm can thus be viewed as an emulsion, where phase-separated compartments organize biochemical processes in space. Droplets that carry chemical activity are active systems that maintained away from thermodynamic equilibrium by chemical energy input. I will discuss the physics of such active droplets and active emulsions and show that they exhibit unusual properties and behaviors. Examples are the arrest of coarsening and the suppression of Ostwald ripening, spontaneous droplet division and droplet positioning by concentration gradients. The physics of active droplets could play important roles in fundamental cellular processes of many organisms and could have emerged early in the evolution of life.

CPP 109: Closing Talk: Roland Wiesendanger (joint session O/CPP/DS)

Time: Friday 14:00–14:45 Location: HSZ 02

Topical Talk CPP 109.1 Fri 14:00 HSZ 02

Surface Science Aspects of Topological States of Matter — •Roland Wiesendanger — Universität Hamburg

Topological states of matter have raised great excitement in solid state physics in the past years, e.g. in the fields of topological insulators, topological spin textures (magnetic skyrmions), and topological superconductors hosting Majorana states. Surface and interface science plays a crucial role for all these fields, as has been demonstrated, e.g., by the discovery of ultimately small-scale skyrmions stabilized by interfacial Dzyaloshinskii-Moriya interactions [1,2] or the direct real-space observation of the emergence of Majorana states in atomic-scale magnet-superconductor hybrid systems [3,4]. In particular, the preparation of extremely clean surfaces of elemental s-wave superconductors, such as Re, Ta, La, and Nb has boosted recent studies of topological superconductivity in bottom-up constructed 1D and 2D hybrid systems, allowing for the atomic-scale design of Majorana states and a one-to-one comparison between results of theoretical toy models and experimental observations. Bringing together surface science concepts and advanced techniques for the fabrication of atomically well defined magnet-superconductor hybrid systems is a key ingredient for this exciting new research area which ultimately will allow for the realization of topological quantum computation schemes. [1] N. Romming et al., Science 341, 6146 (2013). [2] S. Heinze et al., Nature Physics 7, 713 (2011). [3] H. Kim et al., Science Advances 4, eaar5251 (2018). [4] A. Palacio-Morales et al., Science Advances 5, eaav6600 (2019).

CPP 110: Nano- and Optomechanics (joint session TT/HL/CPP)

Time: Friday 9:30–10:30 Location: HSZ 03

Invited Talk CPP 110.1 Fri 9:30 HSZ 03

Microwave Optomechanics with Superconducting Quantum Interference Cavities — •Daniel Bothner, Ines C. Rodrigues, and Gary A. Steele — Kavli Institute of Nanoscience, Delft University of Technology, PO Box 5046, 2600GA Delft, The Netherlands

Within the recent decade, cavity optomechanics has achieved tremendous breakthroughs regarding the detection and control of macroscopic mechanical oscillators with electromagnetic radiation. Among the most groundbreaking results are displacement sensing beyond the standard quantum limit, quantum ground-state sideband cooling and the generation of non-classical states of motion in massive mechanical objects. With most current approaches for optomechanical systems, however, the nonlinear single-photon regime seems still far out of reach.

Here, I will introduce a recently realized, novel approach for coupling microwave fields in a superconducting circuit to mechanical motion: flux-mediated microwave optomechanics. In this approach, mechanical motion is transduced to magnetic flux, which couples into a superconducting quantum interference device (SQUID). The SQUID forms the inductor of a superconducting microwave circuit and the coupling strength between the microwave circuit and the mechanical displacement is tunable and scales with the magnitude of the magnetic transduction field. Due to the linear scaling behavior, this flux-mediated approach has been predicted to have the realistic potential to reach the fully nonlinear regime of the optomechanical coupling, opening the door for the preparation of mechanical quantum states and a new generation of optomechanical devices.

