CPP 22: Poster Session III - Charged Soft Matter and Theory and Simulation

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

CPP 22.1 Wed 16:30 CPPp

In-situ investigation of the thermal stability of thermoelectric thin films based on ionic liquid post-treated PEDOT:PSS — •Anna Lena Oechsle[1], Julian E. Heger[1], Nian Li[1], Shanshan Yin[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]ELETTRA Sincrotrone Trieste S. C. p. A., 34149 Basovizza TS, Italy — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

In total around 66% of the global produced primary energy is lost as waste heat, for example from industrial or everyday life processes. Thermoelectric generators, as they enable the direct conversion of a temperature gradient into electrical power, are therefore considered a promising technique to recycle these large amounts of heat waste. Especially, organic thermoelectric polymers are attractive, owning some advantages like low cost, lightness and high mechanical flexibility, low or no toxicity, as well as a usually low thermal conductivity. In our work we research the positive effect of ionic liquid (IL) treatment on the thermoelectric properties of semi-conducting PEDOT:PSS thin films. Therefore, we measure parameters, like the Seebeck coefficient, electrical conductivity, and furthermore examine the inner film morphology with scattering techniques like grazing incidence small angle x-ray scattering (GISAXS). In addition to find the influence of ILs treatment on the morphology-function relation of the PEDOT:PSS thin films, we also investigate the thermoelectric performance stability these films under operation at elevated temperatures.

CPP 22.2 Wed 16:30 CPPp

Structural and Dynamic Insights in the Conduction of Lithium-Ionic-Liquid Mixtures in Nanoporous MOFs as Solid-State Electrolyte — Micaela Vazquez[1], •Modan Liu[2], Zejun Zhang[1], Abhinav Chandresh[1], Anemar Bruno Kanj[1], Wolfgang Wenzel[2], and Lars Heinke[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Metal-organic framework (MOF) based separators in Li-ion-battery (LIB) help stabilize the solid electrolyte interphase and strongly affect the battery performance. The mobility and conduction of the Lithium-ion and organic ionic liquids (ILs) in these materials is crucially dependent on the MOF structures and the IL loading factors.

Here, via both experiments and all-atom molecular dynamics (MD) simulations, we observe complex conduction behaviors of Li-IL in the MOF with loading and composition dependence, particularly the presence of Li-ion prevents the conductivity collapse at high IL loading. MD reveals a vehicular transport for the IL and a Grotthuss-like conduction for Li-ions. At small pore fillings, the Li conduction is limited by the large separation between anions. At high pore fillings, the conduction is governed by the bunching of IL. In contrast to the Li-free IL, the bunching effect is attenuated by the formation of charge-neutral Li-anion complexes, which results in a tremendously increased conductivity at maximum filling. This tuning mechanism may contribute to development of advanced batteries.

CPP 22.3 Wed 16:30 CPPp

Quantitative prediction of charge regulation in peptides and model ampholytes — •Peter Košovan, Raju Lunkad, Anastasiia Murmiliuk, Pascal Hebbeker, Zdeněk Tošner, and Miroslav Štěpánek — Department of Physical and Macromolecular Chemistry, Charles University

Weak ampholytes are ubiquitous in nature and commonly found in artificial pH-responsive systems. However, our limited understanding of their charge regulation and the lack of predictive capabilities hinder the bottom-up design of such systems. Here, we used a coarse-grained model of a flexible polymer with weakly ionisable monomer units to quantitatively analyse the ionisation behaviour of two oligopeptidesmodel ampholytes. Our simulations predict differences in the charge states between oligopeptides and monomeric amino acids, showing that not only electrostatic interactions between charged groups but also conformational flexibility plays a key role in the charge regulation. By comparing our simulations with experimental results from potentiometric titration, capillary zone electrophoresis and NMR, we demon-

strated that our model reliably predicts the charge state of various peptide sequences. Ultimately, our simulation model is the first step towards understanding the charge regulation in flexible ampholytes, and towards predictive bottom-up design of charge-regulating systems.

CPP 22.4 Wed 16:30 CPPp

Investigating the surface charge of microplastic particles with Colloidal Probe-Atomic Force Microscopy — •Thomas Witzmann and Andreas Fery — Leibniz-Institute of Polymer Research Dresden, Germany

To date, plastic particles have mainly been categorized by polymer type, shape, and size. But there is another important issue arising when investigating microplastic and its interaction with cells. With decreasing size, the surface-volume ratio increases which makes surface properties more important to consider. It is generally believed that the surface properties of the particles influence the cell interaction. Therefore, we investigated un-functionalized polystyrene particles with the size of 3 micrometer with different surface properties of two different manufactures. We found out that the cellular interaction and uptake of microplastic particles (polystyrene) differs for the two particle types. Using Colloidal Probe-Atomic Force Microscopy (CP-AFM) we could show a significant difference in the electric surface properties: homogeneously charged particles vs. heterogeneously charged particles. The heterogeneous surface charge manifests itself in an electrostatic interaction of the particles that depends on the mutual orientation of the particles. CP-AFM is therefore a magnificent tool to obtain additional information*s about surface charge and its distribution on microplastic particles.

CPP 22.5 Wed 16:30 CPPp

Investigation of Cononsolvency Phase Transition of Poly(sulfobetaine)-based Diblock Copolymer Thin Films — •Peixi Wang[1], Christina Geiger[1], Lucas P. Kreuzer[1], Tobias Widmann[1], Suzhe Liang[1], Robert Cubitt[2], André Laschewsky[3], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]Technische Universität München, Garching, Germany — [2]Institut-Laue-Langevin, Grenoble, France — [3]Universität Potsdam, Potsdam-Golm, Germany

Co-nonsolvency occurs if a mixture of two good solvents causes the collapse or demixing of polymers into a polymer-rich phase in a certain range of compositions of these two solvents. The nonionic thermo-responsive polymer, poly(N-isopropylmethacrylamide) (PNIPMAM), has been widely used to investigate its collapse transition behavior in a mixture of two competing good solvents. However, co-nonsolvency response of its block copolymer containing the zwitterionic poly(sulfobetaine)s, especially poly(4-((3-methacrylamidopropyl)dimethyllammonio)butane-1-sulfonate)) (PSBP), shows a strong swelling transition in aqueous media, is newly studied. We focus on the co-nonsolvency behavior of PSBP-b-PNIPMAM thin films in water/acetone mixtures by in situ time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance (SR). Furthermore, Fourier transform infra-red (FTIR) spectroscopy is applied to investigate the interactions between the polymer thin film and water/co-solvent, which strongly alters dependend on their deuteration level.

