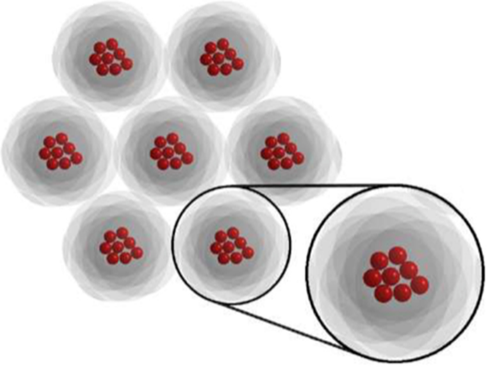

Structure formation in soft colloids

September 19 - 22, 2016
TU Wien

Gerhard Kahl, TU Wien, Austria
Primoz Ziherl, University of Ljubljana, Slovenia

Structure formation in soft colloids

September 19-22, 2016 @ TU Wien

Day 1 - September 19, 2016 (Monday)

13.30 - 14.30	Welcome Reception & Registration
14.30 - 15.00	Introduction & Motivation
15.00 - 15.30	**Hajime Tanaka**, *The University of Tokyo, Japan*
15.30 - 16.00	**Mark Miller**, *Durham University, UK*
16.00 - 16.30	Tea/Coffee Break
16.30 - 17.00	**Alan Denton**, *North Dakota State University, USA*
17.00 - 17.30	**Christos N. Likos**, *University of Vienna, Austria*
17.30 - 18.00	**Goran Ungar**, *The University of Sheffield, UK*
18.00 - 18.30	Open Discussion: Day 1

Day 2 - September 20, 2016 (Tuesday)

09.00 - 09.30	**Nigel Wilding**, *University of Bath, U.K.*
09.30 - 10.00	**Silvano Romano**, *University of Pavia, Italy*
10.00 - 10.30	Tea / Coffee Break
10.30 - 11.00	**Martial Mazars**, *University Paris Sud, University Paris Saclay, France*
11.00 - 12.00	Open Discussion: Day 2A
12.00 - 13.30	Lunch Break
13.30 - 14.00	**Michael Engel**, *Friedrich-Alexander-University Erlangen-Nürnberg, Germany*
14.00 - 14.30	**Matthew Glaser**, *University of Colorado, USA*
14.30 - 15.00	**Xiangbing Zeng**, *The University of Sheffield, UK*
15.00 - 15.30	Tea/Coffee Break
15.30 - 16.00	**Orlin D. Velev**, *North Carolina State University, USA*
16.00 - 16.30	**Albert Philipse,** *University of Utrecht, The Netherlands*
16.30 - 17.00	**Alberto Fernandez Nieves**, *Georgia Institute of Technology, USA*
17.00 - 17.30	**Davide Pini**, *University of Milan, Italy*
17.30 - 18.00	Open Discussion: Day 2B
19.00 - 21.00	Workshop Dinner

Day 3 - September 21, 2016 (Wednesday)

09.00 - 09.30	**Werner Krauth,** *École Normale Supérieure, Paris, France*
09.30 - 10.00	**Georg Maret**, *University of Konstanz, Germany*
10.00 - 10.30	Tea/Coffee Break
10.30 - 11.00	**Michael Grünwald**, *The University of Utah, USA*
11.00 - 12.00	Open Discussion: Day 3A
12.00 - 13.30	Lunch Break
13.30 - 14.00	**Primoz Ziherl**, *University of Ljubljana, Slovenia*
14.00 - 14.15	**Niels Boon**, *Lund University, Sweden*
14.15 - 14.30	**Jonas Riest**, *Forschungszentrum Jülich GmbH, Germany*
14.30 - 14.45	**Massimo Pica Ciamarra**, *Nanyang Technological University, Singapore*
14.45 - 15.00	**Takamichi Terao**, *Gifu University, Japan*
15.00 - 15.30	Tea/Coffee Break
15.30 - 15.45	**Maria Sammalkorpi**, *Aalto University, Finland*
15.45 - 16.00	**Priti Mohanty**, *Lund University, Sweden*
16.00 - 16.15	**Hayato Shiba**, *Tohoku University, Japan*
16.15 - 18.00	Posters & Open Discussion: Day 3B

Day 4 - September 22, 2016 (Thursday)

09.00 - 09.30	**Michel Cloître**, *ESPCI ParisTech, France*
09.30 - 10.00	**Jan Dhont**, *Forschungszentrum Jülich GmbH, Germany*
10.00 - 10.30	**Frederike Schmid**, *Johannes-Guttenberg University Mainz, Germany*
10.30 - 11.00	Tea/Coffee Break
11.00 - 11.20	Summary of Workshop
11.20 - 12.00	Closing Remarks & Feedback

Structure formation in soft colloids

September 19-22, 2016 @ TU Wien

Day 1 - September 19, 2016 (Monday)

13.30 - 14.30	Welcome Reception & Registration
14.30 - 15.00	Introduction & Motivation

15.00 - 15.30 Hajime Tanaka, *University of Tokyo, Japan*

Roles of Local Structural Ordering of a Supercooled Liquid in Crystal Nucleation

Coauthors: John Russo [2], Flavio Romano [3]
[2] School of Mathematics, University of Bristol, [3] Department of Molecular Sciences and Nanosystems, Ca`Foscari University of Venice

Abstract

When a liquid is cooled below the melting point, it is either crystallized or vitrified depending upon the cooling rate. However, it is not clear what physical factors control the ease of crystallization, or the glass-forming ability. For hard and soft spheres, we found that crystal-like bond orientational order grows in both size and lifetime when the degree of supercooling is increased [1]. Furthermore, we revealed that such structural order plays a crucial role in crystal nucleation and polymorph selection [2-5]: In the early stage of crystal nucleation, the ordering proceeds with the enhancement of spatial coherence of crystal-like bond orientational order and is primarily 'not' driven by translational order. Translational ordering plays a crucial role only in the late stage. This indicates the importance of pre-ordering of a supercooled liquid, which takes place before crystal nucleation is initiated. We also show [6] that the degree of local structural ordering is a major controlling factor of the ease of crystallization (or, glass-forming ability): Stronger tendency of local crystal-like structural ordering leads to the lower energy barrier for crystal nucleation. We note that this tendency of local structural ordering is weaker for a system of a softer potential.

Our study indicates that liquid-state theories at the two-body level may not be enough for the description of the phenomena taking place below the melting point and it is crucial to take into account many-body correlations [1].

References

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15.30 - 16.00 Mark Miller, *Durham University, UK*

Nucleation of Deformable Hard Spheres

Coauthors: Vera M. O. Batista[2], Laura Filion[3]
[2] University of Lisbon, Portugal, [3] Utrecht University, The Netherlands

Abstract

An important advantage of describing colloidal systems with simple archetypal models is that such models help to explain why a range of apparently disparate systems have more in common than may be obvious at first sight. For example, in the case of hard spheres, the key feature is the well-defined excluded volume of impenetrable particles, and this is a reasonable description of many different systems. When it comes to modelling soft colloidal particles, one can envisage cases where the softness arises from penetrablity of the particles, in the sense that their individual volumes can overlap and occupy some of the same space. Alternatively, softness could arise if the particles are essentially impenetrable yet deformable. An example of the latter case might be a globular protein, which is compact but not rigid.

We have introduced a simple model to begin probing the effect of softness that arises exclusively from deformability. The particles are always hard (impenetrable) and have an unchanging volume, but they may change their aspect ratio, adopting the shape of an ellipsoid of revolution that can be prolate or oblate with a restoring force of adjustable strength towards a preferred spherical shape. In my talk, I will review our work on the phase diagram of these deformable spheres, which shows that flexibility shifts crystallisation to higher packing fractions. I will then move onto unpublished and more recent work on the nucleation of the crystallisation transition. Perhaps surprisingly, for a given supersaturation, the free energy barrier for nucleation changes nonmonotonically with the flexibility of the particles, exhibiting a minimum for intermediate flexibilities. The origin of this effect lies in the surface free energy.

16.00 - 16.30 Tea/Coffee Break

16.30 - 17.00 Alan Denton, *North Dakota State University, USA*

Structure and Stability of Soft Colloids in Crowded Environments

Abstract

Soft colloidal particles have inspired much recent interest for their unusual and tunable properties, both on individual and collective levels. Interdisciplinary research is driven by applications in the chemical, biomedical, food, consumer care, petroleum, and pharmaceutical industries. The simplest example of a soft colloid is a linear polymer coil, which can be modeled as a deformable particle, whose size and shape respond to confinement. Another example, with many practical applications, is a microgel particle -- a microscopic porous network of cross-linked polymers that, when dispersed in water, swells in size and can acquire charge through dissociation of counterions. Their ability to encapsulate cargo, such as dye or drug molecules, make microgels and microcapsules especially useful as chemical sensors and vehicles for targeted drug delivery. The equilibrium size of a microgel is governed by internal osmotic pressure, which can be tuned by varying particle properties and externally controlled conditions, such as pH, ionic strength, temperature, and concentration. Combining theory and simulation, we demonstrate that (1) crowding by nanoparticles affects the sizes and shapes of polymer coils, with implications for the structure and function of biopolymers [1, 2], and (2) self-crowding of microgels induces deswelling [3, 4], affecting the structure and phase behavior of suspensions and facilitating penetration through small pores, with relevance for filtration, drug delivery, and microfluidics.