CPP 110.2 Fri 10:00 HSZ 03

Magnetoelastic readout concepts — •Daniel Schwienbacher[1,2,3], Nynke Vlietstra[1,2], Thomas Luschmann[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, München, Germany

Nanostring resonators are prime candidates for mechanical sensing applications. Typically, they are used for mass and force sensing. However, it is also possible to use these resonators for the investigation of solid state properties of materials, like magnetoelastics. We investigated the mechanical motion of a 60 μm long SiN/Co bi-layer nanostring resonator with a resonance frequency in the MHz range. Here, we simultaneously use optical and electrical readout techniques. We observe the well known impact of the magnetoelastics, due to the presence of Co, on the resonance frequency of the nanostring. In addition, we study the impact of electrical transport through the string resonator on the mechanical properties of the system.

CPP 110.3 Fri 10:15 HSZ 03

Magnetomechanical Crystals — •T. Luschmann[1,2,3], D. Schwienbacher[1,2,3], J. Graf[4], F. Engelhardt[4], S. Viola Kusminskiy[4], R. Gross[1,2,3], and H. Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, München, Germany — [4]Max Planck Institute for the Science of Light, Erlangen, Germany

Optomechanical crystals have become an established platform for the investigation of light-matter interaction, specifically in the context of optomechanical interaction. The success of this concept is founded in the simultaneous localization of GHz frequency phonons alongside THz photons in a suspended nanostructure [1]. We expand this concept with the introduction of magnetic materials capable of supporting spin-wave resonances in the GHz frequency range. We present finite element studies of phononic crystal cavities alongside micromagnetic simulations of spin-waves in nanostructured magnetic materials to tailor the geometries towards the realization of resonant, artificial magnon-phonon coupling. In addition, we will quantitatively compare numerical simulations with early experimental data.

[1] Eichenfield et al. Nature **462**, 7882 (2009).

CPP 111: Data analytics for dynamical systems II (joint session SOE/CPP/DY)

Time: Friday 9:30–10:00 Location: GÖR 226

CPP 111.1 Fri 9:30 GÖR 226

A Variational Perturbative Approach to Graph-based Multi-Agent Systems — •Dominik Linzner, Michael Schmidt, and Heinz Koeppl — TU Darmstadt, Germany

Understanding the behavior of multiple agents is a difficult task with numerous applications in the natural and social sciences. However, the number of possible configurations of such systems scales exponentially in the number of agents leaving many queries intractable – even if limiting interactions to a static interaction graph.

Variational approaches pave a principled way towards approximations of intractable distributions. Here, traditional approaches focus on directly constraining the class of variational distributions, e.g. in naïve mean-field statistical independence of all random variates is assumed. Variational perturbation theory (VPT) offers a different approach. Here, the similarity measure itself is approximated via a series expansion. A prominent example of this approach is Plefka's expansion [1,2]. The central assumption is that variables are only weakly coupled, i.e. the interaction of variables is scaled in some small perturbation parameter.

We derive a novel VPT for stochastic dynamics on static interaction graphs and use it to develop methods for different (inverse) problems such as system identification from data or optimal planning of coordination tasks.

[1] Plefka, T. (1982). Journal of Physics A, 15, 1971-1978. [2] Bachschmid-Romano et al. (2016). Journal of Physics A: Mathematical and Theoretical, 49(43), 434003-434033.

CPP 111.2 Fri 9:45 GÖR 226

A differentiable programming method for quantum control — •Frank Schäfer, Michal Kloc, Christoph Bruder, and Niels Lörch — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Precise control of quantum systems is highly desirable in many current experimental setups and quantum information technologies. In quantum control, by optimization of control pulse sequences, protocols that maximize a case-specific figure of merit are obtained. To solve quantum state control problems, we treat (closed) quantum systems as differentiable programs. Within a framework that combines machine learning and the knowledge of the differential equations governing the dynamics of the physical system, we employ predictive models for optimal parameter estimation. We analyse the sensitivity of this approach against noise in the initial states and verify the robustness of the method.

CPP 112: Active Matter V (joint session DY/BP/CPP)

Time: Friday 10:00–11:30 Location: ZEU 160

CPP 112.1 Fri 10:00 ZEU 160

A particle-field approach bridges phase separation and collective motion in active matter — •Robert Grossmann[1,2], Igor Aranson[3], and Fernando Peruani[2] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Laboratoire J.A. Dieudonné, Université Côte d'Azur, Nice, France — [3]Department of Chemistry, Pennsylvania State University, University Park (PA), United States of America

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.

