8th Liquid Matter Conference
September 6-10, 2011
Wien, Austria

Conference Book

Volume Editors

I. Coluzza, R. Blaak, B. Capone, S. Jungblut

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Sponsors

The organizers of the 8th Liquid Matter Conference thank all sponsors for their generous support.

Preface

On behalf of the International Program Committee and the Local Organizing Committee we welcome all participants to the 8th Liquid Matter Conference. The conference is organized jointly by the Liquids Section of the Condensed Matter Division of the European Physical Society, the Universität Wien, and the Technische Universität Wien. Previous conferences were held in Lyon (1990), Firenze (1993), Norwich (1996), Granada (1999), Konstanz (2002), Utrecht (2005), and Lund (2008). The aim of the conference is to bring together scientists working on the liquid state of matter and on closely related topics. Ever since the first conference of this series, the spectrum of scientific topics addressed in these conferences has substantially changed. Concepts and methods originally developed for simple and complex fluids have been systematically extended to investigate and understand properties of more complex systems, including nowadays soft matter and biophysical systems. The scientific contributions submitted to this conference demonstrate that the meeting covers a wide spectrum of scientific topics, including the physics, chemistry, biology, and chemical engineering of liquid matter as well as several areas of applied research. We hope that this conference will contribute to intensify these interdisciplinary collaborations.

At this meeting the Liquid Matter Prize of the European Physical Society will be awarded for the third time. The recipient of this prize, awarded for ”outstanding contributions to the science of liquid matter”, is Professor David Chandler of the University of California at Berkeley (USA). Further, we are pleased to host the second edition of the EPJE – Pierre Gilles De Gennes Lecture Prize; the recipient of this prize is Professor Michael E. Cates of the University of Edinburgh (UK) in recognition of his ”outstanding and deeply influential contribution in soft matter science”.

Overall, the conference features 2 prize lectures, 9 further plenary talks, 26 invited keynote and 96 contributed oral presentations, which have been selected by the International Program Committee. As of July 18, 2011, 787 poster contributions have been submitted.

The organizers gratefully acknowledge support from various organizations. In particular, we would like to thank the Universität Wien who offered us to stage the scientific program of this conference in one of the most attractive venues of Wien. We gratefully acknowledge the invitation of the Mayor of Wien to the Rathaus, where the Conference Dinner will take place. Finally, we thank all sponsors for generous financial support.

Christoph Dellago
Universität Wien
International Program Committee

Gerhard Kahl
Technische Universität Wien
Local Organizing Committee

Committees

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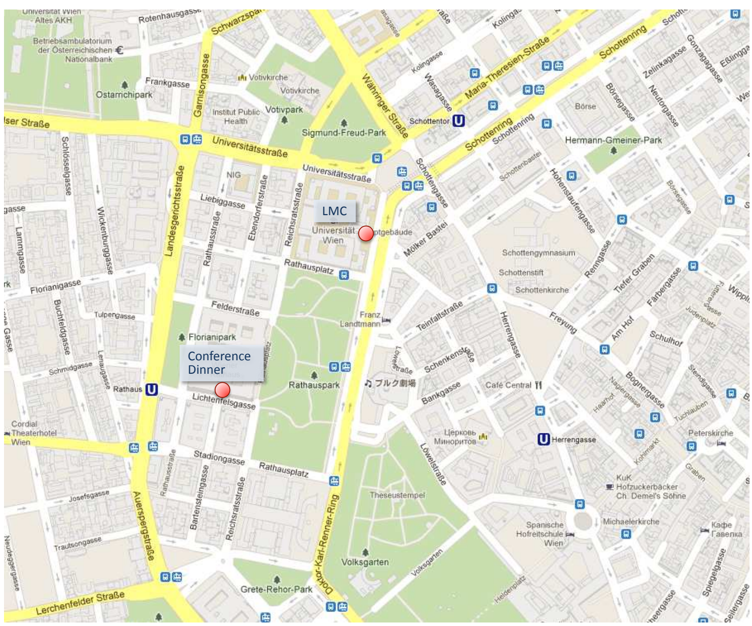
Social Program

Welcome Reception

The Welcome Reception, co-sponsored by *Soft Matter*, will take place on Monday, September 5, 2011, from 18:00-21:00 in the Arcades (Arkadenhof) of the Universität Wien, located close to the registration area. Snacks and drinks will be served.

Conference Dinner

The Conference Dinner will be held on September 7, 2011, at 19:00 in the Festsaal of the City Hall, which is located within five minutes walking distance from the conference site (see map below). The address of the Vienna City Hall is: Lichtenfelsgasse 2, A-1010 Wien.



Practical Informations

Venue

The conference will take place in the main building of the Universität Wien, Dr.-Karl-Lueger-Ring 1, A-1010 Wien, Austria.

All plenary lectures will be held in the Auditorium Maximum. The parallel sessions will take place in the Auditorium Maximum, the Small Ceremonial Hall (Kleiner Festsaal) and the Lecture Hall 28 (Hörsaal 28).

The poster sessions and the accompanying coffee breaks will take place in the Arcades. In this area also lunch will be served.

Floor plans of the conference site are included on pages 13-15 of this booklet.

Registration

The registration desk and the conference office are located in the Aula of the main-building of the Universität Wien (see floor plan on page 14). Registration starts on Monday, September 5, 2011; on this day, the conference office is open from 15:00-20:00.

If you have not paid your conference fee yet, you will have the possibility to do so at the conference office. Furthermore, you can purchase tickets for the conference dinner if places are still available (for technical reasons, the number of participants is limited to 800).

On Tuesday, September 6, 2011, the conference office opens at 8:00. From Wednesday, September 7, to Saturday, September 10, 2011, our staff is available from 8:30 onwards at the conference office . The office closes 15 minutes after the last lecture.

As you register you will receive the following documents:

- the conference booklet;
- a CD containing all the abstracts of the poster contributions as a pdf-file;
- a name badge; all participants are kindly requested to wear this name badge when attending the meeting; only participants who are wearing their name badges will be admitted to the lecture halls, coffee breaks, and lunches;
- a letter certifying your attendance.

Oral and poster presentations

Oral presentations

Oral presentations will be given in the Auditorium Maximum, the Smalll Ceremonial Hall (Kleiner Festsaal) and Lecture Hall 28 (Hörsaal 28) as indicated in the floor plans on pages 13-15.

Contributors are kindly requested to upload their contributions at the Editor's Desk (which is part of the conference office) **half a day before the respective session**. In case your contribution is scheduled for Tuesday morning (September 6, 2011), you are kindly asked to upload your contribution already on Monday evening at the registration. When transferring your files to the editor's computer, please check your contribution for a proper presentation; this holds in particular, if you plan to show videos.

No overhead projectors are available.

For technical reasons only ppt(x) and pdf files are accepted.

Use of personal laptops for presentations is not possible.

Prize winner and plenary lectures are scheduled for 45 (= 35 + 10) minutes, keynote contributions are scheduled for 30 (= 23+7) minutes, and contributed presentations are scheduled for 20 (=16+4) minutes, including discussion as indicated in brackets. Chair persons are instructed to follow the time schedule rigorously.

Poster presentations

The poster sessions will take place in the Arcades of the main-building of the Universität Wien. We kindly ask the presenters to stay close to their respective posters during the poster sessions.

Posters will be on display according to the following time schedule:

Tuesday, September 6

- Session 2: Water, solutions and reaction dynamics
- Session 9: Non-equilibrium systems, rheology, nanofluidics
- Session 10: Biofluids, active matter

Wednesday, September 7

- Session 5: Colloids

Thursday, September 8

- Session 7: Confined fluids, interfacial phenomena
- Session 8: Supercooled liquids, glasses, gels

Friday, September 9

- Session 1: Ionic and quantum liquids, liquid metals
- Session 3: Liquid crystals
- Session 4: Polymers, polyelectrolytes, biopolymers
- Session 6: Films, foams, surfactants, emulsions, aerosols

The list of all posters (titles and authors) is reproduced in this conference booklet. Please be sure that you display your poster at the poster wall assigned to your contribution (i.e., according to the assigned code).

The abstracts of the poster contributions are available on the CD distributed with the conference material and on the conference webpage.

The poster boards are 200 cm high and 100 cm wide. Adhesive tapes will be provided to fix the posters.

Posters should be mounted in the morning and dismounted in the evening of the respective day. Posters that have not been dismounted in time will be removed by the organizers.

Poster prizes

The three best posters presented by young researchers at the Liquid Matter Conference will be awarded with poster prizes sponsored by *Soft Matter*. Prize winners, selected by the International Program Committee, will receive a certificate, an online subscription to *Soft Matter*, and will be featured on the *Soft Matter* webpage. The poster prizes will be awarded on Saturday, September 10, at 10:30 preceding the first plenary lecture.

Other useful information

Internet

WLAN will be available for all participants during the conference.

To access WLAN, start a browser and use the following access codes:

- user-name: lmc8
- password: v1enna

Personal Computers with internet access are available in Lecture Hall 27 during lunch breaks (for the exact times of the lunch breaks see program).

Coffee break and lunch

Coffee breaks will take place in the Arcades according to the time schedule at the back of the booklet.

Lunch will be served in the Arcades. Lunch is free of charge for conference participants (please wear your name badge) and will be available from 12:15 to 13:45.

Additional informations

Conference staff will be happy to assist participants during the whole conference. Conference staff responsible for technical issues in the lecture halls will wear T-shirts with the conference logo.

Tables and chairs in the Large Ceremonial Hall (Grosser Festsaal) will offer you the possibility to meet with your colleagues.

Possible changes in the program will be announced on a message board close to the conference office.

An additional message board will be available close to the registration desk/conference office, displaying messages to participants. You may also leave messages for your colleagues at this board.

A cloakroom (close to the Auditorium Maximum) will be available on Saturday, September 10, from 8:30 until 12:30.

Proceedings

Following a longstanding tradition, we kindly invite contributors of **oral contributions** to publish their results in a special issue of Journal of Physics: Condensed Matter.

As you submit your contribution via the journal website at `http://iopscience.iop.org/0953-8984` please use the following specifications:

- Article type = special issue article
- Special issue = Liquid matter

At this website also general submission rules of the journal are summarized.

The length of your article should lie between a minimum of five and a maximum of ten journal pages. Your article will be refereed by one or more external referees. The special issue should become a standard reference for recent progress in liquid matter science. Thus only articles containing original, yet unpublished material will be accepted.

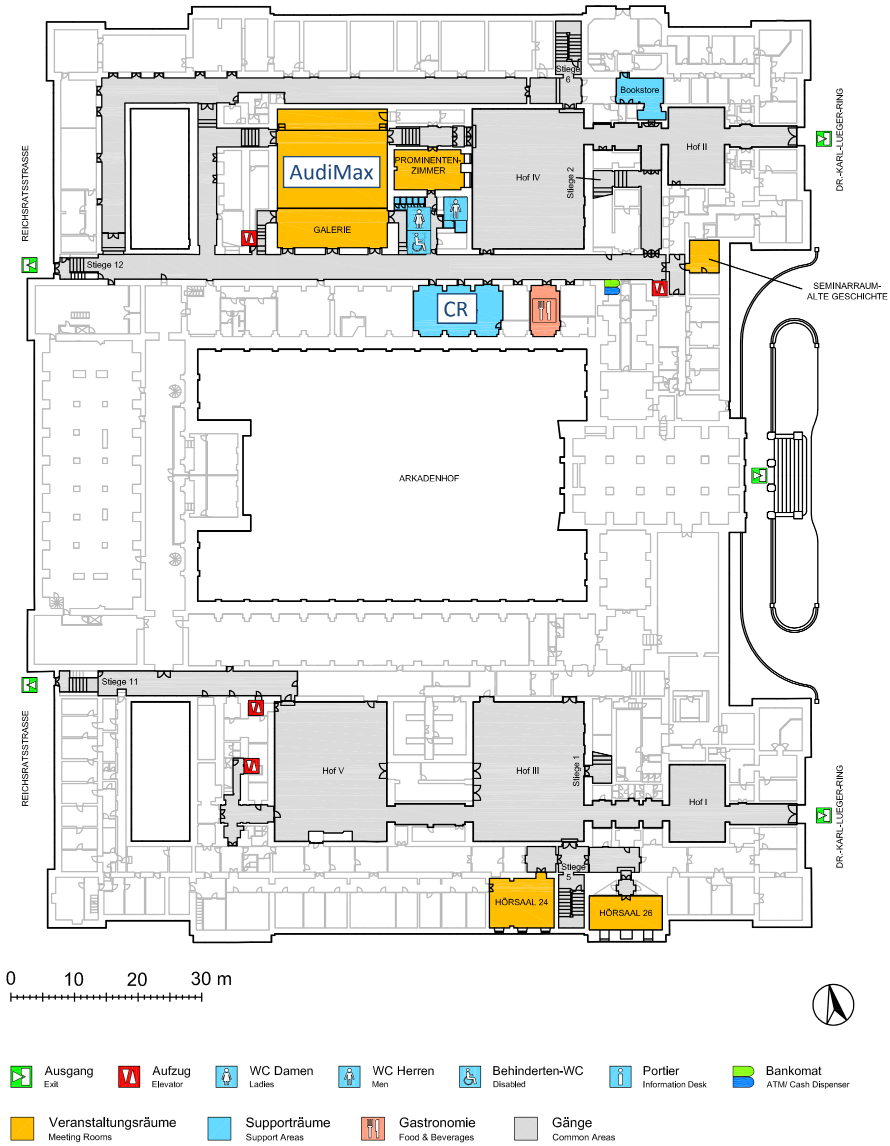
In an effort to guarantee a timely production of this special issue, the deadline for the manuscript submission is October 15, 2011.

Every conference participant will receive a copy of the issue.

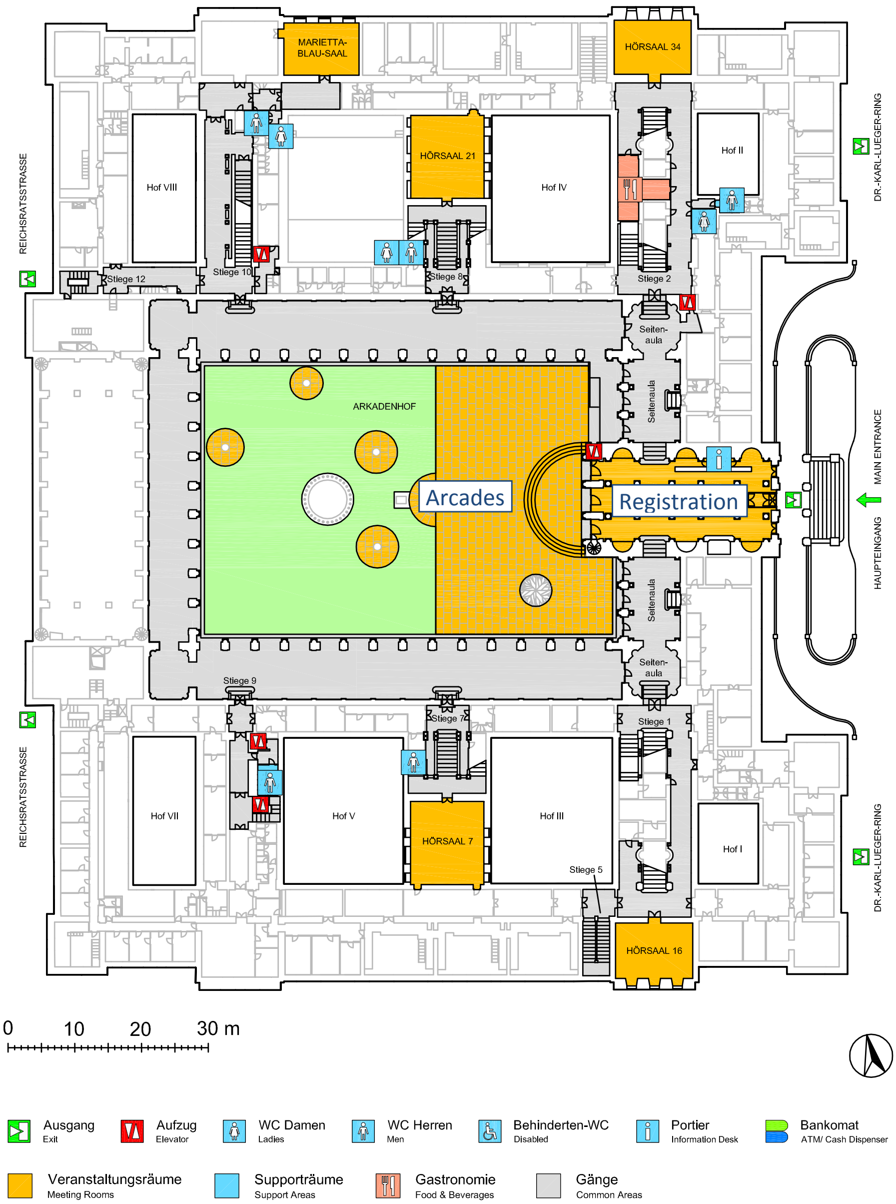
Floor Plans

Ground Floor

AudiMax = Auditorium Maximum
CR = Cloak Room

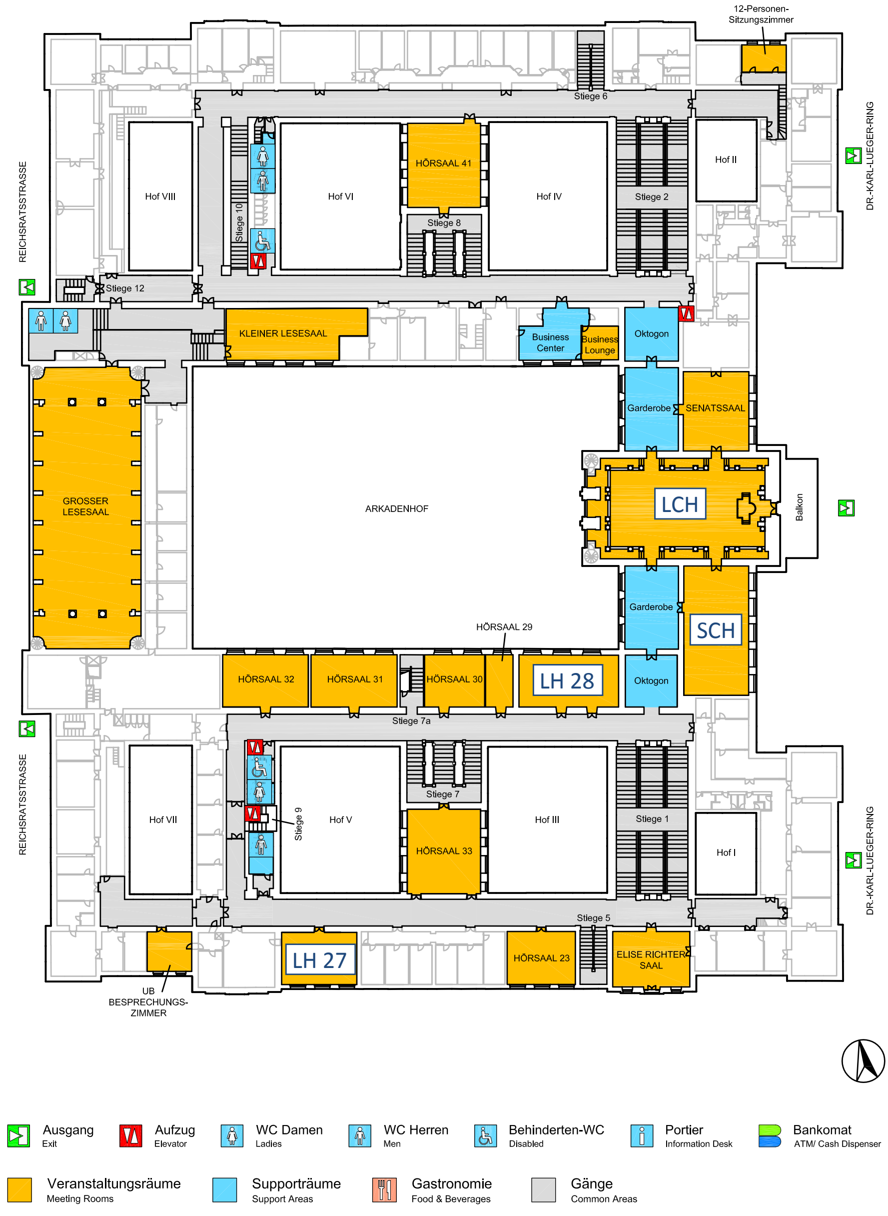


Raised Ground Floor



First Floor

LCH = Large Ceremonial Hall (Großer Festsaal)
SCH = Small Ceremonial Hall (Kleiner Festsaal)
LH 27 = Lecture Hall 27 (Hörsaal 27), *Computer Room*
LH 28 = Lecture Hall 28 (Hörsaal 28)



Program

Monday 5 September – Afternoon

18:00 – 21:00	**Welcome Reception** (Arcades)

Tuesday 6 September – Morning

09:00 – 09:15 **Opening**		
09:15 – 10:00 Auditorium Maximum **S. Glotzer** Self assembly and the role of shape in hard particle fluids and crystals Chair: S. Dietrich		
10:15 – 11:25 Auditorium Maximum **Session 5: Colloids** Chair: H. Löwen	*10:15 – 11:35* Small Ceremonial Hall **Session 1: Ionic and quantum liquids, liquid metals** Chair: Y. Levin	*10:15 – 11:25* Lecture Hall 28 **Session 4: Polymers, polyelectrolytes, biopolymers** Chair: C. Holm
10:15 – 10:45 (keynote lecture) **W. Kegel** Spontaneous formation of finite-size colloidal aggregates	*10:15 – 10:45* (keynote lecture) **M. Wilson** Structure and dynamics of network-forming liquids	*10:15 – 10:45* (keynote lecture) **A. Grosberg** Crumpled globule, melt of rings, and genome folding
10:45 – 11:05 **M. Haw** Onset of mechanical stability in random sphere packings	*10:45 – 11:05* **A. Parola** Liquid-vapor transition in a symmetric binary mixture of charged colloids	*10:45 – 11:05* **D. Démoulin** Measurement of force generated by the growth of actin filaments
11:05 – 11:25 **M. Schmiedeberg** Stability, phase behavior and dynamics of light-induced colloidal quasicrystals	*11:05 – 11:35* (keynote lecture) **A. Meyer** Diffusion of mass in liquid alloys	*11:05 – 11:25* **R. Allen** Exploring the "nucleation" of amyloid fibrils with experiments and computer simulations
11:25 – 14:00 **Posters (Sessions 2, 9 and 10) and Coffee** **Lunch** *(12:15 – 13:45)*		

14:00 – 14:45 Auditorium Maximum **K. Kremer** Topological constraints matter: collapsed polymer globules, chromosome territories, nano composites Chair: A. van Blaaderen		
14:50 – 16:00 Auditorium Maximum **Session 5:** **Colloids** Chair: S. Glotzer	*14:50 – 16:00* Small Ceremonial Hall **Session 9:** **Non-equilibrium systems, rheology, nanofluidics** Chair: R. Winkler	*14:50 – 16:00* Lecture Hall 28 **Session 2:** **Water, solutions and reaction dynamics** Chair: F. Bruni
14:50 – 15:20 (keynote lecture) **U. Gasser** Structural changes and phase behavior of densely packed microgel particles	*14:50 – 15:20* (keynote lecture) **P. Olmsted** Shear banding and related instabilities in entangled polymers	*14:50 – 15:20* (keynote lecture) **F. Caupin** Exploring water at negative pressure
15:20 – 15:40 **A. Philipse** Cubic crystals from cubic colloids	*15:20 – 15:40* **P. Tierno** Transversal dynamics of paramagnetic colloids in a longitudinal magnetic ratchet	*15:20 – 15:40* **X. Noblin** On a use of negative pressures and cavitation to create motion in plants
15:40 – 16:00 **I. Martchenko** Structural and dynamic properties of concentrated suspensions of ellipsoids	*15:40 – 16:00* **V. Blickle** Realization of a µm sized stochastic heat engine	*15:40 – 16:00* **E. Choi** Heat capacity measurements of water at negative pressure
16:00 – 16:30	**Coffee**	
16:30 – 17:50 Auditorium Maximum **Session 5:** **Colloids** Chair: P. Keim	*16:30 – 18:10* Small Ceremonial Hall **Session 9:** **Non-equilibrium systems, rheology, nanofluidics** Chair: P. Olmsted	*16:30 – 17:50* Lecture Hall 28 **Session 2:** **Water, solutions and reaction dynamics** Chair: F. Caupin
16:30 – 16:50 **D. Kraft** Surface roughness directed self-assembly of colloidal micelles	*16:30 – 16:50* **D. Luesebrink** Thermodiffusion of colloids with mesoscopic simulations	*16:30 – 16:50* **C. Chakravarty** Order, entropy and water-like anomalies in tetrahedral liquids
16:50 – 17:10 **H. R. Vutukuri** Colloidal analogues of charged and uncharged polymer chains with tunable stiffness	*16:50 – 17:10* **E. Boek** Colloidal asphaltene aggregation and deposition in capillary flow from multi-scale computer simulation and experiment	*16:50 – 17:10* **G. Stirnemann** Relationship between structural fluctuations and dynamical disorder in water: an explanation for the non-Arrhenius behavior of cold water reorientation
17:10 – 17:30 **M. Dennison** Phase behavior and effective shape of semi-flexible colloidal rods and biopolymers	*17:10 – 17:30* **D. Truzzolillo** Osmotic interactions and arrested phase separation in star-linear polymer mixtures	*17:10 – 17:30* **R. Torre** Time-resolved laser spectroscopy on bulk and confined water
17:30 – 17:50 **N. Ghofraniha** Self-controlled confinement of nanoparticles in the web of grain boundaries of a colloidal polycrystal	*17:30 – 17:50* **M. Giglio** Gradient-driven fluctuations in microgravity	*17:30 – 17:50* **F. Bruni** Water proton’s environment: a new water anomaly at atomic scale?
	17:50 – 18:10 **I. Pagonabarraga** Controlled drop emission by wetting properties in driven liquid filaments	

Wednesday 7 September – Morning

<table>
<tr><td colspan="3">09:00 – 09:45 Auditorium Maximum
E. T. J. Nibbering
Exploring and exploiting photoacids to reveal ultrafast hydrogen bond and proton transfer dynamics in solution
Chair: P. Linse</td></tr>
<tr><td>10:00 – 11:10 Auditorium Maximum
Session 7:
Confined fluids, interfacial phenomena
Chair: V. Lobaskin</td><td>10:00 – 11:10 Small Ceremonial Hall
Session 2:
Water, solutions and reaction dynamics
Chair: A. Baranyai</td><td>10:00 – 11:10 Lecture Hall 28
Session 8:
Supercooled liquids, glasses, gels
Chair: D. Coslovich</td></tr>
<tr><td>10:00 – 10:20
A. A. Verhoeff
Snap-off and coalescence of nematic liquid crystal drops</td><td>10:00 – 10:30 (keynote lecture)
D. Manolopoulos
Competing quantum effects in liquid water</td><td>10:00 – 10:30 (keynote lecture)
M. Guthrie
Manipulating liquid structure with pressure</td></tr>
<tr><td>10:30 – 10:50
C. Rascon
Capillarity and gravity: New phase transitions</td><td>10:30 – 10:50
A. Zeidler
Quantum effects in water</td><td>10:30 – 10:50
M. Mosayebi
Correlated rearrangements in supercooled liquids from inherent structure deformations</td></tr>
<tr><td>10:50 – 11:10
M. Schmidt
Non-additive hard sphere mixtures: from bulk liquid structure to wetting and layering transitions at substrates</td><td>10:50 – 11:10
T. Kühne
Second generation Car-Parrinello molecular dynamics: theory and application to the liquid/vapor interface</td><td>10:50 – 11:10
S. Lang
Liquid-glass phase diagram in confined geometry</td></tr>
<tr><td colspan="3">11:10 – 14:00 Posters (Session 5) and Coffee
Lunch (12:15 – 13:45)</td></tr>
</table>

14:00 – 14:45 Auditorium Maximum **P. Tarazona** Intrinsic structure and capillary waves spectrum at liquid surfaces Chair: J.-P. Hansen		
14:50 – 16:00 Auditorium Maximum **Session 7:** **Confined fluids, interfacial phenomena** Chair: M.M. Buzza	*14:50 – 16:00* Small Ceremonial Hall **Session 6:** **Films, foams, surfactants, emulsions, aerosols** Chair: P. Wagner	*14:50 – 16:00* Lecture Hall 28 **Session 8:** **Supercooled liquids, glasses, gels** Chair: S. Sastry
14:50 – 15:20 (keynote lecture) **O. Paris** Adsorption and phase transitions of fluids in confinement: In-situ studies with X-rays, neutrons and light	*14:50 – 15:20* (keynote lecture) **S. Roke** Small matters: a soap opera of SDS, oil and water at the nanoscopic oil droplet/water interface	*14:50 – 15:20* (keynote lecture) **P. Poole** The liquid-liquid phase transition in simulations of supercooled water: local order parameters, mixturelike behavior, and glass-liquid coexistence
15:20 – 15:40 **M. Blow** Superhydrophobicity on hairy surfaces	*15:20 – 15:40* **C. Raufaste** Interaction of a liquid jet with a soap film	*15:20 – 15:40* **J. M. Tavares** Thermodynamics and structure of fluids with dissimilar patches
15:40 – 16:00 **E. Jamie** Surface effects on the demixing of colloid-polymer systems	*15:40 – 16:00* **S. Cohen-Addad** How is interfacial rheology coupled with 3D foam rheology?	*15:40 – 16:00* **W. Lechner** The role of the prestructured surface cloud in crystal nucleation
16:00 – 16:30	**Coffee**	
16:30 – 17:30 Auditorium Maximum **Session 7:** **Confined fluids, interfacial phenomena** Chair: J. Indekeu	*16:30 – 17:30* Small Ceremonial Hall **Session 6:** **Films, foams, surfactants, emulsions, aerosols** Chair: T. Mason	*16:30 – 17:30* Lecture Hall 28 **Session 2:** **Water, solutions and reaction dynamics** Chair: D. Manolopoulos
16:30 – 16:50 **M. L. Rosinberg** Spontaneous imbibition in disordered porous solids: a theoretical study of helium in silica aerogels	*16:30 – 16:50* **A. Vila Verde** Structure and mechanism of formation of bile salt micelles from molecular dynamics simulations	*16:30 – 16:50* **J. Abascal** Supercooled water: simulation and experiment
16:50 – 17:10 **M. Hishida** Long-range hydration effect of lipid membrane studied by terahertz time-domain spectroscopy	*16:50 – 17:10* **P. L. H. Cooray** Interaction of granular particles on liquid interfaces	*16:50 – 17:10* **M. Kobayashi** Relationship between the phase diagram, the glass-forming ability, and the fragility of a water/salt mixture
17:10 – 17:30 **M. Wolff** Surface slip investigated by scattering techniques	*17:10 – 17:30* **D. Baigl** Photo-actuation of macro- and microfluidic systems	*17:10 – 17:30* **A. Baranyai** A transferable model for water
19:00 – 23:00	**Conference Dinner**	