CPP 22.6 Wed 16:30 CPPp

ToF-NR investigation of cononsolvency in PNIPAM-based block-copolymer thin films — •Christina Geiger[1], Julija Reitenbach[1], Lucas P. Kreuzer[1], Tobias Widmann[1], Peixi Wang[1], Robert Cubitt[2], Cristiane Henschel[3], André Laschewsky[3], Christine M. Papadakis[4], and Christina Geiger[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Institut Laue-Langevin, 38000 Grenoble, France — [3]Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam, Germany — [4]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

The diblock copolymer PMMA-b-PNIPAM forms micelles in aqueous solution that exhibit a reversible shell collapse transition at the lower critical solution temperature (LCST). Apart from a temperature stimulus, the collapse can be induced by the addition of organic co-solvents due to the competitive attachment and detachment of wa-

ter and co-solvent to the PNIPAM chains. We demonstrate that the co-nonsolvency effect is transferrable from solutions to thin film systems. The film swelling and contraction kinetics due to the uptake of water and co-solvent via solvent vapors are investigated with a focus on time-of-flight neutron reflectometry (ToF-NR). Sequential contrasting experiments using protonated and deuterated compounds are performed to differentiate between the distributions of water and co-solvent within the polymer films.

CPP 22.7 Wed 16:30 CPPp
Layer-by-layer Spray-oating of Cellulose Nanofibrils and Silver Nanoparticles for Hydrophilic Interfaces — •QING CHEN[1,2], CALVIN BRETT[1,3], ANDREI CHUMAKOV[1], MARC GENSCH[1,4], MATTHIAS SCHWARTZKOPF[1], VOLKER KÖRSTGENS[4], DANIEL SÖDERBERG[3], ANTON PLECH[5], PENG ZHANG[6], PETER MÜLLER-BUSCHBAUM[4], and STEPHAN ROTH[1,3] — [1]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [2]University of Science and Technology of China, 230026 Hefei, China — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [4]Technische Universität München, 85748 Garching, Germany — [5]Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [6]Sun Yat-sen University, 510275 Guangzhou, China

Silver nanoparticles (AgNPs) and AgNP-based composite materials have attracted growing interest due to their structure-dependent optical, electrical, catalytic and stimuli-responsive properties. In this work, the fabrication of AgNP/cellulose nanofibril (CNF) thin-films via layer-by-layer (LBL) spray-coating is reported. The CNF substrate contributes to a more uniform distribution of AgNPs by its network structure, and by absorbing the partially dissolved AgNP agglomerates. Our approach provides a platform for a scalable production of AgNP/CNF films with low agglomeration rate by two different methods: (1) multi-step layer-by-layer (LBL) spray coating; and (2) direct spray coating of the AgNP/ CNF mixture. We also obtained a uniform AgNP layer with tailorable wettability and plasmonic properties, suggesting their potential applications in anti-fouling coatings and label-free biosensors.

CPP 22.8 Wed 16:30 CPPp
Charge-Dependent Microphase Separation in Thin Films from a Multiresponsive Pentablock Quaterpolymer — •FLORIAN A. JUNG[1], DORTHE POSSELT[2], DETLEF-M. SMILGIES[3], PANAYIOTA A. PANTELI[4], CONSTANTINOS TSITSILIANIS[5], COSTAS S. PATRICKIOS[4], and CHRISTINE M. PAPADAKIS[1] — [1]Physics Department, Soft Matter Group, Technical University of Munich, Garching, Germany — [2]Department of Science and Environment, Roskilde University, Roskilde, Denmark — [3]Wilson Laboratory, Cornell University, Ithaca, USA — [4]Department of Chemistry, University of Cyprus, Nicosia, Cyprus — [5]Department of Chemical Engineering, University of Patras, Greece

Multiblock copolymers and block copolymers with charged segments are attractive candidates for tunable self-assembly of complex morphologies, but their understanding is still at an early stage. In this contribution, we present an investigation of the self-assembly behavior of a pentablock quaterpolymer with (C- *co*-D)-A-B-A-(C- *co*-D) architecture containing ionizable A blocks in thin films using grazing-incidence small-angle X-ray scattering (GISAXS). The two-dimensional scattering patterns were analyzed using simulations combined with a multistep fitting procedure. Furthermore, we performed in-situ swelling experiments to explore the impact of solvents with different selectivities and polarities on the morphology. We find that varying the degree of ionization of the ionizable blocks allows altering of the segregation strength between the blocks. The nature of the solvent used for swelling gives the opportunity to tune the structures in a wide range.

CPP 22.9 Wed 16:30 CPPp
Hybrid Energy Harvester based on Triboelectric Nanogenerator and Solar Cell — •TIANXIAO XIAO[1], WEI CHEN[1], WEI CAO[1], STEPHAN V. ROTH[2,3], and PETER MÜLLER-BUSCHBAUM[1,4] — [1]TUM, Garching, Germany — [2]DESY, Hamburg, Germany — [3]KTH, Stockholm, Sweden — [4]MLZ, Garching, Germany

Developing clean energy lies the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easily fabricated, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in

the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dots (QDs) based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 22.10 Wed 16:30 CPPp
Dynamics in polymer-fullerene blends for photovoltaic applications — •DOMINIK SCHWAIGER[1], WIEBKE LOHSTROH[2], and PETER MÜLLER-BUSCHBAUM[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien James-Franck-Straße 1, 85748 Garching — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed and excitons are created. After diffusion to a donor-acceptor interface, the excitons are dissipated and charge carriers can be extracted from the electrodes. A promising low-bandgap electron donor material is the conjugated polymer PTB7. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited. We investigated films of PTB7, the fullerene derivate PCBM and different blends of these two, prepared out of chlorobenzene solutions. Quasielastic neutron scattering experiments were done at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching). Hydrogen dynamics of pure compounds as well as the blend films are investigated on a pico- to nanosecond timescale in a temperature range from 150 K to 400 K. Results are set into context of photovoltaic performance studies and increase the knowledge base, which is needed for the design of new materials to push the field of organic photovoltaics.

CPP 22.11 Wed 16:30 CPPp
CNF thin films as sustainable carrier material and their functionalization for energy applications — •MARIE BETKER[1,2], CONSTANTIN HARDER[1,3], MARC GENSCH[1,3], CALVIN BRETT[1,2], MATTHIAS SCHWARTZKOPF[1], ANDREI CHUMAKOV[1], QING CHEN[1], DANIEL SÖDERBERG[2], and STEPHAN ROTH[1,2] — [1]Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, Teknikringen 8, 10044 Stockholm, Sweden — [3]Physik-Department E13, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Sustainable carrier materials will play an important role in the design of future functional items. One matching candidate for that purpose are cellulose nanofibrils (CNF) with their many beneficial properties: It is lightweight, transparent, flexible and recyclable, and can therefore be used as template for thin-film applications. Spray deposition is a suitable technique to fabricated thin, homogeneous films of large scale and with a ultra-low roughness, which make it fitting for industrial applications. It can also be used to functionalize and thus to implement functional, nanostructured films and multi-component systems. The deposition of conductive silver nanowires as flexible electrodes, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate as blocking layer and of the photoactive layer poly(3-hexylthiophene) and [6,6]-phenyl C61-butyric acid methylester on nanostructured CNF thin films was studied in situ using GISAXS. Important insights into possible templating effects of CNF and into the interactions between the CNF-layers and the functional materials could be gained.