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17.00 - 17.30 Christos N. Likos, *University of Vienna, Austria*

Coarse-Graining of Flexible and Stiff Ring Polymers

Abstract

Ring polymers and the properties of both isolated molecules and concentrated solutions of the same have attracted a great deal of interest, since the interplay of polymer behavior and topological constraints gives rise to novel and intriguing structural and dynamical behavior [1- 3]. In this talk, I will be first reviewing recent results pertaining to coarse-graining approaches of isolated ring polymers, which highlight the role of topological constraints and of knotedness on the effective potential between rings [4] and bring forward the key differences they have in comparison to their linear counterparts [5]. Unlike linear chains, the effective potential picture breaks down in a dramatic, qualitative fashion at high concentrations, an effect due to ring shrinking. This property calls for a multiblob coarse-graining approach, which successfully addresses the issue and reproduces the correlations in concentrated solutions [6]. To reduce the shrinking, bending rigidity has been added to the rings [7], a property that brings forward a novel glassy state in which collective dynamics is arrested but self-dynamics is not [8]. Finally, I will be discussing findings of ongoing work on coarse-graining approaches of rigid rings modeled as "soft discs", and the associated cluster- and layer-formation in the bulk and under confinement [9].

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17.30 - 18.00 **Goran Ungar**, *The University of Sheffield, UK*

Chiral Fluids from Non-Chiral Molecules

Coauthors: X. B. Zeng[1], C. Dressel[2], W. Stevenson[1], C. Tschierske[2], C. Welch[3], G. H. Mehl[3]
[1] The University of Sheffield, [2] Martin-Luther-University Halle-Wittenberg, Germany, [3] University of Hull, United Kingdom

Abstract

Most biological molecules and medicines are chiral, lacking mirror symmetry and having handedness (“chiral centres”) built into them. E.g. all natural aminoacids are left-handed (L) and the helical segments of the proteins they build, the α-helix, is right handed. But there is a growing number of examples where mirror symmetry breaking, i.e. chirality, is induced in non-chiral compounds, such as polymers [1] and, more recently, liquid crystals [2]. The induced chirality often emerges due to cooperative synchronized selection of, usually one of two enantiomeric conformers of a bistable molecule that a separated by a sizeable but not unsurmountable energy barrier. But recent studies have revealed more complex and puzzling cases. Thus it was found that some long known cubic liquid crystal phases are always highly optically active, while other cubic phases, often appearing in the same non-chiral compound, never are [3]. Even more puzzling is the recent discovery of a liquid phase, Iso*, containing no chiral molecules and having no long range positional or orientational order whatsoever, displays strong optical activity, hence induced chirality, developed over virtually unlimited distances [4]. Furthermore, the “twist-bend” nematic LC phase in dimers [5] and polymers [6] with an awkward “zigzag” shape will be described. Current models of these intriguing phenomena will be described.

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18.00 - 18.30 Open Discussion: Day 1

Day 2 - September 20, 2016 (Tuesday)

9.00 - 9.30 **Nigel Wilding**, *University of Bath, UK*

Quantifying the Importance of Non-Pairwise Additivity of Interactions in Complex Fluids

Coauthor: Douglas Ashton

Abstract

A simulation technique is described for quantifying the contribution of three-body interactions to the thermodynamical properties of coarse-grained representations of complex fluids. The method is based on a new approach for determining virial coefficients from the measured volume-dependent asymptote of a certain structural function. By comparing the third virial coefficient B_3 for a complex fluid with that of an approximate coarse-grained model described by a pair potential, three body effects can be quantified. The strategy is applicable to both Molecular Dynamics and Monte Carlo simulation. Its utility is illustrated via measurements of three-body effects in models of star polymers and in highly size-asymmetrical colloid-polymer mixtures. The results show that three body effects are much larger for soft colloids than hard ones, a finding which we trace to the ability of soft colloids to overlap.

Reference

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9.30 - 10.00 **Silvano Romano**, *University of Pavia, Italy*

Computer Simulation Study of a Mesogenic Lattice Model Based on Long-Range Dispersion Interactions

Abstract

In contrast to thermotropic biaxial nematic phases, for which some long sought for experimental realizations have been obtained, no experimental realizations are yet known for their tetrahedratic and cubatic counterparts, involving orientational orders of ranks 3 and 4, respectively, extensively studied theoretically over the last few decades, also in their colloidal counterparts; In previous studies, cubatic order has been found for hard-core or continuous models consisiting of particles possessing cubic or nearly-cubic tetragonal or orthorhombic symmetries; in a few cases, hard-core models involving uniaxial and centrosymmetric particles have been shown to produce cubatic order as well. Here we address by Monte Carlo simulation a lattice model consisting of uniaxial particles coupled by long-range dispersion interactions of the London-De Boer-Heller type; the model was found to produce no second-rank nematic but only fourth-rank cubatic order, in contrast to the nematic behavior long known for its counterpart with interactions truncated at nearest-neighbor separation.

10.00 - 10.30 Tea / Coffee Break

10.30 - 11.00 **Martial Mazars**, *Paris Sud, University Paris Saclay, France*

The Polymorphic Behavior of Wigner Bilayers

Coauthors: M. Antlanger[1,2], G. Kahl [2], L. Samaj[3,1], E. Trizac[1]
[2] TU Wien, Austria, [3] Slovak Academy of Sciences, Slovakia

Abstract

Self-assembly into target structures is an efficient material design strategy. Combining analytical calculations and computational techniques of evolutionary and Monte Carlo types, we report about a remarkable structural variability of Wigner bilayer ground states, when charges are confined between parallel charged plates. Changing the inter-layer separation, or the plate charge asymmetry, a cascade of ordered patterns emerges. At variance with the symmetric case phenomenology, the competition between commensurability features and charge neutralization leads to long range attraction, appearance of macroscopic charges, exotic phases, and non-conventional phase transitions with distinct critical indices, offering the possibility of a subtle, but precise and convenient control over patterns.

In this contribution, we discuss the phase diagram found for asymmetric Wigner bilayer and the thermal stability of the ordered phases found with the evolutionary algorithm, analytical computations and Monte Carlo simulations.

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11.00 - 12.00 Open Discussion: Day 2A

12.00 - 13.30 Lunch Break

13.30 -14.00 **Michael Engel**, *Friedrich-Alexander-University Erlangen-Nürnberg, Germany*

New Crystals for Soft Colloids

Abstract

The appearance of crystal structures has been successfully understood for many colloidal building blocks. FCC and HCP are explained with hard sphere packing arguments. BCC and Frank-Kasper phases result from extremal principles and are often found when the interaction softness is increased. Here we demonstrate that the correspondence between models and crystal structures extends beyond previous beliefs. We report the self-assembly of many old and new crystal structures from the disordered fluid in computer simulation. Some crystal structures are highly complex and require crystallographic identification using bond-orientational order parameters and other means. The structures we observe are diverse and are of types commonly found in the elements, including covalently-bonded crystals of carbon, high-pressure alkali metals, and complex unit cell metals. Our models promise insights into the growth, defects, and phase transitions in these systems and discuss ways to reproduce the findings in soft colloid systems.

14.00 - 14.30 **Matthew Glaser**, *University of Colorado, USA*

Soft Rods Make Even More Mesophases

Abstract

Systems of spherically symmetric particles with hard core and repulsive soft shoulder interactions display extraordinarily rich phase behavior, including a wide variety of non-close-packed crystal structures, entropy-stabilized quasicrystals, and lamellar, columnar, and micellar mesophases. This rich polymorphism results from competition between excluded volume interactions and a soft shoulder clustering instability, producing a complex array of cluster phases with morphologies and internal structures that depend sensitively on pressure, temperature, and the ratio of soft shoulder and hard core diameters. The internal structure of cluster phases strongly resembles that of hard particles in confined geometries, with soft shoulder interactions giving rise to an effective mean-field confinement potential whose scale and strength are set by the soft shoulder diameter and height [1]. Anisotropic hard particles with soft shoulder interactions offer a more diverse set of orientationally ordered cluster phases, with, for example, intra-cluster nematic, smectic, or columnar order. We report preliminary NPT Monte Carlo simulations of hard spherocylinders with repulsive square step line interactions, a simple anisotropic hard core/soft shoulder model. These simulations reveal a variety of novel liquid crystalline cluster phases, including stripe and column nematics, a diverse array of modulated smectics, and cluster rotator phases.