Thursday 8 September – Morning

<table>
<tr><td colspan="3">09:00 – 09:45 Auditorium Maximum
R. Piazza
The unbearable heaviness of colloids
Chair: L. Reatto</td></tr>
<tr><td>10:00 – 11:10 Auditorium Maximum
Session 5:
Colloids
Chair: M.M. Telo da Gama</td><td>10:00 – 11:10 Small Ceremonial Hall
Session 3:
Liquid crystals
Chair: R. Kamien</td><td>10:00 – 11:10 Lecture Hall 28
Session 4:
Polymers, polyelectrolytes, biopolymers
Chair: I. Coluzza</td></tr>
<tr><td>10:00 – 10:30 (keynote lecture)
P. Ziherl
Packings of soft colloids</td><td>10:00 – 10:30 (keynote lecture)
C. Tschierske
Design of complex liquid crystals with polyphilic molecules</td><td>10:00 – 10:30 (keynote lecture)
D. Richter
On the dynamics of macromolecules: from synthetic polymers to proteins</td></tr>
<tr><td>10:30 – 10:50
H. Löwen
Crystallization in colloids and complex plasmas: similarities and complementarities</td><td>10:30 – 10:50
J. Yamamoto
Molecular manipulator driven by spatial variation of liquid crystalline order</td><td>10:30 – 10:50
R. Sigel
Dendronized polymers investigated by neutron scattering</td></tr>
<tr><td>10:50 – 11:10
J. Russo
A dissimilar patch model with a ”pinched” phase diagram</td><td>10:50 – 11:10
J. M. Romero-Enrique
Complex fluids at complex surfaces: simply complicated?</td><td>10:50 – 11:10
R. Stehle
Counter ion distribution and polyelectrolyte structure in dilute solutions seen by anomalous small angle scattering</td></tr>
<tr><td colspan="3">11:10 – 14:00 Posters (Sessions 7 and 8) and Coffee
Lunch (12:15 – 13:45)</td></tr>
</table>

14:00 – 14:45 Auditorium Maximum **D. Chandler** Pathways to forming glass: hierarchies, bubbles and order-disorder in space-time Chair: R. Evans		
14:50 – 16:00 Auditorium Maximum **Session 3: Liquid crystals** Chair: A. Imhof	*14:50 – 16:10* Small Ceremonial Hall **Session 7: Confined fluids, interfacial phenomena** Chair: E. Lomba	*14:50 – 16:00* Lecture Hall 28 **Session 4: Polymers, polyelectrolytes, biopolymers** Chair: G. Vliegenhart
14:50 – 15:20 (keynote lecture) **O. Henrich** Amorphous networks and rheological response of blue phases in chiral nematic liquid crystals	*14:50 – 15:20* (keynote lecture) **G. Galli** Ab-initio simulations of water at ambient conditions and under confinement	*14:50 – 15:20* (keynote lecture) **C. Pierleoni** Coarse-graining strategy for polymers in solution
15:20 – 15:40 **A. Fernandez-Nieves** Frustrated nematic order in spherical geometries	*15:20 – 15:40* **V. Lobaskin** Electrokinetics of air bubbles in water	*15:20 – 15:40* **F. Lo Verso** Surface-functionalised nanoparticles: Statics and dynamical properties
15:40 – 16:00 **S. Belli** Biaxial nematic LCs: can polydispersity stabilize them?	*15:40 – 16:10* (keynote lecture) **O. Orwar** Biomembrane shape and volume dynamics to the limit of fractal ruptures	*15:40 – 16:00* **D. Lenz** Dendrimer cluster crystals
16:00 – 16:30	**Coffee**	
16:30 – 18:10 Auditorium Maximum **Session 5: Colloids** Chair: R. Piazza	*16:30 – 18:10* Small Ceremonial Hall **Session 7: Confined fluids, interfacial phenomena** Chair: M.-L. Rosinberg	*16:30 – 17:50* Lecture Hall 28 **Session 4: Polymers, polyelectrolytes, biopolymers** Chair: D. Vlassopoulos
16:30 – 16:50 **J. Dobnikar** Self-assembly of magnetic colloids	*16:30 – 16:50* **J. Indekeu** Wetting transitions of infinite order	*16:30 – 16:50* **C. Holm** Simulation of electrokinetic phenomena with discrete ions and beyond
16:50 – 17:10 **L. Filion** Self-assembly of a colloidal interstitial solid solution with tunable sublattice doping	*16:50 – 17:10* **M. Buzza** Two-dimensional colloidal alloys	*16:50 – 17:10* **J. Farago** Anomalous diffusion of a polymer chain in an unentangled melt
17:10 – 17:30 **I. Coluzza** Theory and simulations of designable modular self-assembling materials	*17:10 – 17:30* **L. Helden** Salt induced changes of interactions in binary liquid mixtures	*17:10 – 17:30* **G. Vliegenthart** Compression, crumpling and collapse of spherical shells and capsules
17:30 – 17:50 **F. Romano** Self-assembly of a photonic colloidal crystal: a simulation study	*17:30 – 17:50* **J. Nase** Hydrate formation at liquid-liquid and liquid-gas interfaces	*17:30 – 17:50* **J.-L. Barrat** Nanoscale buckling instability of layered copolymers
17:50 – 18:10 **F. Martinez-Veracoechea** Design rule for colloidal crystals of DNA-functionalized particles	*17:50 – 18:10* **J. M. Oh** Electric field driven instabilities on superhydrophobic surfaces	

Friday 9 September – Morning

09:00 – 09:45 Auditorium Maximum **S. Nagel** Jamming and the emergence of rigidity Chair: C.N. Likos		
10:00 – 11:30 Auditorium Maximum **Session 9:** **Non-equilibrium systems, rheology, nanofluidics** Chair: E. Boek	*10:00 – 11:10* Small Ceremonial Hall **Session 8:** **Supercooled liquids, glasses, gels** Chair: R. Torre	*10:00 – 11:10* Lecture Hall 28 **Session 3:** **Liquid crystals** Chair: P. Ziherl
10:00 – 10:30 (keynote lecture) **J. Vermant** Effects of medium viscoelasticity on particle dynamics and structures in suspensions	*10:00 – 10:30* (keynote lecture) **K. Winkel** Amorphous ices - the glassy states of water: the calorimetric glass-liquid transition of HDA	*10:00 – 10:30* (keynote lecture) **R. Kamien** Smectics!
10:30 – 10:50 **M. Smith** Stretching dense colloidal suspensions: from flow to fracture	*10:30 – 10:50* **S. Sastry** Structural relaxation and correlation length scales in glass forming liquids	*10:30 – 10:50* **A. Imhof** Monodisperse silica bullets: a new model system that enables the real-space study of rod-like colloids
10:50 – 11:10 **T. Besseling** A real-space study of shear induced order in colloidal hard-sphere fluids	*10:50 – 11:10* **J. Kurzidim** Dynamic arrest of fluids in porous media: crossover from glass- to Lorentz-like behavior	*10:50 – 11:10* **C. De Michele** Self-assembly of DNA duplexes into polymers chains: theory, simulations and experiments
11:10 – 11:30 **R. G. Winkler** Non-equilibrium properties of semidilute polymer solutions in shear flow		
11:10 – 14:00 **Posters (Sessions 1, 3, 4 and 6) and Coffee** **Lunch** *(12:15 – 13:45)*		

14:00 – 14:45 Auditorium Maximum **D. Quere** Leidenfrost state Chair: D. Frenkel		
14:45 – 15:30 Auditorium Maximum **M. Cates** How different are polymeric glasses from glassy simple liquids? Chair: D. Frenkel		
15:30 – 16:00	**Coffee**	
16:00 – 18:00 Auditorium Maximum **Session 6: Films, foams, surfactants, emulsions, aerosols** Chair: S. Egelhaaf	*16:00 – 17:40* Small Ceremonial Hall **Session 10: Biofluids, active matter** Chair: R. Goldstein	*16:00 – 17:40* Lecture Hall 28 **Session 1: Ionic and quantum liquids, liquid metals** Chair: A. Parola
16:00 – 16:30 (keynote lecture) **P. Wagner** Formation of molecular clusters and aerosol particles	*16:00 – 16:30* (keynote lecture) **W. Poon** Bacteria as active colloids	*16:00 – 16:20* **S. Saccani** Soft-disk bosons: a minimal model for supersolidity
16:30 – 17:00 (keynote lecture) **T. Mason** Structuring nanoemulsions	*16:30 – 17:00* (keynote lecture) **F. MacKintosh** Control of biopolymer network elasticity through architecture and molecular-motor activity	*16:30 – 16:50* **S. Hosokawa** Transverse excitations in liquid Sn
17:00 – 17:20 **A. Bogdan** Liquid-coated ice particles in high-altitude clouds	*17:00 – 17:20* **A. Zöttl** Motion of a model micro-swimmer in Poiseuille flow	*17:00 – 17:20* **S. Tazi** Accurate force fields from ab-initio simulations: the case of aqueous ions
17:20 – 17:40 **M. Miller** Structure and stability of electrospray droplets	*17:20 – 17:40* **G. Volpe** Behavior of microswimmers in complex environments	*17:20 – 17:40* **Y. Levin** Ions at air-water interface: surface tensions and surface potentials of electrolyte solutions
17:40 – 18:00 **J. de Ruiter** Drops on functional fibers: from barrels to clamshells and back		

Saturday 10 September – Morning

09:00 – 10:00 Auditorium Maximum **Session 5:** **Colloids** Chair: B.M. Mladek	09:00 – 10:00 Small Ceremonial Hall **Session 10:** **Biofluids, active matter** Chair: W. Poon	09:00 – 10:00 Lecture Hall 28 **Session 8:** **Supercooled liquids, glasses, gels** Chair: T. Loerting
09:00 – 09:20 **B. Van Megen** What nucleates the crystal? Perspectives from studies of the hard sphere system	*09:00 – 09:20* **P. Cicuta** Hydrodynamic synchronisation in driven colloidal systems: a model for micro-pumps and biological flows	*09:00 – 09:20* **C. Klix** Elastic properties of glasses
09:20 – 09:40 **G. Doppelbauer** Ordered equilibrium structures of patchy particles	*09:20 – 09:40* **J. Tailleur** Arrested phase separation in reproducing bacteria: a generic route to pattern formation?	*09:20 – 09:40* **L. Cipelletti** Highly nonlinear dynamics in a slowly sedimenting colloidal gel
09:40 – 10:00 **E. Koos** Particle configurations and gelation in capillary suspensions	*09:40 – 10:00* **R. Di Leonardo** Bacterial ratchet motors	*09:40 – 10:00* **R. Ni** Glassy dynamics, spinodal fluctuations, and the kinetic limit of nucleation in suspensions of colloidal hard rods
10:00 – 10:30	**Coffee**	
10:30 – 11:15 Auditorium Maximum **I. Musevic** Liquid crystal colloids Chair: N.B. Wilding		
11:15 – 12:00 Auditorium Maximum **R. Goldstein** Synchronization of eukaryotic flagella Chair: N.B. Wilding		
12:00 – 12:15	**Closing**	

Plenary Lectures

Pathways to forming glass: hierarchies, bubbles and order-disorder in space-time

EPS Liquid Matter Prize 2011 Lecture

David Chandler

University of California, Berkeley, Department of Chemistry, 94720, Berkeley, CA, USA

The onset to vitrification is characterized by heterogeneous dynamics, which results in singular time-correlations, super-Arrhenius temperature variation, and transport decoupling. The phenomena possess significant degrees of universality, and when viewed in terms of the statistical mechanics of trajectory space, they appear as forms of pre-wetting (in space-time) and precursors to a non-equilibrium phase transition. Numerical simulation and analytical treatment elucidate the nature of heterogeneous dynamics, its associated non-equilibrium transition and its relationship to making glass.

How different are polymeric glasses from glassy simple liquids?

EPJE - Pierre Gilles De Gennes Lecture Prize

Michael Cates,[1] Suzanne Fielding,[2] and R. G. Larson[3]
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[2]Durham University, Durham, United Kingdom
[3]University of Michigan, Michigan, USA

Polymer glasses show emergent features that do not arise either for molten polymers or for simple glassy fluids. Recent years have seen remarkable progress in establishing theories for the deformation response of each of those classes of materials separately; but so far there has been limited success in unifying such approaches. Here we show that one striking emergent property of polymer glasses – the time evolution of their segmental mobility under elongational flow – can be explained by compling one of the simplest models of polymer dynamics to a minimal model of an aging glass. This suggests that at least some features of polymeric glasses, though initially mysterious, may have simple explanations.

Self assembly and the role of shape in hard particle fluids and crystals

Sharon Glotzer

University of Michigan, 2300 Hayward St, 48109-2136, Ann Arbor, USA

While the structural diversity of colloidal fluids and crystals has grown substantially in recent years, it still aspires to that of atomic and molecular systems. Ionic colloidal crystals and binary nanoparticle superlattices, by exploiting electrostatic interactions in mixtures of particles of opposite charge, have substantially broadened the diversityof structures beyond those obtainable in traditional hard sphere systems, but rely on energetic interactions as well as entropy for their stability. Here we explore the role of shape and entropy in phase transitions of hard particle fluids and their crystals. Using computer simulations, we show that particle shape alone can suffice to produce a rich diversity of colloidal crystal structures whose complexity rivals that of atomic analogues.

Synchronization of eukaryotic flagella

Raymond Goldstein

University of Cambridge, DAMTP/Centre for Mathematical Sciences, CB3 0WA, Cambridge, United Kingdom

One of the most fundamental issues in biology is the nature of evolutionary transitions from single cell organisms to multicellular ones. Not surprisingly for microscopic life in a fluid environment, many of the processes involved are related to transport and locomotion, for efficient exchange of chemical species with the environment is one of the most basic features of life. This is particularly so in the case of flagellated eukaryotes such as green algae, whose members serve as model organisms for the study of transitions to multicellularity. In this talk I will focus on recent experimental and theoretical studies of the stochastic nonlinear dynamics of these flagella, whose coordinated beating leads to graceful locomotion but also to fluid flows that can out-compete diffusion. A synthesis of high-speed imaging, micromanipulation, and three-dimensional tracking has quantified the underlying stochastic dynamics of flagellar beating, allowed for tests of the hydrodynamic origins of flagellar synchronization, and revealed a eukaryotic equivalent of the run-and-tumble locomotion of peritrichously flagellated bacteria. Challenging problems in applied mathematics, fluid dynamics, and biological physics that arise from these findings will be highlighted.

Topological constraints matter: collapsed polymer globules, chromosome territories, nano composites

Kurt Kremer

MPI for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany

The role of topological constraints on conformational as well as relaxational and dynamical properties of open linear and closed ring polymers as well as mixtures thereof is discussed. In the case of polymer melts the conformational statistics can be used to directly determine the entanglement molecular weight in excellent agreement to experiment. By manipulating the entanglements in long chain melts materials with new rheological properties can be achieved. For ring polymers the situation is completely different. While linked rings act like DeGennes' Olympic gels, we find by massive computer simulations employing a specially adapted algorithm that non concatenated polymer rings segregate and form individual collapsed objects. We discuss the details of their conformations, which not only is related to one of the very basic problems in polymer science but also has far reaching consequences from the collapse of gels to chromosome territories.

Liquid crystal colloids

Igor Musevic

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Dispersions of solid or liquid particles in liquid crystals show several novel classes of anisotropic forces between inclusions, which do not exist in isotropic solvents [1]. Of particular interest are nematic colloids, where the orientationally ordered nematic liquid crystal provides extremely strong, anisotropic and long-range particle pair interaction [2]. These forces are the consequence of elastic distortion of a liquid crystal around the inclusions. They are responsible for a fascinating variety of colloidal assemblies in nematic liquid crystals, such as 2D [3] and 3D nematic colloidal crystals, colloidal superstructures in the mixtures of large and small colloidal particles [4], and colloidal wires, entangled topological defects [5]. In chiral nematic colloids, entanglement of topological defects loops results in the formation of knots and links. In all cases, the colloidal binding energy is several orders of magnitude stronger compared to water based colloids. The mechanisms of nematic colloidal self-assembly are discussed, as well as the role of topology and geometry of defects in the nematic liquid crystal. It will be shown that nematic dispersions provide a unique platform for soft matter photonics, where liquid tunable optical microresonators [6] and microlasers [7] can be self-assembled in a fraction of a second.

[1] P. Poulin, H. Stark, T. C. Lubensky, D. A. Weitz, Science 275, 1770(1997).
[2] M. Yada, J. Yamamoto, H. Yokoyama, Phys. Rev. Lett. 92, 185501 (2004).
[3] I. Musevic, M. Skarabot, U. Tkalec, M. Ravnik, S. Zumer, Science 313, 954(2006).
[4] M. Skarabot et. al. Phys. Rev. E, 77, 061706(2008).
[5] M. Ravnik et al., Phys. Rev. Lett. 99, 247801(2007).
[6] M. Humar, M. Ravnik, S. Pajk, I. Musevic, Nat. Photonics 3, 595(2009).
[7] M. Humar, I. Musevic, Opt. Express, 18, 26995(2010).

Jamming and the emergence of rigidity

Sidney Nagel

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When a system jams it undergoes a transition from a flowing to a rigid state. Despite this important change in the dynamics, the internal structure of the system remains disordered in the solid as well as the fluid phase. In this way jamming is very different from crystallization, the other common way in which a fluid solidifies. Jamming is a paradigm for thinking about how many different types of fluids - from molecular liquids to macroscopic granular matter - develop rigidity. As the geometrical constraints between constituent particles become important, it is less easy for a fluid to flow. At zero temperature, the jamming transition is unusual - with aspects of both continuous and discontinuous behavior. By studying the normal modes of vibration, we have found that the properties of the marginally-jammed solid are also highly unusual and provide a new way of thinking about disordered systems generally.

Exploring and exploiting photoacids to reveal ultrafast hydrogen bond and proton transfer dynamics in solution

Erik T. J. Nibbering

Max Born Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max Born Strasse 2A, D-10623, Berlin, Germany

Modern discussions of solution phase acid-base reactions have evolved from the seminal studies of Eigen and Weller in the 60s [1]. It was already then realised that the elementary steps of proton transfer between acids and bases occur on ultrafast time scales. Ongoing technological advances in time-resolved spectroscopy in the 80s, 90s and 00s have led to breakthroughs in understanding proton transfer dynamics. In these time-resolved studies a class of organic molecules called photoacids have been used as a means to trigger proton transfer on ultrafast time scales. Photoacids are organic molecules that show a large increase in acidity upon electronic excitation. Recent advances in ultrafast infrared spectroscopy have led to a microscopic insight of aqueous acid-base neutralization reactions. I will present an example of photo-induced aqueous proton transfer generating the world's most abundant acid [2], i.e. carbonic acid, and will indicate the role it plays in the aqueous chemistry of carbon dioxide [3]. Whereas profound insight in aqueous proton transfer pathways in acid-base neutralization have been achieved in recent years, the underlying reasons for photoacidity is still an active research topic. Recent approaches how to tackle this issue by experiment will be discussed.

[1] A. Weller, Progr. React. Kin. 1, 187 (1961); M. Eigen, Angew. Chem. Intl. Ed. Engl. 3, 1 (1964).
[2] K. Adamczyk et al., Science 326, 1690 (2009).
[3] T. Loerting et al., Angew. Chem. Int. Ed. 39, 892 (2000).

Leidenfrost state

David Quere,[1] Mathieu Bancelin,[1] James Bird,[1] Christophe Clanet,[1] Guillaume Dupeux,[1] Guillaume Lagubeau,[1] Marie Le Merrer,[1] and Keyvan Piroird[1]
[1]*ESPCI, France*

As pointed out by Johann Leidenfrost in 1756, a liquid on a very hot solid levitates on a cushion of its own vapour. As a consequence, these drops are ultra-mobile, compared to the ones we can see on window panes or on windshields. We discuss in our talk a few consequences of this mobility: 1) how drops can be put in motion using the tiny forces generated by asymmetric substrates; 2) how they can be manipulated using adapted fields; 3) how they can be stopped and trapped using textures. We conclude by describing ways to generate dynamic Leidenfrost situations, which take advantage of air motion to induce levitation, instead of heat.

The unbearable heaviness of colloids

Roberto Piazza

Politecnico di Milano, Department of Chemistry (CMIC), 20133, Milano, Italy

Colloids are unavoidably prone to settling. Often an experimental annoyance, sedimentation can nonetheless provide a rewarding opportunity to obtain crucial information on the structural and dynamical properties of both equilibrium and metastable structures, which can hardly be probed in homogenous conditions.In particular, I shall show that:

- Measurements of equilibrium sedimentation profiles allow reconstructing the phase diagram and the full equation of state of systems of particles interacting via complex potentials. Even for colloids getting stuck into a gel structure, the steady-state profile provides valuable information on the elastic properties of the an arrested phase, yielding the concentration dependence of the compression modulus [1].

- The investigation of the kinetic settling profile of a settling suspension provides direct information on hydrodynamic interactions over a wide concentration range [2].

- Using as a “flag” the settling enhancement associated to the spinodal decomposition processes taking place within a liquid-liquid demixing gap allows investigating complex depletion phenomena and relate them to the critical Casimir effect [3].

- More generally, a general survey of the birth, collapse and restructuring of depletion gels yields a rich panorama of complex and often unexpected effects [4].

All the former investigations, and in particular the last mentioned, greatly profited from the application of novel optical methods, which I shall comment on, relying on tuning the spatial coherence of the illumination on the image plane.

[1] S. Buzzaccaro, R. Rusconi, and R. Piazza, Phys. Rev. Lett. **99**, 098301 (2007)
[2] S. Buzzaccaro, A.Tripodi, R. Rusconi, D, Vigolo, and R.Piazza, J. Phys.: Cond. Matt. **20**, 494219 (2008)
[3] S. Buzzaccaro, J. Colombo, A. Parola, and R. Piazza, Phys. Rev. Lett. **105**, 198301 (2010)
[4] G. Brambilla, S. Buzzaccaro, R. Piazza, L. Berthier, and L.Cipelletti, Phys. Rev. Lett. **106**, 118302 (2011)

Intrinsic structure and capillary waves spectrum at liquid surfaces

Pedro Tarazona

Universidad Autonoma de Madrid, Depto. Fisica Teorica de la Materia Condensada, 28049, Madrid, Spain

The usual representation of liquid surfaces through smooth density profiles hides most of the details in the molecular structure of these interfaces. The concept of a sharper ”intrinsic structure”, that becomes blurred by the capillary wave fluctuations of the liquid surface, was postulated long time ago [1], but only over the last few years we have got efficient methods to separate the intrinsic structure and the spectrum of capillary waves fluctuations from the molecular configurations sampled in computer simulations of liquid surfaces [2]. These recent advances in an old standing problem are opening a new perspective for the molecular arrangements in fluid surfaces. E.g. we may get a surface compactness index [3], relating the two-dimensional density of the first liquid layer with the bulk density, to characterize the surface structure of different liquids in terms similar to those used for crystal phases. Our description of complex fluid interfaces may also gain from the analysis of their intrinsic structure, e.g. to characterize the hydrophobic gap in water-oil systems [3], or to decompose the fluctuation spectrum in lipid bilayers membranes. The accurate characterization of the undulating (capillary wave) mode may be achieved through the cross-correlation between the nominal intrinsic surfaces, pinned to the molecular positions of two different molecular layers. The full characterization of the capillary waves spectrum may be done in terms of three physical parameters: the low-q limit of the (macroscopic) surface tension, a bending modulus and a soft cut-off that sets the molecular limit for the undulations of the surface as a whole. The talk will also comment on the new experimental and theoretical challenges [5], to measure and predict the features observed through the intrinsic analysis of liquid surfaces in computer simulations.

[1] FP Buff, RA Lovett and FH Stillinger (1965), PRL 15, 621; FH Stillinger (1982), J. Chem Phys 76, 1087.
[2] E Chacon and P Tarazona (2003), PRL 91, 166103; P Tarazona and E Chacon (2004), PRB 70, 235407; J. Chowdhary and BM Ladanyi, (2006) J. Phys, Chem. B 110, 15442; M Jorge and NNDS Cordeiro (2007) J. Phys. Chem. C 111, 17612; LB Partay et al. (2008) J. Comp. Chem. 29, 945.
[3] E Chacon et al. (2009), PRB 80, 195403.
[4] F. Bresme et al. (2008), PRL 101, 056102
[5] P Tarazona, R Checa and E Chacon (2007), PRL 99, 196101.

Keynote Lectures

Session 1:
Ionic and quantum liquids, liquid metals

Diffusion of mass in liquid alloys

Andreas Meyer

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Atomic diffusion is a fundamental property for an understanding of liquid dynamics, nucleation, vitrification, and crystal growth. Diffusion data serve as a vital input to the modeling of microstructure evolution and are an essential control to molecular dynamics simulation results. A common method to measure diffusion coefficients in liquid alloys is the long capillary (LC) technique and its variations. There, a diffusion couple of different composition, in the case of interdiffusion, or containing a different amount of isotopes, in the case of self diffusion, is annealed in the liquid state and subsequently quenched to ambient temperature. The diffusion profiles are analyzed post mortem. This technique exhibits several drawbacks, that in most cases prevent an accurate measurement of diffusion coefficients - convectice contributions during diffusion anealing are the most prominent ones. Recently, the field of liquid diffusion experiments advanced through the use of quasielastic neutron scattering (QNS) on levitated metallic droplets for accurate measurements of self diffusion coefficients in high temperature metallic liquids. For the accurate measurement of interdiffusion we combine LC experiments with an in situ monitoring of the entire interdiffusion process by the use of X-ray and neutron radiography. These experiments are accomponied by diffusion experiments in space in order to benefit from the purely diffusive transport under microgravity conditions for a large variety of alloy systems. In this presentation recent experimental results are discussed in the context of the relation of self- and interdiffusion, the relation of self diffusion and viscosity, as well as the relation of properties of mass transport and the atomic melt structure.

Structure and dynamics of network-forming liquids

Mark Wilson

University of Oxford, Physical and Theoretical Chemistry Laboratory, Oxford, United Kingdom

Intermediate-range order (IRO), in which systems exhibit structural ordering on length-scales beyond the nearest-neighbour (short-range), has been identified in a wide range of materials and is characterised by the appearance of the so-called first sharp diffraction peak (FSDP) at low scattering angles. The precise structural origin of such ordering remains contentious and a full understanding of the factors underlying this order is vital if such materials (many of which are technologically significant) are to be produced in a controlled manner. Simulation models, in which the ion-ion interactions are represented by relatively simple potential functions which incorporate (many-body) polarisation and which are parameterised by reference to well-directed electronic structure calculations, have been shown to reproduce such IRO and allow the precise structural origin of the IRO to be identified. Furthermore, the use of relatively simple (and hence computationally tractable) models allows for the study of the relatively long length- and time-scales required. Two typical systems, zinc chloride (which is usually considered as 'ionic') and germanium selenide (considered as having 'covalent' character) have been recently modelled as key target systems deliberately chosen so as to potentially represent two different bonding 'types' whilst both displaying FSDPs at $\sim 1\text{Å}^{-1}$. Both have received recent significant experimental and computational (electronic structure) attention. The underlying structures are analysed with reference to both recent (neutron scattering) experimental results and high level electronic structure calculations and the origin of the FSDP in the Bhatia-Thornton $\mathrm{S}_{CC}(k)$ function discussed. The role of key structural units (corner and edge sharing polyhedra) in determining the network topology is investigated in terms of the underlying dynamics and the relationship to the glass transition considered.

Session 2:
Water, solutions and reaction dynamics

Exploring water at negative pressure

Frédéric Caupin,[1] Arnaud Arvengas,[2] Kristina Davitt,[2] Mouna El Mekki,[1] Claire Ramboz,[3] David A. Sessoms,[4] and Abraham D. Stroock[4]
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[2]Laboratoire de Physique Statistique ENS-UPMC-Paris Diderot-CNRS, Paris, France
[3]Institut des Sciences de la Terre d'Orléans, Orléans Cedex 2, France
[4]Cornell University, Ithaca, USA

Water is famous for its anomalies, most of which become dramatic in the supercooled region, where the liquid is metastable with respect to the solid. Another metastable region has been hitherto less studied: the region where the pressure is negative. We will review the work on the liquid in the stretched state. Most of the research has been focused on determining the limit of rupture of the liquid by the nucleation of bubbles. Our groups have recently investigated this cavitation limit by three techniques: focused ultrasound, artificial trees, and liquid inclusions in quartz. A puzzling discrepancy between experiments and theory remains unexplained. Analysis of the cavitation probability with the nucleation theorem [1] provides the size of the critical bubble and may help us to understand the nucleation mechanism. Characterization of the properties of the metastable liquid before it breaks is a challenging task that has been less tackled. The recent measurement of the equation of state of the liquid at room temperature down to -26 MPa [2] opens the way to more detailed information on the liquid at low density. We will conclude with a discussion of our current efforts to complete a map of the thermodynamic, dynamic, and structural properties of this liquid water at negative pressure.