CPP 22.12 Wed 16:30 CPPp
Oxygen plasma effects on the nanoscale morphology of polyzwitterion-gold interfaces during gold sputtering — •APOSTOLOS VAGIAS[1,2], SIMON J. SCHAPER[1], JULIAN E. HEGER[1], YUQIN ZOU[1], SHANSHAN YIN[1], CHRISTINA GEIGER[1], MATTHIAS SCHWARTZKOPF[3], MARC GENSCH[1,3], ANDRÉ LASCHEWSKY[4,5], STEPHAN V. ROTH[3,6], and PETER MÜLLER-BUSCHBAUM[1,2] — [1]Fachgebiet Physik weicher Materie/Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), D-22607 Hamburg, Germany — [4]Institut für Chemie, Universität Potsdam,14476 Potsdam-Golm, Germany — [5]Fraunhofer Institut für Angewandte Polymerforschung IAP,

14476 Potsdam-Golm, Germany — [6]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Sulfobetaine-based polyzwitterions are efficient interlayers for organic photovoltaics, but their polymer-metal interfacial morphology remains elusive. Moreover, plasma pretreatment of organic solar cells can bypass operational degradation from prolonged light exposure. By in-situ grazing incidence small angle X-ray scattering, we probe the evolution of gold cluster growth on thin polysulfobetaine films during metal sputtering, the latter being an industrially-relevant metal deposition technique. We present differences on the sputtered gold nanostructural morphology with and without oxygen plasma pretreatment.

CPP 22.13 Wed 16:30 CPPp
Morphology investigation of the active layer of hybrid solar cells with TOF-GISANS — •Volker Körstgens[1], Lautaro Diaz Piola[1], Christina Geiger[1], Julian Heger[1], Lucas Kreuzer[1], Anna-Lena Oechsle[1], Tobias Widmann[1], Matthias Nuber[2], Klara Stallhofer[2], Gaetano Mangiapia[3], Hristo Iglev[2], Reinhard Kienberger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Physik Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching — [3]Helmholtz-Zentrum Geesthacht am Heinz Maier- Leibnitz Zentrum, Lichtenbergstr. 1, 85747 Garching

One aspect for the development of non-conventional solar cells should be the sustainability of the production process of devices. Following this idea, we developed hybrid solar cells which can be processed out of aqueous solution. The active layer of these devices is based on laser-processed titania nanoparticles dispersed in a water-soluble thiophene-based polyelectrolyte. The active layers were produced with two of the most common deposition techniques: spray deposition and slot die coating. With these techniques the thickness of layers can be easily controlled and the scale-up toward the coating of large areas is done with low effort. We investigated the morphology of the deposited active layers with time of flight - grazing incidence small angle neutron scattering (TOF-GISANS). The difference of the morphology of these layers is presented and its impact on the performance of devices is discussed.

CPP 22.14 Wed 16:30 CPPp
In-situ GISAXS Investigation of Sprayed Drugs on a Cellulose Based Matrix — •Elisabeth Erbes[1,2], Naireeta Biswas[1,2], Stephan V. Roth[1,3], Simone Techert[1,2], Matthias Schwartzkopf[1], Calvin Brett[1,6], Jose Velazquez Garcia[1], Sreevidya Thekku Veedu[1], Korneliya Goordeyeva[3], Andrei Chumakov[1], and Peter Müller-Buschbaum[4,5] — [1]DESY, 22607 Hamburg, Germany — [2]Institute for X-ray Physics, Goettingen University, 37077 Goettingen, Germany — [3]Department of Fibre and Polymer Technology, KTH, 100 44 Stockholm, Sweden — [4]Department of Physics, Technical University Munich, 85748 Garching, Germany — [5]MLZ, Technical University Munich, 85748 Garching, Germany — [6]Department of Mechanics, KTH, 100 44 Stockholm, Sweden

These experiments show the first steps to a novel drug carrier strategy for a controlled dosage of anti-COVID-19 drugs. The drugs were embedded into a matrix made of a mixture of hydrophilic carboxymethylated nanocellulose (CMC) hydrogel and disordered hydrophobic peptide hydrogel (P). This gives the opportunity to vary the local uptake in hydrophobic or hydrophilic compartments in the matrix. The structural intercalation and the time-resolved process were investigated with in-situ grazing incidence small angle X-ray scattering (GISAXS) experiments. By using the spraying technique the drug concentration can be tuned for a personalized treatment of the patients. This poster focuses only on the structural change analysis of the CMC fibers. For the analysis of the peptide part please see the poster of Naireeta Biswas.

CPP 22.15 Wed 16:30 CPPp
Wrinkled Functional Hybrid Multilayers Between Order and Disorder — •Lukas Wolfram[1], Regine Frank[1,2], and Thomas Fuhrmann-Lieker[1] — [1]Institute of Chemistry, University of Kassel, Germany — [2]Department of Physics and Astronomy, Rutgers, the State University of New Jersey, USA

Multilayer systems of thin films give the opportunity to produce self-structured surfaces via thermal annealing. The corrugations build, so-called wrinkles, are directional isotropic. Wrinkles can be compared to the surface structure of raisins, compressed tissues, or mountain

ranges. A possible application for these structures in thin film technology is the use as a periodic random resonator [1] or previously shown by N.M. Hoinka with spiro compounds.

This Poster will present the first results in testing for a proper material system. So far, experiments with spiro bilayers showed wrinkling over a wide range of surface area. The use of a metallic layer sputtered in a magnetic field can be used to align wrinkles parallel in sucha system.My work concentrates on the conditions causing random lasing in these systems and whether there is any systematic correlation existing between the sample morphology and the spectrum observed. For this purpose, python scripts were written to analyse the shape of the corrugation and their directionality to correlate them with imaged spectra in the future.

[1] Shen, Z. *et al.*, Appl. Phys. Lett. 105, 021106, **(2014)**.
[2] N. M. Hoinka, Doctoral Thesis, **2020**.

CPP 22.16 Wed 16:30 CPPp
Co-nonsolvency-type behavior of a poly(sulfobetaine) and a poly(N-isopropylmethacrylamide) thin film in water / methanol vapor — •Lucas P. Kreuzer[1], Christoph Lindenmeier[1], Christina Geiger[1], Tobias Widmann[1], Viet Hildebrand[2], André Laschewsky[2], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik- Department, LS Funktionelle Materialien, 85748 Garching — [2]Universität Potsdam, Institut für Chemie, 14476 Potsdam Golm

The behavior of a poly(sulfobetaine) (PSPE) and a poly(Nisopropylmethacrylamide)(PNIPMAM) thin film in pure water and in mixed water/methanol vapor is studied in-situ with spectral reflectance and Fourier-transform infrared spectroscopy. While PSPE is insoluble in methanol, PNIPMAM is soluble but exhibits a co-nonsolvency behavior in water/methanol mixtures. In thin film geometry, both the PSPE and PNIPMAM swell in pure water vapor, while upon methanol addition, they contract. Their behavior differs significantly regarding the amount of absorbed water in pure water vapor, and the contraction mechanism in mixed water/methanol vapor. The PSPE thin film shows an abrupt one-step contraction, while the PNIPMAM contraction occurs in two steps. When changing to a pure methanol vapor, both, the PSPE and PNIPMAM thin film, show a higher swelling degree than in mixed water/methanol vapor, which indicates a co-nonsolvency-type behavior in polymer thin films.