References

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14.30 - 15.00 **Xiangbing Zeng**, *The University of Sheffield, UK*

Micellar and Columnar Liquid Quasicrystals

Coauthors: Ruibin Zhang, Feng Liu [1,2], Goran Ungar, Virgil Percec [3], Benjamin Glettner [4], Carsten Tschierske [4]
[2] Xi'an Jiaotong University, P. R. China, [3] University of Pennsylvania, USA, [4] Martin-Luther-University Halle-Wittenberg, Germany

Abstract

The first Liquid Quasicrystal (LQC) with "forbidden" dodecagonal symmetry was discovered in 2004. This thermotropic phase was formed by spherical micelles self-assembled from monodendrons [1]. This was the first example of a quasicrystal whose building block were on nanometre rather than atomic scale. Since then, a number of examples were reported of quasicrystalline structures based on building blocks much larger than atoms. These include block copolymers (BCPs) [2,3], nanoparticles [4], colloidal particles [5] and porous silica [6].

The 12-fold symmetry shown by the micellar LQC phase, like its counterpart in metal alloys, is believed to be created through a tiling of square and triangular tiles. However, many questions still remain about the structure: e.g the exact tiling rule, the "decoration" of tiles, i.e. how micelles are positioned in each tile, the existence of phonon and phason defects in the structure, and their relation to the stability of the LQC phase. We have recently carried out a high resolution AFM study of the micellar LQC, capable of resolving individual self-assembled micelles. The results confirm experimentally the square-triangle tiling model, and previously proposed decoration rules of the tiles. We are also able to examine the tiling rules and defects in the structure in detail.

While the LQCs so far found (about 20 reported examples) are all 3-dimensional structures formed from spherical objects, we present here also a new kind of liquid quasicrystals which are 2-dimensional and are formed from self-assembled columns. Previous studies on polyphilic T- and X-shaped molecules have revealed their ability to form complex two dimensional honeycomb-like structures of columns with polygonal cross-sections. The polygons found in those structures so far are triangles, squares, rhombi, pentagons, hexagons and, more recently, giant squares and octagons. The quasicrystalline symmetry of the new phase is clearly shown by the "forbidden" 12-fold symmetry of the grazing incidence small-angle X-ray scattering (GISAXS) pattern obtained from a thin film. With the help of the structure determination of an approximant, a structural model of the columnar LQC phase, consisting of square, triangular and trapezoidal shaped columns, has been proposed.

References

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15.00-15.30 Tea/Coffee Break

15.30 - 16.00 **Orlin D. Velev**, *North Carolina State University, USA*

Structure Formation and Gelation at Ultra-Low Particle Volume Fractions Induced by Reversible Nanocapillary Binding and by "Gecko Leg" Adhesion

Abstract

We will discuss two unusual gel systems formed by inducing strong and reversible physical bonds between particles in suspensions of ultra-low volume fraction. The first is a new responsive gel of ultraflexible filaments formed by field-driven directed assembly [1-5] of magnetic nanoparticles coated by condensed, surface-anchored lipid shells [6,7]. The magnetic field collects the super-paramagnetic particles into filaments by magnetophoresis [7,8], while the lipid shells form on contact nanocapillary liquid bridges between them. After switching off the field the particles retain their structural arrangement by a soft attractive potential induced by the liquid bridges. The binding was correlated to the thermodynamic phase of the lipid shells, its fluidity and nanoparticle wettability. The nanocapillary binding allows for easy particle rolling and sliding and the

resulting ultrahigh flexibility was measured to be orders of magnitude higher than other linear structures reported to date [6]. This soft, "snappable" capillary interaction enables the making of magnetically self-repairing networks and gels and directed binding and structuring of metallo-dielectric Janus and patchy microspheres.

The second principle of making highly adhesive particles that will be discussed is enabled by our scalable process for synthesis of polymer nanomaterials by biphasic precipitation under shear [9]. By controlling the shear conditions and the solvent/antisolvent composition and polymer interaction parameters, we can make polymer rods [10], nanofibers [9], nanoribbons, and nanosheets. We will first discuss the extraordinary structure building ability of the nanosheets, deriving from the propensity of the crumpled sheets to occupy large excluded volumes. The most interesting new material formed by this process, however, is nanofibrilated dendrimeric polymer particles (DPPs). These dendrimeric particles are hierarchically structured, with a big branched corona of nanofibers spreading out in all directions. The DPPs have very high excluded volume because of their hierarchical structure. The DPPs’ morphological similarity to the gecko lizards’ legs setae enables their strong adhesion to almost any surface and to each other. Due to van der Waals attraction between the nanofiber coronas, the DPPs dramatically modify the rheology of liquids and gels. These new classes of particles are expected to find a broad range of applications.

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16.00 - 16.30 **Albert Philipse**, *University of Utrecht, The Netherlands*

Shape-Sensitive Dipolar Structure Formation in Magnetic Cube Fluids

Abstract

The recently developed [1-4] monodisperse colloidal cubes with rounded corners, also known as colloidal superballs, display a rich phase behavior that critically depends on the shape details of these colloids [1,4]. Cubes containing a (micron-size) hematite core [1,2,4] have a significant permanent magnetic dipole moment that induces chain formation [1,4], with morphologies that markedly differ from the dipolar structures observed for colloidal magnetic spheres [5]. A survey will be given of preparation and properties of magnetic cube fluids, followed by a discussion of experimental cube chain formation in comparison to recent simulations [6].

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16.30 - 17.00 **Alberto Fernandez Nieves**, *Georgia Institute of Technology, USA*

Microgels at High Packing Fractions: Osmotic Pressure, Crystallization and the Role of Ions

Abstract

Microgels are an interesting class of colloidal soft particles that can deform and compress. When suspended in a solvent at large number density, they are able to crystalize, form glasses and exhibit peculiar self-healing behavior. In this talk, we will use ionic microgels with different amount of crosslinker to address the role of single-particle stiffness over the fluid-crystal phase transition. In the process, we will determine the suspension osmotic pressure and discuss the significance of ions and their possible role in determining the suspension behavior.

17.00 - 17.30 **Davide Pini**, *University of Milan, Italy*

An Unconstrained DFT Study of Self-Assembly in One- and Two-Component Fluids with Spherically Symmetric Interactions

Coauthor: Alberto Parola, *University of Insubria, Italy*

Abstract

Among several mechanisms leading to self-assembly in fluids, one which has been under the spotlight for quite some time is the formation of mesoscopic aggregates of particles interacting via potentials whose Fourier components display a negative absolute minimum at non-vanishing wave vector q [1]. While this will obviously favor modulations of the density profile with wavelength $\lambda \approx 2\pi/q$, several different scenarios may arise, depending on the additional features of the interaction.

Here we will present some results for this class of interactions obtained by a fully numerical implementation of density-functional theory tailored to periodic phases, which does not rely on any additional assumption on the functional form of the density profile [2,3]. This makes it useful in the study of mesophases, when it is difficult to have an inkling on the configurations actually chosen by the system, and the preferred structures are often non-trivial.

For one-component systems, our findings confirm the wealth of evidence which has been obtained in previous studies: on the one hand, for mutually penetrable particles such that the density can increase indefinitely with a small penalty in free energy, three-dimensional cluster crystals with multiple occupancy are always the preferred phase at suitably high density [4]. On the other hand, for hard-core particles the necessity to curb the growth of the density inside the aggregates as the overall density increases leads to the sequence clusters-bars-lamellae-inverse bars-inverse clusters [5] which has been known for quite some time in the context of block copolymers melts [6]. In the latter case, bicontinuous phases are also found in a narrow domain squeezed between the bar and lamellar regions, whereas they are altogether absent for penetrable-core particles.

A new and potentially promising scenario emerges as one turns to binary mixtures of soft particles, e.g. Gaussian particles [7], such that the tendency towards self-assembly in either species appears because of the effective interaction mediated by the other species. Compared to one-component systems, these mixtures appear to have a much greater propensity towards the formation of bicontinuous phases, such as the gyroid, the double diamond, or other more exotic structures with non-cubic primitive cells [3].

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17.30-18.00 Open Discussion: Day 2B

19.00-21.00 Workshop Dinner
@ Heuriger Schübl-Auer
1190, Kahlenberger Straße 22

Day 3 - September 21, 2016 (Wednesday)

9.00 - 9.30 **Werner Krauth**, *École Normale Supérieure, Paris, France*

Fast Irreversible Monte Carlo Simulations Beyond the Metropolis Paradigm: 2D Melting and Long-Range Systems

Abstract

I show how the lifting principle and a new pairwise decomposition of the Metropolis filter (1) allows one to design a class of powerful rejection-free Markov-chain Monte Carlo algorithms that break detailed balance yet satisfy detailed balance. These algorithms generalize our recent hard-sphere event-chain Monte Carlo method (2). The new approach breaks with all the three paradigms of common Markov-chain methods: 1/ Moves are infinitesimal rather than finite; 2/ Detailed balance is broken yet global balance is satisfied; 3/ Rejections are replaced by liftings, and moves are persistent.

Monte Carlo algorithms belonging to this class have allowed us to understand the melting transition in two-dimensional hard-disk (3) and in soft-disk systems (4), and I will discuss the different physical transition scenarios. I also outline a promising new approach to the treatment of long-range systems (5) using the event-chain paradigm.