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[2] K. Davitt et al., J. Chem. Phys. **133**, 174507 (2010).

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Wed 7
10:00

Competing quantum effects in liquid water

David Manolopoulos

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I will begin with an overview of the ring polymer molecular dynamics (RPMD) method for including quantum mechanical (zero point energy and tunneling) effects in molecular dynamics simulations. I will then use this method to investigate the role of quantum effects in the dynamics of room temperature liquid water, using a flexible water model that has been parameterized to agree with a wide variety of experimental measurements in quantum mechanical (path integral-based) simulations [1]. If time allows, I will also mention some more recent work from the group of Angelos Michaelides [2]. This work confirms what we have found for liquid water and generalizes our main result (the existence of a competition between intra- and intermolecular quantum effects) to a wide variety of other hydrogen-bonded systems.

[1] S. Habershon, T. E. Markland and D. E. Manolopoulos, J. Chem. Phys. **131**, 024501 (2009).
[2] X-Z. Li, B. Walker and A. Michaelides, Proc. Natl. Acad. Sci. **108**, 6369 (2011).

Session 3:
Liquid crystals

Amorphous networks and rheological response of blue phases in chiral nematic liquid crystals

Oliver Henrich,[1] Kevin Stratford,[2] Davide Marenduzzo,[3] and Michael E. Cates[3]
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[2]Edinburgh Parallel Computing Centre, Edinburgh, United Kingdom
[3]University of Edinburgh, Edinburgh, United Kingdom

Blue Phases (BPs) are equilibrium phases in thermotropic cholesteric close to the cholesteric-isotropic transition. They consist of a lattice of disclination lines with typical length scales around the wavelength of visible light. While older experiments typically observed BPs only in a very narrow temperature range of about 1 K, more recent ones have created BPs over a strikingly wide temperature window of 50 K. However, for this potential for future applications to be fully realized we need our understanding of BPs to advance at the same pace. In this work we show that large scale simulations can help settle important physical question.

The structure of BPIII has been the subject of a long debate in liquid crystal research. Our findings provide strong evidence that BPIII is an amorphous disclination network [1,2] and appear to rule out competing explanations invoking a quasi-crystal icosahedral symmetry. Remarkably, we find that within a certain window of chirality and with a standard choice of free energy functional, individual aperiodic structures exist that are more stable than any other ordered BP. Depending on the sign of the dielectric anisotropy we also observed transitions of the network to new, field-induced BPs as in experiments. More recently we were able to gain first insights into the rheological response of cubic BPI and BPII. In simple shear flow both phases exhibit a pronounced permeative motion of the disclination network in the direction of vorticity, whereas the sense of motion depends on the helicity of the underlying cholesteric. While BPII remains closer to its affinely transformed equilibrium configuration, BPI shows intriguing flow induced structures, which are possibly indicate the onset of rheochaos.

[1] O. Henrich, K. Stratford, D. Marenduzzo, M.E. Cates, Phys. Rev. Lett. **106**, 107801 (2011).
[2] O. Henrich, K. Stratford, D. Marenduzzo, M.E. Cates, Proc. Nat. Acad. Sci. USA **107**, 13212-13215 (2010).

Smectics!

Randall Kamien

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The homotopy theory of topological defects in ordered media fails to completely characterize systems with broken translational symmetry. We argue that the problem can be understood in terms of the lack of rotational Goldstone modes in such systems and provide an alternate approach that correctly accounts for the interaction between translations and rotations. Dislocations are associated, as usual, with branch points in a phase field, whereas disclinations arise as critical points and singularities in the phase field. We introduce a three-dimensional model for two-dimensional smectics that clarifies the topology of disclinations and geometrically captures known results without the need to add compatibility conditions. We use this to uncover a formerly unknown structure in focal conic domains.

Design of Complex Liquid Crystals with Polyphilic Molecules

Carsten Tschierske,[1] M. Prehm,[1] B. Glettner,[1] C. Nürnberger,[1] H. Ebert,[1] G. Ungar,[2] F. Liu,[2] and X.-B. Zeng[2]
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[2]University Sheffield, Sheffield, United Kingdom

Recent progress in the design of complex liquid crystalline phases based on self assembly of polyphilic molecules will be reviewed. First, the concept of T-shaped polyphiles is shortly introduced which form series of fluid honeycomb phases based on polygons with cross sectional shapes ranging from triangles via squares and pentagons to hexagons and beyond [1]. Main focus will be on X-shaped polyphiles composed of four different and incompatible units which produce honeycomb cells with distinct composition (multicolour tilings), leading to a wide range of complex nano-scale morphologies with new superlattices and increased periodicities [2]. In all these ordered liquids space is divided into a number of distinct nanometer sized compartments separated by walls formed by p-conjugated aromatics. The number of distinct compartments can be further increased by local mixing of incompatible units in distinct fixed ratios, in this way creating new ”colors”. Thus, fine-tuning of geometric frustration and miscibility frustration allows formation of structures with a number of distinct compartments exceeding the number of incompatible units actually combined in the molecular tectons; in this way up to seven distinct compartments have been created using polyphiles incorporating only four distinct units. Besides the honeycomb structures also other modes of self assembly, like bicontinuous networks, crossed columns and different combinations of layers and columns can be achieved. This illustrates the enormous potential of the concept of polyphilic liquid crystal engineering for creating new highly complex and also regular soft self-assembled nano-scale structures.

[1] C. Tschierske, Chem. Soc. Rev. **36**, 1930 (2007).
[2] X. Zeng, R. Kieffer, B. Glettner, C. Nürnberger, F. Liu, K. Pelz, M. Prehm, U. Baumeister, H. Hahn, H. Lang, G. A. Geringer, C. H. M. Weber, J. K. Hobbs, C. Tschierske, G. Ungar, Science **311**, 1302 (2011).

Session 4:
Polymers, polyelectrolytes, biopolymers

Crumpled globule, melt of rings, and genome folding

Alexander Grosberg

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Crumpled globule, initially hypothesized as a long lived intermediate state on the path of a long polymer chain collapse transition, is now considered a likely candidate model for large scale organization of DNA in an interphase nucleus of an eukaryote cell. It is also supposed to be the equilibrium state of a ring squeezed between other unconcatenated rings in the melt of rings. Crumpled state has peculiar and as yet incompletely understood fractal properties. In this talk, the current understanding of crumpled globule will be reviewed from both the point of view of its applications and its fundamental understanding.

Coarse-graining strategy for polymers in solution

Carlo Pierleoni
INFN, Italy

I review the basis of the coarse-graining strategy for polymers in solution which maps groups of monomers into effective monomers with monomer-averaged effective interactions [1]. The level of coarse-graining, that is the number of effective monomer per chain, defines the length scale below which structural details are lost. At the highest level of coarse-graining, chains are mapped onto soft particles interacting by density dependent pair potentials. Although it is essential to reproduce the thermodynamic behavior expected by scaling laws, the dependence of the effective potential from the density makes the extension of this model to more complex situations impractical. For solutions of diblock-copolymer, the minimal coarse-grained model maps a single copolymer onto a dumbbell of soft effective monomers [2]. In this simple model the effective interactions can be obtained with the RISM theory at zero density only, and an extension at finite density can only be obtained by iterative numerical inversion of the full-monomer generated structure, limiting very much its applicability. Nonetheless, this simple model exhibits a reach phenomenology when studied at finite density, presenting a CMC for the formation of spherical micelles and a crystalline phase of micelles at even higher density, a phenomenology which is also found in experiments on diblock copolymer solutions [3,4,5]. A less-grained model can in principle be adopted to extend the use of density independent potential to finite density. I will present several attempts in this direction [6,7,8] and discuss future directions of research.

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On the dynamics of macromolecules: from synthetic polymers to proteins

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Neutron Spin-Echo-Spectroscopy accesses the dynamics of macromolecules in space and time on the level of the chains. In the past most of the efforts were focussed on the dynamics of synthetic polymers that to a large extend the determine their rheological and mechanical properties. Recently such studies were extended towards the domain dynamics of proteins that are detrimental for their function. My lecture addresses some key challenges in the field. First on the example of polymer nanocomposites I'll discuss the dynamics of synthetic polymers in a complex environment. I will display neutron scattering data addressing length and time scales from the single monomer to the entanglement network and beyond. These experiments reveal the basic relaxation processes related to monomeric friction, the intermediate scale Rouse dynamics as well as the entanglement controlled dynamics. I will discuss the effects of the filler concentration on the polymer conformation as well as on the dynamics on the various important length scales. Finally the microscopic data are related to results from rheology. Thereafter I will turn to proteins and present neutron spin-echo experiments on the inter domain motions that are important in promoting biochemical function. I shall discuss the cleft opening dynamics of alcohol dehydrogenase that enables the binding and release of the functional important cofactor. Furthermore, I will address the large scale motions in phosphoglycerate kinase, an important enzyme in the glycolitic pathway that catalyses the recharging of ADP to ATP. The observed dynamics show that the protein has the flexibility to allow fluctuations and displacements that seem to enable the function of the protein.

Session 5:
Colloids

Structural changes and phase behavior of densely packed microgel particles

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Colloidal suspensions of microgel particles are systems of great interest for applications and fundamental studies due to their reversible responsiveness to changes of their environment, such as temperature or hydrostatic pressure. Although it has been shown that microgel particles behave like hard spheres under many circumstances [1], they can reach states that are far beyond hard spheres due to their softness, especially at high concentrations [2]. We focus on highly concentrated poly(N-isopropylacrylamide) (pNIPAM) microgels and their volume transition as a function of temperature and hydrostatic pressure [3] and their form factors in highly overpacked states with effective volume fractions above random close packing. SANS and confocal microscopy measurements show that the particles shrink to some extent and interpenetrate in very densely packed suspensions. The SANS studies were carried out using contrast matching methods allowing the direct measurement of the form factor at very high concentrations [4]. The confocal microscopy study was done with particles dyed with two fluorescent dyes to allow the observation of particle overlap via color discrimination. Furthermore, small-angle X-ray scattering investigations of the formation and structure of crystal in dense pNIPAM suspensions are presented and compared to expectations from theoretical work and simulations [5] as well as the behavior of hard spheres.

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Spontaneous formation of finite-size colloidal aggregates

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An overview is given of finite-size structures formed by colloids or macromolecular objects. These structures can be stabilized by electrostatics, geometry ('patchy interactions'), or both. In particular, I will address: (1) two-dimensional structures of polyoxometalates (POMs) and apoferritin [1]; (2) a new class of solid-stabilized emulsions [2]; and (3) colloidal molecules with well-defined bond angles [3]. As relevant to (1) and (2), it will be argued that the relatively long-range nature of electrostatic interactions as well as the entropy associated with ionization are determining factors in stabilizing finite-size structures.

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Packings of soft colloids

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The ever broader palette of micro- to nanometer-size particles with pronounced softness has changed the way we think about structure formation in colloids. Polymer microspheres, hydrogel particles, star polymers, dendrimer micelles, etc. all exhibit a considerable degree of deformation or interpenetration at large densities where the soft interparticle repulsion is more prominent than in the fluid phase. What are the main qualitative features of the phase diagram of soft spheres? How are the details of the potential reflected in the phase sequence? We review the experimental studies as well as the theoretical predictions, and we discuss the unifying aspects of both observations and models. In particular, we focus on particles with core-corona architecture and on the various variants of the penetrable sphere potential as the simplest model of soft colloids.

Session 6:
Films, foams, surfactants, emulsions, aerosols

Structuring nanoemulsions

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Long-lived metastable oil-in-water nanoemulsions having controlled droplet sizes down to micellar dimensions can be produced through a combination of high-flow emulsification and evaporative ripening. Condensation, separation, and recirculation of a low molecular weight oil component provide a green process that eliminates the undesirable potential impact of solvent release. Self-assembly of viral capsid protein around nanodroplets that are as small as wild-type virions yields virus-like droplets, a platform for displaying proteins in ordered and disordered dense states. Alternatively, by tuning the molecular properties of synthetic block copolypeptides that have hydrophilic and hydrophobic segments, it is possible to form sub-100 nm double water-in-oil-in-water nanoemulsions that can carry both oil-soluble and water-soluble cargos. Structuring nanoemulsions through a combination of molecular design and physical processes is yielding advanced out-of-equilibrium soft matter systems.

Small matters: a soap opera of SDS, oil and water at the nanoscopic oil droplet/water interface

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Surfactants such as sodium dodecylsulphate (SDS) consist of a hydrophobic and a hydrophilic part. The mixing of the hydrophilic part with water and the mixing of the hydrophobic part with oil is lowering the interfacial tension on planar oil/water interfaces. It is commonly expected that interfacial tension lowering should also take place on the interface of nanoscopic oil droplets in water. Surprisingly, nonlinear light scattering [1] experiments show otherwise. In these experiments we have measured the unique and exclusive interfacial response of SDS surfactant [2], hexadecane oil [3] and water [4] at the interface of nanoscopic oil droplets in water. We have measured both the molecular conformation of the mentioned species, as well as the interfacial adsorption isotherm of SDS. We find that the interfacial density of adsorbed SDS is at least one order of magnitude lower than that at a corresponding planar interface [2]. The derived maximum decrease in interfacial tension is only 5 mN/m, instead of the 40 mN/m that is found at the equivalent planar interface. The resulting molecular conformation of oil and surfactant indicates that the hydrophobic part of the surfactant does not appear to interact with the oil. Further measurements on the neat oil-water interface, in combination with zeta potential measurements show that the average interfacial structure of water at the surfactant-free droplet interface is identical to the water orientation on a negatively charged oil/droplet water interface. There is, however, no evidence of OH-adsorption.

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Formation of molecular clusters and aerosol particles

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Gas to liquid phase transitions are important processes in materials science, fluid dynamics, aerosol physics and atmospheric science including cloud microphysics and chemistry. The recent decade of atmospheric observations has demonstrated nucleation to be a frequent phenomenon in the global atmosphere [1]. Observations suggest that nucleation and condensational growth are uncoupled [2]. Therefore the activation mechanism of small clusters is of vital importance. Here we are presenting some of our recent studies of nucleation and condensation processes at the Vienna expansion chamber system [3]. Measurements of drop growth kinetics provided a direct determination of the strongly debated mass accommodation coefficient for water vapour [4]. Experiments on heterogeneous nucleation in n-propanol vapour allowed for the first time to bridge the scale from molecular clusters to nanoparticles [5]. The onset vapour supersaturations required for activation of nanoparticles were found to be well below the Kelvin prediction. This observation is particularly important in connection with the detection efficiency of Condensation Particle Counters. Furthermore, for charged seed particles an enhancement of heterogeneous nucleation and a significant sign preference were observed. Studies of the temperature dependence of heterogeneous nucleation resulted in unexpected behaviour [6]. Recently we became interested in the heterogeneous nucleation on single ion molecules. Evaluations based on the nucleation theorem enabled us to obtain the size of critical clusters and we found satisfactory agreement with the Kelvin-Thomson equation.

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Session 7:
Confined fluids, interfacial phenomena

Ab-initio simulations of water at ambient conditions and under confinement

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The first principles description of the properties of liquid water is an ongoing challenge, originating from the presence of several different bonding configurations which are not equally well described by any of the known density functionals. We will discuss results for pure water and water confined within non polar surfaces obtained with ab-initio simulations using several local and non local density functionals, and we will use these results to highlight the major challenges involved in the simulation of hydrogen fluids from first principles.

Biomembrane shape and volume dynamics to the limit of fractal ruptures

Owe Orwar

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Organelles are nano-scale, pleiomorphic systems with a capacity for shape changes that are essential for their function as exemplified in mitochondrial biogenesis. In these systems, transport, mixing, and shape changes can be achieved at or very close to thermal energy levels. In further contrast to macroscopic systems, mixing by diffusion is extremely efficient, and the kinetics of embedded reactions can be controlled by shape- and volume changes. The coupling between shape changes, and chemical activity is often strong, and cases will be presented where chemistry affect reactor geometry, where reactor geometry affect chemistry, and cases where the two properties feed back on each other in self-regulating systems. We will show several non-intuitive and fascinating dynamic properties in a variety of artificial systems including front propagation in reaction-diffusion networks consisting of nanotube-conjugated containers, oscillatory behavior for reversible reactions in volume-fluctuating systems, and filtering of chemical signals in small networks. Using volume fluctuations in mitochondria as an example, we show that the rate of product formation of an enzymatic reaction can be regulated by simple volume transitions. Finally, we will report on a new rupture mechanics in bilayer membranes spreading on solid supports resembling the double bilayer membranes of mitochondria: in one instance fingering instabilities were seen resulting in floral-like pores and in another, the rupture proceeded in a series of rapid avalanches causing fractal membrane fragmentation. The intermittent character of rupture evolution and the broad distribution in avalanche sizes is consistent with crackling-noise dynamics. Such noisy dynamics appear in fracture of solid disordered materials, in dislocation avalanches in plastic deformations and domain wall magnetization avalanches. We also observed similar fractal rupture mechanics in spreading cell membranes.

Adsorption and phase transitions of fluids in confinement: In-situ studies with X-rays, neutrons and light

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Mesoporous silica materials with cylindrical pores of some nanometres in diameter on a highly ordered hexagonal pore lattice are used as model systems to assess the behaviour of fluids in confinement experimentally. Synchrotron radiation based small angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) are very powerful tools to investigate in-situ liquid film formation and capillary condensation of fluids as well as their freezing and melting in these systems. Combined with in-situ spectroscopic techniques such as Raman scattering, these methods can for instance be uniquely combined to shine new light on the phase behaviour of water in strong confinement.

Besides its influence on the phase behaviour, confinement induces strong interaction of the fluids with the solid pore walls, which manifest themself in a fluid pressure dependent, non-monotonous deformation of the solid host material. This deformation can be monitored in-situ by measuring the pore lattice strain with X-ray diffraction, allowing for instance to obtain nanomechanical properties of the materials. The basic mechanisms of the adsorption induced deformation can be understood by combining fundamental principles of fluid thermodynamics with solid mechanics.

Session 8:
Supercooled liquids, glasses, gels

Manipulating liquid structure with pressure

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Pressure is a powerful modifier of structure. In addition to inducing substantial changes in the local molecular arrangements in the liquid state, it is also capable of fundamentally altering the character of molecules themselves. In terms of characterising these changes in structure, diffraction is a powerful tool that spans all of the relevant length scales a liquid. Early in situ high-pressure diffraction studies of glasses included synchrotron x-ray studies of the structure of SiO_2 glass. In recent years, this approach has been extended with an emphasis on not only reaching higher pressures and temperatures, but also achieving higher quality data. In addition, we have made substantial progress towards developing high-pressure neutron diffraction capability in order to examine how light, molecular liquids respond to compression. In this overview, the development of high-pressure diffraction from liquids and amorphous materials will be outlined, including work on H_2O as well as our recent diffraction studies of liquid ammonia and ammonia-water mixtures.

K8.2

LH 28
Wed 7
10:00

The liquid-liquid phase transition in simulations of supercooled water: local order parameters, mixturelike behavior, and glass-liquid coexistence

Peter Poole

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In simulations of a waterlike model (ST2) that exhibits a liquid-liquid phase transition, we examine a number of structural local order parameters for their ability to distinguish the low density liquid (LDL) from the high density liquid (HDL). We thereby test for the occurrence of a thermodynamic region above the liquid-liquid critical temperature in which the liquid can be modeled as a two-component mixture. We find that the best choice is to assign each molecule to one of two species based on the distance to its fifth-nearest neighbor. We then evaluate the concentration of each species over a wide range of temperature and density. Our concentration data compare well with mixture-model predictions based on a modified regular solution theory in a region between the liquid-liquid critical temperature and the temperature of maximum density. Fits of the model to the data in this region yield accurate estimates for the location of the critical point. We also show that the liquid outside the region of density anomalies is poorly modeled as a simple mixture. Below the critical temperature, local order parameters facilitate the visualization of LDL-HDL coexistence, including under conditions of glass-liquid coexistence, where the HDL phase remains a liquid, whereas the LDL phase has become an amorphous solid on our computational time scale.

M. Cuthbertson and P.H. Poole, Phys. Rev. Lett. **106**, 115706 (2011).

Amorphous ices - the glassy states of water: the calorimetric glass-liquid transition of HDA

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The discovery of high- (HDA) and low-density amorphous ice (LDA) [1] prompted the question whether this phenomenon of polyamorphism is connected to the occurrence of more than one supercooled liquid. Alternatively, amorphous ices have been suggested to be of nanocrystalline nature, unrelated to liquids. In case of LDA the connection to the low-density liquid (LDL) was inferred from several experiments including the observation of the calorimetric glass → liquid transition at ambient pressure [2], whereas for HDA experimental evidence for a thermodynamic connection to the high-density liquid (HDL) has been missing so far.

We here present calorimetric measurements on HDA, showing for the first time that HDA transforms into a liquid upon heating even at ambient pressure. Differential scanning calorimetry (DSC) is an established experimental method to investigate vitrification and devitrification transitions between glasses and liquids. Using a relaxed form of high-density amorphous ice [3, 4] we detect the glass → liquid transition HDA → HDL as a sudden increase in heat capacity. Additionally we repeatedly cycle between the ultraviscous high-density liquid state HDL and the non-crystalline solid state HDA. This switching between solid-like and liquid-like behaviour confirms the existence of an ultraviscous high-density bulk liquid at ambient pressure. These findings strengthen the two-liquid theories of water.

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Session 9: Non-equilibrium systems, rheology, nanofluidics

Shear banding and related instabilities in entangled polymers

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Shear banding is now well established in emulsions, pastes, surfactant solutions, colloidal suspensions, and liquid crystalline materials. The variety and range of these phenomena continue to astonish. Arguably the first prediction of shear banding was the Doi-Edwards theory for entangled polymers, in the 1970s. However, it took until the 2000s before convincing evidence of banding was established in polymer solutions, by which time the theory and understanding of the dynamics of entangled polymers had advanced considerably. I will discuss how the new experimental and theoretical results in this area (shear banding, edge fracture, etc) have helped us understand (1) the dynamics of entangled polymeric materials (including wormlike micelles), and more generally (2) structure formation, instabilities, and dynamics of viscoelastic shear banding materials with very strong elastic behaviour.

[Work performed in collaboration with JM Adams (Surrey), OS Agimelen (Leeds), SM Fielding (Durham), and S Skorski (Leeds)].

Effects of medium viscoelasticity on particle dynamics and structures in suspensions

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Hydrodynamic forces play a central role in suspension mechanics and rheology. For suspending media with Newtonian properties, the hydrodynamic effects are fairly well understood. However, when particles are dispersed in a fluid with a complex rheological behaviour, there are some intriguing differences to be observed. A long standing observation is that particles in viscoelastic matrices, such as polymer solutions, will form particle chains in shear flow even at concentrations which would be considered dilute in a Newtonian matrix [1,2]. In some other cases, suspensions will exhibit shear thickening at extremely low volume fractions. An understanding of the changes in the hydrodynamic forces acting upon particles suspended in a range of viscoelastic properties will be discussed. The effect of the suspending fluid rheology on the motion of single particles (rotation and migration), the interactions between particles and the mechanisms by which particle necklaces and sheets form will be discussed by comparing experiments with recent simulation results [3,4]. To evaluate the effects of differences in rheological properties of the suspending media, fluids have been selected which highlight specific constitutive features, including a reference Newtonian fluid, a single relaxation time wormlike micellar surfactant solution, a broad spectrum shear-thinning elastic polymer solution and a constant viscosity, highly elastic Boger fluid. Experiments using video-microscopy and rheology will be compared to simulation results using a finite element method.

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Session 10:
Biofluids, active matter

Control of biopolymer network elasticity through architecture and molecular-motor activity

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Much like the bones in our bodies, the cytoskeleton consisting of filamentous proteins largely determines the mechanical response and stability of cells. In addition to their important role in cell mechanics, cytoskeletal networks have also provided new insights and challenges for polymer physics and rheology. There is increasing evidence that the network response of these systems is governed by the compliance and dynamics of the cross-links, many of which are transient in nature. Here we study the effects of both local network architecture and dynamic cross-linking in disordered fibrous networks. In the cell, biopolymer gels are far from equilibrium in a way unique to biology: they are subject to active, non-thermal internal forces generated by molecular motors. We also describe recent theoretical and experimental results on active networks in vitro that demonstrate significant non-equilibrium fluctuations due to motor activity.

K10.2

SCH
Fri 9
16:00

Bacteria as active colloids

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I will review the physics of suspensions of motile bacteria as active colloids. In particular I will examine the behaviour of such suspensions with added non-adsorbing polymer, causing a depletion attraction between the cells. Experiments show that the added polymer is still able to cause phase separation, but at a higher concentration. This can be interpreted as the motile bacteria having a higher 'effective temperature'. Pre-transition clusters rotate coherently - they are self-assembled 'motors'. I will also introduce a new technique for the high-throughput characterisation of the motility of motile colloids (bacteria or synthetic), and demonstrate the use of this technique in a study of the effect of motile bacteria on the diffusivity of non-motile cells in the same suspension.

Selected Oral Lectures

Session 1:
Ionic and quantum liquids, liquid metals

Transverse excitations in liquid Sn

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In 1973, pioneering molecular dynamics (MD) simulations carried out by Levesque et al. [1], predicted the existence of transverse acoustic (TA) excitation modes in simple liquid systems. However, they were not detected by inelastic scattering experiments. Thus, it was considered that the TA modes in simple liquids could not be experimentally observed. Recently, the TA modes were observed by a careful inelastic x-ray scattering (IXS) experiment on liquid Ga [2]. An orbital-free ab initio MD simulation clearly supported this finding. From the detailed analysis for the $S(Q,\omega)$ spectra, a lifetime of 0.5 ps and the propagating length of 0.5 nm could be estimated for the TA modes. These may correspond to the lifetime and size of cages formed instantaneously in liquid Ga.In order to determine if the TA mode may be detected more generally in liquid metals, we carried out IXS experiments and ab initio MD simulation on liquid Sn near the melting point. The experiment was performed using high energy resolution IXS spectrometer installed at BL35XU/SPring-8. The ab initio MD calculation was based on the density functional method with 64 Sn atoms. The simulation was performed for 30,000 steps with a time step of 3.6 fs. TA excitation modes were observed in liquid Sn, and the excitation energies are, again, in good agreement with the results of the MD simulation. By comparing current correlation spectra between the experimental and theoretical results quantitatively, we concluded that the TA mode are detected through the quasi-TA branches in the LA current correlation spectra. In the presentation, we will show detailed results of the data analysis, and discuss microscopic dynamics of liquid Sn in relation to cage effects and microscopic elastic properties.

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Ions at air-water interface: surface tensions and surface potentials of electrolyte solutions

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Availability of highly reactive halogen ions at the surface of aerosols has tremendous implications for the atmospheric chemistry. Yet neither simulations, experiments, nor existing theories are able to provide a fully consistent description of the electrolyte-air interface. In this talk a new theory will be presented which allows us to explicitly calculate the ionic density profiles, the surface tension, and the electrostatic potential difference across the solution-air interface [1,2]. The theory takes into account both ionic hydration and polarizability [3]. The theoretical predictions are compared to experiments and are found to be in excellent agreement. Finally, the implications of the present theory for stability of lyophobic colloidal suspensions will be considered [4], shedding new light on one of the oldest puzzles of physical chemistry the Hofmeister effect.

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Liquid-vapor transition in a symmetric binary mixture of charged colloids

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Binary mixtures of equal-sized hard spheres interacting via Yukawa potentials, repulsive between like and attractive between unlike molecules, can be taken as a model of a dispersion of two charged colloidal species in an electrolyte solution. In the limit of zero screening, one recovers the restrictive primitive model (RPM) of a Coulomb gas, which is known to exhibit peculiar properties, such as a very low critical density and a strongly asymmetric coexistence curve. The critical behavior of this model, namely, whether it would belong to the Ising universality class or rather would remain mean-field-like even asymptotically close to the critical point, was debated for a long time, and eventually settled in favor of Ising criticality only by numerical simulation. In this work the hierarchical reference theory (HRT) is applied to a symmetric mixture of charged Yukawa spheres. We employ the smooth cut-off formulation of HRT, which is very well suited to Yukawa potentials, and already proved to be quite accurate in the one-component case. The critical point and phase diagram for different values of the screening parameter are compared with simulation results. Interestingly, the renormalization-group structure of HRT enables one to ascertain that the critical behavior does indeed remain Ising-like even in the unscreened limit, thereby providing a theoretical support to the evidence from simulation. The issue of the crossover to the asymptotic Ising scaling is also addressed.

O1.4

LH 28
Fri 9
16:00

Soft-disk bosons: a minimal model for supersolidity

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Using exact numerical techniques, a system of Bose soft-disks in two dimensions is studied. This can be considered as the quantum version of classical systems of repulsive particles displaying crystalline cluster phases at sufficiently high densities. The low-temperature phase diagram is explored, and it is shown that a phase, called supersolid, displaying both a finite superfluid fraction and a cluster crystal structure exists within a range of the model parameters. The excitation spectrum of the system in the various phases is studied: an additional acoustic mode, peculiar to the supersolid, is found. We believe that these properties are common to a wide range of Bosonic system interacting via repulsive bounded potentials giving rise to clustering instability, therefore our system can be considered a ”minimal model” for continuous-space supersolidity.

