Computational statistical physics in the 21st century: The legacy of Kurt Binder

September 11, 2023 - September 13, 2023
Mainz, Germany (MPI for Polymer Research, Hermann-Staudinger lecture hall)

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1. Conference Venue

Hermann-Staudinger-Hörsaal at Max Planck Institute for Polymer Research
Ackermannweg 10, 55128 Mainz

How to reach the MPI-P by public transport
Mainz main station (Mainz Hauptbahnhof) is serviced daily by several Intercity (IC), Eurocity (EC) and Intercity Express (ICE) trains.
From the main station take the tram lines number 51 or 53 to reach the Max Planck Institute for Polymer Research. The journey will take about 10 minutes.

Fares: Single fare tickets can be bought at a vending machine or from the driver. A one-way ticket costs 2.80 Euros. You can find more information about the fares at Mainzer Verkehrsgesellschaft.

If you arrive at Mainz central station with a RMV or RNN ticket, no extra ticket is needed to reach the institute. The same applies, if you have a long-distance train ticket with the addition "Mainz+City".

Tram lines number 51 and 53 (direction Lerchenberg/Hindemithstraße)
Tram number 51 departs from platform A, number 53 from platform L. Get off at the stop "Hochschule Mainz". The institute can be reached after a two-minute walk across Koblenzer Strasse into Ackermannweg.

Conference Dinner Venue:
Restaurant “Goldisch”, Fischtorstr. 1, 55116 Mainz
Tuesday, 12 September, 7 pm
Bus stop: “Fischtor” or “Höfchen”

2. Program

Day 1 - Monday September 11th 2023

Registration & Reception 09:00 to 10:30

Opening remarks 10:30 to 11:00

Presentations (Phase Transitions) 11:00 to 12:30

- 11:00 to 11:30 - **David P. Landau**

  A half century journey with Kurt Binder: from bicritical points to 1st order universality

- 11:30 to 12:00 - **Robert Evans**

  Understanding the physics of hydrophobic solvation

- 12:00 to 12:30 - **Christoph Dellago**

  Non-equilibrium pattern formation in nanocrystal cation exchange: insights from an elastic lattice model

Lunch break 12:30 to 14:00

Presentations (Nucleation & Crystallization I) 14:00 to 15:30

- 14:00 to 14:30 - **Antonia Statt**

  Influence of particle shape on heteroaggregation of colloids

- 14:30 to 15:00 - **Martin Oettel**

  Droplet condensation in the lattice gas with classical density functional theory

- 15:00 to 15:30 - **Yafang Cheng**

  Convergence of dissolving and melting at the nanoscale

Coffee break 15:30 to 16:00

Presentations (Polymers I) 16:00 to 17:30

- 16:00 to 16:30 - **Wolfgang Paul**

  Crystallization in melts of semi-flexible hard polymer chains: an interplay of entropies and dimensions

- 16:30 to 17:00 - **Zhen-Gang Wang**

  Origin of the entropic driving force in polyelectrolyte complex coacervation

- 17:00 to 17:30 - **Jens-Uwe Sommer**

  Polymer assisted condensation: from polymer physics to epigenetics

Day 2 - Tuesday September 12th 2023

Presentations (Colloids & Active Matter) 09:00 to 10:30

- 09:00 to 09:30 - **Nigel Wilding**

  Active wetting

- 09:30 to 10:00 - **Subir Das**

  Mpemba effect in a few magnetic and active matter systems

- 10:00 to 10:30 - **Annette Zippelius**

  Active droplets

Coffee break 10:30 to 11:00

Presentations (Confinement & Surfaces and Interfaces) 11:00 to 12:30

- 11:00 to 11:30 - **Sauro Succi**

  Computer simulations of soft flowing matter under strong confinement

- 11:30 to 12:00 - **Rolf Schilling**

  Strongly confined fluids in a slit pore

- 12:00 to 12:30 - **Andreas Troester**

  New insights into hard antiphase domain boundaries in strontium titanate

Lunch break 12:30 to 14:00

Presentations (Surfaces and Interfaces & Friction) 14:00 to 15:30

- 14:00 to 14:30 - **Andrey Milchev**

  Unidirectional droplet propulsion onto gradient brush-coated substrates without external energy supply

- 14:30 to 15:00 - **Florian Müller-Plathe**

  Polymer interfaces and interphases - the priority programme Kurt Binder helped create

- 15:00 to 15:30 - **Martin Muser**

  Using computer simulations to unravel the origins of friction between solids

Coffee break 15:30 to 16:00

Presentations (Friction) 16:00 to 17:30

- 16:00 to 16:30 - **Hans Herrmann**

  Frustrated bearings

- 16:30 to 17:00 - **Luis MacDowell**

  On slippery ice

- 17:00 to 17:30 - **Jacob Klein**

  Multi-lipid synergy in cartilage boundary lubrication: insights from nanotribology and molecular dynamics

Dinner 19:00 to 22:00

Day 3 - Wednesday September 13th 2023

Presentations (Nucleation & Crystallization II) 09:00 to 10:30

- 09:00 to 09:30 - **Tanja Schilling**

  How to make noise

- 09:30 to 10:00 - **Juergen Horbach**

  Yielding in crystals towards the quasistatic limit: a slip-plane condensation transition