CPP 22.17 Wed 16:30 CPPp
Pore-network model for polymer electrolyte membranes — •Peter Berg and Philippe Nadon — Department of Science, University of Alberta

A random pore-network model for polymer electrolyte membranes (PEM) is presented that couples the flow of protons and water through cylindrical channels (bonds) to the swelling of the membrane. While the flows are determined by closed-form solutions of the Poisson-Nernst-Planck-Stokes equations, the fluid-structure interaction is described by a pressure balance at the channel walls. Macroscopic membrane properties, such as the conductivity, permeability and electro-osmotic coefficient, are computed and compared to experimental data in the literature. In light of the model simplifications, the results compare favourably to data but they also point to the importance of describing proton diffusion in PEM nanopores accurately

CPP 22.18 Wed 16:30 CPPp
Coarse-grained MD simulations of nanoplastic particles interacting with a non-polar environment in aqueous solution — •Lorenz Dettmann, Ashour Ahmed, and Oliver Kühn — University of Rostock, Albert-Einstein-Str. 23-24, 18059 Rostock

Plastic waste in form of small particles is an emerging threat for marine and terrestrial ecosystems. Little is known about the fate and potential impacts of plastic nanoparticles in the environment. In this work, an attempt for understanding the molecular level interaction behavior between nanoplastics (NPs) and non-polar environments in aqueous solution is introduced. Here, NPs are simulated with different polymers, namely polyethylene oxide (PEO), polyethylene (PE), polypropylene (PP) and polystyrene (PS). On the other hand, carbon nanotubes (CNTs) are used to mimic non-polar environmental molecular systems. Moreover, hydrophobicity of CNTs is modified by introducing different hydrophobic and hydrophilic functional groups into the inner surface of CNTs. The interaction of the modeled NPs with bare and modified CNTs in the presence of water is investigated via MARTINI force field based coarse-grained molecular dynamics simulations. The results show that hydrophobic polymers have a relatively

strong affinity to CNTs, especially PE. The hydrophobic functional groups introduced into CNTs increased the interaction between hydrophobic polymers and CNTs. In contrast, PEO showed the lowest affinity towards CNTs. Therefore, one can expect that hydrophobic polymers have a higher tendency to accumulate at non-polar environmental molecular systems.

CPP 22.19   Wed 16:30   CPPp

A mesoscopic approach to magnetostriction of magnetic gels and elastomers — •Lukas Fischer and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Our focus is on magnetic gels and elastomers, consisting of rigid magnetizable particles embedded in an elastic polymeric environment. While the particles are discrete objects on the mesoscopic scale, the polymeric body represents an elastic continuum. When magnetized, the particles are subject to magnetic forces and push against the polymeric environment, inducing macroscopic magnetostrictive distortions.

Using analytical theory and numerical evaluations, we determine the overall distortion resulting for different discrete particle arrangements enclosed by a finite-sized, linearly elastic sphere [1–3]. Overall changes in volume and shape are evaluated. In contrast to many other approaches, our formalism includes the basically infinite number of internal degrees of freedom of deformation of the elastic environment.

We assume well-separated particles, all identically magnetized from outside. Depending on the particle arrangement and the compressibility of the elastic material, overall contraction or elongation along the magnetization axis results [1]. Twisted particle structures can lead to overall twist deformations [2], while targeted positioning of particles of different size can tune the overall response [3]. We presume that our approach can support the design of magnetostrictive actuation devices.
[1] L. Fischer and A. M. Menzel, *J. Chem. Phys.* **151**, 114906 (2019).
[2] L. Fischer and A. M. Menzel, *Phys. Rev. Research* **2**, 023383 (2021).
[3] L. Fischer and A. M. Menzel, *Smart Mat. Struct.* **30**, 014003 (2021).

CPP 22.20   Wed 16:30   CPPp

In situ GISAXS Observation of Sputter-Deposited Gold Nanostructure on Mesoporous Titanium Dioxide Template — •Suzhe Liang[1], Wei Chen[1], Shanshan Yin[1], Simon J. Schaper[1], Thomas Strunskus[2], Matthias Schwartzkopf[3], Stenphan V. Roth[3,4], and Peter Müller-Buschbaum[1,5] — [1]TU München, Garching, Germany — [2]CAU,Kiel, Germany — [3]DESY, Hamburg, Germany — [4]KTH, Stockholm, Sweden — [5]Heinz Maier-Leibniz Zentrum (MLZ), TU München, Garching, Germany

Gold/titanium dioxide (Au/TiO_2) nanohybrid materials have attracted significant attention due to the outstanding optical, photocatalytic and photovoltaic performance. Compared to chemical synthesis and lithography, sputter deposition is a facile and scalable method to produce metallic thin films and nanoparticles on substrates in precise controllability. Using nanostructured templates, ordered metal nanostructures were achieved through the sputter deposition approach. Herein, we propose a strategy to fabricate nanostructured Au/TiO_2 hybrid thin films by sputter-depositing Au on mesoporous TiO_2 template. The mesoporous TiO_2 template is prepared by a typical sol-gel synthesis approach with the assistance of diblock copolymer (PS-b-PEO). In order to investigate the kinetics of the sputter-deposited Au growth on the TiO_2 template, in situ grazing-incidence small-angle X-ray scattering (GISAXS) during sputter deposition is measured.

CPP 22.21   Wed 16:30   CPPp

Modeling and molecular dynamics studies on induced helical polymers — •Montserrat Penaloza-Amion and Wolfgang Wenzel — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Helical conformation plays an important role in biological functions, such as recognition, catalysis and structural support of superstructures. Synthetic helical polymers depend on their inversion barrier and obtaining structural information of dynamic helical polymers requires advanced experimental techniques. Yashima et.al. showed that chiral amines can induce one-handed helical structure in stereoregular cis-transoid poly((4-carboxyphenyl)acetylene) (poly-1), showing intense bands of circular dichroism (CD). Helical models were created based on poly-1. Scan calculations over the dihedral backbone using density functional theory (DFT) on dimers and tetramers of poly-1 backbone were performed to understand the helicity. From these results, Counterclockwise twist with values of -41 and 130 degrees (CCW), and Clockwise twist with values of 42 and -134 degrees (CW) for backbone dihedral were obtained. Molecular Dynamics simulations were per-

formed for 20 ns for both helical models of 20mer with chiral amines and DMSO. Our results show lowest values for RMSD for complexes polymer-R2(CCW) with 0.942 Å, and polymer-S3(CW) with 1.654 Å corresponding to the systems with higher CD intensity in the work of Yashima et.al and indicating that R2 chiral amines could induce a CCW conformation and S3 chiral amines a CW conformation on poly-1.