Accurate force fields from ab-initio simulations: the case of aqueous ions

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The development of classical force fields for aqueous ions is a long-standing issue, due to their importance in many fields. Specific effects, i.e. the effect of the chemical nature of the ion, play an important role e.g. on DNA solvation [1] and on the sorption of ions onto mineral surfaces [2]. Molecular dynamics simulations are an effective tool in the analysis of the chemical and physical properties of solvated ions in solutions [3]. However, the reliability of their predictions depends on the quality of the force field used. We discuss here a method to derive a force field from ab-initio calculations, based on the force-fitting procedure [4]. Some of the parameters are fitted to ab-initio forces while others are directly calculated using maximally localized Wannier functions [5,6]. After describing the method, we illustrate its application to aqueous chloride, alkaline (Li+, Na+, K+, Rb+ and Cs+) and alkaline-earth (Mg2+, Ca2+ and Sr2+) ions. We validate the force field, by comparing its predictions to experimental structural (radial distribution function and EXAFS spectrum), dynamical (diffusion coefficient) and thermodynamical (Gibbs free energy of hydration) properties. Attention was also paid to ion-ion interactions so that the force fields are also able to reproduce crystalline structure of the corresponding series of chloride compounds.

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Session 2:
Water, solutions and reaction dynamics

Supercooled water: simulation and experiment

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In the 1970's, Angell and coworkers presented strong evidence that the compressibility along isobars seems to diverge in the supercooled region of water. In 1992, Poole et al. proposed the existence of a liquid-liquid critical point (LLCP). Certain experiments seem to support the existence of the LLCP but there is not yet a conclusive experimental evidence. In this way, computer simulation may be of great help. Since simulation results are based on approximate water models, some checking is required to demonstrate that the model represents the behaviour of real water. Recent experimental work allows for the first time to check the predictive ability of the models in the region where the LLCP is expected to appear. The comparison of these experimental results with the predictions for the TIP4P/2005 model show an excellent agreement[1]. Thus, it should be expected that the simulation results for this model are close (quantitatively) to those of real water. We have carried out extensive simulations with this model to locate the line of compressibility maxima (Widom line) and the LLCP[2]. The Widom line has a negative slope in a p-T diagram and approaches progressively the line of density maxima (TMD) and, eventually, both lines converge at negative pressures. It is seen that the locus of the TMD retraces at the crossing point. This fact has important consequences because it has been demonstrated from thermodynamic considerations that a reentrant TMD line cannot reach the liquid-vapor spinodal and, thus, the latter cannot be retracing. Besides, beyond the crossing point between the Widom line and the TMD, it should appear a line of compressibility minima. All of these theoretical predictions have been confirmed and numerically evaluated in our simulations of the TIP4P/2005 model[3].

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A transferable model for water

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The two most frequently used models of water, TIP3P and SPC/E, form false geometries of gas phase clusters. [1] We have shown that this problematic behavior is also present in their many-body structure of ambient liquid water. [2] For correct results the position of the negative charge for classical models should be shifted from the oxygen atom towards the hydrogen atoms. [2] We developed a new model for the water molecule [3] which contains only three Gaussian charges. Using the gas phase geometry, the dipole moment of the molecule matches, the quadrupole moment closely approximates the experimental values. The negative charge is connected by a harmonic spring to its gas-phase position. The polarized state is identified by the equality of the intermolecular electrostatic force and the spring force acting on the negative charge. In each timestep the instantaneous position of the massless negative charge is determined by iteration. Using the technique of Ewald summation, we derived expressions for the potential energy, the forces, and the pressure for Gaussian charges. [3] Our model is capable to provide good estimate for the properties of gas clusters, ambient water, hexagonal ice, ice III, ice VI, and several ice VII phases. [3,4] The high-pressure phases are modeled by using two simple exponentials with r^{-6} attractions and a switch function. One of the exponentials represents the repulsion under low pressure, the other is the repulsion under high pressure. The switch function varies between 0 and 1 and portions the two repulsions among the individual particles. The argument of the switch function is a virial-type net force acting on the molecule. [4]

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Water proton's environment: a new water anomaly at atomic scale?

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We find, by means of a Deep Inelastic Neutron Scattering (DINS) experiment, a significant excess of proton mean kinetic energy, E_k, in supercooled water, compared to that measured in stable liquid and solid phases. The observed excess of proton mean kinetic energy, with respect to theoretical predictions and measurements in water stable liquid and solid phases, points to a possible link between the anomalous temperature dependence of water density and the temperature dependence of E_k. In particular, E_k shows a maxima at 277 K, the temperature of the maximum density of water. This anomalous behavior is confirmed by the shape of the measured momentum distribution, thus supporting a likely occurrence of ground state quantum delocalization of a proton between the oxygen atoms of two neighboring molecules. These results strongly suggest a transition from a single-well to a double-well potential felt by the delocalized proton, with a reduced first neighbor O-O distance, in the supercooled state, as compared to ambient condition. New DINS data on D_2O provide evidence for isotope quantum effects in the proton single particle dynamics along the hydrogen bond. These DINS data support the observation that even small changes in the short range environment of a water proton have strong influence on its quantum behavior.

Order, entropy and water-like anomalies in tetrahedral liquids

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Tetrahedral liquids can display a number of liquid-state anomalies in comparison to simple liquids, such a rise in density on isobaric heating and an increase in molecular mobility on isothermal compression. Using molecular dynamics simulations, the interplay between short-range orientational and pair correlation order in such liquids is compared for three different categories of tetrahedral liquids: (a) water (b) ionic melts (SiO_2, BeF_2, GeO_2) and (c) liquid phases of Group IV elements (C, Si and Ge). By studying the evolution of thermodynamic and structural anomalies as the degree of tetrahedrality is tuned within the Stillinger-Weber (SW) family of liquids, it is shown that water-like anomalies emerge at intermediate degrees of tetrahedrality but are absent in the low- and high-tetrahedrality limits. In the specific case of water, we consider both atomistic and coarse-grained models of water to understand how the order-entropy-mobility relationships characteristic of tetrahedral liquids influence bulk liquid properties as well as hydration.

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Heat capacity measurements of water at negative pressure

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Liquid water exhibits many anomalous properties. Despite extensive study, the origin of these anomalies remains unclear. Among the most intriguing of these properties are the measured divergences in thermodynamic and dynamic parameters of liquid water in the supercooled state [1]. Several observations motivate the pursuit of analogous measurements in the stretched, superheated state of liquid water: 1) there is a dearth of experimental data of any type in this regime [2], 2) theoretical [3] and computational [4] studies point to the possibility of unusual features in the phase diagram at negative pressures, and 3) controversy remains about the locations and shapes of the kinetic stability limit and the spinodal that bound this metastable regime [5]. In this presentation, we will report on our measurements of the heat capacity of water in this stretched regime. Our method exploits the metastable equilibrium between liquid water and sub-saturated vapors through an organic hydrogel membrane [6]. This technique allows for macroscopic volumes of liquid water to be put into a stretched state at well-defined temperature and chemical potential. We will present heat capacity measured in such a system and compare with predictions based on extrapolations of an empirical equation of state. Finally, we will conclude with a discussion of the relevance of these measurements to the global understanding of water's thermodynamic properties.

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Relationship between the phase diagram, the glass-forming ability, and the fragility of a water/salt mixture

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Water is known to be an exceptionally poor glass former, which is a significant drawback in the low-temperature storage of food and biomatter. This is regarded as one of the anomalous features of water, but its link to other anomalies remains elusive. We experimentally show that the glass-forming ability and the fragility of a water/salt mixture is closely related to its equilibrium phase diagram [1]. The relationship found in this study can naturally be explained by consistency between local tetrahedral order stabilized by hydrogen bonding and the equilibrium crystal structures. The key underlying concept is frustration between crystallization and local tetrahedral ordering, which we propose controls both glass-forming ability and fragility [2,3]. Relying on the same role of salt and pressure, which commonly breaks tetrahedral order, we may apply this finding in a water/salt mixture to pure water under pressure. This scenario not only explains unusual behavior of water-type liquids such as water, Si and Ge under pressure, but also may provide a general explanation on the link between the equilibrium phase diagram, the glass-forming ability, and the fragility of various materials.

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Second generation Car-Parrinello molecular dynamics: theory and application to the liquid/vapor interface

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A new computational method [1] to accelerate density functional theory-based ab-initio molecular dynamics simulations is presented. In the spirit of the Car-Parrinello [2] approach during the dynamics the electronic wavefunctions are not self-consistently optimized. However, in contrast to the original scheme, large integration time steps can be used. By this means the best of the Born-Oppenheimer and the Car-Parrinello methods are unified, which not only extends the scope of either approach, but allows for ab-initio simulations previously thought not feasible. The effectiveness of this new approach is demonstrated on liquid water at ambient conditions [3], and on the corresponding liquid/vapor interface [4].

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On a use of negative pressures and cavitation to create motion in plants

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Negative pressures are used by trees to move water from roots to leaves. Unfortunately this is at risk for plants when water is lacking. Here we present another beautiful example taken from plants where cavitation is not a drawback but the triggering mechanism of a fast motion: the use of water under negative pressures by ferns. In these organisms, the reproductive particles (spores) are ejected at a speed around 10 m/s in air. The mechanism consists in the fast released of a spring-like structure, the sporangium, after its opening due to dehydration. Thirteen cells constitute the sporangium's annulus that surrounds the spores over 500 microns. Through a thin membrane, water inside these cells evaporates and due to cohesive forces, it imposes strong stresses on the annulus which get deformed. When the negative pressure in the cells can no more be sustained, violent nucleation of cavitation bubbles leads to the fast closure of this natural catapult. We have studied the mechanism of opening, bubble nucleation and closing using high speed imaging. From our model, we have determined that the negative values reached for the water pressure in the cells that can be of the order of – 100 bar. We also show here how cavitation is used to generate a global motion of the structure.

Relationship between structural fluctuations and dynamical disorder in water: an explanation for the non-Arrhenius behavior of cold water reorientation

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In this contribution, we study the water reorientation mechanism and dynamics below room temperature down to the supercooled regime, where it exhibits a non-Arrhenius behavior, with an increasing activation energy at lower temperatures [1, 2]. Based on molecular dynamics simulation results in quantitative agreement with the available experimental data (femtosecond infrared anisotropy [3, 4], NMR [5], SAXS [6]), we find that the jump reorientation mechanism determined at room temperature and involving large amplitude jumps [7] remains the dominant reorientation pathway for water at lower temperatures. We show that the jump kinetics sensitively depends on the local water structure, as measured through the Voronoi cell sphericity. The distribution of such local structures is unimodal at all investigated temperatures, and no evidence is found of two distinct water structures in equilibrium. Our results suggest that the non-Arrhenius behavior is not due to enhanced structural fluctuations at low temperature. Through a kinetic model, we establish the origin of the broadening distribution of jump rate constants at low temperature. The resulting increasing dynamical disorder can simultaneously explain the non-Arrhenius behavior of the reorientation dynamics and the non-exponential anisotropy relaxation.

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O2.10

LH 28
Tue 6
17:10

Time-resolved laser spectroscopy on bulk and confined water

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Despite the paramount importance and the continuous research effort, water remains a cryptic liquid. The water anomalies did not find a complete explanation and still a large debate is present about the physic models able to describe them. The supercooled phase remains the benchmark of water understanding where the structural and dynamic features are expected to give clear indications on the elusive water nature. Unfortunately supercooling of bulk water is limited by the homogeneous nucleation limit (- 42 C at atmospheric pressure) so that the direct investigation of deep supercooled bulk water is presently impossible. Differently if water is confined in nano-pores its supercooling can be extended below the nucleation limit giving access to the, so called, water “no-man land”. Nevertheless the diameter of the nano-pores must be very small, typically $<$ 2 nm, in order to avoid freezing. Here an extra issue is added: how much are the properties of confined water different from that of its bulk phase? In this scenario, we studied the water dynamics by new time-resolved laser techniques [1] that enable to achieve new valuable information on water physics, both on the supercooled bulk phase [2] and the nano-confined water [3]. In particular, we will report on the investigation the vibrational and structural dynamics of supercooled bulk and confined water by ultra-fast optical Kerr effect and the results interpretation on the base of mode-coupling theory.

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Quantum effects in water

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Despite the multitude of experimental and theoretical methods applied to water many details of its structure are still poorly understood. Here we introduce the method of oxygen isotope substitution in neutron diffraction as a structural probe of disordered materials. This technique is employed to measure the structure of light and heavy water, thus circumventing the assumption of isomorphism between H and D as used in more traditional neutron diffraction methods. The intra-molecular and inter-molecular O-H and O-D pair correlations are found to be in excellent agreement with path integral molecular dynamics simulations, both techniques showing a difference of 0.5 between the O-H and O-D intra-molecular bond distances and essentially no change in the average hydrogen bond length. The results demonstrate both the effectiveness of our approach and the validity of a competing quantum effects model for water in which its structural and dynamical properties are governed by an offset between intra-molecular and inter-molecular quantum contributions.

Session 3:
Liquid crystals

Biaxial nematic LCs: can polydispersity stabilize them?

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Since its first prediction in the early 70s, the biaxial nematic phase has been considered the "Holy Grail" of liquid-crystal science. The reason for this relies in its higher orientational order with respect to the usual uniaxial nematic, which determines a potential higher efficiency in technological applications. Unfortunately, the development of such applications has been so far forbidden by the very little stability of this liquid crystal phase. In fact, its first experimental observation dates back to just few years ago.In lyotropic liquid crystals, a stable biaxial nematic phase was recently observed in a colloidal suspension of goethite particles with brick-like shape [1]. However, the relative stability of this phase was surprisingly wide, thus contradicting every theoretical prediction. We claim that the reason of this disagreement lies on the oversimplified theoretical assumption that particles have all exactly same size and dimensions.This unexpected result motivates our interest in studying the effect of polydispersity on the stability of the biaxial nematic phase. By using a density functional theory approach at second virial order (Onsager theory) with discretized orientations (Zwanzig model), we analyze the phase diagram of a mixture of brick-like particles. Surprisingly enough, we show that when polydispersity is high enough "rod-like" bricks behave like "plate-like". Moreover, a crossover region between these two regimes exists, when the stability of the biaxial nematic is considerably increased at expenses of the uniaxial. We claim that this effect plays an important role in order to interpret the experimental results. Moreover, in a wider perspective this work offers an important example of using polydispersity to control the phase behavior of colloids.

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Self-assembly of DNA duplexes into polymers chains: theory, simulations and experiments

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End-to-end stacking of short DNA duplexes (monomers) formed by complementary B-form DNA oligomers, 6 to 20 base pairs in length, by virtue of hydrophobic interactions gives rise to nematic and liquid crystal phases [1]. Duplex oligomers aggregate into poly-disperse polymers chains with a significant persistence length. Experiments show that liquid crystals phases form above a critical volume fraction, which depends on the number of basis composing the duplex. We introduce and investigate, theoretically and via numerical simulations, a coarse-grained model of DNA duplexes [2]. Each monomer is represented as a hard quasi-cylinder whose bases are decorated with two identical reactive sites, which may interact with any other reactive site in the system via a short-range attractive interaction, modeled by a square-well potential. We propose a free energy functional which successfully provides a quantitative description of the phase diagram, i.e. of the location of the isotropic and nematic phases, as well as a description of the system structure, e.g. the polymer length distributions. We also compare with previous studies of equilibrium polymerization in dense systems [3-6]. Finally, the comparison of the numerical and theoretical results with the experimental findings concerning the isotropic-nematic phase boundaries allows us to give an estimate of the stacking energy.

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Frustrated nematic order in spherical geometries

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When an ordered material lives in a curved space, topological defects are often required, even in the ground state. The north and south poles in the Earth's globe and the pentagonal units in the soccer ball provide familiar realizations of this fact. When the order is nematic and the space is a spherical shell, a variety of defect structures all comply with the topological constraints imposed by the sphere. However, the arrangement of the defects depends on the geometry and in particular on the shell thickness inhomogeneity. We will present recent experimental results on these questions and elastic energy calculations to rationalize them [1]. In addition, we will also present our recent progress on generating [2] and stabilizing [3] non-zero genus surfaces, which we plan on using as templates to address the interplay between order and topology.

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O3.4

LH 28
Fri 9
10:30

Monodisperse silica bullets: a new model system that enables the real-space study of rod-like colloids

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Rod-like systems are known for their liquid crystal phases, but existing rod-like colloidal model systems do not allow in situ observation of single particles. Therefore, experimental studies of liquid crystal phases have been mainly on the many-particle level, using properties such as birefringence. We developed a new rod-like colloidal model system, consisting of silica bullets that are tuneable in length and aspect ratio, which does allow for real-space 3D observation on the single particle level in highly concentrated dispersions [1]. The anisotropic particles form at the interface of water droplets in a higher alcohol. Using confocal microscopy, we studied the phase behaviour of the rods in gravity and external electric fields, resulting in the observation of isotropic, (para-) nematic and smectic liquid crystal phases quantitatively on the single particle level.

[1] Journal of the American Chemical Society 133, 2346 (2011).

Molecular manipulator driven by spatial variation of liquid crystalline order

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Previous studies on liquid crystal systems containing impurities such as colloidal particles have focused on the collective long-range interactions among micron-scale impurities, resulting from elastic distortion of the liquid crystalline order. When the impurity size decreases substantially, the coupling between the scalar nematic order parameter S and the polymer concentration f becomes relevant instead of the elastic interaction mechanism. The coupling between S and f originates from local molecular interaction, but becomes long-ranged because the total polymer concentration is conserved over the whole sample. Here, we propose a novel mechanism in which the spatial variation of S generates a 'force' that transports nano-scale polymeric impurities mediated by the coupling between S and f. We have successfully designed a prototype of a molecular manipulator that transports molecules along spatial variations of the scalar order parameter, modulated in a controlled manner by spot illumination of an azobenzene-doped nematic phase by UV light. We also demonstrate the use of the manipulator for the measurement of the anisotropic diffusion constant of a polymer in a nematic phase. The manipulator can control the spatial variation of the polymer concentration; therefore it shows promise for use in the design of novel hybrid soft materials. However, since the low molecular weight azo dye can freely walk out from the illuminated area by UV light, then the edge of the low order parameter region become diffuse. Recently, we have drastically improved the resolution of the manipulator up to several micron by the polymerization of the azo dye molecules. Thus, we got elemental tools to make a regular arrangement of the functional macro-molecules or nano-particles in the liquid crystals.

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Session 4:
Polymers, polyelectrolytes, biopolymers

Exploring the ”nucleation” of amyloid fibrils with experiments and computer simulations

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Amyloid fibrils are ordered aggregates of misfolded protein. These fibrils are of great interest because of their role in degenerative diseases including Alzheimer’s and Type-2 diabetes. Their physical properties also make them potentially useful in the development of novel materials. It is well known that fibril formation occurs with ”nucleation-like” kinetics in which a long lag phase is followed the rapid appearance of fibrils. However, despite much work, the molecular mechanisms responsible for fibril formation and growth remain unclear. This is particularly important because it is believed that pre-fibril oligomeric species present during the lag time may be the cytotoxic agents responsible for amyloid associated pathologies. Much recent debate has focussed on whether fibril formation is a stochastic nucleation process and the possible role of secondary processes such as fibril fragmentation. We have used a combination of high throughput experiments and computer simulations to investigate in detail the kinetics of fibril formation in bovin insulin. Our experiments reveal different kinetic behaviour in the regimes of high and low protein concentration, as well as stochasticity in the fibril growth rates. Using a series of computer simulation models with different early stage fibril formation mechanisms, we show that this behaviour is not fully explained by any of the current models, but may point to the presence of multiple competing or sequential assembly processes during the lag and growth phases of fibril formation.

O4.2

LH 28
Thu 8
17:30

Nanoscale buckling instability of layered copolymers

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In layered materials, a common mode of deformation involves buckling of the layers under tensile deformation. This undulation of the layers under deformation is well known in smectic crystals, where it arises from the need to keep a constant period of the lamellae. Another mechanism, which is thought to operate in elastic materials from geological to nanometer scales, involves the elastic contrast between different layers. If the material is made of a regular stacking of "hard" and "soft" layers, the tensile deformation is first accommodated by a large deformation of the soft layers. The Poisson effect implies that compressive stress develops in the direction transverse to the tensile deformation axis. The "hard" layers sustain this transverse compression until buckling takes place and results in an undulated structure. In general, elasticity predicts buckling to take place on the largest wavelength compatible with the boundary conditions imposed to the system. We study this generic scenario by means of molecular dynamics simulations, for a material made of triblock copolymers in their lamellar phase. The contrast in elasticity is provided by a different glass transition temperature of the different blocks. The buckling deformation is observed to take place at the nanoscale, at a wavelength that depends on sample size and strain rate. In contrast to what is commonly assumed, the wavelength of the undulation is not determined by pre-existing defect in the microstructure of the material. Rather, it results from kinetic effects, with a competition between the rate of strain and the growth rate of the buckling instability. We propose a simple model for understanding this competition.

Measurement of force generated by the growth of actin filaments

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The actin cytoskeleton is a complex network of proteic filaments directly involved in cellular motility: in a moving cell, the plasma membrane is pushed forward by the formation of actin filaments polymerizing against it. We study this phenomenon with an original experimental set-up based on superparamagnetic colloids that self-assemble into chains when an external magnetic field is applied. Under field, colloids with actin filaments anchored on their surface are pushed apart by the filaments growing in the interspace between them. The observation of this dynamic process allowed us to measure for the first time the force versus velocity transduction profile of a small number of actin filaments [1]. In our model system, the number and the organization of the filaments can be precisely controlled, reproducing different biologically relevant situations. We show how these changes in geometry and structure alter the filaments' response to the applied load and discuss this response in the light of theoretical models for force generation by actin polymerization.

[1] C. Branbour, O. du Roure, E. Helfer, D. Demoulin, et al. PLoS Biol 9(4), 2011

Anomalous diffusion of a polymer chain in an unentangled melt

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Contrary to common belief, the hydrodynamic interactions (HI) in polymer melts are not screened beyond the monomer length and are important in transient regimes. We show that the viscoelastic HI effects (VHI) lead to anomalous dynamics of a tagged chain in an unentangled melt at $t < t_N$ (t_N, the Rouse time). The chain centre-of-mass (CM) mean-square displacement is enhanced (as compared to the Rouse diffusion) by a large factor increasing with chain length. We develop an analytical theory of VHI-controlled chain dynamics yielding negative CM velocity autocorrelation function which quantitatively agrees with our MD simulations without any fitting parameter. It is also shown that the Langevin friction force, when added in the model, strongly affects the short-t CM dynamics which, however, can remain strongly enhanced. The transient VHI effects thus provide the dominant contribution to the subdiffusive CM motion universally observed in simulations and experiments on polymer melts.

Simulation of electrokinetic phenomena with discrete ions and beyond

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Electrokinetic phenomena are very interesting since their range of applications is broad, ranging from polyelectrolye and colloidal electrophoresis over to microfluidic devices like pumps up to DNA translocation through nanopores. Over the last years a plethora of mesoscopic methods have been developed to simulate electrokinetic effects. We present recent progress in the development of discrete ion based simulation methods that extend mesoscopic fluid dynamics methods such as the Lattice Boltzmann Method or Dissipative Particle Dynamics. This allows to take into account ion correlations in vicinity of highly charged interfaces beyond the electrokinetic equations and thus allows to study phenomena beyond the standard model of electrokinetics. In particular we present a method that allows to take dielectric boundary forces into account[1]. As an application of this method we will discuss the translocation process of a simple polyelectrolyte through a synthetic nanopore [2]. When the Debye length is small with respect to other length scales of the system the electrostatic interaction can be treated implicitly which allows a very efficient calculation of complex phenomena. We present a Lattice-Boltzmann-based implicit treatment that allows to simulate complex effects beyond the capabilities of explicit-ion methods. As an example we present the unusual motion of overall charged neutral object in an electric field[3]. This method allows to study various fancy electrokinetic effects predicted long time ago [4].

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O4.6

LH 28
Thu 8
15:40

Dendrimer cluster crystals

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We study systems of amphiphilic dendrimers of second generation with regards to their predicted capability [1-3] of building stable cluster crystals, by employing monomer-resolved Monte Carlo simulations. By varying parameters according to the predictions made in an coarse-grained level description [1], we artificially create several cluster crystal systems in the computer. Although the predictions are based on the zero-density limit effective pair-interaction, we discover that at sufficiently high densities (and corresponding cluster occupation numbers), cluster crystals remain stable. To put the validity of this result under scrutiny, we further investigate the behavior of the stable systems under several conditions, such as crystal and cluster occupation defects or variations of the pressure. Since spontaneous cluster hopping behavior is too slow to be observed within simulation times, [4] we further investigate the response of the system under forced hopping (i.e., pulling) of single dendrimers through the crystal. In addition we examine the melting behavior of both the whole crystal systems and single clusters as they occur in the crystal under several conditions, as well as the structure and cluster distribution of the associate cluster-forming liquids at lower dendrimer concentrations [5].

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Surface-functionalised nanoparticles: Statics and dynamical properties

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Nanoparticles functionalized by polymers have found biomedical and therapeutic applications. The functionalization by polymers has been used to alter the physicochemical properties of the particular nanoparticle. In the case of viral vectors, e.g., polymer functionalization tunes the biocompatibility, suppressing the binding of antibodies and conferring the nanoparticle with stealth properties. By contrast, the inorganic nanoparticles comprise materials in a form that is not normally encountered in the human body, and polymer functionalization is necessary to ensure biocompatibility. By means of molecular dynamic simulations and density functional theory we try to clarify some of the mechanism driving specific properties, shape and response to the environment of these polymeric materials. The main purpose of the present work is to give a detailed quantitative description of the spherical brush behavior when the radius of gyration of the corona is comparable with the size of the core. A coarse-grained bead-spring model is used to describe the macromolecules, and purely repulsive monomer-monomer interactions are taken throughout, restricting the study to the good solvent limit. The structural characteristics are discussed (density profiles, average end-to-end distance of the grafted chains, etc.) and the potential of mean force between the particles as function of their distance is computed, varying both the radius of the spherical particles and their distance, as well as grafting density and chain length of the end-grafted flexible polymer chains. When the nanoparticles approach very closely, some chains need to be squeezed out into the tangent plane in between the particles, causing a very steep rise of the repulsive interaction energy. Finally we analysed in detail the monomer/polymer dynamics for several values of the surface density and length of the chains. The limit of applicability of the different models and approaches is also discussed.

O4.8

LH 28
Thu 8
10:30

Dendronized polymers investigated by neutron scattering

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A dendrimer is built up by regularly arranged chemical branching units, which form a fractal object. Attached as side groups to a polymer chain, the dendrimers affect the chain stiffness and cross section. Based on neutron scattering investigations, we quantified these changes for dendronized polymers of generation 1 to 5. We also investigated the conformational changes that occur upon charging the side groups and transferring the polymers to aqueous solvents with different ionic strength.

Counter ion distribution and polyelectrolyte structure in dilute solutions seen by anomalous small angle scattering

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Polyelectrolytes are common structures in nature. But the distribution and correlation of counterions around polyelectrolytes is still a challenging problem. In solution only parts of the counterions are dissociated. Due to electrostatic interactions parts of the counterions are condensated to the polymer chain [1]. Anomalous small angle scattering is a feasible method to seperate the resonant signal of appropriate counterions from the nonresonant contributions of the polyion [2]. Rod like polyelectrolytes were investigated sucessfully by this method [3]. Polyacrylic acid is a flexible polyion, widely used for different applications. The Rb^+ counterion distribution around polyacrylic acid with two different narrowly distributed chain lengths is analysed. From the quantitative analysis of the resonant invariant, Rb^+ concentrations were calculated.

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Compression, crumpling and collapse of spherical shells and capsules

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The deformation of thin spherical shells by applying an external pressure or by reducing the volume is studied by computer simulations and scaling arguments. The shape of the deformed shells depends on the deformation rate, the reduced volume V/V_0 and on the Föppl-von-Kármán number γ. For slow deformations the shell attains its ground state, a shell with a single indentation, whereas for large deformation rates the shell appears crumpled with many indentations. The rim of the single indentation undergoes a shape transition from smooth to polygonal that depends on the indentation depth and the Föppl-von-Kármán number. For the smooth rim the elastic energy scales like $\gamma^{1/4}$ whereas for the polygonal indentation we find a much smaller exponent, even smaller than the $1/6$ that is predicted for stretching ridges. The relaxation of a shell with multiple indentations towards the ground state follows and Ostwald ripening type of pathway and depends on the compression rate as well as on the Föppl-von-Kármán number.

Session 5: Colloids

Theory and simulations of designable modular self-assembling materials

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We present a novel theoretical framework to design new experimentally realizable materials with tunable self-assembling properties. Our designable self-assembling system is based on a small set of realistic modular sub-units, which, thanks to the wide range of options offered by state of the art nano-particle manipulation, allow for a direct translation of the theoretical predictions to experiments. Our results point towards the identification of an optimal set of modular sub-units, and introduce a general design procedure [1] necessary to choose a sequence of units that, once bonded into a chain,will spontaneously collapse to a specific target structure. Subsequently, the collapsed chains will themselves self-assemble into complex super structures, again controlled by the same sequence selection criterion. We show how patchy colloidal particles are an optimal choice for the sub-units, as they have proven to posses a rich set of self-assembling properties [2, 3] and allow real space tracking by means of confocal microscopy.