- 10:00 to 10:30 - **Christos Likos**

  Cluster crystals: from a theorist’s toy model to experimental realization

Coffee break 10:30 to 11:00

Presentations (Ising Model & Magnetic Systems) 11:00 to 12:30

- 11:00 to 11:30 - **Wolfhard Janke**

  Coarsening and aging in the long-range ising model with power-law interactions

- 11:30 to 12:00 - **Martin Weigel**

  Magnetic systems with quenched disorder: results from (quasi) exact ground states

- 12:00 to 12:30 - **Andres De Virgiliis**

  Phase behavior and structure of a lattice model for microemulsions

Lunch break 12:30 to 14:00

Presentations (Polymers II) 14:00 to 16:00

- 14:00 to 14:30 - **Fathollah Varnik**

  Shape memory polymers, experiments and modelling

- 14:30 to 15:00 - **Claudio Pastorino**

  Liquid and droplet flow on nanochannels coated by polymer brushes

- 15:00 to 15:30 - **Alexander Grosberg**

  TBA

- 15:30 to 16:00 - **Marcus Mueller**

  Simulation of block copolymer membrane fabrication

Closing remarks 16:00 to 16:15

Coffee 16:15 to 17:00

3. Abstracts

A half century journey with Kurt Binder: from bicritical points to 1st order universality

David P. Landau
Center for Simulational Physics, The University of Georgia, Athens, United States

Active droplets

Annette Zippelius
Institute for Theoretical Physics, University of Goettingen, Germany

Controlled locomotion on micro- or nanometer scales is of great interest for both cell biology and microrobotics. In the former case, one aims to understand the swimming motion of microorganisms and cell motility. In the latter case, the goals are control and design of microrobots optimized for a variety of biomedical applications. We focus here on the propulsion of a liquid droplet which is driven by an active slip or active tractions. We show that the dynamics in the interior of the flow is in general chaotic in contrast to regular motion of the droplet as a whole. We also discuss compound droplets driven by an encapsulated swimmer, and show that active droplets in general deform – even in the limit of a strong surface tension.

Active wetting

Nigel Wilding
University of Bristol, United Kingdom

We study non-equilibrium analogues of surface phase transitions in a minimal model of active particles in contact with a purely repulsive potential barrier that mimics a thin, porous membrane. Under conditions of bulk motility-induced phase separation, the interaction strength ε_w of the barrier controls the affinity of the dense phase for the barrier region. We uncover clear signatures of a wetting phase transition as ε_w is varied. In common with its equilibrium counterpart, the character of this transition depends on the system dimensionality: a continuous transition with large density fluctuations and gas bubbles is uncovered in 2d while 3d systems exhibit a sharp transition absent of large correlations.

[1] F. Turci, N. Wilding, Phys. Rev. Lett., ***127****, 238002 (2021)*
[2] F. Turci, N. Wilding, Phys. Rev. Lett., ***126****, 038002 (2021)*

Cluster crystals: from a theorist's toy model to experimental realization

Christos Likos[1], Emmanuel Stiakakis(2)[2]
[1]University of Vienna, Austria
[2]Forschungszentrum Jülich, Germany

Crystals are orderly states of matter in which particles with sizes ranging from sub-nanometer to micron are arranged in a periodic lattice. Crystalline solids epitomize the notion of rigidity, lying at the antipode of fluidity that is embodied by liquids. Accordingly, hybrid, exotic phases that combine crystallinity with (super-)fluidity have fascinated researchers both in the classical realm of soft matter physics and in the quantum domain. In usual crystals, the lattice constant a and the particle concentration c obey the proportionality $a \propto c^{-1/3}$, dictated by the condition that the (conventional) unit cell be populated by a fixed number of particles determined by the lattice geometry. Cluster crystals, a newer concept, are unconventional states of matter whose lattice sites are occupied by clusters of fully or partially overlapping particles rather than single ones. In these states, the number of overlapping particles within a cluster, the lattice-site occupancy N_{occ}, is a fluctuating quantity, with its expectation value scaling with concentration as $N_{\mathrm{occ}} \propto c$ and thus resulting in a concentration-

independent lattice constant, the latter being the salient structural characteristic of both cluster crystals and cluster quasicrystals. In this talk, I will briefly review 20 years of theoretical work that led to a recent, theory-informed, experimental discovery [1] of this new state of matter.