CPP 112.2 Fri 10:15 ZEU 160

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 numerically investigate turbulent flows in a two-dimensional dense suspension of active nematic liquid crystals. We qualitatively compare numerical simulations with and without nonlinear advection of the flow field. We find that for sufficiently high activity, the simulations considering the advection term display large-scale motion not observed when excluding inertia. 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 slows down the large-scale motion.

CPP 112.3 Fri 10:30 ZEU 160

Active Brownian particles show motility-induced spatially periodic patterns — •Samuel Grimm[1], Andreas Fischer[2], Thomas Speck[2], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physics Institute, University of Mainz, 55099 Mainz, Germany

We suggest and investigate a model for active Brownian particles, that shows motility induced pattern formation. We complement a model of motility induced phase separation (MIPS) [J. Chem. Phys. 142, 224149 (2015)] by the dynamics of auto-inducer molecules. This results in a prototype model for spatially periodic patterns under conservation constraints, here the conservation of Brownian particles. By increasing the chemotactic sensitivity of active Brownian particles a transition from MIPS to motility induced periodic patterns takes place. They are found in a wide parameter range. Besides the phase diagrams for the onset of spatially periodic patterns also their nonlinear behavior beyond onset is investigated for selected parameter ranges.

CPP 112.4 Fri 10:45 ZEU 160

The role of advection in the diffusioosmosis of an active micropump — •Gonçalo Antunes[1,2], Paolo Malgaretti[1,2], Jens Harting[3,4], and Siegfried Dietrich[1,2] — [1]MPI-IS, Stuttgart, Germany — [2]U. Stuttgart, Stuttgart, Germany — [3]HI-ERN, Forschungszentrum Jülich, Nürnberg, Germany — [4]TU/e, Eindhoven, The Netherlands

Diffusioosmosis can be exploited to fabricate active colloids that swim in a fluid/solute mixture through a self-generated inhomogeneous concentration of solute [1]. Using the same mechanism, an active channel can be fabricated such as to pump fluid in a way that is tunable via the geometry and chemistry of the channel.

In this talk, we study the flow inside an active hourglass-shaped channel. Our Lattice Boltzmann simulations are combined with a finite-difference solver for the advection-diffusion equation that determines the solute dynamics [2]. We find that even when the channel is fore-aft symmetric, advection can lead to the pumping of fluid, in analogy to the steady motion of isotropic colloids [3,4]. Furthermore, sustained oscillations are found where the magnitude of the flow oscillates with a tunable frequency. Our findings are thus relevant for those who wish to exploit surface-driven flows at small scales.

[1] J. L. Anderson, Ann. Rev. Fluid Mech. **21** 61-99 (1989) [2] T. Peter, P. Malgaretti, N. Rivas, A. Scagliarini, J. Harting, S. Dietrich, arXiv:1911.06324 (2019) [3] S. Michelin, E. Lauga, and D. Bartolo, Phys. Fluids **25** 061701 (2013) [4] P. de Buyl, A. S. Mikhailov, and R. Kapral, EPL **103** 60009 (2013)

CPP 112.5 Fri 11:00 ZEU 160

Dynamical states in underdamped active matter — •Dominic Arold and Michael Schmiedeberg — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Many active matter systems 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 in active matter is 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 of polar orientations whereas long-ranged correlations of orientational order are suppressed. 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 in a certain parameter regime, 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.

[1] Scholz C et al. 2018 *Nature communications* **9** 5156

[2] Archer A J 2009 *The Journal of chemical physics* **130** 014509

CPP 112.6 Fri 11:15 ZEU 160

Predictive local field theory for interacting active Brownian spheres in two spatial dimensions* — Jens Bickmann and •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

We present a predictive local field theory for the dynamics of interacting spherical active Brownian particles in two spatial dimensions. Alongside the general theory, which includes configurational order parameters and derivatives up to infinite order, we present reduced models that are easier to apply. We show that our theory contains popular models such as Active Model B + as special cases and that it provides explicit expressions for the coefficients occurring in these models. As further outcomes, the theory yields analytical expressions for the density-dependent mean swimming speed and the spinodal corresponding to motility-induced phase separation of the particles. The analytical predictions for the spinodal are found to be in very good agreement with the results of Brownian dynamics simulations. Furthermore, the critical point predicted by our analytical results agrees excellently with recent computational results from the literature.