CPP 22.22   Wed 16:30   CPPp

Co-nonsolvency effect on phase segregation of polymer solution — •Zahra Mohammadyarloo and Jens-uwe Sommer — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

Phase segregation of polymer solution in the presence of cosolvent (CNS) is studied by molecular dynamics simulations, where CNS particles are preferential solvent for the polymers. Simulation results for different attraction strengths are compared with the prediction of the adsorption-attraction mean-field theory under constant osmotic pressure. The osmotic pressure has been simulated by a semi-permeable wall in the simulation box. The polymer solution without cosolvent was prepared in the semi-dilute state. Polymer concentration increases until reach a peak by adding more CNS particles, then decreases in higher concentrations of CNS. The radius of gyration of individual chains also display as non-monotonic behavior which in part be explained by the scaling law in semi-dilute solutions, and with the increasing effective excluded due to adsorption of cosolvent. At higher attraction strengths a jump-like collapse of the polymer volume can be observed which corresponds to a type-II phase transition of the polymer solution. For interaction strengths greater than critical, two states of polymer solution coexists. Furthermore we have calculated the single-chain and collective structure factors. The dynamics was studied and the monomer diffusion coefficient was presented as a function of attraction strength.

CPP 22.23   Wed 16:30   CPPp

Challenges and limits of Mechanical Stability in 3D Direct Laser Writing — •Elaheh Sedghamiz, Modan Liu, and Wolfgang Wenzel — Karlsruhe Institute of Technology, Karlsruhe, Germany

Direct laser writing is an effective technique for the fabrication of complex polymeric 3D polymer networks using ultrashort laser pulses. Practically, it remains a challenge to design and fabricate high-performance materials with different functions that possess a combination of high strength, substantial ductility, and tailored functionality, in particular for small feature sizes. To date, it is difficult to obtain a time-resolved microscopic picture of the printing process in operando. To close this gap, we have developed a molecular dynamics simulation approach to model direct laser writing and investigate the effect of writing condition and aspect ratio on the mechanical properties of the printed polymer network. We show that writing condition provides a possibility to tune the mechanical properties and an optimum writing condition can be applied to fabricate structures with improved mechanical properties. We reveal that beyond the writing parameters, aspect ratio plays an important role to tune the stiffness of the printed structures.

CPP 22.24   Wed 16:30   CPPp

Periodic Boundary Calculations of photosensitive $Ru(bpy)_3$ complexes attached to polymer chains — •Miftahussurur Hamidi Putra and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Polymers are considered as potential candidate materials for the photocathodes of p-type dye sensitized solar cells (p-DSSCs), as they can be easily synthesized and are robust under operation conditions [1]. To optimize the performance of such solar cells, a better understanding of the structural and electronic coupling between the dyes and the polymer matrix is necessary which can be obtained through first-principles total energy calculations. However, dyes attached to polymer chains represent a challenge for quantum chemistry calculations because of their large system size. Here we present a first-principles computational study based on density functional theory of a $Ru(bpy)_3$ dye, one of the common dyes in p-DSSCs, attached to a polymer chain using a periodic boundary approach [2].

We will particularly address the geometrical and electronic coupling between the dye and the polymer chain and elucidate the changes in the optical properties of the dye upon the attachment to the polymer chain.
[1] Y. Pellegrin, L. Le Pleux, E. Blart, A. Renaud, B. Chavillon, N.

Szuwarski, M. Boujtita, L. Cario, S. Jobic, D. Jacquemin, and F. Odobel, J. Photochem. PhotobiolA: Chem. **219**, 235 (2011).
[2] A. Sen and A. Groß, Int J Quantum Chem. **119**, e25963 (2019).

CPP 22.25   Wed 16:30   CPPp
Machine learning approach to long time step molecular dynamics for hard sphere systems — ● KA CHUN CHAN and WOLFGANG WENZEL — Institute of Nanotechnology Technology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

Atomistic simulation techniques such as molecular dynamics (MD) provide an accurate and precise description of atomic motion, molecular structure and permit the prediction of the physical and chemical properties of molecular system. However, MD requires expensive computation of energy and force which leads to significant computational effort. This severely limits MD applications to biological system and soft matter physics on long time scales.

The usual MD time step is approximately 1/10 of the fastest frequency of the molecular system. In order to accelerate the MD computation, we propose a machine learning approach to propagate the molecular system instead of the usual MD time step. As a first step we developed a machine learning (ML) propagator for hard-sphere systems that propagates the molecular system with each atomic collision as a new time step. The proposed algorithm learns the time evolution of the atomic motion and the collision between atoms, such that the neural network are able to predict the system trajectory, identify the collided atomic pairs and correct the trajectory of the collided pairs for each collision time step. We will discuss the perspective of this newly ML propagator for the acceleration of MD simulations and further application to the molecular system with long time scales.

CPP 22.26   Wed 16:30   CPPp
Kinetic Monte Carlo modeling of graphene growth on chemical vapor deposition. — ●MEYSAM ESMAEILPOUR, MARIANA KOZLOWSKA, and WOLFGANG WENZEL — Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany

Chemical vapor deposition (CVD) is the most promising method for high quality, large area graphene synthesis. Optimization of this chemical process will enable control over crucial properties, such as graphene quality and domain size. This requires the development of a detailed atomistic understanding of the underlying processes guiding the growth mechanism. In particular there is a need to understand the mechanism behind graphene nucleation and growth during CVD and its dependence on the synthetic parameters: temperature, CVD pressure, catalyst type, facet etc.

The complexity of CVD prohibits a complete description of all reaction mechanisms at the DFT level. Using the library of surface reaction rates, we have developed a Kinetic Monte Carlo (KMC) method to study the process of CVD of graphene from methane on Cu(111) under different synthesis conditions. It explains how synthesis parameters *affect the quality and domains size of graphene. The results are compared with experimental measurements, enabling better understanding of the CVD mechanism.

CPP 22.27   Wed 16:30   CPPp
A theoretical and computational study of ionic liquid mixtures in front of charged surfaces — ●TAKESHI KOBAYASHI, MARIA FYTA, and JENS SMIATEK — Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The properties of the electric double layer formed in front of charged surfaces in room temperature ionic liquids (RTILs) solutions are studied by means of atomistic Molecular Dynamics simulations and the theory of the Lattice Boltzmann Gas model. We study 1-Ethyl-3-methylimidazolium dicyanamide ([EMIm]+[DCA]-) with water or dimethyl sulfoxide (DMSO) mixtures at different concentrations in order to investigate the solvent effects on the IL structuring in front of the surfaces. Our results reveal clear differences between water and DMSO mixtures at the interfaces. By applying the Lattice Boltzmann Gas model, the entropic and enthalpic contributions to the accumulation of the solvent molecules are discussed. The differences mainly appear in front of the positively charged interface where water accumulation but DMSO depletion occurs. Such outcomes are assigned to the combination of size and polarity of water or DMSO and the corresponding interactions with the cations or the anions in the solution. Overall, our results provide a deep understanding of the ionic liquid (IL) behavior close to interfaces and links to a proper selection of IL-based mixtures in order to optimize specific technological applications.