*[1] E. Stiakakis, N. Jung, N. Adžić, T. Balandin, E. Kentzinger, U. Rücker, R. Biehl, J. Dhont, U. Jonas, C. Likos, Nat. Commun., **12**, 7167 (2021)*

Coarsening and aging in the long-range ising model with power-law interactions

Wolfhard Janke[1], Henrik Christiansen[2], Fabio Müller[1], Suman Majumdar[3], Malte Henkel[4]
[1]Institut für Theoretische Physik, Universität Leipzig, Germany
[2]NEC Laboratories Europe GmbH, Germany
[3]Amity Institute of Applied Sciences, Amity University, India
[4]Laboratoire de Physique et Chimie Théoriques (CNRS UMR 7019), Université de Lorraine Nancy, France

Our current understanding of coarsening and aging phenomena is mainly confined to systems with short-ranged interactions. Particularly little is known about aging of long-ranged systems. Thanks to recent algorithmic improvements [1,2] we were able to perform extensive Monte Carlo simulations of phase-ordering (nonconserved) [1,3] and phase-separating (conserved) [4] kinetics of the two-dimensional Ising model with long-range power-law interactions on large lattices up to sufficiently long time scales. We observe dynamical scaling, confirm theoretical predictions for the asymptotic scaling of the characteristic coarsening length scale, and obtain in the nonconserved case from analyses of the two-time spin-spin autocorrelator estimates for the autocorrelation exponents depending on the decay strength of the power-law interactions.

*[1] H. Christiansen, S. Majumder, W. Janke, Phys. Rev. E, **99**, 011301 (2019)*
[2] F. Müller, H. Christiansen, S. Schnabel, and W. Janke, Phys. Rev. X (2023, in print)
*[3] H. Christiansen, S. Majumder, M. Henkel, W. Janke, Phys. Rev. Lett., **125**, 180601 (2020)*
*[4] F. Müller, H. Christiansen, W. Janke, Phys. Rev. Lett., **129**, 240601 (2022)*

Computer simulations of soft flowing matter under strong confinement

Sauro Succi
Istituto per le Applicazioni del Calcolo (IAC), CNR, Rome, Italy

We present recent computational studies of soft mesoscale flowing systems, such as dense emulsions and soft granular materials under strong micro-geometrical confinement. The prospects of tuning the rheological properties of the flowing system, as well as their dynamic morphology, by suitable geometrical changes of the experimental apparatus, is explored via systematic Lattice Boltzmann simulations. We also comment on the use of machine-learning algorithms for the automatic identification of droplet within the microflow and tracking of their trajectories within the microflows. Besides automatizing the task of droplet tracking, this may also help the formulation of reduced models of droplet dynamics under complex microflow conditions.

Convergence of dissolving and melting at the nanoscale

Yafang Cheng, Chuchu Chen, Xiaoxiang Wang, Hang Su, Ulrich Pöschl
Max Planck Institute for Chemistry, Germany

Phase transition of water and its mixtures are of fundamental importance in physical chemistry, pharmaceutical industry, materials sciences, and atmospheric sciences. However, current understanding remains elusive to explain relevant observations especially at the nanoscale. Here, by using molecular dynamics simulations, we investigate the dissolution of sodium chloride (NaCl) nanocrystals with volume equivalent diameters from 0.51 to 1.75 nm. Our results show that the dissolution of NaCl in aqueous nanodroplets show a strong size dependence, and its solubility can be predicted by the Ostwald-Freundlich equation and Gibbs-Duhem equation after considering a size-dependent solid-liquid surface tension. We find that the structure of dissolved ions in the aqueous nanodroplet resembles the structure of molten NaCl nanoparticle. With decreasing nanodroplet size, this similarity grows and the average potential energy of NaCl in solution, molten phase and crystal phase converges.

*[1] X. Wang, C. Chen, K. Binder, U. Kuhn, U. Pöschl, H. Su, Y. Cheng, Atmos. Chem. Phys., **18**, 17077-17086 (2018)*
*[2] X. Wang, K. Binder, C. Chen, T. Koop, U. Pöschl, H. Su, Y. Cheng, Phys. Chem. Chem. Phys., **21**, 3360-3369 (2019)*
*[3] Y. Cheng, H. Su, T. Koop, E. Mikhailov, U. Pöschl, Nat. Commun., **6**, 5923 (2015)*

Crystallization in melts of semi-flexible hard polymer chains: an interplay of entropies and dimensions

Wolfgang Paul, Timur Shakirov
Martin Luther University, Halle-Wittenberg, Germany

Morphology selection upon crystallization of long-chain polymers is governed by an intricate and so far unresolved interplay between thermodynamic and kinetic effects. We argue, that the thermodynamic driving forces for this phase transition can be studied looking at short enough chains as well. For a melt of short, semi-flexible polymer chains with purely repulsive intermolecular interactions, Stochastic Approximation Monte Carlo (SAMC) simulations [1] (a variant of flat-histogram Monte Carlo simulations [2]) can be employed to obtain the complete thermodynamic equilibrium information. Thermodynamics is obtained based on the density of states of a simple coarse-grained model. We show that our polymer melt undergoes a first-order crystallization transition upon increasing the chain stiffness at fixed density [3].
The lyotropic three-dimensional orientational ordering transition drives the crystallization and is accompanied by a two-dimensional hexagonal ordering transition in the plane perpendicular to the chains. While the three-dimensional ordering can be understood in terms of Onsager theory, the two-dimensional transition is similar to the liquid-hexatic transition of hard disks. Due to the domination of lateral two-dimensional translational entropy over the one-dimensional translational entropy connected with columnar displacements, the chains form a lamellar phase.