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CPP 113: Nanostructured Surfaces and Thin Films III: Dots, Particles, Clusters (joint session O/CPP)

Time: Friday 10:30–13:00 Location: WIL B321

CPP 113.1 Fri 10:30 WIL B321

Reconfigurable Polaritonics using Phase Change Materials — •Christina M. Spägele[1], Xinghui Yin[1], Michele Tamagnone[1], Kundan Chaudhary[1], Stefano L. Oscurato[1,2], Jiahan Li[3], Christoph Persch[4], Ruoping Li[1], Noah A. Rubin[1], Luis A. Jauregui[5], Kenji Watanabe[6], Takashi Taniguchi[6], Philip Kim[1], Matthias Wuttig[4], James H. Edgar[3], Antonio Ambrosio[1,7], and Federico Capasso[1] — [1]Harvard University, USA — [2]Unina, Italy — [3]KSU, USA — [4]RWTH, Germany — [5]UCLA, USA — [6]NIMS, Japan — [7]CNST-IIT, Italy

Polaritons garnered significant interest due to their ability of confining light to the nanoscale. They arise when light couples strongly to material excitations such as excitons, plasmons or phonons. To date, methods to control these highly confined states of light are not well-suited for free-form manipulation of polaritons. Moreover, they create systems that are unalterable after the initial fabrication process.

Placing the hyperbolic vdW-material hexagonal boron nitride on the phase change material (PCM) Ge3Sb2Te6, we successfully achieved spatial control of the propagation of surface phonon polaritons (SPhP) by structuring the PCM. The exponentially decaying tail of the guided SPhP modes interacts with the PCM, which can be optically switched to a higher refractive index crystalline phase, slowing the SPhP. We demonstrate rewritable waveguides and refractive optical elements such as lenses and prisms for mid-IR polaritons. Moreover, we will discuss reconfigurable metalenses that allow for precise wavefront engineering and diffraction-limited focusing.

CPP 113.2 Fri 10:45 WIL B321

Synthesis of 3D ZnO nanostructures on different substrates for gas sensor applications — Hanaa Seso, Stefan Ostendorp, •Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische-Wilhelms-Universität, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Three-dimensional (3D) ZnO nanostructures have been synthesized via atomic layer deposition (ALD) on different types of templates to act as a gas sensing active material. The used template structures range from anodic aluminum oxide (AAO) template synthesized by a two-step anodization method, a polymer template prepared by infiltration of a polymer solution into an AAO structure to a porous gold template fabricated by de-alloying of an Au-Ag solid solution. The morphology of the templates and the nanostructured ZnO-based carbon monoxide (CO) sensors were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The gas-sensing performance of sensors based on the different templates was measured successfully in terms of electrical response to detect CO as a hazardous gas. The tremendously increased surface to volume ratio of ZnO on an AAO (alike) template or porous gold template is thereby supposed to provide an enhanced sensing capability compared to 2D thin film or bulk sensor structures.

CPP 113.3 Fri 11:00 WIL B321

Thinking inside the box: Quantum corrals as artificial atoms and molecules — •Saoirse Freeney, Jaap Harteveld, Sam Borman, and Ingmar Swart — Utrecht University, Utrecht, Netherlands