CPP 22.28   Wed 16:30   CPPp
A computational model for the study of catalysts in the Supported Ionic Liquid Phase in mesoporous media — ●TAKESHI KOBAYASHI[1], HAMZEH KRAUS[2], NIELS HANSEN[2], and TAKESHI KOBAYASHI[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart, Germany

We set-up a model for the investigation of a linker-free immobilization of catalysts in confined media in an ionic liquid (IL)-mixture. Specifically, we study the mixture of n-heptane and 1-Butyl-3-methylimidazolium trifluoromethanesulfonate ([BMIm]+[Otf]-) in a closed pore geometry with a pore diameter of 5nm. The inner walls of the pore are functionalized in order to tune the polarity of the pore and its interaction with the solvent. The immobilization of the catalyst is expected to lead to higher turnover rates in the catalysis. Using Molecular Dynamics simulations, we model the catalyst in the IL-heptane mixture within the nanopore. Our simulations reveal that the IL accumulates within the pore, while we also follow the dynamics of all molecules involved in the system. Using quantum mechanical calculations, we parameterize a force-field for the catalyst, which is being further used for a more accurate model of the catalyst within the IL-mixture. Our results provide important information on the influence of steric and IL-specific effects, the structuring of a varying solvent environment, the pore functionality, and their interactions with the catalytic center. These aspects promote a rational design of the catalyst immobilization and point to the relevant conditions.

CPP 22.29   Wed 16:30   CPPp
Self-assembly of silica nanoparticles guided by directional crystallization of grafted polymers — ●ASWATHY MUTTATHUKATTIL[1], AFSHIN NABIYAN[2], FEDERICO TOMAZIC[1], FELIX HELMUT SCHACHER[2], and MICHAEL ENGEL[1] — [1]Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg, Cauerstrasse 3, 91058 Erlangen, Germany — [2]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich-Schiller University Jena, Lessingstraße 8, 07743 Jena, Germany

Self-assembly of nanoparticles (NP) is an efficient bottom-up approach to produce nanostructures with complex architectures. Here, we report the formation of an inorganic-organic hybrid network by self-assembly of silica NPs grafted by poly(2-iso-propyl-2-oxazoline)(PIPOX) at elevated temperatures. To resolve the underlying molecular mechanism, we utilize coarse-grained molecular dynamics simulations. Earlier reports stated that PIPOX polymers crystallize into long fibers guided by directional dipolar interactions between amide groups. Building on this information, we represent PIPOX monomers by spherical, patchy beads. Chains of patchy beads represent polymer is attached to NP sphere. Our simulations of this NP-polymer system characterize the two steps of the self-assembly process: (1) rapid formation of amorphous aggregates via gelation, mediated by interaction between NPs through grafted polymers; (2) slower formation of diverging fibers via directional crystallization of unbound polymers with the grafted polymer matrix. The understanding of the molecular mechanism is a step towards targeted self-assembly for catalysis and other applications.

CPP 22.30   Wed 16:30   CPPp
Low-symmetry phases in attraction-driven assembly of nanotriangles — ●MARCO KLEMENT and MICHAEL ENGEL — Institute for Multiscale Simulation, IZNF, FAU Erlangen, Erlangen, Germany

Hard triangles at high packing density spontaneously order into high-symmetry phases [1,2] with wallpaper groups p6 and p6mm. Recent experiments with coated nanotriangles [3] observed additional phases with wall paper groups pmg and p2. The appearance of these low-symmetry phases depends on the contour length and grafting density of surfactant polymer ligand molecules. We develop a novel simulation algorithm for anisotropic interacting nanoparticles, which attribute a majority of the observations to effective rounding of triangle vertices. The remaining observation, a p2 symmetric phase for the shortest molecules in use is a consequence of a soft attractive interaction of surfactant molecules.

[1] Gantapara, A. P., Qi, W., and Dijkstra, M. "A novel chiral phase of achiral hard triangles and an entropy-driven demixing of enantiomers". Soft Matter 11, 8684-8691 (2015).
[2] Walker, D. A., Browne, K. P., Kowalczyk, B., and Grzybowski, B. A. "Self-Assembly of Nanotriangle Superlattices Facilitated by Repulsive Electrostatic Interactions." Angewandte Chemie International

Edition 49, 6760*6763 (2010).

[3] Liu, Yang and Klement, Marco and Zhong, Yaxu and Chen, Jun and Engel, Michael and Ye, Xingchen, "Using Ligand Engineering to Control Self-Assembly of Polysterol Coated Nano Triangles", in preparation (2021)

CPP 22.31   Wed 16:30   CPPp

Pendant drop tensiometry: A machine learning approach —
•FELIX KRATZ and JAN KIERFELD — Department of Physics, TU Dortmund University, Dortmund, Germany

Modern pendant drop tensiometry relies on the numerical solution of the Young-Laplace equation and allows us to determine the surface tension from a single picture of a pendant drop with high precision. Most of these techniques solve the Young-Laplace equation many times over to find the material parameters that provide a fit to a supplied image of a real droplet. Here, we introduce a machine learning approach to solve this problem in a computationally more efficient way. We train a deep neural network to determine the surface tension of a given droplet shape using a large training set of numerically generated droplet shapes. We show that the deep learning approach is superior to the current state of the art shape fitting approach in speed and precision, in particular if shapes in the training set reflect the sensitivity of the droplet shape with respect to surface tension. In order to derive such an optimized training set, we clarify the role of the Worthington number as a quality indicator in conventional shape fitting and in the machine learning approach. Our approach demonstrates the capabilities of deep neural networks in the material parameter determination from rheological deformation experiments, in general.

CPP 22.32   Wed 16:30   CPPp

Magneto-mechanical response of nanoscale magnetic filaments —
DENIZ MOSTARAC[1], PEDRO A. SÁNCHEZ[1,2], and •SOFIA KANTOROVICH[1,2] — [1]University of Vienna, Vienna, Austria. — [2]Ural Federal University, Ekaterinburg, Russia.