*[1] B. Werlich, T. Shakirov, M. Taylor, W. Paul, Computer Physics Communications, **186**, 65-70 (2015)*
*[2] W. Janke, W. Paul, Soft Matter, **12**, 642-657 (2016)*
*[3] T. Shakirov, W. Paul, Phys. Rev. E, **97**, 042501 (2018)*

Droplet condensation in the lattice gas with classical density functional theory

Martin Oettel
University of Tübingen, Germany

A density functional for the lattice gas with next-neighbor attractions (Ising model) from fundamental measure theory is applied to the problem of droplet states in three-dimensional, finite systems. The density functional is constructed via an auxiliary model with hard lattice gas particles and lattice polymers to incorporate the attractions. Similar to previous simulation studies, the sequence of droplets changing to cylinders and to planar slabs is found upon increasing the average density in the system. Owing to the discreteness of the lattice, additional effects in the state curve for the chemical potential are seen upon lowering the temperature away from the critical temperature [oscillations in the slab portion and spiky undulations in the cylinder portion as well as an undulatory behavior of the radius of the surface of tension in the droplet region]. This behavior in the cylinder and droplet region is related to washed-out layering transitions at the surface of liquid cylinders and droplets. The analysis of the large-radius behavior of the surface tension shows a dominant term proportional to the inverse square of the radius and a logarithmic term which is smaller than a universal value derived with field-theoretic methods.

Frustrated bearings

Hans Herrmann
ESPCI Paris, France

A bearing is a system of spheres (or disks) in contact. If in a bearing every loop must be even, one can obtain “bearing states”, in which touching spheres roll on each other without slip. We frustrate a system of touching spheres by imposing two different bearing states on opposite sides and search for the configurations of lowest energy dissipation. For Coulomb friction (with random friction coefficients) in two dimensions, a sharp line separates the two bearing states and we prove that this line corresponds to the minimum cut. Astonishingly however, in three dimensions, intermediate bearing domains, that are not synchronized with either side, are energetically more favourable than the minimum-cut surface. This novel state of minimum dissipation is characterized by a spanning network of slip-less contacts that reaches every sphere. Such a situation becomes possible because in three dimensions bearings of loops of size four have four degrees of freedom. By considering spheres of different size, packings with bearing states can even be made space-filling. The construction and mechanical properties of such space-filling bearings will be discussed. Space-filling bearing states can be viewed as a realization of solid turbulence exhibiting Kolmogorov scaling and anomalous heat conduction. Bearings states can be perceived as physical realizations of networks of oscillators with asymmetrically weighted couplings. These networks can exhibit optimal synchronization properties through tuning of the local interaction strength as a function of node degree or the inertia of their constituting rotor disks through a power-law mass-radius relation. As a consequence, one finds that space filling bearings synchronize fastest, when they are hollow.

How to make noise

Tanja Schilling
University of Freiburg, Germany

In physics, we hardly ever describe a system in terms of all of its microscopic degrees of freedom. We usually resort to effective coarse-grained models, which predict the behaviour of "relevant" system properties. One widely used effective equation of motion for coarse-grained variables is the Langevin equation, a stochastic differential equation, in which the effect of the neglected degrees of freedom is encoded in friction terms and stochastic noise.
I will review the steps of derivation and approximation that are required to obtain the Langevin equation from a system's microscopic description. I will discuss the interplay between the potential of mean force and the memory kernel, the range of validity of the second fluctuation dissipation theorem, and the stochastic interpretation of the fluctuating force, i.e. the noise.

Influence of particle shape on heteroaggregation of colloids

Antonia Statt
University of Illinois Urbana-Champaign, United States

Nano and microplastics, i.e., non-spherical colloids, are a growing threat to the environment, particularly in aqueous habitats. However, the impact of the shape and flow conditions of microplastics on their aggregation with other organic matter is not well understood. In this talk, we present molecular dynamics simulations of heteroaggregation of various shapes of microplastic particles with smaller spherical organic matter using molecular dynamics simulations. We show that the shape has a strong influence on the aggregate structure. Microplastics with mostly smooth surfaces (e.g., spheres, round cubes) form compact structures with many neighbors with weak connections and a high fractal dimension with many neighbors and high fractal dimension. Microplastics with edges and corners (e.g., cubes, plates) aggregate into more fractal structures with fewer neighbors but stronger connections. Using multi-particle collision dynamics, we also investigate aggregate behavior under shear flow. To accelerate our simulations, we use a fully connected neural net to learn the interaction of pairs between particles of different shapes to replace the need to calculate many distances and forces between shapes made of smaller composite beads. Use a feedforward neural network. We will discuss the resulting pair-correlation functions and the overall performance of this approach.

Liquid and droplet flow on nanochannels coated by polymer brushes

Claudio Pastorino[1], Kevin Speyer[2], Marcus Müller[2]
[1]National Scientific and Technical Research Council, Argentina
[2]Georg-August University Göttingen, Germany

We study the liquid flow through nanochannels coated by polymer brushes of varying stiffness. We use molecular-dynamics simulations of the Kremer-Grest coarse-grained model for polymers, and the dissipative particle dynamics thermostat, to keep constant temperature under the action of external forces on the system. We focus on the flow properties and the liquid structure produced by the polymers grafted to the confining walls in conditions of poor liquid-polymer chemical affinity and narrow channels. We characterize the flow of droplets or continuous threads as a function of grafting density and flow intensity. We find that when the polymer chains can interact from opposing channel walls, a very interesting gating effect takes place, with a significant change in flow rate, from a threshold of liquid intensity. It is also observed, a dynamic transition from a flow of droplets to a continuous liquid thread, as a function of force intensity, for nanochannels of cylindrical geometry.