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9.30 - 10.00 **Georg Maret**, *University of Konstanz, Germany*

The 2D Glass Transition in Soft Colloids

Abstract

Binary mixtures of spherical colloidal particles confined by gravity to a horizontal plane are excellent model systems to study the glass transition in 2D, because the inherent experimental time and length scales are well suited for real time video microscopy monitoring at the individual particle level [1]. In this talk, we review work on our 2D system of superparamagnetic colloids pinned at the air-water interface in a hanging drop setting [2] whose soft dipole-dipole interactions is induced by a vertical magnetic field B. This provides an effective system temperature which can be tuned through the glass transition by simple variation of B. Emphasis will be on the interplay between structural order and dynamics on local and non-local length scales and on the systems elasticity near the glass transition. In particular we discuss how competing local crystalline structures build up a glassy state [3-5], how such local structural order correlates with dynamic heterogeneities [6-7], how the shear elasticity abruptly changes near the glass transition [8,9] and that 2D glasses exhibit long range (Mermin-Wagner type) density fluctuations very similar to 2D crystals [10].

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10.00 - 10.30 Tea / Coffee Break

10.30 - 11.00 **Michael Grünwald**, *The University of Utah, USA*

Nucleation and Growth in Metal-Organic Frameworks

Abstract

Classical nucleation theory paints a simple and intriguing picture of the early stages of crystal formation, in which a nucleus of the stable crystal structure forms in the metastable mother phase. Mounting evidence from in-situ spectroscopy suggest that more complex, non-classical processes of crystal formation are widespread, in particular in the crystallization from dilute solution. Here we present our recent efforts to model and understand the nucleation behavior of ZIF-8, a prototypical metal-organic framework (MOF). MOFs are highly porous crystalline materials that have been synthesized in a large variety of topologies. Their formation process, however, is poorly understood and can display pronounced polymorphism and strong sensitivity to experimental conditions. Recent experiments have suggested non-classical nucleation scenarios for ZIF-8, including the formation of amorphous precursor clusters that grow and crystallize at later stages. Our model sheds light on these experiments and highlights the sensitivity of MOF topology to details of molecular shape.

11.00 - 12.00 Open Discussion: Day 3

12.00 - 13.30 Lunch Break

13.30 - 14.00 **Primoz Ziherl**, *University of Ljubljana, Slovenia*

Bronze-Mean Hexagonal Quasicrystal

Coauthors: Tomonari Dotera, Shinichi Bekku
Kinki University, Japan

Abstract

The most striking feature of conventional quasicrystals is their nontraditional symmetry characterized by icosahedral, dodecagonal, decagonal, or octagonal axis. The symmetry and the aperiodicity of these materials stem from an irrational ratio of two or more length scales controlling their structure, the best-known examples being the Penrose and the Ammann-Beenker tilings as two-dimensional models related to the golden and the silver mean, respectively. Surprisingly, no other metallic-mean tilings have been discovered so far. We propose a self-similar bronze-mean hexagonal pattern, which may be viewed as a projection of a higher-dimensional periodic lattice with a Koch-like snowflake projection window. We use numerical simulations to demonstrate that a disordered variant of this quasicrystal can be materialized in soft polymeric and colloidal particles with a core-shell architecture. Moreover, by varying the geometry of the pattern we generate a continuous sequence of structures, which provide an alternative interpretation of quasicrystalline approximants observed in several metal-silicon alloys. Thus the new tiling relates to both materials science and the mathematical basis of quasicrystals.

14.00 - 14.15 **Niels Boon**, *Lund University, Sweden*

Charge Regulation and Swelling of Microgels with a Cross-Linker Gradient

Coauthor: Sofi Nöjd, Peter Holmqvist, Peter Schurtenberger
Lund University, Sweden

Abstract

The swelling of cross-linked poly(N-isopropylacrylamide) (PNIPAM) microgels can be enhanced significantly by adding ionizable groups to the polymer backbone. This is because the counterions will gain entropy if the gel swells. The degree of swelling may be strongly dependent on the acidity of the solvent, salt concentration, and the volume fraction. In this combined theoretical and experimental work we combine various models to calculate equilibrium single-particle swelling profiles,, i.e. the polymer solubility, network elasticity, charge regulation, and the ionic osmotic pressure balance each other throughout the particle. We focus on so-called 'fuzzy spheres' that have a relatively dense core and a softer outer shell. We demonstrate how the microscopic properties relate to experimentally obtained quantities such as the effective charge, the pH, and the form factor.

14.15 - 14.30 **Jonas Riest**, *Forschungszentrum Jülich GmbH, Germany*

Dynamics and Filtration of Permeable Particles Dispersions: From Non-ionic to Ionic Microgels and Proteins

Coauthor: Gerhard Nägele

Abstract

We have developed and applied a toolbox of versatile theoretical methods of calculating structural, and short-time and long-time dynamic properties of suspensions of hydrodynamically structured colloidal particles [1], dispersions of submicron sized charge-stabilized colloidal globules [2], and globular protein solutions [3]. The considered dynamic properties include short- and long-time self-diffusion and sedimentation coefficients, the wavenumber-dependent diffusion function determined routinely in dynamic scattering experiments, and the zero- and high-frequency shear viscosities.

The accuracy of our toolbox methods is assessed by the comprehensive comparison with experimental measurements of, and simulation results for static and dynamic properties. In particular, we provide various analytic transport coefficient expressions for rigid permeable particles that can be readily used for the analysis of dynamic scattering and rheology data [1].

The good performance of the toolbox methods is demonstrated by comparison with dynamic light scattering experiments on concentrated suspensions of solvent permeable non-ionic microgels. Furthermore, we quantify the effect of particle softness and permeability on the dynamics of ionic microgel suspensions [4].

The results for the transport, structure, and thermodynamic properties of charge-stabilized colloids are used as input in our realistic macroscopic diffusion-advection modeling of the membrane cross-flow ultrafiltration of silica particles dispersions. The importance of using accurate inputs to the macroscopic modeling is demonstrated by the excellent agreement of our theoretical model predictions with UF measurements of the permeate flow for low-salinity silica suspensions [2].

Our work bridges thus the gap from the theoretical exploration of intra-particle properties such as solvent permeability, particle softness, and surface charge, to the calculation of transport, structural, and thermodynamic properties of concentrated dispersions, and to the modeling of a technologically important filtration process.

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14.30 - 14.45 **Massimo Pica Ciamarra**, *Nanyang Technologcial University, Singapore*

Jamming of Compressible Microgel Suspensions

Abstract

The jamming transition has been mostly investigated in systems of in-deformable particles, that interact via a well defined two-body interaction potential. Here [1] we consider how jamming occurs in systems of soft polymeric particles, that shrink and deform when compressed. Specifically, we investigate experimentally and theoretically jamming in systems of soft microgel particles. In these systems, the bulk and the shear modulus have a complex and system dependent concentration dependence, but the two moduli result to be always proportional. We show that these observations are rationalized assuming the particles to deform affinely upon compression, which implies that the concentration dependence of the elastic constants is fixed by the dependence of the osmotic pressure of a particle on its size. We determine the size dependence of the osmotic pressure developing a mechanical model for the particles that combines Flory's mean field and the Alexander-de Gennes model for polymer brushes. The model successfully reproduces the observed concentration dependence of the elastic constants of three different sets of microgel particles.

Reference

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14.45 - 15.00 **Takamichi Terao**, *Gifu University, Japan*

Monte Carlo Simulation of Dendritic Spherical Polymer Brushes

Abstract

Polymer-nanoparticle composites, also called as spherical polymer brushes, are typical soft colloidal systems. The features of the polymer-induced repulsive potential are essential for colloidal stability and lubrication. An array of these composites has industrial applications such as photonic crystals with photonic band gaps that forbid the propagation of light belonging to a certain frequency range. Therefore, it is important to study the effective interaction and structural formation of these systems (crystallization and phase diagram). The crystallization of polymer-nanoparticle composites occurs when the density of the system is sufficiently high and the number of polymer chains per each particle is large [1]. Recently, the structure of dendritic polymer brushes has been investigated by means of theoretical approaches and computer simulations [2]. In this presentation, dendritic spherical polymer brushes under confinement is investigated by Monte Carlo simulations. Further, the effective interaction between a pair of dendritic spherical polymer brushes and the structural formation, order–disorder transition, and phase diagram of this system are studied. We introduce a computer simulation method suitable for the analysis of soft colloidal systems [3,4]. Furthermore, the properties of binary soft colloids are discussed.

References

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15.00 - 15.30 Tea/Coffee Break

15.30-15.45 **Maria Sammalkorpi**, *Aalto University, Finland*

Controlling Colloidal Assembly Structure and Aqueous Dispersion via Lipid and Polymer Shape

Abstract

Phospholipids and block-copolymers offer efficient, noncovalent functionalization and dispersion of hydrophobic objects, e.g., therapeutic molecules and nanoparticles. However, the relation of the aggregates in bulk solution and in the presence of the object, and the properties of the resulting soft colloidal system and dispersion remain open questions. We have examined via molecular modelling methodology in coarse-grained and all-atom detail lipid and polymer aggregates at interfaces, the resulting colloidal solutions, and the dispersion efficiency.