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Phase behavior and effective shape of semi-flexible colloidal rods and biopolymers

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The fd-virus is a semi-flexible virus particle that is often used as an experimental model of colloidal rods. A recent study of thick-thin fd-virus mixtures [1] has shown a diverse range of phase behaviour, with isotropic-nematic, nematic-nematic, and isotropic-nematic-nematic phase coexistence regions found. Due to the fd-virus' long, thin shape and low polydispersity, one would expect the phase diagrams to match those predicted by Onsager theory. However, standard Onsager theory of binary mixtures gives surprisingly poor agreement with experiments [2]. We present a generalized model to describe binary mixtures of semi-flexible rod-like colloids, calculating full phase diagrams for fd-virus mixtures of a range of diameter ratios. By incorporating flexibility we find quantitative and qualitative agreement with experimental results [3]. We explore the effects of particle stiffness on the phase diagram, and show how that the observed phase behaviour becomes richer upon increasing the flexibility of the particles. Our model can also be used to calculate the state-point dependent effective shape of the rods, which we find to vary widely throughout the phase diagrams.We apply our model also to single semi-flexible polymers dissolved in an fd-virus solution, which experimentally have been shown to stretch out over the isotropic-nematic transition of the fd-virus [4]. Our model shows that sufficiently stiff polymers will stretch out, and that the effect may be tuned by varying the stiffness of the background solution.

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Self-assembly of magnetic colloids

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Large fraction of colloidal science is recently focused on self-assembly of novel structures. The shape of the particles, their interactions and the kinetics are the main factors determining the types of structures we can observe. Paramagnetic colloids driven by external magnetic fields are easily tunable and feature an extremely rich variety of behavior. Therefore, such systems can provide a valuable insight into the self-assembly process. Here we report experiments that probe assembly of superparamagnetic micrometer size spherical colloids in precessing external fields. In a magic-angle geometry the external fields induce an isotropic attraction between two isolated colloids in bulk, similar to the van der Waals force between atoms. However, the strong many-body polarization interactions among them steer an ordered aggregation pathway consisting of growth of chains, cross-linking, network formation, and consolidation of one colloid thick membranes. We theoretically explain the membrane stability, their elastic and self-healing properties and the observed aggregation pathway. Geometrical confinement provides an additional control over the self-assembly process. We investigate the 2D systems with induced interactions ranging from purely repulsive to purely attractive. We observe curious arrested networks and analyze the kinetics of their formation by first constructing effective pair interactions. We also study the transition from 2D towards 3D in the case of soft repulsive interactions. Finally, we discuss possible applications of our results to the nano and atomic length scales.

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[3] PRL 99 248301 (2007)

Ordered equilibrium structures of patchy particles

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[2] *Instituto de Química Física Rocasolano, Madrid, Spain*

We have investigated the self-assembly scenarios of spherical colloidal particles decorated by four attractive patches of finite extension [1,2]. The positions of the patches on the colloidal surface form the tips of a pyramid, whose lateral extension can be triggered by a geometrical parameter g. Varying g and the external pressure, we identify ordered equilibrium structures that the system is able to form. This is achieved by minimizing the Gibbs free energy at $T = 0$ by an optimization tool based on ideas of genetic algorithms [3]. This optimization strategy copes very well with the large parameter space (defined by the unit cell parameters as well as particle positions and orientations within the unit cell) and the rugged energy landscape. The variety of ordered structures turns out to be very rich. It is governed by a competition between patch saturation (minimizing energy) and packing (minimizing volume): at low pressure values we find rather open structures, realized via staggered honey-comb lattices, bcc-type, or layered structures, all of them being characterized by a high degree of saturated bonds between the patches; at high pressure, on the other hand fcc- and hcp-like, close-packed structures dominate, leaving many patches unsaturated. For a particular patch decoration, which is more elongated than a the tetragonal arrangement, a relatively open bcc-type structure is able to survive until particularly high pressure values. Via Monte Carlo simulations and thermodynamic integration we obtain results for the Gibbs free energy at finite temperature to calculate phase diagrams, including both ordered and disordered phases [4].

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Self-assembly of a colloidal interstitial solid solution with tunable sublattice doping

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Hard sphere mixtures are arguably one of the simplest systems for modelling and explaining the phase behaviour in colloidal, nanoparticle, and atomic systems. Comparisons between theory, simulations, and experimentally realized hard sphere mixtures have provided a wealth of information regarding e.g. nucleation processes, entropy driven crystal formation, and the glass transition. In this work we present a novel phase appearing in colloidal hard sphere mixtures, namely, an interstitial solid solution (ISS). We demonstrate theoretically and experimentally the self assembly of a purely entropic ISS in a binary hard sphere mixture of size ratio 0.3. The ISS phase is constructed by filling the octahedral holes of an FCC crystal of large particles with small particles. We find that the fraction of octahedral holes filled with a small particle can be completely tuned from 0 to 1. Interestingly, this ISS was likely seen but misidentified in previous theoretical and experimental work. We also study the hopping of the small particles between neighboring octahedral holes, and surprisingly, we find that the diffusion increases upon increasing the density of small spheres. The existence of an ISS in such a simple model system demonstrates the possibility of ISSs in many other colloidal and nanoparticle systems.

O5.6

AudiMax
Tue 6
17:30

Self-controlled confinement of nanoparticles in the web of grain boundaries of a colloidal polycrystal

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Composites materials comprising nanoparticles dispersed in a matrix are of great scientific and technological interest, since nanoparticles can enhance dramatically the matrix properties or even impart new functionalities, and because the matrix can act as a template that structures the particles at the nanoscopic level. However, controlling the three-dimensional spatial distribution of nanoparticles in a molecular or macromolecular matrix is a challenging task, as particle segregation usually depends crucially on the surface chemistry of the particles. Here, we present a model hybrid material, obtained by dispersing nanoparticles in a colloidal crystalline matrix, composed of thermoresponsive micelles. Using confocal microscopy, we show that the nanoparticles segregate in a network of thin sheets, in analogy to impurities confined in the grain boundaries of atomic polycrystals. We demonstrate that the size of the colloidal crystallites is tuned by varying independently the nanoparticle concentration (regardless of their composition and surface chemistry) and the crystallization rate, because they both determine the number of critical nuclei during the nucleation process and we quantify our findings using classical nucleation theory. Remarkably, we find that the efficiency of the segregation of the nanoparticles in the grain-boundaries is dictated solely by the typical size of the crystalline grains, due to the fact that the larger a grain can grow, the higher the concentration of the impurities progressively expelled from the crystallites during their growth and eventually trapped in the grain boundary, as we clearly show. Our method provides a general approach for confining nanoparticles in absence of any external field and in a controlled and tunable fashion in a three-dimensional soft colloidal matrix.

Onset of mechanical stability in random sphere packings

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[3] *The University of Edinburgh, Edinburgh, United Kingdom*

Particulate systems are widespread in nature and industry, and display complex packing properties. Their load-bearing properties, especially how they respond to gravity, are poorly understood. In systems as diverse as sand piles and cornflakes, the density of a random particulate pile under gravity depends sensitively on preparation (pouring, shaking, tapping…), but experimentally always falls within a limited range between the so-called random loose- and random close-packed states (denoted RLP and RCP). This behaviour can be reproduced by model sphere systems, which have stable packing fractions $\Phi_{RLP} \simeq 0.55 \leq \Phi \leq \Phi_{RCP} \simeq 0.64$. The microscopic explanation as to why random sphere packings first become stable at such repeatable packing fractions is of fundamental interest. We study the stability of individual particles in real experimental three-dimensional packings, and show that in a large number of experimental random sphere packings larger than but encompassing the range Φ_{RLP}–Φ_{RCP}, a system-spanning stable 'backbone' emerges at a well-defined packing fraction. At this point, individually mechanically stable particles become sufficiently connected to form a globally stable pile. We show that this state is 'overstabilised', in keeping with recent theoretical and simulation results. Using our results for experimental colloidal and granular sphere packings, as well as for simulated spheres, we highlight general aspects of the load-bearing behaviour of random sphere packings.

O5.8

AudiMax
Sat 10
9:40

Particle configurations and gelation in capillary suspensions

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When a small amount (less than 1 of a second immiscible liquid is added to the continuous phase of a suspension, the rheological properties of the admixture are dramatically altered and can change from a fluid-like to a gel-like state. This transition is attributed to the capillary forces of the two fluids on the solid particles and two distinct states are defined: the 'pendular state' where the secondary fluid preferentially wets the particles and the 'capillary state' where the secondary fluid wets the particles less well [1]. This current research investigates the capillary state suspensions in more detail using a computational model to evaluate the lowest energy states of small particle number clusters. These clusters are used as building blocks for the formation of sample-spanning networks within the admixture, where the constituent structures have limited regions of stability based on the wetting angle and volume of the secondary fluid leading to changes in the strength of the network. The influence of the capillary force in the formation of these networks is further substantiated using rheological measurements. For a series of glass bead suspensions with varying particle radii, the expected reciprocal radius scaling of yield stress is found. These mixtures also reduce in strength with increasing temperature (trending with interfacial tension) and are completely reversible if the secondary fluid is removed. Capillary suspensions have numerous technical applications including the formation of tunable, stable suspensions of lyophobic solids. The strong network of particles may be used as a template for the manufacturing of various porous materials, like lightweight ceramics, thermal insulators, or catalyst carriers.

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Surface roughness directed self-assembly of colloidal micelles

Daniela Kraft,[1] Ran Ni,[2] Frank Smallenburg,[2] Michiel Hermes,[2] Kisun Yoon,[3] David Weitz,[3] Alfons van Blaaderen,[2] Jan Groenewold,[1] Marjolein Dijkstra,[2] and Willem Kegel[1]

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Self-assembly of colloidal particles into larger structures bears potential for creating materials with unprecedented properties, such as full photonic band gaps in the visible spectrum. For self-assembly uniform colloids are quite limited as building blocks since their shape is the only control parameter. Much more promising in this respect are colloids with site-specific attractions. Here a novel experimental realization of such "patchy" particles based on surface roughness specific depletion attraction is reported. Colloids with one attractive patch are experimentally shown to assemble into clusters resembling surfactant micelles. Similarities as well as differences between the colloidal model system and molecular surfactants are discussed and quantified by employing computational and theoretical models. The observed extremely long equilibration times reveal a fundamental challenge for self-assembly on the colloidal scale, which needs to be accounted for in the future.

O5.10

AudiMax
Thu 8
10:30

Crystallization in colloids and complex plasmas: similarities and complementarities

Hartmut Löwen

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Colloidal dispersions and complex plasmas are ideal model systems to study nonequilibrium phenomena on the fundamental particle-scale. These two systems share the classical many-body character of strongly coupled systems but differ in their dynamics which is overdamped in the colloidal and almost ballistic in the complex plasma case. While equilibrium freezing behaviour is therefore quite similar for colloids and complex plasmas, nonequilibrium crystallization processes can be vastly different. Using simulations and experiment [1,2], the role of the latent heat for crystallization is emphasized. For colloidal dispersions, the latent heat produced upon solidification is immediately transported away by the solvent, but it is kept locally for complex plasmas leading to a completely different crystallization scenarios.

[1] K. R. Sutterlin, A. Wysocki, A. V. Ivlev, C. Rath, H. M. Thomas, M. Rubin-Zuzic, W. J. Goedheer, V. E. Fortov, A. M. Lipaev, V. I. Molotkov, O. F. Petrov, G. E. Morfill, H. Lowen, Phys. Rev. Letters 102, 085003 (2009).
[2] A. Wysocki, C. Rath, A. V. Ivlev, K. R. Sutterlin, H. M. Thomas, S. Khrapak, S. Zhdanov, V. E. Fortov, A. M. Lipaev, V. I. Molotkov, O. F. Petrov, H. Lowen, G. E. Morfill, Phys. Rev. Letters 105, 045001 (2010).

Structural and dynamic properties of concentrated suspensions of ellipsoids

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[2]INSA de Lyon, Villeurbanne, France
[3]Physical Chemistry, Lund University, Lund, Sweden

Despite extensive numerical simulations [1, 2], limited systematic experimental data is currently available on the volume fraction dependence of the structural and dynamic properties of non-spherical colloids and the onset of dynamical arrest. This is partly due to the difficulties of finding appropriate model systems. We have probed the morphology, dynamics and structural ordering of nearly monodisperse ellipsoidal nanoparticles, with an average aspect ratio of 2.7 by a combination of scattering and microscopy techniques in an extended range of volume fractions, Φ. The particles are obtained by growing a uniform silica layer on a spindle-type hematite core [3], and then fully removing the core. This yields silica capsules of moderate negative buoyancy and reduced turbidity, retaining the shape of the initial core-shell system. At low volume fractions, the dynamics (translational and rotational diffusion) as measured by dynamic and depolarized dynamic light scattering was found to be reproduced quantitatively by the theoretical predictions for ellipsoids with linear dimensions given those determined from TEM [4]. The evolution of the structure factor S(q) with increasing volume fractions was determined using small-angle X-ray scattering, where volume fractions were determined independently through a combination of thermogravimetric analysis and TEM. The resulting structural correlations are analyzed and compared to numerical simulations [2, 5].

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[3] Ch. Rufier et al. Accepted, Langmuir (2011)
[4] I. Martchenko et al. In preparation (2011)
[5] D. Frenkel et al. Phys. Rev. Lett. 52, 4, 287 (1984)

Design rule for colloidal crystals of DNA-functionalized particles

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[2]Department of Structural and Computational Biology, Max F. Perutz Laboratories, Campus Vienna Biocenter 5, 1030, Vienna, Austria

We report a Monte Carlo simulation study of the phase behavior of colloids functionalized with a few long DNA chains. We find that an important qualitative change appears in the phase diagram when the number of DNAs per colloid is decreased below a critical value. Above this threshold, the system exhibits a normal vapor-liquid-crystal phase diagram, but below it, the triple point disappears completely. In this case, the condensed phase that coexists with the vapor at low temperatures and low osmotic pressures is always an amorphous liquid, and crystallization can therefore only take place under applied pressure. Such behavior is well known for Helium but is, to our knowledge, unprecedented for soft matter. Our simulations thus explain why, in the dilute solutions typically used in experiments, colloids coated with a small number of DNA strands cannot crystallize. We observe that the disappearance of the triple point for low DNA coverage is a direct consequence of the discrete nature of DNA binding and this allows us to formulate a simple rule of thumb to estimate whether a given system of DNA-coated colloids can crystallize.

Cubic crystals from cubic colloids

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[2]*New York University, New York, USA*

We have found that colloidal cubes, driven by tunable depletion forces, crystallize into cubic, lego-like structures with a symmetry set by the size of the depletant polymers [1]. Our colloidal system consists of novel micron-sized cubes prepared by silica deposition on hematite templates, and various non-adsorbing water-soluble polymers as depletion agents. The dynamics of cubic crystal nucleation and growth is directly imaged in situ via optical microscopy. Furthermore, by using temperature sensitive micro-gel particles, the depletion attractions can be fine-tuned which allows observation of reversible melting of cubic crystals. Assisting crystallization with an alternating electric field improves the uniformity of the cubic pattern allowing the preparation of macroscopic (almost defect-free) mosaic crystals that exhibits visible Bragg colors.

[1] Laura Rossi, Stefano Sacanna, William T. M. Irvine, Paul M. Chaikin, David J. Pine and Albert P. Philipse , Soft Matter (2011)

O5.14

AudiMax
Tue 6
16:50

Colloidal analogues of charged and uncharged polymer chains with tunable stiffness

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A quest for colloidal particles with more complex shapes and interactions is fueled by applications in self-assembly, advanced functional materials design, but also by the demand for more realistic model systems for molecular analogues. The assembly of colloids into polymer-like chains would constitute a significant step in the design of colloidal molecules. Here, we present a general methodology to produce model systems of colloidal analogues of (bio-)polymer chains with a tunable flexibility from smaller dielectric-colloids using electric fields and a simple bonding step. The combination of soft repulsions with induced dipolar interactions gives rise to high yields and purity of the permanent bead chains or strings of the original starting particles. We demonstrate that chain conformations can be controlled by manipulating interactions between the particles in a chain through electrostatic repulsions, as in polyelectrolytes, and/or using depletion attractions. Furthermore, our method is used to mimic more complex polymer chains such as block-polymers and a-tactic chains.

Self-assembly of a photonic colloidal crystal: a simulation study

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Patchy particles are promising building blocks for the fabrication of new materials via self-assembly [1]. Recently, triblock Janus particles were rationally designed and built to self-assemble into a two-dimensional Kagome lattice [2], providing a test-case of a complete bottom-up approach to the fabrication of a colloidal structure. We show that the Kern-Frenkel model provides an accurate modeling of these particles [3] and that in three directions, triblock Janus particles are compatible with the formation of a technologically relevant three-dimentional open cubic structure, the photonic tetrastack crystal [4]. The self-assembly of the tetrastack structure is unfortunately hindered by the formation of stacking faults alternating planes of cubic and hexagonal symmetry, a phenomenon analogous to the random stacking of fcc and hcp for hard-sphere colloids; the stacking alters the global symmetry of the self-assembled structures disrupting their photonic properties. Interestingly, this is the same problem that arises in the self-assembly of tetrahedral patchy particles in the diamond structure [5]. Building on the possibilities offered by the surface patterning technique used to realize Janus particles [6], we propose to modify the patch shape, from circular to roughly triangular, to lower the particles symmetry and to suppress the local structure responsible for the hexagonal ordering. We then prove, in silico, that these rationally designed patchy particles readily self-assemble in the desired tetrastack structure.

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[2] Q. Chen, S. C. Bae and S. Granick, Nature **469**, 381–384 (2011).
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A dissimilar patch model with a ”pinched” phase diagram

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[3] Centro de Física Teórica e Computacional, Lisbon, Portugal
[4] Dipartimento di Fisica and CNR-ISC, Rome, Italy

Simple models of patchy particles offer the possibility to investigate with a combination of theoretical and numerical approaches unconventional gas-liquid phase diagrams [1,2]. In this contribution we introduce a microscopic model particles functionalized with dissimilar patches which exhibits self-assembly into chains connected by Y-junctions [2,3]. The model presents both in the theoretical calculations based on Wertheim theory and in extensive numerical simulations a ‘pinched” phase diagram, in which the density of the coexisting liquids, at low temperature, approaches the density of the gas phase. Such pinched phase diagram, originally proposed by Tlusty and Safran in the context of dipolar fluids [4], arises from a subtle interplay between the entropy of chaining and branching and the associated energies. To our knowledge, this is the first model in which the predicted topological phase transition between a fluid composed of short chains and a fluid rich in Y-junctions is actually observed. Interestingly, both theory and simulations suggest that above a certain threshold for the energy cost of forming a Y-junction, condensation ceases to exist. We discuss the relevance of our finding in respect to the longly debated possibility of a gas-liquid critical point [5] in dipolar hard-spheres and other network forming systems.

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[2] J. Russo, J. M. Tavares, P. I. C. Teixeira, M. M. Telo da Gama, and F. Sciortino, Phys. Rev. Lett. **106**, 085703 (2011)
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Stability, phase behavior and dynamics of light-induced colloidal quasicrystals

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[2] *Technische Universität Berlin, Berlin, Germany*

Quasicrystals are non-periodic solids which nevertheless possess long-range positional and orientational order. We study a 2D charge-stabilized colloidal suspension in quasicrystalline potentials with decagonal or tetradecagonal symmetry that in experiments are realized by five or seven interfering laser beams. By using Monte-Carlo simulations, we explore the rich phase behavior of the colloidal particles in the decagonal potentials and analyze the surprising phases that can be found when the colloidal ordering results from a competition of the colloidal interaction and the substrate potential [1]. Further studies using quasicrystalline potentials with both decagonal and tetradecagonal symmetry provide a new insight into the question why many five-fold symmetric quasicrystals have been identified in nature while not a single quasicrystal with seven-fold symmetry has been observed so far [2]. Finally, we study the dynamics of the colloids in response to a phasonic drift. Phasons are unique to quasicrystals and like phonons they are hydrodynamic modes since they do not increase the free energy in the long wavelength limit. The properties of phasons are still intensively discussed in the field. By using Brownian dynamics simulations, we find that in a potential with constant phasonic drift individual particles move in different directions. However, there is a net drift of the colloids that sensitively depends on the direction and velocity of the phasonic drift. Our observations help to get a deeper insight into the properties of phasonic displacements in colloidal as well as in atomic quasicrystals.

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O5.18

AudiMax
Sat 10
9:00

What nucleates the crystal? Perspectives from studies of the hard sphere system

Bill Van Megen[1] and Gary Bryant[1]

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The growing sophistication of computational and experimental techniques has led to an increasingly detailed microscopic picture of the structural evolution of the crystal from the melt. While there is now exquisite detail on the steps by which the rotational symmetry of the fluid phase is broken, the basic question that remains is; what causes this to occur? In anthropomorphic terms one might ask; how do the spheres know that lattice modes comprise a new source of entropy? In endeavouring to answer these questions we consider; (A) Structures precursory to crystal nuclei observed in metastable suspensions of hard spheres. (B) Emergence of a negative algebraic tail in the velocity auto-correlation function (VAF) at the freezing density. In the classical Lorentz gas such decays are caused by the structural memory provided by the fixed scatterers. (C) The observation that the classical (positive) t -3/2 hydrodynamic "tail" of the VAF, a property of the bulk fluid dictated by momentum conservation, is cancelled by the reaction field in the presence of a wall. This results not only in faster algebraic decays, but in the case of motion perpendicular to the wall, the VAF is negative. For a suspended particle to attain Brownian motion, or more generally for a fluid to attain thermodynamic equilibrium, there must be no impediment to the transfer of its instantaneous, thermally activated momentum to the surrounding fluid. It is proposed that the structural precursors present just such an impediment that breaks, locally, the rotational invariance of the diffusing part of the momentum current. Consequences of this proposal vis-a vis crystallization and glass formation are explored.

Session 6:
Films, foams, surfactants, emulsions, aerosols

Photo-actuation of macro- and microfluidic systems

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We have designed a photosensitive surfactant, called AzoTAB, which allows us to modulate surface tension using light. We are implementing this unique molecule for the photo-actuation of macroscopic and microscopic liquid systems. At the macro-scale, we use light to induce interfacial tension gradients between an oil droplet and a water phase containing AzoTAB. This results in light-induced Marangoni flows able to make macroscopic droplets move in a controlled fashion. This phenomenon, which we call the chromocapillary effect, allows us to manipulate millimetric droplets using light, at a controllable speed (up to 0.3 mm/s) and along any desired trajectories.[1] This can be applied for manipulation of biological objects, safe handling of liquids, and development of light-driven soft machines.[2,3] At the micro-scale, it allows us to induce by light reversible switches from a continuous two-phase laminar flow to a droplet generating regime, in microfluidic devices with a usual water-in-oil flow focusing geometry. It consists in adding AzoTAB to the aqueous phase to modulate using light the interfacial energy between flowing liquids and the microfluidic substrate. We found that UV irradiation induced liquid fragmentation into monodisperse water microdroplets and that many cycles of reversible and rapid switches ($<$ 2 s) between continuous laminar flows and stable droplet regimes can be realized.[4] By spatially controlling the application of the light stimulus, we also achieved the first spatially resolved remote induction of droplet generation.[4]

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[3] X. Laloyaux, A. M. Jonas, Angew. Chem. Int. Ed. **49**, 3262 (2010)
[4] A. Diguet, H. Li, N. Queyriaux, Y. Chen, D. Baigl, submitted

Liquid-coated ice particles in high-altitude clouds

Anatoli Bogdan[1] and Thomas Loerting[1]
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High-altitude clouds, which include polar stratospheric clouds (PSCs) and upper tropospheric (UT) cirrus clouds, participate in many atmospheric physical and chemical processes. PSCs are thought to be culprits of the formation of polar stratospheric ozone holes in winter/spring time. The UT cirrus clouds regulate solar and terrestrial radiation. They also redistribute moisture to lower altitudes and supply surface for heterogeneous destruction of UT ozone. Water vapour and UT ozone are dominant greenhouse gases. Naturally, these processes are governed by the microphysical properties of cloud particles, i.e., by the composition, surface phase state, and shape of particles. Until recently it was believed that cloud particles are liquid droplets and/or solid ice and acid/salt hydrate crystals. However, our laboratory experiments demonstrate that PSCs and UT cirrus can be composed also of mixed-phase particles [1, 2]. Such particles can be formed by freezing aqueous aerosol droplets. As aqueous droplets freeze, ions or/and soluble neutral components are expelled from the ice lattice to form a residual freeze-concentrated coating around ice core. If the coating freezes at the atmospheric temperature (above $\sim$183 - 185 K) then the formed cloud particles will be solid. If it freezes at temperature below $\sim$183 K then the cloud particles will be mixed-phase. Our experiments also show that (i) the character of phase transitions and the number of freezing and melting events depend on the size of droplets [3] and (ii) lanolin surfactant may impact on the freezing behaviour of emulsified aqueous droplets.

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[3] Bogdan, A.; Molina, M. J.; Tenhu, H.; Mayer, E.; Bertel, E.; Loerting, T. J. Phys: Condensed Matter, 23, 035103 (2011).

How is interfacial rheology coupled with 3D foam rheology?

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Aqueous foams are complex fluids constituted of gas bubbles densely packed in a surfactant solution. Their structure involves a hierarchy of length scales, set by the surfactant molecules adsorbed at the liquid-gas interfaces, the soap films and the bubbles. Their rheological properties result from a coupling between processes at these different length scales. Below the yield stress, foams exhibit a linear viscoelastic behavior that involves multiple relaxation processes [1]. While slow relaxations are coupled to the coarsening dynamics, fast relaxations may arise from viscous flow in the films or in their junctions as well as from the intrinsic dilatational surface viscosity of the liquid-gas interfaces. Indeed, interfacial relaxations exhibit characteristic times that can vary by three orders of magnitude depending on the surfactants [2]. Moreover, due to the structural disorder, these relaxations may be collective, at the scale of a few bubbles, as reported in the case of concentrated emulsions [3]. I will present experiments that probe the linear viscoelastic complex shear modulus of 3D foams, in the frequency range corresponding to fast relaxations. Using foams with controlled physico-chemical properties I will show how the dominant dissipative processes depend on the rigidity of the liquid-gas interfaces [4]. To get more insight into the role of the disorder of the packing, I will compare the viscoelastic response of ordered bubble monolayers with either rigid or mobile interfaces to the one of disordered 3D foams.

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Interaction of granular particles on liquid interfaces

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[2]University of Oxford, Oxford, United Kingdom

Granular particles floating on water deform the liquid surface, such that the surface tension and gravity forces are balanced. Minimising these deformations often results in inter-particle attraction, leading to aggregation into surface clusters. This problem is studied experimentally, and modelled numerically. Working on a confined system, images of aggregating particles were recorded at regular intervals. Different granular systems (varying grain size, roughness and material) were investigated. Forces of attraction between individual pairs of particles were determined using particle tracking, balancing the velocity to the drag coefficient. A numerical simulation was developed to determine the three-dimensional shape of the liquid surface around particles, by solving the nonlinear Young-Laplace equation using mesh-free finite difference method. Inter-particle attractions for pairs of particles were determined for different distances and contact angles. These results were compared with asymptotic analytical results. At small meniscus slopes and large inter-particle separations, good agreement was found between the simulation and the analytical result obtained from linearized Young-Laplace equation. For steeper menisci and near-range particles, the simulation was a better model because it properly treats the nonlinear nature of the Young-Laplace equation and does not rely on linear superposition.

Drops on functional fibers: from barrels to clamshells and back

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Drops on fibers are a familiar sight, for instance in the form of dew drops on spider webs. They can exist in two competing morphologies, a cylindrically symmetric barrel state completely engulfing the fiber and an asymmetric clamshell state, in which the drop touches the fiber only sideways. Despite their omnipresence and their practical relevance, e.g. for the adherence of drops to fibers in separation technology and filter materials, the physical mechanisms governing the stability of the two morphologies remained elusive. Using electrowetting-functionalized fibers we can tune the wettability of fibers and thereby reversibly switch between the two states. This allows determination of the stability limits of both morphologies as a function of the two relevant control parameters, namely the contact angle and the volume. While clamshells are found to prevail for large contact angles and small volumes and barrels prevail for small angles and large volumes, there is also a wide range of intermediate parameter values, for which both morphologies are mechanically stable. Mapping out the energy landscape of the system by numerical minimization of the free energy we find that the barrel state is easily deformed by non-axisymmetric perturbations. Such perturbations facilitate the transition to the clamshell state and thereby the removal of drops from the fibers. From a general perspective, the demonstration of electrowetting-based reversible switching of liquid morphologies on fibers opens up opportunities for designing functional textiles and porous materials for various applications in detergency, filtering, and controlled absorption and release of liquids.

O6.6

AudiMax
Fri 9
17:20

Structure and stability of electrospray droplets

Mark Miller

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Electrospray ionisation is a popular and versatile method for obtaining gas phase droplets containing a solute for analysis in mass spectrometry. The technique causes minimal fragmentation of the analyte and can be used to study molecules as large as proteins or even protein complexes. Despite the wide applicability of electrospray ionisation, some important aspects of the process are not fully understood, particularly the mechanism by which the solvent evaporates from the solute, thereby depositing charge onto it. Some of the key results relating to the stability of charged droplets date back to the work of Lord Rayleigh in the 19th century. I will present a fresh look at the stability of charged droplets, showing that Rayleigh's results are not usually applicable in the regime relevant to electrospray ionisation. I will also examine the statistics of the charge location in the droplets, showing that instability usually intervenes before the repulsion between charges is strong enough to drive them to the surface, as envisaged in the celebrated "Thomson problem."