Magnetic systems with quenched disorder: results from (quasi) exact ground states

Martin Weigel
TU Chemnitz, Germany

Quenched impurities are ubiquitous in laboratory samples of magnetic systems. Depending on the type and strength of disorder, the effects on the type of ordering as well as the persistence and order of the accompanying phase transitions can be dramatic, ranging from shifts in transition temperature in disordered ferromagnets to the replacement of conventional long-range order by a locally frozen state in spin glasses. Due to the presence of excessively large relaxation times and the need to perform an average over disorder (sometimes complicated by a lack of self-averaging), numerical studies of such systems are exceedingly difficult. With the help of mappings of the ground-state problems to well known combinatorial optimization problems as well as, where needed, generalized-ensemble Monte Carlo methods meaningful studies of such systems become feasible.
In this lecture I will illustrate how such problems can be tackled with the help of a combination of Monte Carlo methods as well as exact and heuristic optimization methods, and I will illustrate this approach with a range of results for spin glasses and random-field systems in two and three dimensions.

[1] L. Münster, M. Weigel, Phys. Rev. E, ***107****, 054103 (2023)*
[2] M. Kumar, V. Banerjee, S. Puri, M. Weigel, Phys. Rev. Research, ***4****, L042041 (2022)*
[3] A. Vasilopoulos, N. Fytas, E. Vatansever, A. Malakis, M. Weigel, Phys. Rev. E, ***105****, 054143 (2022)*
[4] D. Perera, F. Hamze, J. Raymond, M. Weigel, H. Katzgraber, Phys. Rev. E, ***101****, 023316 (2020)*
[5] M. Vaezi, G. Ortiz, M. Weigel, Z. Nussinov, Phys. Rev. Lett., ***121****, 080601 (2018)*
[6] H. Khoshbakht, M. Weigel, Phys. Rev. B, ***97****, 064410 (2018)*

Mpemba effect in a few magnetic and active matter systems

Subir Das
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, India

"The fact that the water has previously been warmed contributes to its freezing quickly ...", said Aristotle. This forgotten fact was rediscovered by Erasto Mpemba, about 60 years ago, in the context of milk, while preparing ice-cream as a part of an assignment in his school in Tanzania. Later, Mpemba and Osborne published results from controlled experiments supporting the existence of it in water. Nevertheless, the observation, now referred to as the Mpemba effect (ME), remains a puzzle. In fact, the scientific literature is somewhat divided on the issue of the very existence of ME. Despite this there are efforts to identify it in other systems and positive observations are being reported. I will present results on ME from the investigations of far-from-steady-state dynamics in a few (*favorite*) magnetic and active matter systems (*of Kurt Binder*). It will be argued that for a class of systems the differences in spatial correlations at the starting state points can lead to ME.

Multi-lipid synergy in cartilage boundary lubrication: insights from nanotribology and molecular dynamics

Jacob Klein, Yifeng Cao, Di Jin, Nir Kampf

Weizmann Institute of Science, Israel

Uniquely efficient lubrication of cartilage in the major human joints is essential for its well being and its breakdown is associated with osteoarthritis, a debilitating disease affecting millions. it is believed to be mediated by lipid layers at the cartilage surface acting through the hydration lubrication mechanism. In natural joints however there are over a 100 different lipids and the question is: is this natural redundancy or natural evolution. Here we present surface force balance studies showing a marked synergy when certain lipid mixtures are used. Moreover, using molecular dynamics simulations we are able to account for this synergy via consideration of the factors promoting hemifusion, the main cause of lubrication breakdown in our experiments.

New insights into hard antiphase domain boundaries in strontium titanate

Andreas Troester
University of Vienna, Austria

Recently [1] the emergence of polarity of so-called hard antiphase boundaries in strontium titanate was investigated using atomistic simulations based on machine-learned force fields. Comparing order parameter (OP) and polarization profiles to those numerically obtained from a standard Landau-Ginzburg-Devonshire (LGD) parametrization produces good agreement of the structural order parameter amplitudes, but fails dramatically in reproducing the domain wall polarization properties. While the atomistic simulations yield a non-zero domain wall polarization up to at least 120 kbar, LGD theory would predict a sharp transition to zero at a pressure as low as 4.6 kbar. A semi-quantitative agreement can be restored by adding so-called rotopolar couplings [2, 3] to the LGD potential and by considering the effects of nuclear quantum fluctuations. Additional evidence for the correctness of this approach is provided by comparing the temperature dependence of the domain wall polarization to recent experimental depolarization pyrocurrent measurements [4]. New results [5] illustrate the importance of ac counting for nuclear quantum effects beyond standard atomistic approaches in the investigation of domain wall properties.