By varying lipid and substrate surface curvature, and for PEGylated lipids the PEG chain length, in the simulations we find the assembled morphology varies from micellar-like to tubular coating (phospholipids) and micellar to monolayer-like (PEGylated lipids) with the transition depending on lipid curvature and for PEGylated lipids also on the PEG chain length and CNT diameter. We find the aggregation morphology directly influences the colloidal behavior and dispersion ability. Finally, we generalize the findings on properties of soft colloidal systems to lipid and polymer shape and discuss the implications to tailoring colloidal suspensions of hydrophobic objects, size-selective separation of hydrophobic particles, and experimental observations.

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15.45 - 16.00 **Priti Mohanty**, *Lund University, Sweden*

Probing Phase Transition Kinetics in Solid-to-Solid Transformations Using Soft-Repulsive Colloids as a Model System

Coauthors: Sofi Nöjd[1], Payam Bagheri[2], Anand Yethiraj[3], Peter Schurtenberger[1]
[2] KIIT University, India, [3] Memorial University, Canada

Abstract

In spite of the importance of solid-to-solid transformations in many areas of material science and the numerous experimental and theoretical studies, a deep understanding of the micro-structural changes and the underlying kinetic mechanisms is still missing. In this workshop, we will introduce a versatile model system composed of micron-scale soft-repulsive colloids [1-2] where we not only probe the single-particle kinetics in real space and real time using confocal laser scanning microscopy, but also tune the phase transition in a multiple-parameter space (effective volume fraction, alternating electric field and temperature). We discuss our recent discovery that the kinetics of crystal-to-crystal transformations is either diffusive or martensitic depending on the path, which we believe to be the first real-space, particle-level demonstration of diffusive and martensitic transformations respectively in a single system [3].

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16.00 – 16.15 **Hayato Shiba**, *Tohoku University, Japan*

Apparent Dimensionality Dependence of Glassy Dynamics: Infinite Growth of Acoustic Vibrations in Two Dimensions

Abstract

Dimensionality plays a key role in the physics of solids and liquids – from high to low dimensions, and fluctuation shows up differently, as typically observed in phase transitions. Indeed, two-dimensional (2D) systems often exhibit enhanced fluctuations, leading to various anomalies that are not experienced in three-dimensional (3D) systems. The melting of a 2D solid is a marked example, where the long-wavelength structural correlation is induced by thermal fluctuations stemming over an infinite length [1]. However, for the glass transition from supercooled liquids to amorphous solids, the dimensionality dependence of the fluctuation has become the issue only recently. Gigantic fluctuation in 2D supercooled liquids has been observed that is far stronger than that in their 3D counterparts [2,3].

In this paper, the dynamics of 2D supercooled liquids turns out to be dependent on the system size, while the size dependence is not pronounced in 3D systems, by using molecular dynamics simulations with up to 10^7 particles. It is demonstrated that the strong system size effect in 2D amorphous systems originates from the enhanced fluctuations at long wavelengths, which are similar to those of 2D crystal phonons. This observation is further supported by the frequency dependence of the vibrational density of states, consisting of the Debye approximation in the low-wavenumber limit. However, the system size effect in the intermediate scattering function becomes negligible when the length scale is larger than the vibrational amplitude. This suggests that the finite-size effect in a 2D system is transient and also that the structural relaxation itself is not fundamentally different from that in a 3D system. In fact, the dynamic correlation lengths estimated from the bond-breakage function, which do not suffer from those enhanced fluctuations, are not size dependent both in 2D and 3D systems [4].

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16.15 - 18.00 Posters & Open Discussion: Day 3B

Swetlana Jungblut, *University of Vienna, Austria*

Heterogeneous Crystallization on Pairs of Pre-Structured Seeds

Coauthor: Christoph Dellago

Abstract

Studying the effects of small pre-structured seeds on the crystallization transition in an undercooled monodisperse Lennard-Jones fluid, we analyze the impact of the simultaneous presence of two seeds with various structures. In the presence of seeds with face- and body-centered cubic structures, we find that decreasing the inter-seed distance enhances the probability of the crystalline clusters formed on one of the seeds to grow beyond the critical size, thus, increasing the crystal nucleation rates. In contrast, when seeds have an icosahedral structure, the crystalline clusters form mostly in the bulk. The crystal nucleation rate, however, is also determined by the distance between the seeds with regular structure in which the lattice spacing is equal to the bulk lattice constant, pointing to a heterogeneous crystal nucleation that occurs away from the icosahedrally structured seeds. For slightly squeezed seeds, the effects of the presence of seeds with face- and body-centered cubic structures are reduced in comparison to the regular seeds, and we do not see any effect of the presence of the second seed for seeds with squeezed icosahedral structure.

Christian Leitold, *University of Vienna, Austria*

Nucleation and Structural Growth of Cluster Crystals

Coauthor: Christoph Dellago

Abstract

We study the nucleation of crystalline cluster phases in the generalized exponential model with exponent $n = 4$. Due to the finite value of this pair potential for zero separation, at high densities the system forms cluster crystals with multiply occupied lattice sites. Here, we investigate the microscopic mechanisms that lead to the formation of cluster crystals from a supercooled liquid in the low-temperature region of the phase diagram. Using molecular dynamics and umbrella sampling, we calculate the free energy as a function of the size of the largest crystalline nucleus in the system, and compare our results with predictions from classical nucleation theory. Employing bond-order parameters based on a Voronoi tessellation to distinguish different crystal structures, we analyze the average composition of crystalline nuclei. We find that even for conditions where a multiply-occupied fcc crystal is the thermodynamically stable phase, the nucleation into bcc cluster crystals is strongly preferred. Furthermore, we study the particle mobility in the supercooled liquid and in the cluster crystal. In the cluster crystal, the motion of individual particles is captured by a simple reaction-diffusion model introduced previously to model the kinetics of hydrogen bonds.

Maddalena Mattiello, *ESPCI ParisTech, France*

The Role of Softness in Associative Microgels Suspensions

Coauthors: Raphaël Hepiegne, Michel Cloître

Abstract

Microgels suspensions are known to be an excellent example of soft materials, thanks to their capability to adjust volume and shape in order to obey to the topological constraints imposed by their neighbors above the glass and the jamming transition [1,2]. In this work we explore the main properties of a novel class of soft polyelectrolyte loosely crosslinked microgels that, thanks to the presence of associative moieties, are able to interact via attractive short range potentials. We compare the dynamics of concentrated and dilute suspensions to the behavior of analogous systems with purely soft repulsive interactions. Our results show how softness and associations can interplay in giving the final properties to the material.

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Jonas Riest, *Forschungszentrum Jülich GmbH, Germany*

The Elasticity of Polymeric Nanocolloidal Particles

Coauthors: Labrini Athanasopoulou[2], Sergey A. Egorov[3], Christos N. Likos[4], Primoz Ziherl[2,5]
[2] Jozef Stefan Institute, Slovenia, [3] University of Virginia, USA, [4] University of Vienna, Austria,
[5] University of Ljubljana, Slovenia

Abstract

Softness is an essential mechanical feature of macromolecular particles such as polymer-grafted nanocolloids, polyelectrolyte networks, cross-linked microgels as well as block copolymer and dendrimer micelles. Elasticity of individual particles directly controls their swelling, wetting, and adsorption behaviour, their aggregation and self-assembly as well as structural and rheological properties of suspensions. Here we use numerical simulations and self-consistent field theory to study the deformation behaviour of a single spherical polymer brush upon diametral compression. We observe a universal response, which is rationalised using scaling arguments and interpreted in terms of two coarse-grained models. At small and intermediate compressions the deformation can be accurately reproduced by modelling the brush as a liquid drop, whereas at large compressions the brush behaves as a soft ball. Applicable far beyond the pairwise-additive small-strain regime, the models may be used to describe microelasticity of nanocolloids in severe confinement including dense disordered and crystalline phases [1].

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Robert Salazar, *Universidad de los Andes, Colombia*

The Melting of the Classical Two-Dimensional Crystals with Long-Ranged Interactions

Coauthor: Martial Mazars
University Paris-Sud, University Paris-Saclay

Abstract

The melting of crystal phases in two-dimensional systems has been the subject of a large amount of theoretical, numerical and experimental works. Several mechanisms to describe the melting in two dimensional, including, in particular, the KTHNY theory and the melting induced by formation of grains boundaries, have been proposed. There are strong evidences that the melting in two dimensions depends crucially on the form and range of the interaction potentials between particles.

In this contribution, we report extensive Monte Carlo studies of the melting of the classical two-dimensional crystal for systems of point particles interacting via the $1/r^n$ potential [1,2] for $n = 1$, 2 and 3; the long ranged interaction is taken into account with the Ewald method [3,4]. For the Wigner crystal ($n = 1$), a hexatic phase is found in large enough systems. With the multiple histograms method and the finite-size scaling theory, we show that the fluid/hexatic phase transition is weakly first order. No set of critical exponents, consistent with a Kosterlitz-Thouless transition and the finite-size scaling analysis for this transition, has been found.