Nanoscopic magnetic filaments (MFs) are magnetic, nano-sized colloids, crosslinked into polymer-like linear chains. They are a promising platform for engineering new magnetically controlled filtering and flow control elements in micro-fluidic devices. Recent advances, advocating an assembly mechanism where the structure building instructions are embedded into nanoparticles via DNA origami frames, synthesis of MFs with desirable mechanical properties.[2,3] Using MD simulations we have studied how possible crosslinking scenarios and magnetic nature of monomers (ferromagnetic or super-paramagnetic) influence equilibrium properties of MFs.[4] In this contribution, we elucidate an interesting phenomenology of MFs, by examining their behaviour in a Langevin thermostat (equilibrium properties) and explicit solvent representations using the Lattice Boltzmann method (dynamics in rotating magnetic fields). Magnetization of super-paramagnetic monomers is taken into account in an accurate manner, inclusive of non-linear contributions. [1] Sánchez, P. A., et al. Macromolecules 48.20 (2015): 7658-7669. [2] Liu, W., et al. Nature chemistry 8.9 (2016): 867. [3] Tian, Y., et al. Nature mate- rials 15.6 (2016): 654. [4] Mostarac, D., et al. Nanoscale (2020).

CPP 22.33   Wed 16:30   CPPp

Directing the Diffusion of a Nonmagnetic Nanosized Active Particle with External Magnetic Fields —
•MARTIN KAISER[1] and SOFIA KANTOROVICH[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Ural Federal University, Lenin Av. 51, Ekaterinburg 620000, Russian Federation

With the help of molecular dynamics simulations we show that an arbitrary non-magnetic active particle with a size below one micrometer, being immersed in a polydisperse system of magnetic nanoparticles, can diffuse twice faster along the direction of the applied field than perpendicular to the latter, whereas, for a monodisperse system, the ratio between diffusion coefficients parallel and perpendicular to the field approaches two orders of magnitude, even for magnetic fields of moderate strength. The ability to direct a non-magnetic active particle along the magnetic field stems from the formation of chains of magnetic nanoparticles aligned with the field direction. Such chains form effective channels through which the active particle can diffuse. We find that the ability to direct an active particle of a given size can be maximised by changing magnetic particle concentration so that the tunnels formed by the change have a mean width of approximately the active particle size.

CPP 22.34   Wed 16:30   CPPp

CPP 22.34   Wed 16:30   CPPp

Deformation of Azo-Polymer Droplets by Light: Modeling the Effects of Light on Glassy Azobenzene Materials —
•MARKUS KOCH, MARINA SAPHIANNIKOVA, and OLGA GUSKOVA — Institute Theory of Polymers, IPF Dresden, Germany

Azobenzene (azo) is the most widespread light-responsive molecule due to its well-studied trans-cis photoisomerization mechanism. This compound has gained prominence due to the possibility to create surface relief gratings in azo-polymer materials using light interference patterns. However, it remains an open question how light induces mechanical stresses in the material. To study this process we consider a model system: A droplet composed of PMMA with azobenzene side chains is exposed to linearly polarized UV-Vis light. Experiments demonstrate, that such droplets deform along the polarization direction [1]. Here, using all-atom MD simulations two different approaches are applied: In the first case, the angle-dependent photoisomerization of azobenzene is simulated explicitly. In the second case, an effective orientation potential acts on the azo groups [2]. We demonstrate that both approaches lead to the reorientation of azobenzene in the polymer matrix and discuss the induced deformation of the droplet.

[1] Loebner, S. et al., J. Phys. Chem. B, 122 (6), 2001-2009 (2018)
[2] Toshchevikov, V. et al. J. Phys. Chem. Lett., 8 (5), 1094-1098 (2017)

CPP 22.35   Wed 16:30   CPPp

End-Adsorbing Chains in Polymer Brushes: Pathway to Highly Metastable Switchable Surfaces —
•MARKUS KOCH[1], DIRK ROMEIS[1], and JENS-UWE SOMMER[1,2] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute Theory of Physics, TU Dresden, Germany

Polymer brushes are promising systems for the design of stimulus-responsive surfaces. In addition, it is often highly desirable to controllably hide or expose functional groups. To this end, we investigate monodisperse polymer brushes, which contain a small fraction of end-modified minority chains [1]. The length of these chains is variable and their end groups can adsorb to the grafting surface. We study these systems using Scheutjens-Fleer SCF calculations [2], MD simulations, and analytical theory. The conformational changes of the admixed chains are explored, which depend on their length and the attraction between their end groups and the surface. Based on the free energy profiles of the adsorption transition, free energy barriers are extracted, which are in good agreement with our theoretical predictions. The barriers are strongly reduced upon the collapse of the brush and can be tuned to attain reversible or irreversible switching behavior.

[1] Koch, M., Romeis, D., Sommer, J.-U., Macromolecules, 53 (17), 7356-7368 (2021)
[2] Fleer, G. J., et al. Polymers at Interfaces. London, Chapman and Hall, 1993

CPP 22.36   Wed 16:30   CPPp

Fast high-accuracy optimization of delocalized Gaussian sets for eigenfunctions —
MOHAMMADREZA EIDI, •BENJAMIN RABE, and JAN-MICHAEL ROST — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Gaussian basis sets are widely used to represent the wave function of atomic and molecular systems due to their great advantage that matrix elements with Gaussians at different locations can often be calculated analytically [1]. However, it is not trivial to optimize for a large set of Gaussians $\{exp(-\alpha_i(x - x_i)^2 | i = 1, ..., N\}$ the parameters $\{\alpha_i, x_i\}$. Procedures with predefined positions following a geometric series, so called even tempered basis sets (e.g. [2]), have been put forward. Here we introduce an iterative scheme which optimizes positions and widths simultaneously for a given number N of s-type Gaussians. To this end we use only during the optimization process auxiliary Gaussians which have in 3D angular momentum p and d character. This way one gets highly accurate results at low computational cost, even for small numbers of Gaussians. We will demonstrate how the method works with explicit 1D examples for various potentials representing atomic and molecular scenarios. [1] Mitroy, Jim, et al., Rev. Mod. Phys. 85.2 (2013): 693. [2] Cherkes, I., Klaiman, S., and Moiseyev, N., Int. J. Quantum Chem. 109, 2996 (2009).

CPP 22.37   Wed 16:30   CPPp

Phase behavior of polymeric microemulsion in ternary

A+B+AB blends — •RUSSELL SPENCER[1] and MARK MATSEN[2] — [1]Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — [2]Department of Chemical Engineering, Department of Physics & Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

Ternary blends of AB diblock copolymers with A and B homopolymers microphase segregate into lamellae (LAM) for copolymer-rich blends and macrophase segregate into A- and B-rich regions for homopolymer-rich blends. Mean-field theory predicts that these regions are separated by three-phase coexistence of the LAM, A-rich, and B-rich phases, which terminates at a Lifshitz critical point. Experiments, however, report that the Lifshitz point is destroyed by fluctuations and that the three-phase coexistence is replaced by a channel of bicontinuous microemulsion (BμE). Using field-theoretic simulations, we show that fluctuations do indeed destroy the Lifshitz point, but that three-phase coexistence continues to exist. However, at high temperatures, the LAM+A+B coexistence predicted by mean-field theory is replaced by BμE+A+B coexistence. We speculate that the single-phase BμE observed in experiments is a result of kinetic trapping as the blend is cooled from the mixed state.