*[1] A. Tröster, C. Verdi, C. Dellago, I. Rychetsky, G. Kresse, W. Schranz, Phys. Rev. Materials, **6**, 094408 (2022)*
*[2] W. Schranz, C. Schuster, A. Tröster, I. Rychetsky, Phys. Rev. B, **102**, 184101 (2020)*
*[3] A. Schiaffino, M. Stengel, Phys. Rev. Lett., **119**, 137601 (2017)*
*[4] R. Cabassi, S. Checchia, G. Trevisi, M. Scavini, Materials Today Communications, **28**, 102742 (2021)*

Non-equilibrium pattern formation in nanocrystal cation exchange: insights from an elastic lattice model

Christoph Dellago[1], Layne Frechette[2], Phillip Geissler †[3]
[1]University of Vienna, Austria
[2]Brandeis University, United States
[3]University of California Berkeley, United States

Cation exchange - the replacement of one species of ions with another - is an efficient method to modify the composition of nanocrystals post-synthesis. This process can lead to a variety of patterned heterostructures with core/shell, segmented and striped morphologies. Here, I will discuss the microscopic mechanism governing cation exchange using an elastic lattice model that captures the key ingredients of pattern formation: the lattice mismatch caused by the different sizes of the exchanging ions and the differing time scales of surface exchange and internal diffusion. The long-ranged interactions arising upon integrating out mechanical fluctuations lead to an equilibrium phase diagram with both uniform and spatially modulated phases, whose coexistence is determined by the extensive mechanical cost of segregation. The key features of the model can be understood in terms of a mean field theory applied to the resulting effective Hamiltonian. Kinetic Monte Carlo simulations of the non-equilibrium exchange process further reveal that the rapid exchange of cations on the nanocrystal surface generates effective boundary conditions that transiently stabilize spatially modulated structures akin to those observed in experiments. Our results help explain the varied patterns observed in heterostructured nanocrystals produced by cation exchange and suggest strategies for leveraging elasticity to design patterned nanoscale materials.

On slippery ice

Luis MacDowell[1], Lukasz Baran[2], Pablo Llombar[3], Wojciech Rzysko[2]
[1]Universidad Complutense de Madrid, Spain
[2]Maria-Curie-Sklodowska University, Poland
[3]Universidad Autónoma de Madrid, Spain

Sliding on ice is a familiar experience, but the reason why ice has such a low friction has a long and controversial history. For many years, it has been assumed that the main reason for the low friction of ice is due to the formation of a thick lubrication layer of melt water. However, there is no consensus on the origin of the melt water film. Among the different hypothesis enumerated are pressure melting, ice premelting and frictional heating of the surface [1]. Very recently, however, it has been suggested that lubrication plays no role whatsoever, and that ice friction is mainly given by adhesive and mechanical properties of ice [2].
Unfortunately, these hypothesis cannot be easily confirmed by macroscopic experiments. What is the actual thickness of the watery lubrication film under static conditions? Does it change significantly with the nature of the substrate? Does it become thicker upon increasing the pressure or shearing? Is the resulting thickness sufficient for the establishment of a lubricating Couette flow?
In our work we borrowed tools from our recent investigations on the structure of ice premelting in order to understand better the microscopic origin of the low friction coefficient of ice [3-4]. We found that ice friction is the result of spontaneous surface premelting, pressure melting and frictional heating operating simultaneously during sliding [5].

*[1] R. Rosenberg, Physics Today, **58**, 50-54 (2005)*
*[2] R. Liefferink, F. Hsia, B. Weber, D. Bonn, Phys. Rev. X, **11**, 011025 (2021)*
*[3] P. Llombart, E. Noya, L. MacDowell, Sci. Adv., **6**, (2020)*
*[4] D. Sibley, P. Llombart, E. Noya, A. Archer, L. MacDowell, Nat. Commun., **12**, 239 (2021)*
*[5] Ł. Baran, P. Llombart, W. Rżysko, L. MacDowell, Proc. Natl. Acad. Sci. U.S.A., **119**, (2022)*

Origin of the entropic driving force in polyelectrolyte complex coacervation

Zhen-Gang Wang
California Institute of Technology, United States

Mixing two solutions of oppositely charged polyelectrolytes under appropriate conditions results in a liquid–liquid phase separation into a polymer-rich coacervate phase and a coexisting polymer-poor supernatant phase. This polyelectrolyte complex coacervation (PCC) has received considerable attention in recent years due to its relevance to membraneless organelles in biology, and applications in biomedical and biomimetic systems. The complexation of oppositely charged polymers has been widely believe to be driven by the entropy gain due to counterion release. In this talk, we show that a large portion of the entropy change is due to solvent (water) reorganization, which we can extract by exploiting the temperature dependence of the dielectric constant. For weakly-to-moderately charged systems under common conditions (monovalent ions, room temperature in aqueous solvent), the solvent reorganization entropy, rather than the counterion release entropy, is the primary entropy contribution. We use this framework to examine the two elementary stages in the symmetric PCC—the complexation between a polycation and polyanion, and the subsequent condensation of the polycation–polyanion pairs by computing the potential of mean-force (PMF) using molecular dynamics simulation. From the calculated PMF, we find that the supernatant phase consists predominantly of polyion pairs with vanishingly small concentration of bare polyelectrolytes, and we provide an estimate of the spinodal of the supernatant phase. Finally, we show that prior to contact, two neutral polyion pairs weakly attract each other by mutually induced polarization, providing the initial driving force for the fusion of the pairs.