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Huzaifa Shabbir, *University of Vienna, Austria*

Effect of Cross-Links Coordination on the Mechanical Response of Polymeric Structures

Coauthor: M. A. Hartmann

Abstract

(Reversible) cross-linking is a common strategy to specifically tailor the mechanical properties of natural and synthetic polymeric systems. In biological materials, cross-links are often weaker than the covalent bonds holding the structure together. Thus, upon loading these bonds rupture before the covalent backbone fails, providing an efficient energy dissipation mechanism. Furthermore, the reversibility of the cross-links provides the material with a self healing mechanism because broken cross-links may reform after release of the load. In the context of biological materials such crosslinks are often called “sacrificial bonds” and they can be found in a large variety of structures like bone, wood, silk and the mussel byssus [1].

While the coordination of cross-links (i.e. the number of monomers participating in one cross-link) often varies in real systems (e.g. depending on pH the Fe-DOPA complex in the mussel byssus is known to exist in the mono-, bis- and tris-state), theoretical and simulation work dealing with the effect of cross-links on the mechanics of polymeric structures (aligned fiber bundles and random polymer networks) mostly investigate the effect of two fold coordinated cross-links only. In the current study, we aim at closing this gap by explicitly investigating the mechanical response of a polymeric system as a function of the coordination of reversible cross-links.

In the study presented, the Monte Carlo method is used to investigate the mechanical properties of cross-linked polymeric systems. The coordination of cross-links is controlled using the framework given by potentials of the REBO (Reactive Empirical Bond Order) type. In these potentials, the strength of an individual bond depends on the coordination of the involved atoms. The current study investigates the effect of different cross-links coordination on the mechanical properties of polymeric systems including random fiber networks and aligned fiber bundles. We present computational loading experiments performed at different cross-links densities and different spatial arrangement of cross-links and discuss the most important mechanical properties (stiffness, strength and toughness). As previous work on two-fold coordinated cross-links was showing a strong dependence of the mechanical performance on the topology of formed cross-links [2-4], in the present investigation special emphasis is put on the interplay of topology and mechanics.

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Susanne Wagner, *TU Wien, Austria*

Bonding Pattern Formation in a Two-Dimensional System of Patchy Particles

Coauthor: Gerhard Kahl

Abstract

We consider a two dimensional ensemble of patchy particles that carry one patch: while the particles are impenetrable we assume for the patch-patch interaction a Kern-Frenkel type potential. The density is fixed to close packing conditions thus particles form a hexagonal lattice and are only allowed to rotate. The system is studied with standard Monte Carlo simulations. Depending on the opening angle of the patch (i.e., the only degree of freedom left to the particles) typical bonding patterns are identified at low temperatures (see also [1]). We investigate via suitable order parameters how these bonding patterns change as the temperature is increased.

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Labrini Athanasopoulou, *Jozef Stefan Institute, Slovenia*

Phase Diagram of Elastic Spheres

Coauthor: Primoz Ziherl[1,2]

[2]University of Ljubljana, Slovenia

Abstract

At large enough densities, polymeric colloidal nanoparticles like star polymers, dendrimers, self-organized micelles often form open crystal lattices as well as quasi-crystalline phases [1]. By assuming that this behavior may be attributed to the deformability of the particles, we model them as homogeneous elastic spheres which interact with each other only upon a contact. We describe their deformation using two finite-deformation theories of elasticity, the Saint-Venant--Kirchhoff and the neo-Hookean model. We determine the range of indentations where the interaction between the balls is pairwise additive and described by the well-known Hertzian theory. By computing the free energies of 9 trial crystal lattices, we construct the phase diagram of the spheres which features the face- and body-centered cubic lattices, the A15 lattice and the simple hexagonal lattice. These results are compared to previous studies in the field [2,3].

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Day 4 - September 22, 2016 (Thursday)

9.00 - 9.30 **Michel Cloître**, *ESPCI ParisTech, France*

Flow and Structure of Soft Amorphous Solids: A Microscopic Perspective

Abstract

Soft amorphous solids are made of deformable particles jammed into a glass-like structure like concentrated emulsions, microgel suspensions, vesicles, star polymers, copolymer micelles and laponite suspensions. In spite of their great variability in composition, architecture, and interactions these materials exhibit generic dynamical properties intermediate between those of solids and liquids. They behave like weak elastic solids at rest but yield and flow with complex shear-rate dependence at large stresses. Although such materials are ubiquitous in nature and relevant in applications, a theory connecting macroscopic flow behavior to microstructure and particle properties remains a formidable challenge.

Repulsive suspensions can be modeled as packings of athermal, frictionless, elastic spheres, which are dispersed in a solvent at volume fractions well above the random close-packing of hard spheres. The particles are in contact and interact via elastohydrodynamic repulsive forces only [1]. Using a combination of particle scale 3D simulations, rheology, real space microscopy experiments, and theory, we analyze the microscopic mechanisms at the origin of yielding [2], flow [1], and aging [3]. Our results provide quantitative predictions of the microstructure in terms of particle scale properties as well as constitutive equations for the shear stress and normal stress differences. We will discuss the relevance of the model in relation with the behavior of well-defined microgel suspensions. A special emphasis will be given to the importance of the internal architecture of the particles and the role of the softness [4].

Attractive interactions add a higher degree of complexity. To explore this question we use a novel class of associative particles obtained by decorating the surface of microgels with functional hydrodrophobic macromonomers. The macromonomers have a controlled architecture and composition allowing for a fine tuning of the interactions. The phase diagram, the linear rheology and the flow properties are now entirely modified. We will discuss in details the new and unique phenomena that take place in relation with the strength of the interactions.

References

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9.30 - 10.00 **Jan Dhont**, *Forschungszentrum Jülich GmbH, Germany*

Rod-Like Colloids with Long-Ranged Electrostatic Interactions in Electric Fields and Shear Flow

Coauthors: Kyongok Kang[1], Dimitris Vlassopoulos[2]

[2] FORTH, Greece

Abstract

Highly charged rod-like colloids (fd-virus particles) at low ionic strength, and for concentrations within the two-phase isotropic-nematic coexistence region, exhibit various phases and dynamical states when subjected to alternating electric fields, depending on the field amplitude and frequency [1]. A non-chiral nematic, a chiral nematic and a homeotropically aligned homogeneous phase are observed, as well as a dynamical state where nematic domains persistently melt and form. The phase/state diagram in the field-amplitude versus frequency is determined by means of polarization microscopy, and the nature of the various transition lines is characterized with birefringence, dynamic light scattering and image-correlation spectroscopy. The microscopic origin for the existence of these various phases and dynamical states will be discussed, and a theory will be presented that explains and describes the origin of the dynamical state [2].

For concentrations above the isotropic-nematic coexistence region, a chiral-nematic phase and different types of equilibrated orientation textures are observed. At such high concentrations, a glass transition is found where not only the dynamics of the fd-particles is arrested (as probed with dynamic light scattering), but also the dynamics of the nematic texture freezes (probed with video image time-correlation) [3,4]. The flow behavior around the glass transition will be discussed. Contrary to glasses of spherical colloids, highly inhomogeneous flow profiles are observed. Fracture and plug flow is attributed to the response of the nematic texture, while gradient-banding is due to the response of single nematic domains.

References
[1] K. Kang and J. K. G. Dhont, Soft Matter **6**, 273 (2010)
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[3] K. Kang and J. K. G. Dhont, Phys. Rev. Lett. **110**, 015901 (2013)
[4] K. Kang and J. K. G. Dhont, Soft Matter **9**, 4401 (2013)

10.00 - 10.30 **Friederike Schmid**, *Johannes-Guttenberg University Mainz, Germany*

Nonequilibrium Self-Assembly of Polymeric Nanoparticles in Flow

Abstract

Polymeric nanoparticles are of increasing interest in nanotechnology and nanomedicine. One promising approach to preparing nanoparticles in a controlled manner is to use microfluidic devices. Nanoparticles then form as the result of a self-assembly process under conditions far from equilibrium, and parameters like mixing speed and shear rate can be used to control the size and shape of the particles. Here we use field-based simulations to investigate some of the main physical mechanisms underlying this control. First, we examine the size control in the so-called co-solvency method, where a collapse of polymeric nanoparticles from solution is induced by mixing bad solvent into a polymer dispersion. Experimentally, it is found that the particle size can be controlled by varying the mixing speed. We show that this control essentially happens in the initial stage of polymer-solvent demixing and derive scaling laws which are in agreement with experiments. Then, we study the effect of high shear rates on self-assembly. Shear mainly affects the later stages of self-assembly. It can reduce potential barriers for particle fusion, and thus assist the production of larger particles. Furthermore, it can induce irreversible shape changes in the particles and be exploited to make particles with unconventional shapes.