Interaction of a liquid jet with a soap film

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[1]*University of Nice, LPMC, LPMC - UMR6622 CNRS UNSA, Parc Valrose, 06108, Nice, France*

Situations where liquid foams are driven far from equilibrium and for which Plateau's laws [1] do not hold anymore are still not fully understood. Such is the case of the impact of an obstacle [2] or of a liquid jet on a liquid foam, two situations that arise in many natural or industrial conditions. The knowledge of the response of such a solicitation is a prerequisite to build criteria on foam deformation and stability. An experimental study at the film scale is performed: a laminar jet of aqueous surfactant solution is projected towards a liquid film of the same composition. Typical jet characteristics are the following: diameter ranges between 0.15 and 0.27 mm, and velocity between 1 and 5 m/s. These values hold for high Reynolds numbers and inertia dominated flows. The film is initially horizontal and maintained by a circular frame, 10 cm in diameter. The whole dynamics of the impact is then recorded by a high speed camera. Depending on the jet velocity and impact angle, different behaviors are observed. For high velocities or quasi-normal jet, the jet pierces the film without any visual change in their respective geometries. For lower velocities or more inclined jet, a deflection of the jet is observed and an analogy with transmission in optics can be made. For further changes in velocity or angle, neither transmission nor reflection are observed, but the jet is catch and absorbed by the film and gives rise to a surprising undulating pattern. The different regimes and the transitions between each other are well characterized by using a Weber number which balances inertia and capillarity respective contributions. Scaling approaches and a simple model based on momentum balance are used to quantify the phenomena.

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Structure and mechanism of formation of bile salt micelles from molecular dynamics simulations

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Bile salts (BS) play a key role in the absorption of fats and fat soluble nutrients by intestinal cells: they form dietary mixed micelles (DMMs) into which these nutrients are solubilized, transported near the intestinal cell wall and then released. The molecular scale mechanisms associated with these processes are still unclear, and to study them we require coarse-grained (CG) models of each of the components of DMMs. Bile salts are among the least studied DMM components and have atypical structure for surfactants (concave steroid ring group with hydrophilic and hydrophobic faces, attached to which is a short and flexible tail), so we focus on them. Here report our simulation study of the structure and mechanism of formation of micelles of pure di- or trihydroxy (2OH; 3OH) BSs at physiological bile salt and NaCl concentration, using a CG model of these molecules. Grand-canonical parallel tempering simulations ensure adequate sampling of equilibrium static properties. Our results agree with reported experiments and point to the origin and biological significance of the bile salts' unusual surfactant properties. The micelle size distribution shows the typical qualitative surfactant behavior, but dimers and trimers are abundant even far from the critical micellar concentration (CMC), the peak of the distribution is broad and a shallow minimum separates micelles from monomers. These observations indicate that BSs are poorly cooperative micelle formers and that the free energy barrier to disassembly is low. The bile salts' high CMC and low micelle stability mean DMMs may rapidly aggregate and then easily release nutrients near the intestinal wall. The interior of bile micelles is rich in hydrophilic groups, and molecules may pack in many different orientations in the micelle. These features may reduce the incidence of undesired smectic phases in the intestine and may facilitate formation of micelles with nutrients with diverse shapes, sizes and hydrophilicity.

Session 7:
Confined fluids, interfacial phenomena

Superhydrophobicity on hairy surfaces

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There is widening interest in the interaction of fluid streams and drops with micropatterned surfaces. For example, rough surfaces can exhibit superhydrophobicity, characterised by contact angles near 180○ and easy roll-off. The bodies of some plants and animals are covered with tiny hairs that show strong water repellency. There have also been recent advances in the microfabrication of hairy surfaces. To exploit these possibilities fully, it is important to gain a better theoretical understanding of how fluids interact with such surfaces. The leaves of the Lady's Mantle are superhydrophobic, despite being patterned with hydrophilic hairs, and it has been proposed that the flexibility of the hairs provides the mechanism to superhydrophobicity. To quantitatively understand the role of elasticity, we formulate a model of a large drop in contact with an array of elastic hairs and, by minimising the free energy, identify the stable and metastable states. In particular, we concentrate on states where the hairs bend to support the drop and find the limits of stability of these configurations in terms of the material contact angle, hair flexibility, and system geometry. We solve the model analytically for a 2D system, and for a 3D system in restricted circumstances, and find that for hair rigidity within a given range, the drop can remain suspended for hydrophilic contact angles, and that the robustness of such states is improved if the hairs have a small uniform inclination. Some aquatic arthropods carry a layer of air against their bodies (plastron), to facilitate underwater respiration. We study the performance of different shapes and spacings of plastron hairs. We find that bent hairs with a section tangential to the interface can withstand a high Laplace pressure whilst providing a large interfacial area for respiration. The plastron is vulnerable to depinning from the tips of the hairs but this can be suppressed by making the hairs more hydrophobic.

Two-dimensional colloidal alloys

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We study both experimentally and theoretically the structure of mixed monolayers of large (3μm) and small (1μm) very hydrophobic silica particles at an octane/water interface as a function of the number fraction of small particles. We find that a rich variety of two-dimensional hexagonal super-lattices of large and small particles can be obtained in this system experimentally due to strong and long-range electrostatic repulsions through the non-polar oil phase. These represent the first experimental results for long-range order in a 2D binary colloidal system. The structures obtained for the different compositions are in good agreement with zero temperature lattice sum calculations and finite temperature Monte Carlo simulations [1]. Our theoretical analysis also reveals that the melting behaviour of these super-lattice structures is very rich, proceeding via a multi-stage process, with melting temperatures that show a very strong and non-monotonic dependence on composition [2].

[1] A.D. Law, D.M.A. Buzza, T.S. Horozov, Phys. Rev. Lett., 106, 128302 (2011)
[2] A.D. Law, T.S. Horozov, D.M.A. Buzza, submitted to Soft Matter

Salt induced changes of interactions in binary liquid mixtures

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Aggregation phenomena of colloidal particles in binary liquid mixtures are a topic of current interest. We recently demonstrated that critical Casimir forces can account for such aggregation in a water 2,6-Lutidine critical mixture without additional ions [1]. We now study the influence of ions in these systems by direct measurements of interaction potentials using total internal reflection microscopy. Strong attraction is observed already several degrees away from the critical temperature. Depending on boundary conditions an unexpected sign reversal from strong attraction to repulsion could be observed. This indicates that beyond Debye screening effects ions play an essential role in such systems. A possible coupling between the distribution of ions and the concentration profiles near the surfaces which consecutively affects the interaction potentials is discussed.

[1] Hertlein et. al, Nature 451,(2008), 172

Long-range hydration effect of lipid membrane studied by terahertz time-domain spectroscopy

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The hydration state of biomolecules has been believed to affect their self-assembly and functions. However, due to a lack of definitive experimental method, the hydration states of biomolecules have not been clarified precisely. On the other hand, very recently, the method to measure precisely the physical properties of hydration water has been suggested using terahertz time-domain spectroscopy (THz-TDS), with which collective rotational dynamics of water molecules is directly measured in ultrafast time scale (sub picosecond) [1]. With using this technique, the evaluated hydration water includes even slightly perturbed water molecules by solute compared to bulk water, which offers quite different results from the previous technique such as NMR that observe only the strongly perturbed water. In the present study, we applied the THz-TDS for multilamellar vesicles of phospholipid, the model of biomembrane, and investigated the dynamical state of water between the bilayers (water layer thickness ∼2.5 nm). By analysing the complex dielectric constant of the lipid solution in terahertz region, we evaluated the state of the hydration water on the surface of lipid membrane. Further, by combining the THz TDS results with the structural information of multilamellar structures of the lipid observed by small-angle x-ray scattering (SAXS), we clarify that the layer of hydration water at a phospholipid bilayer is much larger than that considered in earlier studies, and over 75 of water molecules between bilayers are concluded as the hydration water [2]. This indicates that the water molecules at a phospholipid membrane surface have much different physical properties than bulk water in a large extent on up to 1 nm from the surface, and we need to reconsider the phenomenon took place through water layer at the lipid membrane in meso-scale.

[1] T. Arikawa, M. Nagai, K. Tanaka, Chem. Phys. Lett., 457 (2008) 12
[2] M. Hishida, K. Tanaka, Phys. Rev. Lett., 106 (2011) 158102

Wetting transitions of infinite order

Joseph Indekeu

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We consider a state-of-the-art mean-field density-functional model for three-phase equilibria and wetting. The model features two densities and two control parameters, one of which is related to order parameter asymmetry or spatial anisotropy. The global wetting phase diagram in the space of these two parameters features first-order, second-order, continuously-varying-order and infinite-order wetting transitions. We argue that varying the spatial anisotropy of the magnetic interaction in ferromagnets with cubic anisotropy may well lead the way towards an experimental realization of infinite-order wetting. We also discuss renormalization group ”corrections” beyond mean-field theory to the wetting phase diagram. Co-authors: Kenichiro Koga (Okayama) and Benjamin Widom (Cornell)

Surface effects on the demixing of colloid-polymer systems

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We study the effect of a wetting surface upon the fluid-fluid phase separation of a colloid-polymer mixture. Using Confocal Scanning Laser Microscopy, we obtain real space images of demixing from both the unstable and metastable regions of the phase diagram. The presence of a wall breaks the symmetry of the phase separation morphology in the direction perpendicular to the surface, due to the interplay between the competing processes of wetting and demixing. We analyse the thickening of the wetting layers and demonstrate that hydrodynamic transport processes can significantly increase the rate of wetting layer growth. We also consider the possibility of a different cross-over between demixing regimes in bulk and at a wall. We interpret our findings in light of previous experiments and simulations.

Electrokinetics of air bubbles in water

Vladimir Lobaskin

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In micro and nanofluidic applications involving complex fluids, the ionic components and Coulomb forces are often of primary importance. Due to the competition of main lengthscales: Gouy-Chapman length, Debye length, and the system size, as well as of diffusive and convective timescales, the character of ionic motion and of the emerging flows is determined by a rich interplay of hydrodynamic, electrostatic, and diffusive effects. A quantitative study of such systems demands a careful inclusion of all the relevant factors.In this work we perform computer simulation of electrophoresis of nanoscale air bubbles in a liquid.The charge on the bubble is induced by preferential adsorption of one ion type at the interface. We use primitive electrolyte model for all ion types and coarse-grained DPD solvent that takes care of hydrodynamics.The ion adsorption potential is tuned to reproduce the experimentally observed pH-dependence of the bubble mobility in water. We further analyse the bubble and ion motion under applied DC and AC electric field as a function of the reduced screening parameter a (a being the bubble radius).We show that the bubble mobility at different salt concentrations differs from the mobility of a solid colloidal particle of the same size and charge both due to the surface slip and due to charge equilibrium condition at the interface. However, we find that a number of non-trivial effects observed in colloidal electrophoresis: the mobility dependence on the surface potential, mobility inversion in presence of multivalent ions can be observed for the bubbles as well. Finally, we discuss the possibility of inferring the zeta potential of the air-water interface from the mobility data.

O7.8

AudiMax
Wed 7
16:30

Spontaneous imbibition in disordered porous solids: a theoretical study of helium in silica aerogels

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We present a theoretical study of spontaneous imbibition in nanopores using a lattice-gas description and a dynamical mean-field theory. We first consider the case of a slit pore and investigate the influence of precursor films on the speed of the imbibition front due to liquid mass conservation. We then study the much more complex case of a three-dimensional disordered solid in order to interpret recent experiments with liquid helium in silica aerogels showing a striking influence of the gel porosity on the fluid dynamical behavior. As in recent phase-field models of spontaneous imbibition, we assume that capillary disorder predominates over permeability disorder. Our results reveal a remarkable connection between imbibition and adsorption as also suggested by experiments. Irrespective of porosity, we find that the first stage of the imbibition process corresponds to the advance of a liquid film along the silica strands and in the small crevices of the microstructure. The main front is associated to the filling of the largest cavities in the gel. The classical Lucas-Washburn scaling law is generally recovered, although some deviations may exist at large porosity. Moreover, the interface roughening is modified by wetting and confinement effects. Our results suggest that the interpretation of the experiments should be revised.

Complex fluids at complex surfaces: simply complicated?

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We study wetting and filling of patterned surfaces by a nematic liquid crystal. We focus on three important classes of periodic surfaces: saw-toothed, sinusoidal and stepwise, which have been considered in the literature as promising candidates to develop less-consuming zenithal bistable switches for practical applications. For saw-toothed substrates, geometry induces the nucleation of disclination lines on the wedges and apexes of the substrate, so the nematic surface free energy density develops an elastic contribution which scales as $q \ln q$ (with q being the wavenumber associated with the substrate periodicity). This leads to a large departure from Wenzel's prediction for the wetting transition. For the sinusoidal substrate, the interplay of geometry, surface and elastic energies can lead to the suppression of either filling or wetting, which are observed for a same substrate only for a narrow range of roughness parameters. Finally, periodic stepwise surface displays re-entrant transitions, with a sequence dry-filled-wet-filled, in the relevant region of parameter space.

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[2] J. M. Romero-Enrique, C.-T. Pham and P. Patricio, Phys. Rev. E **82**, 011707 (2010)
[3] P. Patrício; J. M. Romero-Enrique; N. M. Silvestre; N. R. Bernardino and M.M. Telo da Gama, Molec. Phys. IFirst doi: 10.1080/00268976.2010.542780 (2011)

Hydrate formation at liquid-liquid and liquid-gas interfaces

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[3] ESRF, Grenoble, France

The formation of clathrate hydrates, cage-like water-gas structures, is of great importance in both industries and earth science. However, the formation process is not completely understood so far. We studied hydrate formation at interfaces between water and varying guest molecules. We investigated the structure of these interfaces under quiescent conditions in-situ by means of x-ray reflectivity measurements both inside and outside the zone of hydrate stability. In the first part of our work, we studied liquid-liquid water-alkane systems. The roughness of water-isobutane and water-propane interfaces was in good agreement with capillary wave theory. No indication for hydrate formation was observed. A study of a liquid-liquid water-CO_2 system revealed a rearrangement of the interface when supercooling in the region of hydrate stability. A pronounced mixing layer emerged just before the formation of macroscopic hydrate. A strong accumulation of guest molecules was likewise obseved at the liquid-gaseous water-xenon interfaces, along with spontaneous hydrate formation. We conclude from our experiments that an accumulation of guest molecules at the interface serves as a nucleation spot for hydrate formation. We observed that systems with typically long induction times for hydrate formation do not exhibit an enrichment of guest molecules at the interface, nor the appearance of macroscopic hydrates, within the duration of the x-ray experiments ($\approx$ 10 hours). In contrast, in systems where hydrate was formed during the experiment, we found a mixed layer with a significant supersaturation of guest molecules. The supersaturation increases drastically the local guest offer and thus the probability for hydrate formation. The discovery of nano-thick supersaturated layers at the interface between water and guest molecule phases opens new perspectives for a comprehensive understanding of hydrate formation and may represent the basis for a unified theory of hydrate nucleation.

Electric field driven instabilities on superhydrophobic surfaces

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We study possible mechanisms of the transition from the Cassie state to the Wenzel state on superhydrophobic surfaces under the influence of electric fields as a function of the aspect ratio and the wettability of the surface. It is shown that the equilibrium shape of the composite interface between superhydrophobic surfaces and drops in the superhydrophobic Cassie state under electrowetting is determined by the balance of the Maxwell stress and the Laplace pressure. We demonstrate how reversible switching between the two wetting states can be achieved locally using suitable surface and electrode geometries. A simple analytical model for axisymmetric cavities and small deflections of the liquid menisci within the cavities reveals the existence of a novel electric field driven instability of the liquid surface. Fully self-consistent calculations of both electric field distribution and surface profiles show that this instability evolves from a global one towards a local Taylor cone-like instability for increasing aspect ratio of the cavities. A two-dimensional map is derived indicating the prevalence of the interfacial instability as compared to the depinning scenario of the three-phase contact line, which is well-known from ordinary superhydrophobic surfaces.

O7.12

AudiMax
Wed 7
10:30

Capillarity and gravity: New phase transitions

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Phase transitions of inhomogeneous fluids such as wetting and capillary-condensation that occur when a fluid is confined near a substrate or in parallel-plate geometries have received enormous attention over the last few decades. In most theoretical studies of these transitions, the influence of a gravitational field is either considered secondary or, more often, completely neglected. However, it is clear that gravity plays a central role in many practical situations and, in combination with confinement, induces further interfacial behaviour. Consider, for example, a large volume of a non-volatile liquid in a cylindrical pore which is capped at its bottom. What happens to the liquid when the capillary is slowly turned to the horizontal? Common experience tells us that, if the capillary is wide enough, the liquid will spill from the open end (as water drains from a tipped glass) but, if it is sufficiently narrow, the liquid will remain in the capillary (as in a drinking straw). It is somewhat surprising to find that this rather basic aspect of capillarity has not been investigated in depth. Here, we present theoretical and experimental results illustrating different aspects of this phenomena, including a number of phase diagrams. An unexpected connection of this phenomenon with the theory of wetting is also highlighted.

Non-additive hard sphere mixtures: from bulk liquid structure to wetting and layering transitions at substrates

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An overview of a variety of interesting many-body phenomena that occur in the simple binary liquid mixture of non-additive hard spheres is given. Based primarily on a fundamental measures density functional theory [1], but also on Monte Carlo computer simulations, we investigate the fluid-fluid demixing phase diagram, the partial bulk pair correlation functions via both the Ornstein-Zernike and the test particle routes, the asymptotic (large distance) decay of correlation functions via pole analysis of the complex structure factors [2], as well as behaviour in inhomogeneous situations. A rich variety of interfacial phenomena is found when the mixture is exposed to a planar hard wall (entropic wetting) or in a planar slit (capillary demixing). At a general hard wall adsorption proceeds either through a series of first-order layering transitions, where an increasing number of liquid layers adsorbs sequentially, or via a critical wetting transition, where a thick film grows continuously [3].

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[3] P. Hopkins and M. Schmidt, submitted to Phys. Rev. Letters.

Snap-off and coalescence of nematic liquid crystal drops

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Droplet formation and coalescence are both familiar phenomena in everyday life that are also important in many industrial processes. Furthermore, these intriguing events are of great scientific interest because of the hydrodynamic singularities by which they are accompanied. For that reason, both phenomena have been studied intensively, especially for the case of Newtonian fluids, but more recently also for non-Newtonian liquids. The already rich behavior that these fluids display becomes even more intricate if the liquid possesses liquid crystalline order. We studied both phenomena in suspensions of colloidal gibbsite platelets with nematic liquid crystalline order. The ultra-low interfacial tension in these suspensions, combined with the relatively high viscosity and low density differences, slows down the dynamics of both processes considerably, which allows for detailed investigation with polarized light microscopy. We found remarkable differences in droplet snap-off behavior depending on the anchoring properties of the nematic phase. In the case of weak anchoring droplet snap-off appeared to be determined mostly by the viscous properties of the nematic phase. On the other hand, in the case of strong anchoring the snap-off is hindered due to an energy barrier related to the formation of a topological defect in the separating drop. Next, we studied the coalescence of nematic droplets with the macroscopic isotropic-nematic interface as a function of droplet size. It appeared that coalescence of small drops with a uniform director field proceeds similar to the case of isotropic fluids. However, larger droplets with a non-uniform director field behave rather differently, in fact remarkably similar to the passage of deformable immiscible drops through a liquid-liquid interface.

Surface slip investigated by scattering techniques

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Surface-related anomalies in flowing liquids are quantified by the slip length. However, this phenomenological number is neither simply related to a molecular picture (e. g. specific surface structures or unlike conformations of molecules adjacent to the boundary) nor contains information on the length scale of the anomaly. An analysis of the surface region by scattering techniques can potentially reveal insights on a molecular level. Neutron scattering can be tuned to become surface/interface sensitive for scattering conditions covering the region of total reflection. Thus, it provides a unique probe to elucidate slip-induced structural changes. Following along this line we have obtained recent results that can be summarized as follows: A neutron reflectivity (NR) study on a in situ sheared low viscosity Newtonian liquid in contact with solid interfaces shows that the extent of the depleted layer close to the interface is influenced by the surface energy of the substrate, shear rate and temperature but can not explain the slip length reported earlier and extracted by complementary techniques. For a micellar system we report on a more ordered structure at an interface having a good affinity to the micelles corona. In situ measurements under shear load reveal that shear aligns the crystallites, but decreases long-range correlations. After stopping the shear, a slower relaxation of the crystalline structure is found close to the interface that showed more pronounced ordering. A polymer melt has been investigated with NR in contact to grafted polymer layers at rest and under shear load. We find interdiffusion of the chains from the melt into the grafted layer before shear is applied. This may explain the amount of surface slip and result in ripping off molecules from the grafted surface.

Session 8:
Supercooled liquids, glasses, gels

Highly nonlinear dynamics in a slowly sedimenting colloidal gel

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We use a combination of original light scattering techniques and particles with unique optical properties to investigate the behavior of suspensions of attractive colloids under gravitational stress, following over time the concentration profile, the velocity profile, and the microscopic dynamics [1,2]. During the compression regime, the sedimentation velocity grows nearly linearly with height, implying that the gel settling may be fully described by a (time-dependent) strain rate. We find that the microscopic dynamics exhibit remarkable scaling properties when time is normalized by strain rate, showing that the gel microscopic restructuring is dominated by its macroscopic deformation.

[1] G. Brambilla et al., Phys.Rev. Lett. 106, 118302 (2011).
[2] ”Gels settle down”, in Physics, Spotlighting exceptional research: http://physics.aps.org/synopsis-for/10.1103/PhysRevLett.106.118302

Elastic properties of glasses

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In this contribution, we present experimental results on the elastic properties of a two-dimensional colloidal glass former. Given that glasses are solids, one expects a mechanical behaviour similar to that of crystals, i.e., glasses exhibit a finite shear modulus μ. Using positional data from video microscopy [1], we study the displacement field and connect it to the dynamical matrix $\mathbf{D}(\mathbf{q})$ via the equipartition theorem [2]. The resulting dispersion relation of the system hints at structural change upon decreasing the temperature in the glassy state. Next, this data is used to derive the Lamé coefficients and the corresponding moduli from thermally excited modes in the long wavelength limit [3] using continuum elasticity theory. We consider finite size and time effects and find the expected frequency dependence of the shear modulus μ. By cooling the system, the significant increase of μ allows us to determine the glass transition temperature T_g precisely. Following the method described in [4,5], we compute the short wavelength excitations in our system and analyse the density of states as well as the structure of normal modes in a two-dimensional colloidal system.

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[3] H. H. Von Grünberg, P. Keim, and G. Maret, Phys. Rev. Lett. **93**, 255703 (2004)
[4] A. Gosh, V. K. Chikkadi, P. Schall, J. Kurchan, and D. Bonn, Phys. Rev. Lett. **104**, 248305 (2010)
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Dynamic arrest of fluids in porous media: crossover from glass- to Lorentz-like behavior

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We have used molecular dynamics simulations to study the slow dynamics of a hard-sphere fluid confined to a random array of hard-sphere obstacles. Two arrest mechanisms control the behavior of the fluid: localization is dominant at high obstacle densities, ϕ_m, whereas caging prevails at large fluid densities, ϕ_f. Similar effects exist in real systems like the movement of proteins in cytoplasm [1]. We have investigated the specific case of "quenched-annealed" (QA) systems, where upon varying ϕ_m and ϕ_f we unveiled scenarios of discontinuous and continuous dynamic arrest, subdiffusion, and a decoupling of the time scales for the relaxation of the self and the collective correlators of the system [2]. Our observations are consistent with many phenomena predicted by a recent extension of mode-coupling theory to systems with quenched disorder [3]. To elucidate the origin of the arrest phenomena, we geometrically distinguished individual pores formed by the obstacles [4]. This enabled us to identify particles that are "free" (located in the void percolating through space) and "trapped" (confined in a void of finite volume). We separately evaluated various dynamic correlators for these two classes of fluid particles and demonstrated that they exhibit significant differences [5]. Finally, we investigated how correlations among the fluid particles and among the obstacles influence the subdiffusive behavior, thus contributing to the ongoing debate about the mathematical limits that distinguish the Lorentz gas [6] from QA systems.

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O8.4

LH 28
Wed 7
10:50

Liquid-glass phase diagram in confined geometry

Simon Lang,[1] Vitalie Botan,[2] Martin Oettel,[2] David Hajnal,[2]
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[2] Johannes Gutenberg-Universität, Mainz, Germany

Significant experimental and simulation research has been performed on small pores, films or tubes in order to elucidate the nature of the glass transition. In particular, computer simulations reveal that the wall-fluid interaction significantly alters the transition temperatures and that the diffusivities depend sensitively on the distance of the walls [2]. To achieve a theoretical description, we extend the microscopic mode-coupling theory to a liquid confined between two flat and parallel walls. The essence of our extension consists of an expansion of the assigned space direction into a discrete Fourier spectrum. This ansatz leads to a generalized intermediate scattering function forming a matrix-valued quantity of infinite size. Obeying the mode-coupling approximations adapted to these modifications, a self-consistent description for the generalized intermediate scattering function follows. The theory contains the standard mode-coupling equations for two dimensions and three dimensions as limiting cases and requires as input only the equilibrium density profile and the static structure factors of the fluid in confinement. We evaluate the phase diagram as a function of the distance of the plates for the case of a hard sphere fluid and obtain an oscillatory behavior of the glass transition line as a result of the structural changes related to layering [1]. We find, that the glass transition is facilitated at half-integer values of the distance with respect to the hard-sphere diameter. In contrast, at commensurate packing particles can more easily slide along the walls and therefore the liquid phase remains favored for higher packing fractions.

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The role of the prestructured surface cloud in crystal nucleation

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For the homogeneous crystal nucleation process in a soft-core colloid model we identify optimal reaction coordinates from a set of novel order parameters based on the local structure within the nucleus, by employing transition path sampling techniques combined with a likelihood maximization of the committor function. We find that nucleation is governed by solid clusters that consist of an hcp core embedded within a cloud of surface particles that are highly correlated with their nearest neighbors but not ordered in a high-symmetry crystal structure. The results shed new light on the interpretation of the surface and volume terms in classical nucleation theory.

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O8.6

LH 28
Wed 7
10:30

Correlated rearrangements in supercooled liquids from inherent structure deformations

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We propose that deformations of inherent structures are a suitable tool for detecting structural changes and the onset of cooperativity in supercooled liquids. Following a nonequilibrium thermodynamic theory of glasses [1], we use small, static deformations to perturb the inherent structures -that are local minima of the underlying potential energy landscape- of supercooled liquids approaching the glass transition. By comparing inherent structures before and after applying the deformation, we can extract a non-affine displacement field which shows characteristic differences between the high temperature liquid and supercooled state. The average magnitude of the non-affine displacements is very sensitive to temperature changes in the supercooled regime and is found to be strongly correlated with the mean inherent structure energy. In addition, the non-affine displacement field is characterized by a correlation length that increases upon lowering the temperature. The finite-size scaling analysis of our numerical results indicate that the correlation length has a critical-like behavior and diverges at a temperature Tc, below the temperatures where the system can be equilibrated. Our numerical results are consistent with random first order theory, which predicts such a divergence with a critical exponent $\nu = 2/3$ at the Kauzmann temperature, where the extrapolated configurational entropy vanishes [3].

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Glassy dynamics, Spinodal fluctuations, and the kinetic limit of nucleation in suspensions of colloidal hard rods

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The interest in positionally and orientationally ordered assemblies of anisotropic particles is driven by their great technological potential as they exhibit anisotropic optical properties, but arises from a more fundamental point of view as well. However, the kinetic pathways of the self-assembly of anisotropic particles are not well understood. For instance,the phase diagram of hard rods has been known for around fifteen years, and shows that there are stable isotropic, nematic, smectic and crystal phases depending on the aspect ratio. Only very recently, the kinetic pathway of isotropic-nematic(IN) phase transition for long rods was reported, but the isotropic-smectic(ISm) and isotropic-crystal(IX) phase transitions of short rods still remain unknown. In this work, we study the nucleation of colloidal short rods from isotropic fluid to the crystal and smectic phases by computer simulations. We identify three dynamic regimes in a supersaturated isotropic fluid of short hard rods: (i) for moderate supersaturations, we observe nucleation of multilayered crystalline clusters which is in marked contrast to an earlier study[1] ; (ii) at higher supersaturations, we find nucleation of small crystallites which arrange into long-lived locally favored structures; and (iii) at even higher supersaturations, the dynamic arrest is due to the conventional cage-trapping glass transition. For longer rods we find that the nucleation of the (stable) smectic phase out of a supersaturated isotropic state is strongly suppressed by an isotropic-nematic spinodal instability that causes huge spinodal-like orientation fluctuations.

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Structural relaxation and correlation length scales in glass forming liquids

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The rapid rise of structural relaxation times in supercooled liquids upon decreasing temperature, and their transformation to an amorphous solid state (the glass transition), display many puzzles which have eluded a satisfactory explanation despite decades of experimental and theoretical investigation. A key mystery is the role of structural or other lengthscales in determining dynamical slow down. The conventional view holds that lengthscales associated with structural ordering do not grow appreciably as the glass transition is approached. Nevertheless, the role of growing static and dynamical length scales in determining relaxation times in glass forming liquids has received increasing attention in recent years. New insights into spatial correlations in structure and dynamics, and their relationship with the rapid rise of relaxation times in glass forming liquids, obtained via computer simulations of model liquids, will be described. Specific issues addressed will be the relationship of the short and long time relaxation and corresponding length scales, the validity of the Adam-Gibbs relation and the breakdown of the Stokes-Einstein relation in different spatial dimensions.

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Thermodynamics and structure of fluids with dissimilar patches

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Anisotropic interactions between particles of a fluid promote their aggregation into self-assembled structures that can compete with the clustering that drives condensation. We address this general problem by studying a model of patchy particles, hard spheres whose surface is decorated with ”sticky” spots (or patches). The interaction between two patches results in a bond between two spheres. The type of aggregates in which particles self assemble is tuned by the number of patches in a sphere and by the energy of the bonds. Using Wertheim's perturbation theory and a generalized version of the Flory-Stockmayer percolation theory [1], we analyse the thermodynamics and the equilibrium structure of several realizations of this model: (i) phase separation of dimers, chains and hyper-branched polymers [2] ; (ii) the percolation and the phase behaviour of a system with chaining and branching [3] ; (iii) the emergence (of entropic origin) of re-entrant phase diagrams when branching is energetically unfavourable relatively to chaining [4] ; (iv) the appearance of ”empty” fluids in binary mixtures of patchy particles. Finally, we build up a detailed analogy between a patchy particle model and the dipolar hard sphere fluid (DHS), that enlightens the controversial phase behaviour observed in the DHS [6].