The electronic behaviour that underlies the field of chemistry is essentially a result of the confining potential of an atom's nucleus on its electrons. Due to their confinement, the allowed energies that electrons can take in an atom are quantised, and their wavefunctions are well-defined . If we were to create our own potential that confines electrons within, we could emulate real atoms and change their properties at will. In fact, a quantum corral is exactly this. To create one, adsorbates on a metal surface are accurately manipulated with an STM tip to predetermined positions. Much like a particle-in-a-box, the surface state electrons are then confined, exhibiting discrete energy levels analogous to an atom. We can liken the measured wavefunctions to those of s, p, d etc orbitals in an atom. Beyond this, we can pair two quantum corrals together and observe that bonding and antibonding orbitals arise. Here, we use CO molecules to scatter the Cu(111) surface state and investigate the relation of size and shape on the energy and wavefunction, and secondly we tailor the strength of coupling in "molecular" quantum corrals. Several artificial lattices have been made before with the CO/Cu(111) platform. The information presented is useful for designing such lattices.

CPP 113.4 Fri 11:15 WIL B321

Ordered structures with functional units from artificial alumina membranes — •Wenxin Wang — Photonic Materials Group, College of Physics and Optoelectronic Engineering, Harbin Engineering University,15001 Harbin, China

Constructing ordered structures with functional units (OSFU) gives opportunities to improve, modify intrinsic performances of ordered structures, even render novel properties. Here I report an approach to realize OSFU through artificial alumina membranes (AAMs), single and multi-order structure(s) are functionalized with plasmonic and (or) smart polymer unit to check their mesoscopic optical behaviors. For instance, AAMs are directly used as OSFU to achieve structural color imaging with high reflectivity. Second, functionalize units with plasmonic materials to obtain enhanced local field and resonance modes hybridization, in order to manipulate the linear and nonlinear optical performances. Third, functionalize units with polymer to realize reversible structures for dynamic optical modulation. Finally, multi-order OSFU is designed by inducing diverse lattice arrangements for photonic band engineering. The second-order elements are embedded on special points that corresponding high symmetry points in k-space that will arise Dirac cone and flat band.

CPP 113.5 Fri 11:30 WIL B321

Comsol modeling of the role of nanostructured current collectors in supercapacitor — •Maximilian Kaupenjohann, Long Liu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98393, Ilmenau, Germany

Current collector is an important component in supercapacitors and its main role is to transport charge carriers from/to electroactive materials during the charge-discharge process. The charge transport efficiency is believed to be dominated by the resistance at the electroactive-material/current-collector interfaces. Owing to the large specific surface area, nanostructured current collectors have been designed, fabricated, and investigated intensively for supercapacitors. Especially for pseudocapacitive materials that have theoretically high specific capacitance but intrinsically low electric conductivity, nanostructured current collectors enable one to achieve a much higher specific capacitance even nearly reach the theoretical value. The improved performance is generally attributed to the improved electrical and ionic transport kinetics endowed by nanostructured current collectors. In this work, the role of nanostructured current collectors in supercapacitor electrode is further identified by using COMSOL Multiphysics simulations in combination with the experiment results.

CPP 113.6 Fri 11:45 WIL B321

Global Optimization of Copper Clusters on ZnO Surfaces Utilizing a Neural Network Potential — •Martín Leandro Paleico and Jörg Behler — Universität Göttingen, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

The catalyst used in the industrial synthesis of methanol is composed of large copper and zinc oxide nanoparticles. Studying the structure of this system requires a simulation method capable of handling thousands of atoms with ab initio accuracy, but with computational efficiency comparable to classical empirical potentials. To meet these requirements, a Neural Network Potential (NNP) has been trained to reproduce the potential energy surface of the system based on DFT reference calculations.

We have utilized this potential to carry out the tens of thousands of energy and force evaluations required to perform global optimization searches employing genetic algorithms. With this, we are able to optimize pure copper and binary copper-zinc clusters with up to 30 atoms on two different zinc oxide surfaces. This allows us to investigate structural and energetical trends in cluster growth and cluster-substrate interactions, as well as to identify possible active sites and their distribution in the clusters.