10.30 - 11.00	Tea/Coffee Break

11.00 - 11.20	Summary of the Workshop
11.20 - 12.00	Closing Remarks & Feedback

Structure formation in soft colloids

September 19-22, 2016 @ TU Wien

Description

The insight into structure formation in soft matter from liquid crystals to polymers and colloids relies in many ways on our understanding of how the respective building blocks pack, the best-known examples being hard spheres, rods, and platelets. The insight into packing of soft particles is much less comprehensive, yet during the past decade the body of experimental and theoretical work on systems based on deformable and compressible colloidal particles such as star polymers [1], hydrogel spheres [2], dendrimer micelles [3, 4], and block copolymer micelles [5] reached a level where certain patterns began to appear. For example, the salient features of model dendrimers are cluster crystals [6] as well as the otherwise exotic A15 and σ phase [7-10].

In view of the rich phenomenology reported, the field is in need of rules, mechanisms, and models relating the phase behavior, rheology, and other aspects of physics involved to the interparticle interaction. Ideally, these rules be simple much like the Onsager theory of nematic phase or the clustering criterion [11]. At the workshop, we wish to make a step ahead towards universal models of soft colloids, aiming at identifying a few working hypotheses to be explored in the future. This is a speculative endeavor, and the CECAM workshop will provide a suitable forum for out-of-the-box discussions of the possible form and scope of these models. The aim of the workshop is twofold

- To compare the experimental and theoretical insight into the structure formation in soft nanocolloidal particles, attempting to outline the generic features of their phase diagram to including orientational, bond-orientational, and other partly ordered mesophases.

- To discuss experimental, numerical, and theoretical methods as well as models applicable to these problems so as to identify the most efficient approach leading to as unified an understanding as possible.

Among the more concrete objectives, we wish that the workshop will address the following open questions:

- How to distinguish between the generic and the specific structural features reported both experimentally and theoretically in various soft nanocolloids? For example, what is it that the different shoulder potentials have in common, and in what respect are they different?

- What is the best working definition of softness in nanocolloidal particles? How to distinguish between particle penetrability and deformability?

- How to experimentally quantify soft nanoparticle shape both in dilute solutions and in condensed phases? What is the shape of soft nanocolloids? Is a large-scale parameter such as the aspect ratio sufficient for the description of shape?

- How do particle softness and anisometry affect the nature and the stability of the bond-ordered phases, and how does bond order interfere or correlate with orientational order in mesophases?

- How is clustering affected by particle anisometry?

- In crystals of penetrable anisometric particles, the interplay of positional and orientational order can be quite pronounced yet different than in hard rods. At small anisometry the orientational order should not matter much and positional order should be the defining feature of the crystals, whereas at large anisometries the orientational order should be dominant. Is the phase sequence similar than in hard rods or not?

- One of the neat recent ideas is the Miller-Batista deformable-droplet model and its implementation in a simulation code [12]. Can it be generalized to non-spherical particles?

- How important is the non-pairwise additivity of interactions in real nanocolloids? What are the most evident signatures of non-pairwise additivity?

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Participants

Austria

- Ronald Blaak, University of Vienna
- Benedikt Hartl, TU Wien
- Diego Felipe Jaramillo Cano, University of Vienna
- Martin Jehser, University of Vienna
- Clemens Jochum, University of Vienna
- Swetlana Jungblut, University of Vienna
- Christian Leitold, University of Vienna
- Emanuele Locatelli, University of Vienna
- Christos N. Likos (invited speaker), University of Vienna
- Huzaifa Shabbir, University of Vienna
- Andreas Singraber, University of Vienna
- David Toneian, TU Wien
- Luca Tubiana, University of Vienna
- Evagelos Voyiatzis, University of Vienna
- Susanne Wagner, TU Wien

Colombia

- Robert Salazar, Universidad de los Andes

Finland

- Maria Sammalkorpi, Aalto University

France

- Michel Cloître (invited speaker), ESPCI ParisTech
- Werner Krauth (invited speaker), École Normale Supérieure de Paris
- Maddalena Mattiello, ESPCI ParisTech
- Martial Mazars, University Paris-Sud, University Paris Saclay

Germany

- Jan Dhont (invited speaker), Forschungszentrum Jülich GmbH
- Michael Engel (invited speaker), University Erlangen-Nürnberg
- Georg Maret (invited speaker), University of Konstanz
- Jonas Riest, Forschungszentrum Jülich GmbH
- Friederike Schmid (invited speaker), University of Mainz

Italy

- Silvano Romano (invited speaker), University of Pavia

Japan

- Hayato Shiba, Tohoku University
- Hajime Tanaka (invited speaker), The University of Tokyo
- Takamichi Terao, Gifu University

Mexico

- Alexis Torres-Carbajal, Guanajuato University

The Netherlands

- Albert Philipse (invited speaker), Utrecht University

Singapore

- Massimo Pica Ciamarra, Nanyang Technological University

Slovenia

- Labrini Athanasopoulou, Jozef Stefan Institute

Sweden

- Niels Boon, Lund University
- Priti Mohanty, Lund University

United Kingdom

- Mark Miller (invited speaker), Durham University
- Goran Ungar (invited speaker), University of Sheffield
- Nigel Wilding (invited speaker), University of Bath
- Xiangbing Zeng (invited speaker), University of Sheffield

USA

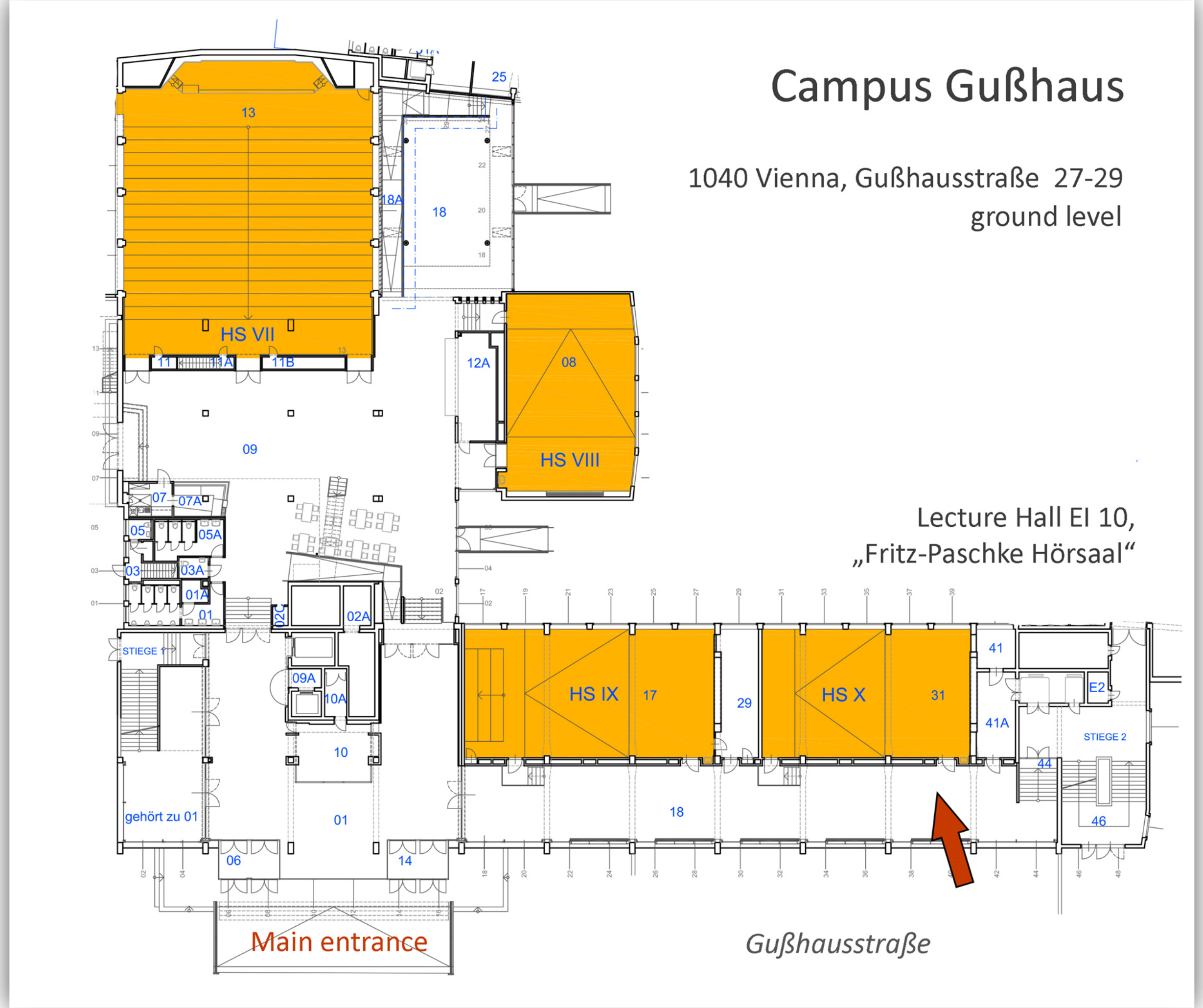
- Ioan Andricioaei, University of California Irvine
- Alan Denton (invited speaker), North Dakota State University
- Alberto Fernandez Nieves (invited speaker), Georgia Institute of Technology
- Matthew Glaser (invited speaker), University of Colorado
- Michael Grünwald, University of Utah
- Orlin D. Velev (invited speaker), North Carolina State University