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Session 9:
Non-equilibrium systems, rheology, nanofluidics

A real-space study of shear induced order in colloidal hard-sphere fluids

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Light scattering experiments have demonstrated that oscillatory shear can induce crystallization in a colloidal hard-sphere fluid below the bulk freezing density [1]. We investigate this non-equilibrium phase behavior in real-space with experiments on density matched PMMA colloids and Brownian Dynamics computer simulations [2]. The zero-velocity plane of the shear cell enables us to experimentally investigate the kinetics of the transition with confocal microscopy while the shear is being applied [3]. Although our computer simulations neglect hydrodynamic interactions and non-linear flow profiles, there is a good qualitative agreement with the experiments. Depending on the amplitude and frequency of the oscillation, we identify the real-space structures of four shear induced phases, including one that has not been reported previously in the experimental literature. This phase consists of lanes of particles that order in a tilted hexagonal array in the gradient-vorticity plane. By calculating the structure factor we also identify the elusive string-phase, both experimentally and with simulations. As an outlook, we present preliminary results on a columnar phase formed in a suspension of rod-like particles under steady shear flow.

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O9.2

SCH
Tue 6
15:40

Realization of a μm sized stochastic heat engine

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The thermodynamical properties of small systems are of central importance for the understanding of many processes at the interface of physics, biology and chemistry. Contrary to the description of large systems which exhibit many internal degrees of freedom, classical thermodynamics fails to properly describe microscopic systems such as molecular machines or micro-mechanical devices where typical energies are on the order of k B T and fluctuations become important. We experimentally demonstrate the realization and operation of a micron-sized heat engine where the working gas and the piston are replaced by a single colloidal particle and an optical laser trap with time-dependent stiffness. When the particle's environment is periodically heated and cooled with an additional laser beam, work is extracted or delivered from and to the system depending on the direction of the working cycle. We demonstrate that in the limit of large cycle times the efficiency of this micro-machine is in agreement with the corresponding Carnot value. When the cycle time is decreased we first observe a maximum in the output power of the machine followed by the stall of the machine.

Colloidal asphaltene aggregation and deposition in capillary flow from multi-scale computer simulation and experiment

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Asphaltenes are known as the 'cholesterol' of crude oil. They may form nano-aggregates and block rock pores, hindering oil recovery and carbon sequestration operations. Here w e have investigated the deposition and aggregation of colloidal crude oil asphaltenes in capillary flow using multi-scale simulations and experiments. First, we use micro-fluidic flow experiments to co-inject an asphaltenic fluid with a precipitant, typically n-heptane, in a glass capillary. The dynamics of asphaltene precipitation, aggregation and deposition in the capillary were monitored using optical microscopy and pressure drop measurements as a function of time. It turns out that the results are dependent on the flow rate imposed. At small flow rates, the pressure drop across the capillary increases slowly, leading to a gradual and complete blocking of the capillary. For high flow rates, on the other hand, we observe a rapid initial blocking, followed by episodes of erosion and re-deposition. These observations are confirmed by microscopy. We hypothesize that the shear forces associated with the high flow rates are strong enough to erode the transient deposits. We have checked this hypothesis using a hybrid computer simulation method: Multi Particle Collision Dynamics for the solvent coupled to Molecular Dynamics (MD) for the asphaltene colloids. We tune the flow rate to obtain Pe flow $>> 1$ (hydrodynamic interactions dominate) and Re $<< 1$ (Stokes flow). Here, we check in detail the effect of the finite size of the asphaltene colloids. We observe that the fraction of particles deposited decreases with increasing flow rate, but does not depend on the potential well depth. We find that the dimensionless conductivity measured in the experiment can be well-matched by simulation results. This implies that the essential physics of the capillary flow deposition experiment has been captured by the computer simulations.

Gradient-driven fluctuations in microgravity

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Equilibrium fluctuations of thermodynamic variables, like density or concentration, are known to be small and occur at a molecular length scale. At variance, theory predicts that non equilibrium fluctuations grow very large both in amplitude and size. On earth, the presence of gravity and buoyancy forces severely limits the development of the anomalous fluctuations. We will present the results of a 14 year long international collaboration on an experiment on non equilibrium fluctuations in a single liquid and in a liquid suspension under microgravity conditions. Non equilibrium conditions are generated by applying a temperature gradient across millimeter size liquid slabs confined by temperature controlled sapphire windows. Phase modulations introduced by fluctuations are measured with a quantitative Shadowgraphy method, with optical axis parallel to the temperature gradient. Random phase modulations picked up by the main beam translate into intensity modulations that are measured by a CCD a meter or so away from the thin liquid slab. Thousands of images are analyzed and their two dimensional power spectra yield the fluctuation structure function S(q), once data are reduced according to the instrumental transfer function T(q). A robust calibration procedure to derive T(q) will be presented. Also, by analyzing time delayed images, accurate description of the q dependent dynamics has been obtained.The mean square amplitude of the fluctuations exhibits an impressive power law dependence at larger q and a low q rolloff, showing that the fluctuation size is determined by the sample thickness. The shape of the structure function, its increase due to gravity removal, and its dependence on applied gradient are in agreement with available theoretical predictions. Diffusive time correlations up to thousands of seconds are observed for the suspension sample. Possible impact on growth mechanism in space will be discussed.

Thermodiffusion of colloids with mesoscopic simulations

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In this work, we present a hydrodynamic simulation study of colloidal dispersions in a temperature gradient. The solvent is implemented through a technique known as multiparticle-collision dynamics (MPC), which properly incorporates hydrodynamic interactions and is able to sustain temperature gradients. With a hybrid model of MPC and molecular dynamics, colloid-solvent and colloid-colloid interactions are included. The Soret coefficient quantifies the thermodiffusive effect. The magnitude of the Soret coefficient depends on the effective force that the particle experiences through the temperature gradient in the solution, and the sign indicates whether the colloid moves to the hot or to the cold area. We analyze the dependence of the Soret coefficient on the particle size and on the average temperature of the solution. The size dependence of the Soret coefficient in colloidal solutions is described by a power law, $S_T \propto a^s$, with a the colloid diameter, which has also been found in experiments. We consider different colloid-solvent interactions, which are tuned from strongly repulsive to strongly attractive. We observe how the exponent and the prefactor of the power law can be related to the nature of the colloid-solvent interactions. The regime of concentrated solutions is investigated with increasing volume fraction. The Soret coefficient is now measured through the concentration and temperature profiles. We analyze the influence of range and strength of the colloid-colloid interactions on the thermodiffusive behavior as a function of the colloid concentration, besides the different colloid-solvent interactions.

Controlled drop emission by wetting properties in driven liquid filaments

Ignacio Pagonabarraga

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The controlled formation of micron-sized drops is of great importance in microfluidic technological applications. Here we present a novel, wetting-based, destabilization mechanism of forced microfilaments on either hydrophilic or hydrophobic dry stripes, that leads to the periodic emission of droplets. The drop emission mechanism is triggered above a critical forcing, where the contact line no longer follows the leading edge of the filament. We propose a dynamical model which includes the effects of wetting, capillarity, viscous friction and the driving force to determine the interface cofiguration at the threshold. We compare our theory to lattice-Boltzmann simulations and microfluidic experiments, accounting for the emission threshold and hence the size and emission period of droplets, which can be controlled independently. Our results show that the critical filament velocity depends strongly on wetting, and exhibits a qualitative different behaviour on hydrophilic and hydrophobic stripes, which arises from the dependency of viscous dissipation on the shape of the advancing interface. Our results suggest that this new kind of instability in contact lines is general to advancing fronts, and opens new possibilities of exploiting wetting to handle interfaces at the microscale.

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[2] C. Duez, C. Ybert, C. Clanet and L. Bocquet, Nature Physics, 3, 180 (2007)

Stretching dense colloidal suspensions: from flow to fracture

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Concentrated suspensions of particles are commonly used in the pharmaceutical, cosmetic and food industries. Manufacture of these products often involves flow geometries that are substantially different from those studied by conventional shear rheology. Using a capillary break-up extensional rheometer we stretch fluids of different volume fraction at strain rates just below, at and above the critical rate required to induce jamming. We show that the jamming of a stretched colloidal column is closely related to that observed during shear rheology. However, fascinating additional effects due to the geometry are also observed. High speed photography of the filament shows evidence of dilatancy and granulation, leading finally to fracture at a critical strain rate. Finally we investigate an intriguing aspect of thin fluid filaments of the colloidal suspension, when stretched below the critical strain rate required to produce jamming. These filaments are observed to thin to a critical diameter before rupturing and displaying visco-elastic recoil.

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Transversal dynamics of paramagnetic colloids in a longitudinal magnetic ratchet

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In this talk I will describe the transversal motion of paramagnetic particles above the magnetic stripe pattern of a uniaxial garnet film, exhibiting a longitudinal ratchet effect in the presence of an oscillating magnetic field [1]. First I will focus on the behaviour of one colloid. Without the field, the thermal diffusion coefficient obtained by video microscopy is $D_0 \sim 10^{-4}$ micron 2 /s. With the field, the transversal diffusion exhibits a giant enhancement by almost four decades and a pronounced maximum as a function of the driving frequency. It is possible to explain the experimental findings with a theoretical interpretation in terms of random disorder effects within the magnetic film [2]. On the second part of this talk I will focus on the collective dynamics of an ensemble of paramagnetic particles organized as a one-dimensional chain and driven above the magnetic film. The centre of mass of the chain shows a diffusive behavior with mean square displacement $\sim t$, while its end-to-end distance shows anomalous kinetics with a sub-diffusive growth $t^{1/2}$. It is possible to extract the potential of mean force between the particles within the chain by invoking the Pope-Ching equation [3]. Thus the experimental data are interpreted by using the Rouse model, originally developed for polymers, and all relevant parameters are extracted experimentally.

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Osmotic interactions and arrested phase separation in star-linear polymer mixtures

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Whereas hard-colloid/polymer mixtures are established as a model system for exploring aspects of gelation and glass formation in soft matter [1], mixtures involving soft colloids have received very little attention so far [2]. Yet, the effect of softness can be very significant and lead to an incredible wealth of phases/states, hence providing ways for tailoring the rhelogy of colloidal dispersions. Here we focus on mixtures of star polymers (as model soft colloids) and linear polymers. Starting from a glassy suspension of star polymers in molecular solvent, we add linear homopolymers of fixed size ratio and ever increasing concentration, hence diluting the glass and eventually approaching the regime of stars in polymer matrix. We show that we can quantitatively decompose the rheology of the mixtures into colloidal star and linear polymer contributions, by accounting for the osmotic shrinkage of the stars due to the added polymers. We show that, when the number of star-star particle contacts decreases due to the addition of linear polymers, the star repulsions weaken and eventually become attractive. The attraction is accompanied by an observed phase separation, pointing to the presence of unstable regions in the star/linear polymer phase diagram, where gelation results from an arrested phase separation. Furthermore, we explore the effect of size ratio at fixed star polymer concentration on the rheology of the mixtures and discover the existence of different glassy states as the linear concentration changes.These results add to the generic picture emerging for soft colloidal mixures, with ultimate aim the molecular design of soft composites with tunable properties.

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[2] Stiakakis E., Vlassopoulos D., Likos C.N., Roovers J., and Meier G., Phys. Rev. Lett., 89, 208302, 2002.

Non-equilibrium properties of semidilute polymer solutions in shear flow

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Polymers in solution exposed to shear flow exhibit a remarkably rich dynamical behavior. In particular, they exhibit tumbling motion, i.e., they undergo a cyclic stretching and collapse dynamics, with a characteristic frequency which depends on shear rate and the internal relaxation time. This behavior has intensively be studied for polymers in dilute solution. Much less is known about the non-equilibrium dynamics of polymers in semidilute solution. While the dynamical behavior of polymers in dilute solution is governed by hydrodynamic interactions, their relevance in semidilute solution is less evident. Employing hybrid mesoscale hydrodynamics simulations, which combine molecular dynamics simulations of the polymer with the multiparticle collision dynamics approach for the fluid, we studied the non-equilibrium behavior of polymer solutions in shear flow. We find that polymers in both, dilute and semidilute solutions exhibit large deformations and a strong alignment along the flow direction. More importantly, in the stationary state, the conformational and rheological properties for various concentrations are universal functions of the Weissenberg number with a concentration-dependent relaxation time. Hence, with increasing concentration, hydrodynamic interactions affect the conformational and rheological properties only via the increasing relaxation time. Moreover, dynamical properties–orientational distribution functions and tumbling times–depend on concentration in excess to the relaxation time, a dependence, which we attribute to screening of hydrodynamic interactions in semidilute solution. In the presentation, the various results will be discussed.

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[2] C.-C. Huang, G. Sutmann, G. Gompper, R. G. Winkler, EPL 93, 54004 (2011)

Session 10:
Biofluids, active matter

Hydrodynamic synchronisation in driven colloidal systems: a model for micro-pumps and biological flows

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Cilia and flagella are biological systems coupled hydrodynamically, exhibiting dramatic collective motions. At the scale of a single filament, it is well understood how momentum is transferred to the fluid, allowing motility and fluid generation. At the scale of assemblies of filaments (swarms and tissues) there are various open questions. The talk will be based on an experimental model system developed in our lab: arrays of colloidal spheres are maintained in oscillation by switching the position of an optical trap when a sphere reaches a limit position, leading to oscillations that are bounded in amplitude but free in phase and period. The interaction between the oscillators is only through the hydrodynamic flow induced by their motion. We prove the general structure of the stable dynamical state, in the absence of stochastic noise, extending previous results on two beads [1] and showing the importance of geometry through the structure of the coupling tensor [2]. These results help to understand the origin of hydrodynamic synchronization and how the dynamics can be tuned. At the colloidal scale, thermal fluctuations are important, and synchronisation needs to be robust against these. We propose that weakly correlated phase fluctuations are characteristic of hydrodynamically coupled systems in the presence of thermal noise.

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O10.2

SCH
Sat 10
9:40

Bacterial ratchet motors

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Self-propelling bacteria are a nanotechnology dream. These unicellular organisms are not just capable of living and reproducing, but they can swim very efficiently, sense the environment, and look for food, all packaged in a body measuring a few microns. Before such perfect machines can be artificially assembled, researchers are beginning to explore new ways to harness bacteria as propelling units for microdevices. Proposed strategies require the careful task of aligning and binding bacterial cells on synthetic surfaces in order to have them work cooperatively. Here we show that asymmetric environments can produce a spontaneous and unidirectional rotation of nanofabricated objects immersed in an active bacterial bath. The propulsion mechanism is provided by the self-assembly of motile Escherichia coli cells along the rotor boundaries. Our results highlight the technological implications of active matter's ability to overcome the restrictions imposed by the second law of thermodynamics on equilibrium passive fluids.

[1] R. Di Leonardo et al. PNAS, 107, 9541 (2010).
[2] L. Angelani, R. Di Leonardo, G. Ruocco, Phys. Rev. Lett., 102, 048104 (2009).

Arrested phase separation in reproducing bacteria: a generic route to pattern formation?

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In this talk I will present a generic mechanism that we uncovered recently [1] by which reproducing microorganisms can form stable patterns. This mechanism is based on the competition between two separate ingredients. First, a diffusivity that depends on the local population density can promote phase separation, generating alternating regions of high and low densities. Then, this is opposed by the birth and death of microorganisms which allow only a single uniform density to be stable. The result of this contest is an arrested nonequilibrium phase separation in which dense droplets or rings become separated by less dense regions, with a characteristic steady-state length scale. I will illustrate this mechanism by considering a model of run-and-tumble bacteria, for which a density dependent diffusivity can stem from either a decrease of the swim speed or an increase of the tumbling rate at high density. No chemotaxis is assumed in this model, yet it predicts the formation of patterns strikingly similar to those believed to result from chemotactic behavior.

[1] M. E. Cates, D. Marenduzzo, I. Pagonabarraga, and J. Tailleur, PNAS, 107, 11715 (2010).

O10.4 SCH Fri 9 17:20

Behavior of microswimmers in complex enviroinments

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Self-propelled Brownian particles take up energy from their environment and convert it into directed motion. Examples range from chemotactic cells and bacteria to artificial systems. Until now most studies have concentrated on the behaviour of microswimmers in homogeneous environments, where one typically observes a crossover from ballistic motion at short times to enhanced diffusion at long times. Under many natural conditions, however, self-propelled particles move inside patterned or crowded environments, e.g., during bioremedation where bacteria spread through contaminated soils or in medical infections where pathogenic microorganisms propagate inside tissues. In a similar way, artificial microswimmers will be employed in patterned surroundings, e.g., in lab-on-a chip devices. As a first step towards more realistic conditions under which such microswimmers will be employed, we studied the motion of microswimmers in simple environments such as single pores, walls and periodically patterned samples. As microswimmers we used an alternative approach where gold-capped colloidal spheres are suspended in a binary liquid mixture. Illumination with light causes a local demixing of the fluid, which leads to self-diffusiophoresis where the swimming speed is easily controlled by the light intensity. Due to rotational diffusion, the swimming direction of such particles changes randomly. We investigated how such particles swim across periodically patterned samples under the influence of an external drift force and observe large differences in their trajectories depending on their swimming speed. While slow swimmers overall follow the direction of the force, fast swimmers swim along directions where the pattern leaves straight channels. We demonstrated that this behaviour can be exploited to effectively sort particles with different swimming behaviour and we expect that this method can be also applied to characterize cells and bacteria.

Motion of a model micro-swimmer in Poiseuille flow

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Many microorganisms in the human body swim in confined environments like sperm cells in the Fallopian tube or *E. coli* bacteria in the colon. Microswimmers exhibit hydrodynamic interactions with bounding surfaces that change their swimming speeds and orientations. In particular, *pushers* and *pullers* show different behavior. Pushers such as sperm cells or bacteria propel themselves with flagella attached at the back of the cell body whereas pullers like the algae *Chlamydomonas* typically have a propelling apparatus in the front. Both create a dipole far-field but with reversed fluid flow directions provoking different hydrodynamic interactions with surfaces. Pushers typically get attracted by a wall and orient parallel to it, pullers get either reflected by a wall or get trapped oriented perpendicular to it. As a simple model microorganism we use the so-called *squirmer*. It has a spherical shape with a prescribed axisymmetric tangential surface velocity, different for pushers and pullers. We systematically investigate the swimming behavior of both pushers and pullers in a cylindrical microchannel with an imposed Poiseuille flow. The hydrodynamics of squirmers including thermal noise is modeled using multi-particle collision dynamics. This method introduces ballistic and collision steps of effective particles in order to solve the Navier-Stokes equations. When the strength of the flow is sufficiently small, pushers swim upstream at the wall. Pullers can also swim upstream, however, in the center of the channel. Increasing the strength of the imposed flow, pushers and pullers now start to tumble. Hydrodynamic interactions with the wall become negligible and both swimmers can also perform periodic motions around the centerline of the channel while drifting downstream. These observations match well with our analytical model reminiscent to the nonlinear pendulum equation.

Posters

Session 1:
Ionic and quantum liquids, liquid metals

P1.1 **Relation between chemical ordering and transport phenomena in binary liquid mixture**
Stefano Amore, Juergen Horbach, Ivan Egry

P1.2 **Universal relations in the dynamics of ionic liquids: self-diffusion and electrical conductivity**
Jeffrey Armstrong, Pietro Ballone

P1.3 **Vapour structure of room temperature ionic liquids**
Markus Bier

P1.4 **Bulk and interfacial properties of room temperature ionic liquids**
Markus Bier

P1.5 **Insight on relaxations in ionic liquids by means of Brillouin light scattering**
Stefano Cazzato, Marco Zanatta, Andrea Mandanici, Eliana Quartarone, Ezio Zanghellini, Aleksandar Matic, Per Jacobsson

P1.6 **Structure and dynamics of ionic liquids entrapped in nanoporous silica**
Benoit Coasne, Lydie Viau, Andre Vioux

P1.7 **Universal solidification behaviour in liquid metals?**
Franz Demmel, Christoph Morkel

P1.8 **Surface tension of electrolyte solutions: a Monte Carlo study**
Alexandre Diehl, Alexandre Pereira dos Santos, Yan Levin

P1.9 **Fingerprints of order and disorder in the microscopic dynamics of liquid metals**
Valentina Giordano, Giulio Monaco

P1.10 **Primary relaxation in 1-alkyl-3-methylimidazolium bromide liquids**
Miguel A. Gonzalez, Bachir Aoun, David Price, Marie-Louise Saboungi, Wolfgang Haussler, Alberto Rivera, Carlos Leon

P1.11 **Intrinsic analysis of the vapour/liquid interface of a room temperature ionic liquid**
Gyorgy Hantal, Miguel Jorge, M. Natalia D. S. Cordeiro

P1.12 **An efficient method of calculating free energies of charged systems**
Robert Horton, Mike Finnis, George Jackson, Amparo Galindo, Andrew Haslam

P1.13 **Detection of collective optic excitations in molten NaI**
Shinya Hosokawa, Masanori Inui, T. Bryk, I. Mryglod, Wolf-Christian Pilgrim, Y. Kajihara, K. Matsuda, Y. Ohmasa, Satoshi Tsutsui, Alfred Q. R. Baron

P1.14 **The single particle dynamics of liquid iodine in the Sachs-Teller regime**
Maria Grazia Izzo, Alessandro Cunsolo, Filippo Bencivenga, Silvia Di Fonzo, Roberto Verbeni, Ramon Gimenez De Lorenzo

P1.15 **Transport properties of tetrahedral, network-forming ionic melts: LiF-BeF$_2$ mixtures**
Shadrack Jabes, Manish Agarwal, Charusita Chakravarty

P1.16 **Computer simulation study on room-temperature ionic liquid/graphene supercapacitor**
YounJoon Jung, Youngseon Shim, Hyung Kim

P1.17 **Dressed counterions: poly- and monovalent ions at charged dielectric interfaces**
Matej Kanduc, Ali Naji, Jan Forsman, Rudolf Podgornik

P1.18 **Porphyrin preparation in the acidic ionic liquids**
Satoshi Kitaoka, Kaoru Nobuoka, Tomoya Matsufuji, Yuichi Ishikawa

P1.19 **Dynamics and transport of ions in supercritical fluids under the action of an electrostatic field**
Andreas Koutselos, Maria Anagnostopoulou, Hercules Litinas, Jannis Samios

P1.20 **A representation of thermal conductivity in molten salts**
Masanobu Kusakabe, Shigeru Tamaki

P1.21 **Relation between structure and thermodynamic properties of anomalous liquid metals**
Guy Makov, Eyal Yahel, Yulia Shor, Yaron Greenberg, Elad Caspi

P1.22 **Network of tetrahedral Hg$_4$ blocks in expanded liquid Hg**
Kenji Maruyama, Hirohisa Endo, Hideoki Hoshino, Friedrich Hensel, Takashi Odagaki

P1.23 **X-ray Compton scattering measurements of expanded fluid rubidium**
Kazuhiro Matsuda, Takena Nagao, Yukio Kajihara, Koji Kimura, Masanori Inui, Kozaburo Tamura, Makoto Yao, Masayoshi Itou, Yoshiharu Sakurai

P1.24 **Inter-cation correlation in molten and superionic (AgxCu1-x)Br**
Shigeki Matsunaga

P1.25 **Structural fluctuations in para-hydrogen clusters studied by the variational path integral molecular dynamics method**
Shinichi Miura

P1.26 **Atomic structure and transport of liquid silver and gold**
Mohamed Mouas, Jean-Georges Gasser, Slimane Hellal, Ahmed Makradi, Salim Belouettar, Benoit Grosdidier

P1.27 **A new visualization method of transverse wave in liquids**
Shuji Munejiri, Fuyuki Shimojo, Kozo Hoshino

P1.28 **Proline based chiral ionic liquids for chiral synthesis**
Kaoru Nobuoka, Satoshi Kitaoka, Yuichi Ishikawa

P1.29 ***Ab initio* molecular dynamics study of pressure-induced metallization of covalent liquid**
Satoshi Ohmura, Fuyuki Shimojo

P1.30 **Magnetic properties of liquid 3d transition metal-Sb alloys**
Satoru Ohno, Shuta Tahara, Tatsuya Okada

P1.31 **Magnetic properties of 3d transition metal-Sb alloys**
Satoru Ohno, Shuta Tahara, Tatsuya Okada

P1.32 **On peculiarities of viscosity of the Co91B9 melt**
Natalya Olyanina, Vladimir Ladyanov, Anatoliy Beltyukov

P1.33 **Structure and short-time dynamics of ionic liquids: a molecular dynamics simulation and Raman spectroscopy study**
Mauro Ribeiro, Sérgio Urahata, Leonardo Siqueira, Luciano Costa, Bruno Nicolau, Tatiana Penna

P1.34 **Densities of EMIM-CnS binary mixtures with ethanol at four temperatures**
Esther Rilo Siso, Montserrat Dominguez-Perez, Juan Vila, Luisa Segade, Sandra García-Garabal, Oscar Cabeza

P1.35 **Short- and intermediate-range structure analysis for liquid Cs-Au mixtures by using Reverse Monte Carlo modeling**
Satoshi Sato

P1.36 **A molecular dynamics simulation study of magmatic liquids**
Nicolas Sator

P1.37 **Longe range fluctuations in ionic liquids**
Wolffram Schröer, Vlad Vale, Bernd Rathke, Stefan Will

P1.38 **The lquid-liquid phase transitions in ionic solutions**
Wolffram Schröer, Jan Köser, Darius Arndt, Vlad Vale, Anna Butka, Abdallah Elshwishin, Bernd Rathke

P1.39 **The dielectric response of charged liquids**
Marcello Sega, Sofia Kantorovich, Axel Arnold, Christian Holm

P1.40 **Nanoporous carbon supercapacitors: Fill'er up!**
Youngseon Shim

P1.41 ***Ab initio* molecular-dynamics study of diffusion mechanisms in liquid $ZnCl_2$ under pressure**
Fuyuki Shimojo, Akihide Koura, Satoshi Ohmura

P1.42 **Computational studies of molecular ionic liquids: from pure solvents to protein solutions**
Othmar Steinhauser

P1.43 **Van der Waals interactions between bodies of classical dipoles**
Joakim Stenhammar, Martin Trulsson, Håkan Wennerström, Per Linse, Gunnar Karlström

P1.44 **Medium range fluctuation in liquid pseudo-binary mixture between non-superionic AgCl and superionic AgI**
Hiroki Ueno, Yukinobu Kawakita, Shuta Tahara, Koji Ohara, Hironori Shimakura, Rosantha Kumara, Akinori Yasunaga, Yuiko Wakisaka, Shunsuke Ohba, Jyunpei Yahiro, Masanori Inui, Yukio Kajihara, Shinji Kohara, Shin'ichi Takeda

P1.45 **Lindemann criterion for nano-clusters and the glass transition**
Alexander Voronel

P1.46 **Structural and dynamic changes of ionic liquids under an external electric field**
Yanting Wang

P1.47 **Collective dynamics of atoms in liquid $Li_{70}Bi_{30}$ alloy**
Jean-François Wax, Mark R. Johnson, Livia E. Bove, Marek Mihalkovic

P1.48 **How strongly ionic are room temperature ionic liquids? A corresponding-states analysis of the surface tension**
Volker C. Weiss, Berit Heggen, Frédéric Leroy

P1.49 **The phase diagram of liquid bismuth**
Eyal Yahel, Guy Makov, Yaron Greenberg, Elad Caspi, Ori Noked, Aviva Melchior

P1.50 **Viscosity of Sn-enriched Co-Sn liquid alloys**
Andriy Yakymovych, Stepan Mudry

P1.51 **Densities of the binary system Trihexyltetradecylphosphonium Bromide + N, N-dimethylformamide from 293.15 to 313.15 K at atmospheric pressure**
Abel Zuñiga-Moreno, Elizabeth Juarez-Camacho, Carmen Reza, Maria Manriquez, Rosa de Lima Gutierrez-Lugo

Session 2:
Water, solutions and reaction dynamics

P2.1 **Liquid water: from symmetry distortions to diffusive motion**
Noam Agmon

P2.2 **Water + tert-butanol mixtures: ultrasonics, hypersonics and molecular dynamics**
Augustinus Asenbaum, Christian Pruner, Emmerich Wilhelm, Aurelien Perera

P2.3 **Structure of the water - alcohol solutions at T=300K**
Nataliya Atamas, Alexander Atamas

P2.4 **Experimental evidence of reaction-driven miscible viscous fingering**
Luis Atilio Riolfo, Yuichiro Nagatsu, Shohei Iwata, Philip M. J. Trevelyan, Anne De Wit

P2.5 **Puckering free energy of pyranoses in solution**
Emmanuel Autieri, Marcello Sega, Francesco Pederiva

P2.6 **Trapping proton transfer reaction intermediates in cryogenic hydrofluoric acid solutions**
Patrick Ayotte

P2.7 **The field experiments on the HTO washout from the atmosphere**
Yuri Balashov, Alexey Golubev, Sergey Mavrin, Valentina Golubeva

P2.8 **The effect of rain characteristics on tritium oxide washout rate from the atmosphere**
Yuri Balashov, Alexey Golubev, Vladimir Piskunov, Sergey Mavrin, Valentina Golubeva, Alexey Aleinikov, Vladimir Kovalenko, Igor Solomatin

P2.9 **Ionic dissociation revisited**
Andy Ballard

P2.10 **Equation of state for water in the small compressibility region**
Vitaliy Bardik, Dmitry Nerukh, Evgen Pavlov, Igor Zhyganiuk