CPP 113.7 Fri 12:00 WIL B321

Deposition and annealing of Fe_xNi_{1-x} nanoparticles on a W(110) surface — •Mahboobeh Ravankhah, Dennis Jagenburg, and Mathias Getzlaff — Institute of Applied Physics, University Düsseldorf

3d bimetallic nanoparticles have received lots of attention because of their technological application. In comparison to pure Fe and Ni, alloys of Fe_xNi_{1-x} have much more complex structural phases under different conditions. Different FeNi alloys are used: $Fe_{0.50}Ni_{0.50}$, $Fe_{0.25}Ni_{0.75}$ and $Fe_{0.75}Ni_{0.25}$. All nanoparticles are prepared by a magnetron sputtering source under UHV condition on a W(110) surface, therefore contaminations are avoided. The deposited nanoparticles are subsequently annealed between 500-800K. Particle's size, shape and structure will be investigated by Transmission Electron Microscopy (TEM) and Scanning Tunneling Microscopy (STM). We report on the influence of different parameters like size of nanoparticles, stoichiometry and annealing temperature on the melting behavior.

CPP 113.8 Fri 12:15 WIL B321

Cu2+ Detection by Carbon Quantum Dots Derived from Water Hyacinth (Eichhornia crassipes) — •Eduardo Magdaluyo Jr[1], Gerald Mari Quiachon[2], and Persia Ada de Yro[2] — [1]Department of Mining, Metallurgical and Materials Engineering, University of the Philippines, 1101 Diliman, Quezon City, Philippines — [2]Materials Science Division, Industrial Technology Development Institute, Department of Science and Technology, Bicutan, Taguig, Metro Manila, Philippines

Preparation of carbon quantum dots (CQDs) was derived from water hyacinth (Eichhornia crassipes) leaves as a carbon source using facile approach of hydrothermal treatment in acidic medium. The as-synthesized CQDs exhibited coagulation in aqueous solution and a strong blue fluorescence under UV light at 365 nm. Infrared spectra analysis confirmed the presence of functional groups such as hydroxyl (OH), carboxyl (COO) and carbonyl (CO) on the surface of the CQDs. The functional groups were analyzed using zeta potential and was found to induce surface charges which allow the attraction of copper ions and bind with the CQDs. These surface charges were utilized in the application of the CQDs as a biosensor for the detection of Cu2+ ions based on ion-induced fluorescence quenching of CQDs. The photoluminescence spectra confirmed this process and it was found to have excellent affinity toward Cu2+ as the PL of CQD with copper solution was quenched relative to pure CQD solution. The highest quantum yield of the CQD sample being measured against deionized water was found to be at 6.48.

CPP 113.9 Fri 12:30 WIL B321

Electronic and optical properties of quantum-confined nanoparticles — •Marius Buerkle and Vladimir Svrcek — National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

We discuss the electronic and optical properties of semiconducting nanoparticles in the quantum-confinement regime. Here we focuse on how do quasi-band-like features emerge from finite electronic states with increasing particle size. This is discussed for Si, SiC, and Sn nanoparticles. Particularly interesting is the transition from an indirect to direct bandgap semiconductor for ultra-small Sn nanoparticles.

CPP 113.10 Fri 12:45 WIL B321

Developing a GAP machine-learned potential for iridium dioxide nanoparticles — •Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Iridium dioxide is currently the preferred material for highly active, yet chemically stable nanoparticle catalysts enabling the electrochemical oxygen evolution reaction (OER) in proton exchange membrane electrolyzers. Full ab initio molecular dynamics (MD) simulations of the reactive processes at the electrified nanoparticle surface would be highly desirable for mechanistic catalyst improvement, but are computationally not tractable for a foreseeable time. To overcome the limitations regarding system size and propagation time, MDs based on machine-learned interatomic potentials are an appealing alternative.

Here, we present a corresponding Gaussian Approximation Potential (GAP) for IrO_2 combining two-body and smooth overlap of atomic positions (SOAP) descriptors to capture the atomic environment. The potential is trained with density-functional theory (DFT) data comprising IrO_2 bulk, various surface slabs, Wulff shape nanoparticles, as well as semi-amorphous structures iteratively obtained from short MD trajectories based on the developing GAP. The final GAP is found to faithfully provide a wide range of static geometric and energetic key parameters. MD simulations based on this GAP now provide first insight into stability and special OER active sites offered by nanoparticles of varying size and shape.