CPP 22.38 Wed 16:30 CPPp
Understanding the static and dynamic behaviour of stars forming reversible networks — •KIRAN SURESH KUMAR[1,2], TONI MÜLLER[1,2], JENS-UWE SOMMER[1,2], and MICHAEL LANG[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Strasse 6, 01069 Dresden, Germany — [2]nstitut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

Reversible networks break and reform continously allowing the material to flow and self-heal on long time scales while being a solid on short times. Recent experiments and simulation studies find an apparent anomalous superdiffusive regime in reversible networks by analyzing Forced Rayleigh Scattering (FRS) data [1-3]. The molecular origin of this superdiffusive regime is not yet fully understood. In our contribution, we approach this problem by computer simulations of FRS experiments in reversible networks using the Bond Fluctuation Model. We analyze the static properties and the connectivity of individual stars and develop an analytic model for the statistics of connections. We analyze dynamic properties of individual stars and compute the collective relaxation as accessible in FRS. Our goal is to develop a model based upon the molecular statistics that allows to quantitatively predict the collective dynamics of the reversible network.

[1] Tang, S.; Wang, M.; Olsen , B. D. J. Am. Chem. Soc. 2015, 137, 3946-3957. [2] Tang, S.; Habicht, A.; Li, S.; Seiffert, S.; Olsen, B. D. Macromolecules 2016, 49, 5599-5608. [3] Ramirez, J.; Dursch, T. J.; Olsen , B. D. Macromolecules 2018, 51, 2517-2525.

CPP 22.39 Wed 16:30 CPPp
Self-Assembly of Copolymers in Presence of Solvent Evaporation — •GREGOR IBBEKEN and MARCUS MÜLLER — Institut für Theoretische Physik, Georg August Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Integral asymmetric block copolymer membranes constitute a fascinating new technology for ultrafiltration. Solvent evaporation aligns and facilitates the long-range order of microphase separating diblock copolymers, which is exploited to form monodisperse pores. More specifically, we are interested in the emergence of perpendicularly oriented, cylindric morphologies. We investigate a system consisting of a diblock copolymer, a solvent and air by use of a continuum model in which the concentrations act as order parameters. This allows us to explore the high-dimensional parameter space with a parameter study. Four parameters turn out to have a dominant influence on emergent morphologies, namely the polymer volume fraction, the surface preference, the incompatibility of polymer blocks and the evaporation rate. Kinetically, the orientation of cylinders is determined immediately after the onset of microphase separation. If cylinders become stable when the evolution zone is wide enough, initially developed spheres elongate vertically. Most notably, this occurs for high evaporation rates. Additionally, we are able to demonstrate that the kinetic pathways taken are describable as paths in a two-dimensional parameter space consisting of effective block ratio f^{eff} and effective segregation strength χN_{ab}^{eff}.

CPP 22.40 Wed 16:30 CPPp
Magnetic nanogels in magnetic field — •IVAN NOVIKAU[1], PEDRO SANCHEZ[1], and SOFIA KANTOROVICH[1,2] — [1]University of Vienna — [2]Ural Federal University

Nanogels (NGs) with multifunctionalized magnetic nanoparticles (MNPs) have demonstrated the ability to effectively destroy cancer cells in vivo, without causing visible damage to healthy organs [1]. The presence of MNPs inside the NGs also offers an additional mechanism to control their properties by means of applied magnetic fields.

Our study of a suspension of NGs loaded with MNPs in zero-field case showed that the structural properties of a single gel, and the self-assembly in the given system, strongly depend on the strength of the dipole-dipole interaction (dipolar coupling parameter) between the MNPs [2].

Here, we investigate a suspension of magnetic NGs in a constant external magnetic field by means of molecular dynamics computer simulations [3]. Each NG is initially modeled as a system of bead-spring polymer chains randomly cross-linked into a polymer network. MNPs are arbitrary incorporated into this network.

We find that even weak fields lead to drastic changes in the structure factors of both, the embedded MNPs and of whole NGs. But what is even more curious, is that the polymer matrix of nanogels enhances the magnetization of free MNPs.
[1] Qing Wu et al., Nat. Commun., 10 (240), 2019.
[2] Novikau et al., JMMM, 498, 2020.
[3] Novikau et al., J. Mol. Liq., 307, 2020.

CPP 22.41 Wed 16:30 CPPp
Water purification with pvdf membrane — •RENÉ HAFNER[1,2] and PETER KLEIN[1] — [1]Fraunhofer ITWM, Kaiserslautern, Deutschland — [2]TUK, Kaiserslautern, Deutschland

We investigate the interaction of crystal and amorphous Polyvinylidenfluorid (PVDF) membranes with the pharmaceutical diclofenac, i.e. an inflammatory pain killer, as a surrogate of a wider class of charged drug molecules via the potential of mean force (PMF) method. While the crystal membrane is in polar beta zigzag form of PVDF, both are created by a structure generator of our own. We further highlight the features of our structure generator. For both membrane and diclofenac the Charmm force field is used. Simulations were conducted using the simulation software NAMD. The PMFs between drug and membrane are obtained via the adaptive biasing force method ABF and its extended version. Comparism is drawn between amorphous and crystal PVDF membranes and their adsorption capabilities are discussed.

CPP 22.42 Wed 16:30 CPPp
Separable intermolecular force fields from first principles — •MANUEL KONRAD and WOLFGANG WENZEL — Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

The decomposition of intermolecular interactions into physically meaningful components can be a useful tool to gain a deeper understanding about non-covalently bonded complexes. However, separable ab initio methods, such as symmetry adapted perturbation theory (SAPT), are limited to small systems. Here we present a systematic approach to derive an analytical force field from a finite number of SAPT calculations while preserving the energy decomposition of the reference method. For several small organic molecules, we apply this model in molecular dynamics simulations to compute thermodynamic properties. The comparison against experimental values shows promising prediction capabilities. Together with the additional insight from the energy decomposition, this makes our method a potentially versatile tool for the in silico discovery of new molecular materials, where force field parametrizations can't rely on experimental target data.

CPP 22.43 Wed 16:30 CPPp
Structure formation in 2D-Copolymer Networks — •GAOYUAN WANG and MARCUS MÜLLER — Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

Two-dimensional polymer networks, characterized by a planar geometry, open new possibilities for the design of polymer molecules with novel properties. Using large-scale simulations, we study microphase separation in two-dimensional, defect-free, interpenetrating phantom networks, obtained by crosslinking symmetric diblock copolymers. The system exhibits a complex interplay between the network structure, characterized by the length (geometry) of a unit cell, and the lamellar microphase with its periodicity that depends on the incompatibility between the blocks. We investigate the incompatibility at which system microphase separates as a function of the size of the (unper-

turbed) unit cell of the network and quantify the network structure in the microphase-separated state. Our findings are compared to the microphase separation linear diblock, triblock and multiblock copolymers as well as to the mechanical properties of networks.