Phase behavior and structure of a lattice model for microemulsions

Andres De Virgiliis
CONICET, Argentina

We performed extensive Monte Carlo simulations of the three dimensional Widom model, one of the simplest lattice models for ternary microemulsions, i.e. solutions made of water, oil and surfactant. It is, effectively, a isotropic spin-1/2 Ising model, with nearest neighbor ferromagnetic interactions, and next-nearest neighbor antiferromagnetic interactions, linear and diagonal.

Our aim is to obtain the phase equilibria for a wide range of temperatures and surfactant concentrations, and to examine the different spatially structured phases. It is found that a continuous phase transition separates the disordered phase from the oil-water coexistence, while a first-order transition separates the structured disordered phase from the modulated, lamellar phase. Also a first-order boundary exists between the lamellar and the oil-rich (or water-rich) phases.

The disordered (but structured) microemulsion phase is studied further by the calculation of the isotropically averaged structure factor $S(q)$. We are able to locate both the Lifshitz line, where the peak position of $S(q)$ goes to zero, and the disorder line at which the correlation length of the typical domain size diverges. The disorder line extends beside the order-disorder boundary right up to the critical end point.

Polymer assisted condensation: from polymer physics to epigenetics

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Liquid-liquid phase separation of proteins is increasingly recognized as a fundamental concept to understand biological functions. We introduce polymer-assisted condensation (PAC) of proteins which can explain the formation of heterochromatin using concepts from polymer physics and phase separation theory [1]. Our work, consisting of mean-field theory and simulations, displays the role of meta-stable states of protein solutions which can be switched into a stable condensed state triggered by a weak attractive interaction with a polymer such as chromatin. A significant increase/decrease in interaction strength between proteins and polymer leaves the properties of the polymer-assisted condensate nearly invariant, and fluctuations in the concentration of the protein outside the droplet are buffered. Both features are essential for the preservation of epigenetic information during the cell cycle. On the other hand, our polymer-physics model is generic and can be extended to other multi-component solutions in the presence of polymers such PNiPAAm in mixtures of water and alcohols [2].

*[1] J. Sommer, H. Merlitz, H. Schiessel, Macromolecules, **55**, 4841-4851 (2022)*
*[2] H. Yong, E. Bittrich, P. Uhlmann, A. Fery, J. Sommer, Macromolecules, **52**, 6285-6293 (2019)*

Polymer interfaces and interphases - the priority programme Kurt Binder helped create

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From 2008 to 2014, the Deutsche Forschungsgemeinschaft funded the Priority Prpogramme 1369 "Polymer-Solid Contacts: Interfaces and Interphases". What is maybe less known that Kurt Binder was among the very first activists to conspire for its creation. In addition to the history leading of it coming into existence, I will review some of the scientific findings that came out.

Shape memory polymers, experiments and modelling

Fathollah Varnik
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Shape memory polymers (SMPs) are a class of smart materials with a large variety of applications ranging from solar panels and wind foils to stents in sclerotic coronary arteries. Common to all shape memory materials is their ability to recover a programmed shape via activation of a switching mechanism, e.g., heating above a certain threshold temperature. In contrast to metallic shape memory alloys, where recovery is triggered via a diffusionless martensitic phase transformation, the shape memory effect in polymers has its origin in entropy: Above the glass transition temperature, stretched polymers, which had been immobilized via cooling, become mobile again and can explore more isotropic conformations which are available in a larger number than the stretched ones. As a result, the sample shrinks back towards its original shape. It follows from this picture that any parameter, which influences the mobility of polymers, can, at least in principle, have an effect on shape recovery process. This presentation addresses this issue - using the example of the effect of small solvent molecules - both from the experimental side and via molecular dynamics computer simulations of simple model systems.

Simulation of block copolymer membrane fabrication

Marcus Mueller
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SNIPS refers to the combination of evaporation-induced self-assembly (EISA) and subsequent, nonsolvent-induced phase separation (NIPS) of block copolymer-solvent systems and provides a bottom-up approach to fabricate integral-asymmetric, isoporous block copolymer membranes. Initially, EISA creates a self-assembled, well-ordered, functional top layer of perpendicular cylindrical domains. Subsequently, as the film contacts the nonsolvent (coagulation bath), NIPS fabricates a macroporous mechanical support. To optimize permeability, selectivity, longevity, and cost, and to rationally design fabrication processes, direct insights into the spatiotemporal structure evolution are necessary.
Using a single, coarse-grained, particle-based model in conjunction with an efficient, multi-GPU-implementation of the SCMF algorithm, we study both processes, EISA and NIPS, focusing on the complex interplay between evaporation and solvent-nonsolvent exchange, micro- and macrophase separation, and kinetic arrest as the plasticizing solvent leaves the dense, polymer-rich domains. The simulations identify a process window that allows for the successful fabrication of integral-asymmetric, isoporous diblock copolymer membranes, and contribute to understanding the role of the different structural and thermodynamic (e.g., solvent selectivity for the block copolymer components) as well as kinetic (e.g., plasticizing effect of the solvent) characteristics.