Location

The workshop takes place at the TU Wien, "Campus Gusshaus",
1040 Vienna, Gußhausstraße 27-29

The Venue

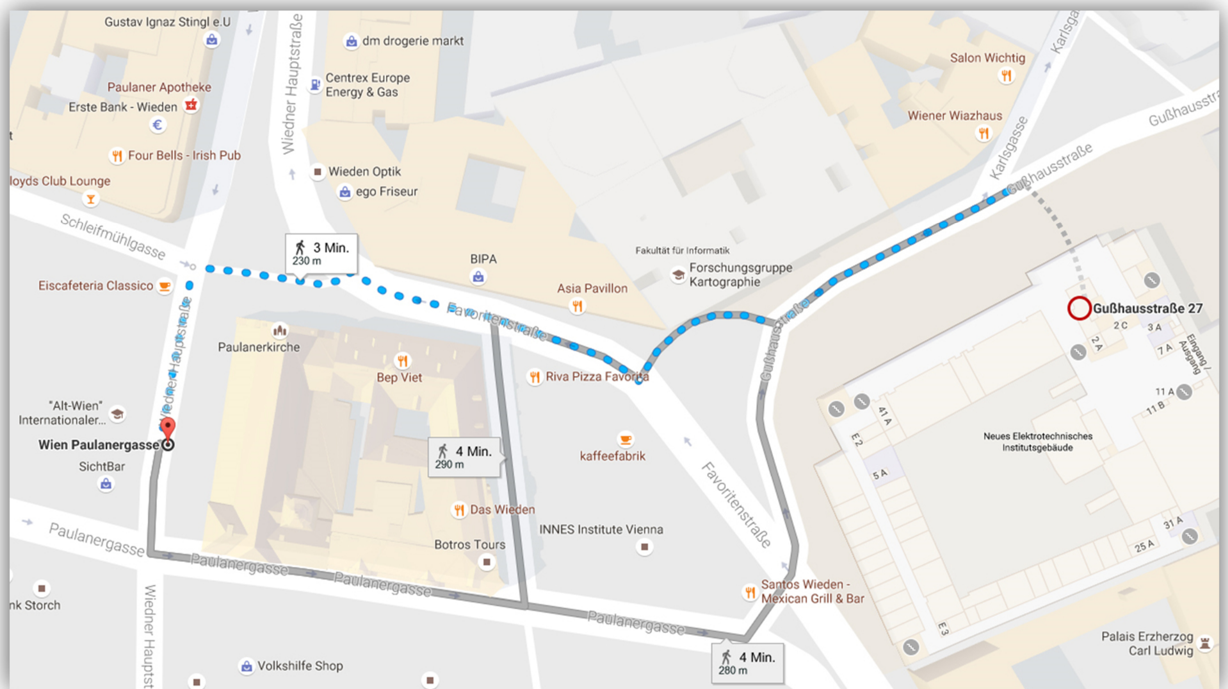
Lecture Hall EI 10, ground floor ("Fritz-Paschke-Hörsaal")



Evening @ Heuriger Schübel-Auer

Tuesday, September 20, 2016, 19:00

Leave Gußhausstraße 27-29 through the main entrance, turn left and go to Wiedner Hauptstraße.
Enter tram at station „Paulanergasse“. Take tram line 1, direction „Prater Hauptallee“,
for three stops, leave at station „Kärntner Ring/Oper“.

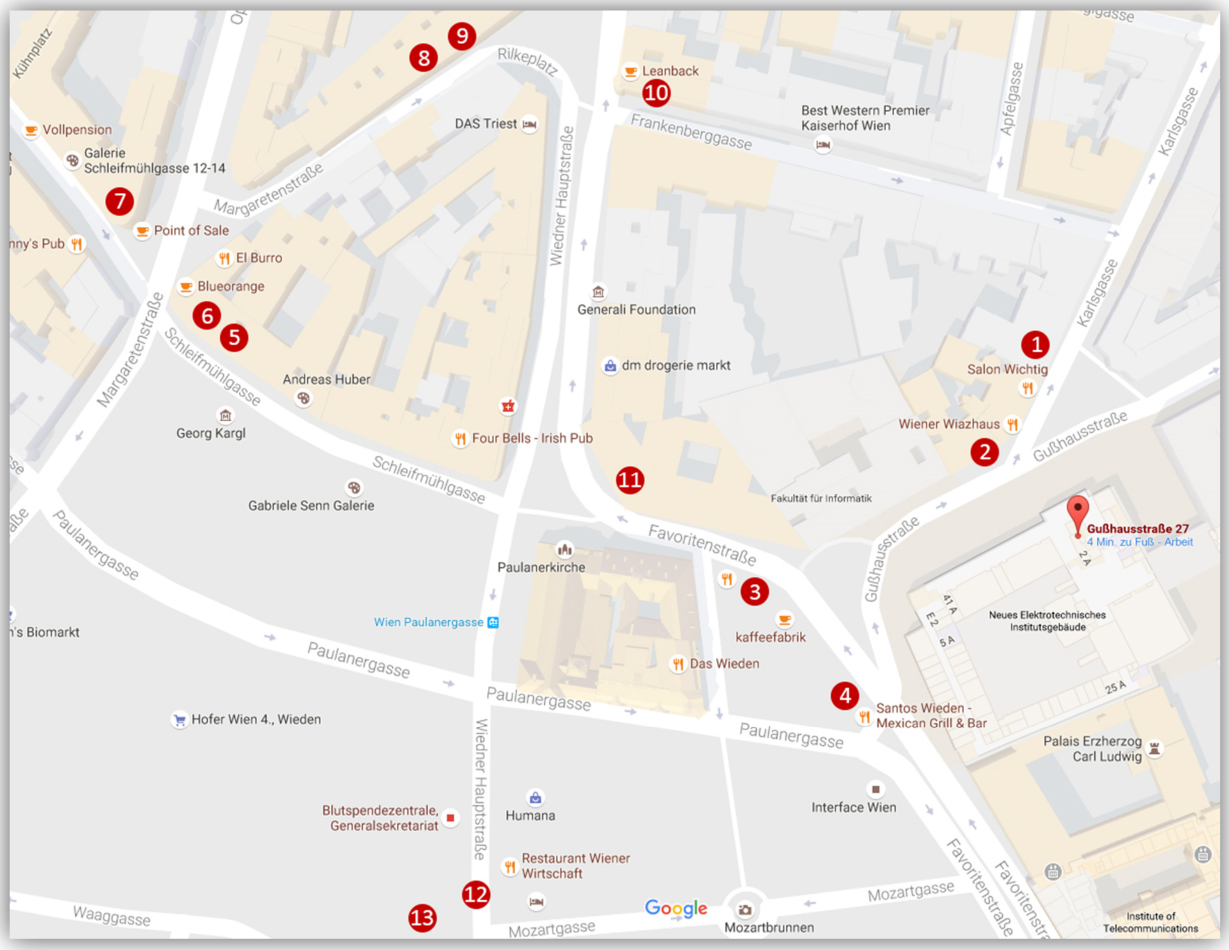


Change to tram line D,
direction „Nußdorf“,
to the terminal stop „Nußdorf“.

Cross the street and enter
the Heurigen‘s 2nd entrance
at Zahnradbahnstraße 17.

Heuriger Schübel-Auer
Kahlenberger Straße 22
1190 Wien-Nußdorf
Phone: +43 1 370 22 22

Possibilities for Lunch



Austrian Cuisine

(2) Wiener Wiazhaus
1040, Gußhausstraße 24
www.wiener-wiazhaus.at

(9) Gasthaus am Rilkeplatz
1040, Rilkeplatz 7
01 / 586 61 77

(12) Restaurant Wiener Wirtschaft
1040, Wiedner Hauptstraße 27
01/22 111 364

(x) Cafe-Restaurant Resselpark
1040, Wiedner Hauptstraße 1
www.restaurant-resselpark.at

Panini & Bagels

(6) Blueorange
1040, Margaretenstraße 9
www.blueorange.co.at

Fusion Cuisine

(1) Salon Wichtig
1040, Karlsgasse 22
www.salonwichtig.com

(7) Point of Sale
1040, Schleifmühlgasse 12-14
www.thepointofsale.at

(10) Leanback / Lanea
1040, Rilkeplatz 3
www.lanea1040.at

(11) Fein Essen
1040, Wiedner Hauptstr. 19
www.feinessen.at

Mexican Cuisine

(4) Santos
1040, Favoritenstraße 4-6
www.santos-bar.com

Pizza & Pasta

(3) Riva Pizza Favorita
1040, Favoritenstraße 4-6
www.riva.pizza

(8) Teigware
1040, Rilkeplatz 7/2
www.teigware.at

Asian Cuisine

(5) Nagoya Sushi
1040, Schleifmühlgasse 8
www.nagoyasushi.at

(13) Chang
1040, Waaggasse 1
www.chang.at

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