Strongly confined fluids in a slit pore

Rolf Schilling[1], Wei Dong[2], Thomas Franosch[3], Simon Lang[3]
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In the first part, earlier work will be reviewed in which we showed that the thermodynamic properties of a fluid in a very narrow slit pore with width, L, can be obtained from a $2D$ fluid with effective interparticle interactions. This allows one to expand the free energy into a power series with nL^2 (n= $2D$ number density) as smallness parameter. Analytical results for the normal pressure, the "surface tension" and the density profile of a hard-sphere fluid will be presented. The latter will be compared with recent MC results.
Motivated by the first part, the second one discusses two possible measures of a surface tension, γ and ($-\Sigma$), defined by the change of the free energy with the surface area at constant volume and constant pore width, respectively. As expected, only γ is a surface tension in case of large pore widths.
Decreasing the width more and more, both quantitites become a L-dependent measure of the tension of a quasi-two-dimensional liquid. Finally, it is shown how the divergencies for $L \to 0$ can be treated properly in order that the thermodynamic quantities of a confined fluid converge to those of a corresponding $2D$ fluid.

Tba

Alexander Grosberg
New York University, United States

Understanding the physics of hydrophobic solvation

Robert Evans

University of Bristol, United Kingdom

The origins of the density depletion and accompanying enhanced density fluctuations that arise in water in the vicinity of an extended hydrophobic solute are investigated. We argue that both phenomena are remnants of the critical drying surface phase transition that occurs at liquid-vapour coexistence in the macroscopic planar limit, i.e., as the solute radius $R_s \rightarrow \infty$. Focusing on the density profile and a sensitive spatial measure of fluctuations, the local compressibility profile (the analogue of the layer magnetic susceptibility χ_n studied by Binder) we develop a scaling theory which expresses the extent of the density depletion and enhancement in compressibility in terms of R_s, the strength of solute-water attraction, and the deviation from liquid-vapor coexistence $\delta\mu$.

Testing the predictions against results of i) classical density functional theory for a simple (LJ) solvent and ii) grand canonical Monte Carlo simulations of a popular water model (mw), we find that the theory provides a firm physical basis for understanding how water behaves at a hydrophobe.

*[1] M. Coe, R. Evans, N. Wilding, Phys. Rev. Lett., **128**, 045501 (2022)*
*[2] M. Coe, R. Evans, N. Wilding, J. Chem. Phys., **158**, 034508 (2023)*

Unidirectional droplet propulsion onto gradient brush-coated substrates without external energy supply

Andrey Milchev

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Using extensive molecular dynamics simulation of a coarse-grained model, we demonstrate the possibility of sustained unidirectional motion of droplets without external energy supply when placed on a polymer brush substrate with a characteristic gradient in a certain direction. For brushes with *stiffness* gradient the droplets move to the stiffer parts of the brush (durotaxis) whereas for coatings with *grafting density* gradient all droplets move towards the more sparsely coated end of the substrate (anti-durotaxis). The governing key parameters for each specific substrate gradient, which determine the propulsion efficiency, are found to be the grafting density of the brush and the droplet adhesion to the brush surface whereas the strength of the gradient, viscosity of the droplet, or the length of the polymer chains in the brush have only minor effect on the process. It is shown that this durotaxial motion is driven by the steady increase in the interfacial energy between droplet and brush as the droplet moves along the gradient direction.

Using computer simulations to unravel the origins of friction between solids

Martin Muser

Saarland University, Germany

When two solids slide against each other, friction occurs. While the laws describing friction are quite simple and have been known for a long time, there can be many different reasons leading to solid friction at the small scale. Computer simulations have helped quite a bit to elucidate them. Some highlights will be presented in my talk. For example, I will address the origin of interfacial water in sliding ice interfaces but also the reasons for why bulk metallic glasses dissipate very little energy when used as great golf rackets but have yet unusually large friction coefficients compared to poly-crystalline metals.

Yielding in crystals towards the quasistatic limit: a slip-plane condensation transition

Juergen Horbach

Heinrich Heine University Duesseldorf, Germany

When a crystalline solid is slowly deformed with a constant deformation rate, plastic flow initiates only at a limiting deformation called the yield point. In this talk, the yielding of a Lennard-Jones fcc crystal with periodic boundary conditions is studied using particle-based simulation techniques. We show that in the quasi-static limit the yielding can be described as a slip-plane condensation transition, a novel type of first-order phase transition that occurs in the limit of very large but finite linear dimension of the system. This transition shares similarities with the droplet condensation transition [1, 2] that is observed in the context of first-order phase transitions. It is associated with a jump of an intensive thermodynamic variable and strongly depends on the boundary conditions and the deformation protocol. For finite deformation rates, we present a theory for the deformation rate dependence of the yield strain which is in excellent agreement with the simulation data.

[1] K. Binder, M. Kalos, J. Stat. Phys., ***22****, 363-396 (1980)*
[2] K. Binder, Physica A: Statistical Mechanics and its Applications, ***319****, 99-114 (2003)*

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5. Additional Information

CECAM website for this workshop:
https://www.cecam.org/workshop-details/1256