P2.11 **High-resolution tandem Fabry-Perot interferometer for Ultra-Violet Brillouin scattering measurements**
Andrea Battistoni, Filippo Bencivenga, Daniele Fioretto, Claudio Masciovecchio

P2.12 **Phase transition and some properties in a water-like model**
Andressa Antonini Bertolazzo, Márcia Cristina Bernardes Barbosa, Márcia Martins Szortyka

P2.13 **"Blue energy" from ion adsorption and electrode charging in sea- and river water**
Niels Boon, René van Roij

P2.14 **Multiscale studies of hydrophobic association**
Aviel Chaimovich, M. Scott Shell, Jacob Israelachvili

P2.15 **Hydration water in diluted aqueous solutions of biological interest: an extended frequency range depolarized light scattering study**
Lucia Comez, Laura Lupi, Stefania Perticaroli, Marco Paolantoni, Paola Sassi, Assunta Morresi, Daniele Fioretto

P2.16 **Dipolar solute rotation in a supercritical polar fluid**
Amit Das

P2.17 **Equation of state of water measured down to -260 bars**
Kristina Davitt, Etienne Rolley, Frederic Caupin, Arnaud Arvengas, Sebastien Balibar

P2.18 **Statical and dynamical structure of water-methanol mixtures**
Simone De Panfilis, Ferdinando Formisano, Federica Venturini, Monica Jimenez-Ruiz, Helmut Schober, Giancarlo Ruocco

P2.19 **Computer simulation of fluids with intrinsic and permanent cavities**
Mario G. Del Popolo, Gavin M. Melaugh, Nicola Giri, Cristine E. Davidson, Stuart L. James

P2.20 **Long-lived sub-microscopic bubbles in very diluted alkali halides water solutions**
Eugène Duval, Sergey Adishchev, Sergey Sirotkin, Alain Mermet

P2.21 **Glass transition and relaxation processes in xylitol-water mixtures**
Khalid Elamin, Johan Sjöström, Helén Jansson, Jan Swenson

P2.22 **Water-like anomalies in core-softened system: relation between different anomalies regions**
Yury Fomin, Valentin Ryzhov, Elena Tsiok

P2.23 **Water in different kinds of hydrophobic nanoconfinements**
Giancarlo Franzese

P2.24 **Study of supramolecular structures in aqueous solutions of diols**
Ziyoyev Gafurdjan, Mirzaev Sirojiddin

P2.25 **Supercooled aqueous solutions: a route to explain water anomalies**
Paola Gallo

P2.26 **Local thermodynamics of hydration: theory and application to the hydration of a hard sphere**
Aljaz Godec, Franci Merzel

P2.27 **High-resolution RIXS on liquids and gases**
Franz Hennies

P2.28 **Ultrasonic evidence for low density water to high density water transition**
Eduardo Hidalgo, Mercedes Taravillo, Valentín Garcia Baonza, Pedro Dimas Sanz, Bérengère Guignon

P2.29 **Pressure-induced poly-amorphism of amorphous ices by molecular-dynamics simulations**
Kozo Hoshino, Takuya Yoshikawa, Shuji Munejiri

P2.30 **The theoretical analysis of water droplets in SDS/(Hexylamine+Heptane)/water system**
Parviz Hossein Khani, H. Moazzami

P2.31 **The theoretical analysis of size, average number of water droplets and electrical conductivity values in SDS/(Hexylamine+Heptane)(1:1)/water ternary microemulsion system**
Parviz Hossein Khani, Hamid Moazzami

P2.32 **High frequency dielectric spectroscopy of polymers, biomolecules and polar liquids**
Pravin Hudge

P2.33 **Cold and ultracold NH + NH collisions**
Liesbeth Janssen, Ad van der Avoird, Gerrit Groenenboom, Piotr Zuchowski, Jeremy Hutson

P2.34 **Towards a molecular theory of hydrophobic hydration: hard spheres in primitive water**
Jan Jirsák, Ivo Nezbeda

P2.35 **Dielectric relaxation study of aqueous binary liquids using picosecond time domain reflectometry**
Yogesh Joshi, Ashok Kumbharkhane

P2.36 **Crystallization of a pure fluid and a binary mixture of Lennard-Jones particles**
Swetlana Jungblut, Christoph Dellago

P2.37 **Sound velocity in aqueous mixtures of N, N-dimethylformamide and tetrahydofuran**
Egamberdiev Kamoliddin, Avdievich Vladimir, Mirzaev Sirojiddin

P2.38 **A study of dielectric behavior of alcohol in non polar solvents**
Kamalakar Kanse, Ashok Kumbharkhane

P2.39 **Accurate evaluation of structural correlations in realistic liquids: a RISM-based approach**
Bernarda Kezic

P2.40 **Virial equation of state of the hard tetrahedron fluid**
Jiri Kolafa, Stanislav Labik

P2.41 **Static dielectric constant of polarizable models from simulations**
Jiri Kolafa

P2.42 **Compensation effect in thermodynamics of hydroperoxides solutions**
Irina Kolyadko, Dina Kamalova, Alexandr Remizov, Roman Skochilov

P2.43 **Subdiffusion in a system with chemical reactions**
Taduesz Kosztolowicz, Katarzyna Lewandowska

P2.44 **The electric properties of ionic solutions at the membrane interface: a molecular dynamics study**
Gianluca Lattanzi, Mauro Lorenzo Mugnai, Giovanni Ciccotti, Ron Elber

P2.45 **Dipolar order in molecular fluids**
Per Linse, Gunnar Karlström

P2.46 **The hydrophobic interaction at high hydrostatic pressure**
Diarmuid Lloyd, Rosalind Allen, Paul Clegg

P2.47 **Experimental evidence for the Yang-Yang anomaly in a binary liquid mixture: high-resolution study by adiabatic scanning calorimetry**
Patricia Losada-Perez, ChandraShekhar Pati Tripathi, Jan Leys, Christ Glorieux, Jan Thoen

P2.48 **Treating hydrophobic hydration on a simple level**
Miha Lukšič, Tomaz Urbič, Barbara Hribar-Lee

P2.49 **Intermolecular polarizability dynamics of sugar aqueous solutions: molecular dynamics simulations and depolarized light scattering experiments**
Laura Lupi, Lucia Comez, Marco Paolantoni, Branka M. Ladaniy, Daniele Fioretto

P2.50 **Correlations in diffusional motion of water molecules: computer simulation**
George Malenkov, Yu. I. Naberukhin, V. P. Voloshin

P2.51 **Alkali and halide ions potential parameters for simulation of ion specific effects in aqueous medium**
Shavkat Mamatkulov, Dominik Horinek, Roland Netz

P2.52 **Hydrogen bond network, effect of solutes and viscosity of aqueous solutions**
Rosaria Mancinelli, Maria Antonietta Ricci, Fabio Bruni

P2.53 **Liquid crystal phase and waterlike anomalies in a core-softened shoulder-dumbbells system**
Márcia Cristina Bernardes Barbosa

P2.54 **Water structure enhancement in water-rich binary solvent mixtures**
Yizhak Marcus

P2.55 **Anion polarizability in solution: does it depend on the environment?**
Marco Masia, Elvira Guardia, Jonas Sala, Ausias-March Calvo

P2.56 **Rationalizing the stereoselectivity of paroline-catalyzed asymmetric aldol reactions in water**
Marco Masia, Jordi Ribas, Maria Angels Carvajal, Alain Chaumont

P2.57 **Local internal pressures in aqueous and alcohol solutions**
Nubia Mendoza, Mercedes Cáceres, Mercedes Taravillo, Valentín Garcia Baonza

P2.58 **Collective behavior of single-file water chains in nanopore membranes**
Georg Menzl, Jürgen Köfinger, Christoph Dellago

P2.59 **The noncoincidence effect of the overtone of the C=O stretching mode of acetone**
Maurizio Musso, Paolo Sereni, Maria Grazia Giorgini, Hajime Torii

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Santosh Mysore

P2.61 **The structure of chaos in liquid water**
Dmitry Nerukh, Vladimir Ryabov

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Paulo Netz, Márcia Cristina Bernardes Barbosa, Juliana Paukowski, Gavazzoni Cristina, Gonzatti Guilherme, Oliveira Alan

P2.63 **A dynamical simulation study of the rotational absorption spectra of HCl diluted in liquid Ar**
Antonio Padilla, Justo Pérez

P2.64 **The micro-structure of liquid water**
Aurélien Perera

P2.65 **Rate determination for precipitation scavenging of HTO vapour**
Vladimir Piskunov

P2.66 **Parameterization of aerosol washout rate by precipitation**
Irina Piskunova, Vladimir Piskunov

P2.67 **Role of the fluid and porosity formation during solvent-mediated phase transformations**
Christophe Raufaste, Bjørn Jamtveit, Timm John, Paul Meakin, Dag K. Dysthe

P2.68 **Is there a riskless way to enter the water's no-man's land?**
Maria-Antonietta Ricci, Fabio Bruni, Rosaria Mancinelli

P2.69 **Temperature and concentration effect on the hydration properties of Cyclodextrin and its substituted form: a depolarized light scattering study**
Barbara Rossi, Lucia Comez, Laura Lupi, Daniele Fioretto, Silvia Caponi, Flavio Rossi

P2.70 **Excess entropy and diffusivity of water in a supercooled aqueous solution of salt**
Mauro Rovere, Dario Corradini, Paola Gallo

P2.71 **Water-like anomalies in core-softened system: trajectory dependence of anomalous behavior**
Valentin Ryzhov, Yury Fomin, Elena Tsiok

P2.72 **Solid/liquid and liquid/vapor equilibria for common water models**
Ryuji Sakamaki, Amadeu Sum, Tetsu Narumi, Kenji Yasuoka

P2.73 **The structure of simple aromatic liquids and solutions by neutron scattering**
Neal Skipper, Tom Headen, Chris Howard, Daniel Bowron, Alan Soper

P2.74 **Percolation line and response functions in supercritical water**
Jiri Skvor, Jan Jirsak, Ivo Nezbeda

P2.75 **Model of a topological rearrangement wave on hydrogen-bonded network of water**
Alexey Solovey

P2.76 **Regularities in the rare earths hydrolytic behaviour**
Sophia Stepanchikova

P2.77 **How the liquid-liquid transition affects hydrophobic hydration of a polymer chain in supercooled water**
Tomonari Sumi, Hideo Sekino

P2.78 **A molecular dynamics study of protonated water clusters**
Yukari Sumita

P2.79 **Effect of protein dynamics on biological proton transfer reactions**
Srabani Taraphder

P2.80 **Complex phase behavior of the system of particles with smooth potential with repulsive shoulder and attractive well**
Elena Tsiok, Yurii Fomin, Valentin Ryzhov

P2.81 **New classical polarizable water model for molecular dynamics simulations of ice**
Linda Viererblová, Jirí Kolafa

P2.82 **Understanding water dynamics near topologically complex solutes from simulation**
Ana Vila Verde, Kramer Campen

P2.83 **Statistics and dynamics of water cavitation in synthetic trees**
Olivier Vincent, Philippe Marmottant, Pedro Quinto-Su, Claus-Dieter Ohl

P2.84 **Guanidinium in aqueous solution studied by quantum mechanical charge field - molecular dynamics (QMCF-MD)**
Alexander Weiss, Thomas Hofer, Bernhard Randolf, Anirban Bhattacharjee, Bernd Rode

P2.85 **Kinetics of thermostatted ice growth from supercooled water in simulations**
Volker C. Weiss, Markus Rullich, Christof Köhler, Thomas Frauenheim

P2.86 **Theoretical study of protein hydration thermodynamics based on the 3D integral equation theory of molecular liquid and the spatial decomposition analysis**
Takeshi Yamazaki, Andriy Kovalenko

P2.87 **Molecular Ornstein-Zernike self-consistent-field approach to hydrated electron**
Norio Yoshida, Fumio Hirata

P2.88 **Effects of interaction potential and hydrodynamic interaction on the diffusion-influenced bimolecular reaction rates**
Chang Yun Son, Sangyoub Lee

P2.89 **Crowding and shear flow effects on diffusion-limited reaction kinetics in liquids**
Alessio Zaccone

Session 3:
Liquid crystals

P3.1 **Calculation of surface elastic constants of a Gay- Berne nematic liquid crystals with prolate molecules from new direct correlation and pair distribution functions**
Abolghasem Avazpour, Mehrnosh Hashemi, Ladan Avazpour, Foroogh Lotfi

P3.2 **Studies in Cds-nanorods doped ferroelectric liquid crystal films**
Ashok Chaudhary, Praveen Malik, Rohit Mehra, KK Raina

P3.3 **Influence of silica nanoparticle on electro-optical and dielectric properties of ferroelectric liquid crystal**
Ashok Chaudhary, Praveen Malik, Rohit Mehra, K. K. Raina

P3.4 **Undulation instabilities in the meniscus of liquid crystal membranes**
Philippe Cluzeau, Jean Christophe Loudet, P. Patricio, Pavel Dolganov

P3.5 **Rod-like viruses in a wedge**
Oliver Dammone, Pavlik Lettinga, Dirk Aarts

P3.6 **Translation diffusion in thermotropic liquid crystals**
Sergey Dvinskikh

P3.7 **Filling and wetting transitions of nematic liquid crystal on rectangular grated surfaces**
Zahra Eskandari, Nuno M. Silvestre, Pedro Patricio, Jose M. Romero-Enrique, Margarida M. Telo da Gama

P3.8 **Electro-optic response and X-ray orientational analysis of anisotropic colloidal liquid crystal particles with applied electric field**
Robert Greasty, Robert Richardson, Susanne Klein, Jana Heuer, Claire Pizzey

P3.9 **Brodband dielectric and infrared spectroscopy studies on confined liquid crystals**
Malgorzata Jasiurkowska, Roxana Ene, Wilhelm Kossack, Ciprian Iacob, Wycliffe Kiprop, Periklis Papadopoulos, Maria Massalska-Arodz, Friedrich Kremer

P3.10 **Isotropic to nematic phase transition in mixtures with double peak specific heat anomaly**
Dalija Jesenek, Samo Kralj, Vlad Popa-Nita, George Cordoyiannis, Zdravko Kutnjak

P3.11 **Interparticle force in nematic colloids**
Yasuyuki Kimura, Takahiro Kishita, Noboru Kondo, Masatoshi Ichikawa, Jun-ichi Fukuda

P3.12 **The influence of suspended nano-particles on the electro-optical behaviour of liquid crystals**
Susanne Klein, Robert Greasty, Robert Richardson, John Rudin

P3.13 **Manipulating gibbsite liquid crystals in an external electric field**
Anke Leferink op Reinink, Bonny Kuipers, Dima Byelov, Andrei Petukhov, Gert-Jan Vroege, Henk Lekkerkerker

P3.14 **Tuning diffusion and phase behaviour with tuneable rod-like viruses**
Pavlik Lettinga, Gerhard Gompper, Emilie Pouget, Eric Grelet

P3.15 **X-ray and dielectric studies of (4-(4-oktylobiphenyl)carboksylan) 4-(2-methylobuthyl) phenol liquid crystal having blue phase**
Gabriela Lewinska, Wojciech Otowski, Andrzej Budziak, Dorota Dardas

P3.16 **Instability patterns in thin nematic films: comparison between theory and experiment**
Oksana Manyuhina, Anne-Marie Cazabat, Martine Ben Amar

P3.17 **Biaxial nematic phases in fluids of hard board-like particles**
Yuri Martinez-Raton, Enrique Velasco, Szabolcs Varga

P3.18 **Study of new polymer-magnetite particles/liquid crystal colloidal composite**
Doina Manaila Maximean, Constantin Rosu, Emil Petrescu, Dan Donescu, Eugeniu Vasile, Cristina Cirtoaje, Octavian Danila

P3.19 **Maier-Saupe nematogenic system near hard wall: field theoretical approach**
Myroslav Holovko

P3.20 **Stereo-specific lateral-pressure profile changes in lipid membranes by general anesthetics**
Georg Pabst, Eva Sevcsik, Michael Rappolt, Thomas Stockner

P3.21 **High-resolution adiabatic scanning calorimetric study of phase transition behavior of some piperidinium and morpholinium ionic liquid crystals**
Chandra Shekhar Pati Tripathi, Jan Leys, Patricia Losada-Pérez, Christ Glorieux, Kathleen Lava, Koen Binnemans, Jan Thoen

P3.22 **Colloidal particles at a cholesteric liquid crystal interface**
Anne Pawsey, Juho Lintuvuori, Job Thijssen, Davide Marenduzzo, Paul Clegg

P3.23 **Lysine based surfactants: relationship between chemical structure and adsorption/aggregation properties**
Ramon Pons, Aurora Colomer, Lourdes Pérez, Aurora Pinazo, Maria-Rosa Infante

P3.24 **Polymorphism of two-dimensional crystals of oppositely charged cylindrical macroions**
VA Raghunathan, A. V. Radhakrishnan, SK Ghosh, Georg Pabst, AK Sood

P3.25 **Liquid crystalline behaviour of cylindrical block copolymer micelles**
Alexander Robertson, Joe Gilroy, Paul Rupar, Laura Senior, Robert Richardson, Ian Manners

P3.26 **Computer simulation study of the surface tension of the vapor-nematic planar interfaces**
Luis F. Rull, Jose Manuel Romero-Enrique

P3.27 **Colloidal particles with planar anchoring in liquid crystals**
Nuno M. Silvestre, Mykola Tasinkevych, Margarida M. Telo da Gama, Siegfried Dietrich

P3.28 **Direct observation of interaction of nanoparticles in a nematic LC**
Miha Skarabot, Igor Musevic

P3.29 **Anisotropy of spatiotemporal decorrelation in electrohydrodynamic turbulence**
Luca Sorriso-Valvo, Francesco Carbone, Giuseppe Strangi

P3.30 **Spatio-temporal dynamics, patterns formation and turbulence in complex fluids due to electrohydrodynamics instabilities**
Luca Sorriso-Valvo, Francesco Carbone, Antonio Vecchio

P3.31 **Fractal aggregates evolution of methyl red in liquid crystal**
Luca Sorriso-Valvo, Federica Ciuchi, Alfredo Mazzulla, José Manuel Redondo

P3.32 **Continuum theory for smectic A liquid crystals**
Iain Stewart

P3.33 **Field responsive anisotropic colloidal dispersions in nematic liquid crystals**
Michael Thomas

P3.34 **Isotropic lasing from cholesteric shell**
Yoshiaki Uchida, Yoichi Takanishi, Jun Yamamoto

P3.35 **Biaxiality and nematic-nematic phase separation in colloidal goethite dispersions**
Esther van den Pol, Andreea Lupascu, Mihai Diaconeasa, Dominique Thies-Weesie, Dmytro Byelov, Andrei Petukhov, Gert Jan Vroege

P3.36 **Effect of polydispersity and soft interactions on the nematic versus smectic phase stability in platelets suspensions**
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P3.37 **Mesophase formation in a system of top-shaped hard molecules: density functional theory and MC simulation**
Franz Vesely, Daniel de las Heras, Szabolcs Varga

P3.38 **Liquid crystalline order of charged colloidal platelets**
Rik Wensink

P3.39 **Generalised van der Waals-Onsager approach for attractive oblate cylinder particles**
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P3.40 **Multiscale simulation of rod-like liquid crystals**
Iori Yonekawa, Kenji Yasuoka

P3.41 **Novel perforated lamellar-nematic phase in binary mixture of amphiphilic and calamitic liquid crystals**
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Sreenath Bolisetty, Jozef Adamcik, Jijo Vallooran, Stephan Handschin, Raffaele Mezzenga

P4.2 **Experiments and theory on the electrophoresis of fd viruses, a finite or an infinite rod?**
Johan Buitenhuis

P4.3 **Self-assembly of block copolymer stars**
Barbara Capone, Federica Lo Verso, Ronald Blaak, Christos Likos

P4.4 **Online monitoring of ultrasonic degradation of poly (sodium styrene sulfonate)**
Huceste Catalgil-Giz, Gokce Onbirler, Ali Akyuz, Ahmet Giz

P4.5 **Potential theory of the polymer-mediated interactions in colloid-polymer mixtures**
Alexander Chervanyov, Gert Heinrich

P4.6 **Single chain dynamics of wormlike polyelectrolyte in flow fields by mesoscale simulations and single molecule imaging**
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P4.7 **A coarse-grained approach to protein design: learning from design to understand folding**
Ivan Coluzza

P4.8 **Helix specific electrostatics in DNA braids and supercoils**
Ruggero Cortini, Alexei Kornyshev, Dominic Lee, Sergey Leikin

P4.9 **Ultrasoft primitive model of polyelectrolytes in solution**
Daniele Coslovich, Jean-Pierre Hansen, Gerhard Kahl

P4.10 **Exploring the structural properties and molecular mechanisms of cryoprotectants**
Lorna Dougan

P4.11 **Molecular transport in liquid polymers**
Henryk Drozdowski, Zdzislaw Blaszczak

P4.12 **Monte Carlo simulations of semiflexible polymer chains. Efficient sampling from compact to extended structures**
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P4.13 **Off-equilibrium response of grafted polymer chains at variable rates of compression**
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P4.14 **Spherical vs periodic boundary conditions. Why and how?**
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P4.15 **Self-association of polymer-polyphenol complexes**
Paola Ferrari, Krassimir Velikov, Dirk GAL Aarts

P4.16 **Structural studies of proton conducting fluorous copolymers: blocks and grafts**
Barbara Frisken, Rasoul Narimani, Ami Yang, Emily Tsang, Steven Holdcroft

P4.17 **Large amphiphilic dendrimers: internal structure and effective pair interactions**
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P4.18 **The influence of light absorption and shadowing among segments of a chain on the kinetics of ultraviolet depolymerization**
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P4.19 **Conformations and interactions of charged dendrimers in implicit and explicit solvents**
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P4.20 **Viscoelasticity of semiflexible fibers in a hydrodynamic solvent**
T. A. Hunt, J. T. Padding, W. J. Briels

P4.21 **Atomistic investigations of P3HT polymers**
Alessandra Imperio, Johannes Padding, Wouter Den Otter, Wim Briels

P4.22 **Competitive adsorption of surfactants and polymers at the free water surface. A computer simulation study of the SDS - PEO system**
Pál Jedlovszky, Mária Darvas, Tibor Gilányi

P4.23 **Diffusion coefficients in binary polymer systems and effective sizes of mobile holes of components**
Dina Kamalova, Irina Kolyadko, Alexander Remizov

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Jan Kobierski, Hubert Haranczyk, Dorota Zalitacz, Monika Marzec, Jacek Niziol

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Christian Koch, Christos Likos, Athanassios Z. Panagiotopoulos, Federica Lo Verso

P4.26 **Diffusion of tracer particles in hydrogel networks**
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P4.27 **Star polyelectrolytes in poor solvents**
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P4.32 **Orientation mobility of dendrimer segments in dilute solutions: comparison of analytical calculations, computer simulation and NMR relaxation experiments**
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Andreas Menzel

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Firestone Millicent, Brombosz Scott, Sungwon Lee

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Sebastian Reddig, Holger Stark

P4.48 **Influence of the sorption of polar and non-polar solvents on Polyamide-6, 6 molecular dynamics**
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P4.49 **Liquid-liquid phase separation in protein solutions controlled by multivalent salts and temperature**
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P4.50 **Application of holographic gratings recorded in nanoparticle-polymer composites as cold-neutron diffractive elements**
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Michael Smith, Volfango Bertola

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P4.56 **Wrinkling labyrinth patterns on elastomeric Janus particles**
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Domenico Truzzolillo, Stefano Sarti, Federico Bordi

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Filip Uhlik

P4.60 **Anomalous structure and scaling of ring polymer brushes**
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P4.61 **Free energy and pressure calculations within two-dimensional Wang-Landau entropic sampling**
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Dean Wood, Philip Camp

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Takashi Yoshidome, Yuko Ito, Mitsunori Ikeguchi, Masahiro Kinoshita

P4.67 **Investigation of interplay between finite size scaling and aspect ratio in continuum percolating networks**
Milan Zezelj, Igor Stankovic, Aleksandar Belic

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Andrew Archer, Paul Hopkins, Andrea Fortini, Matthias Schmidt

P5.7 **The role of boundary conditions on the low-frequency dielectric relaxation of concentrated colloidal suspensions**
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Labrini Athanasopoulou, Primoz Ziherl

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P5.11 **Diffusive motion of nanoparticles under external magnetic field**
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P5.12 **Effect of radiation pressure on the arrangement of colloids**
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P5.13 **Crystallization kinetics in colloidal hard spheres obtained by a combined small angle light and Bragg scattering setup**
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Jean-Marc Bomont, Jean-Pierre Hansen, Dino Costa

P5.19 **Detection of early cluster formation in globular protein solutions: an entropic signature**
Jean-Marc Bomont, Dino Costa

P5.20 **Inhomogeneous colloidal liquids under shear flow**
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P5.24 **Ultra-soft colloid/polymer mixtures: structure and phase diagram**
Manuel Camargo, Barbara Lonetti, Jörg Stellbrink, Christos Likos, Emanuela Zaccarelli

P5.25 **Dielectric response in realistic salt-free concentrated suspensions. Non-equilibrium dissociation-association processes**
Felix Carrique, Emilio Ruiz-Reina, Francisco J. Arroyo, Angel V. Delgado

P5.26 **A DFT study of microphase formation in binary gaussian mixtures**
Marcello Carta, Davide Pini, Luciano Reatto, Alberto Parola

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Ramon Castaneda-Priego, Salvador Herrera-Velarde, Edith Cristina Euan-Diaz, Nestor Enrique Valadez-Perez, Fidel Cordoba-Valdez, Jose Marcos Falcon-Gonzalez

P5.28 **Hydrophobic versus electrostatic interactions: stability of macromolecular clusters**
Jaydeb Chakrabarti

P5.29 **Phase behavior of solvent-free oligomer-grafted nanoparticles**
Alexandros Chremos, Athanassios Z. Panagiotopoulos, Donald L. Koch, Hsiu-Yu Yu

P5.30 **Collisional formulas for molecular dynamics of patchy colloids**
Agnieszka Chrzanowska, Pawel Karbowniczek

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P5.39 **Predicting crystal structures and phase behavior for faceted non-convex colloids and nanoparticles**
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Thomas Fischer

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Jaffar Hasnain

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Peter Keim, Patrick Dillmann, Georg Maret

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José Juan López García, Miguel Jesús Aranda Rascón, José Horno Montijano

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Adam Law, Tommy Horozov, Martin Buzza

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Achim Lederer, Hans Joachim Schöpe

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P5.99 **Thermodynamic properties of non-additive hard-sphere mixtures in d dimensions**
Mariano Lopez de Haro, Andres Santos, Santos B. Yuste

P5.100 **Effective pair potentials for super-paramagnetic colloids in rotating magnetic fields**
Kathrin Müller, Arash Nikoubashman, Natan Osterman, Dušan Babič, Jure Dobnikar, Christos Likos

P5.101 **Consolidation and yielding behaviour of an aqueous nanoscale titanium dioxide system**
Alastair Mailer

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Alexandr Malijevsky, Andrew Archer

P5.103 **Crystallization of charged colloids: shape matters**
Ethayaraja Mani, Peter Bolhuis, Wolfgang Lechner, Willem Kegel

P5.104 **Inhomogeneous fluids of hard dumbbells by fundamental measure theory and Monte Carlo simulations**
Matthieu Marechal, Hanns Hagen Goetzke, Harmut Löwen

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Daniela Marzi, Barbara Capone, Christos N. Likos

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Kristina Milinkovic, Johan T. Padding, Marjolein Dijkstra

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P5.114 **Small-angle X-ray scattering studies of nanoparticles in solution for biological and drug delivery applications**
Christian Moitzi, Heinrich Santner

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Simon Stanley

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Tamara Tóth, Davide Ferraro, Matteo Pierno, Giampaolo Mistura, Ciro Semprebon

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P7.119 **Nucleation on a partially wettable solid substrate: thermodynamics and an interface displacement model**
Dmitry Tatyanenko, Alexander Shchekin

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Takamichi Terao

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Andreas Tröster

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Takuma Akimoto

P8.2 **Hyperacoustic relaxations in liquids: a comparison of renormalized damped oscillator and generalizaed hydrodynamics approaches**
Francesco Aliotta, Rosina Celeste Ponterio, Franz Saija, Mikolaj Pochylski, Jaceck Gapinski

P8.3 **Dynamical and structural heterogeneities in the context of liquid-liquid phase transitions: the case of gallium**
Alex Antonelli, Oscar Macollunco, Diego Jara, Mateus Michelon, Maurice de Koning

P8.4 **Glass transition in thin polymer films**
Laura R. Arriaga, Francisco Monroy, Dominique Langevin

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Paul Bartlett, Lisa Teece, Malcolm Faers

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Silvia Caponi, Silvia Corezzi, Daniele Fioretto, Aldo Fontana, Giulio Monaco, Flavio Rossi

P8.8 **Metastable highly ordered supercooled liquid phase inherited from molecular beam grown glasses**
Simona Capponi, Simone Napolitano, Michael Wubbenhorst

P8.9 **Critical loci emanating from water's second critical point**
Claudio A. Cerdeiriña, Pablo G. Debenedetti

P8.10 **Measurements of the dynamic susceptibility of colloidal suspensions using coherent X-rays**
Heiko Conrad, Louisa Dahbi, Birgit Fischer, Christian Gutt, Gerhard Gruebel

P8.11 **Dynamics of suspensions of anisotropic colloidal particles investigated by X-Ray Photon Correlation Spectroscopy**
Louisa Dahbi, Heiko Conrad, Ingo Steinke, Felix Lehmkühler, Michael Sprung, Gerhard Grübel

P8.12 **Time resolved high energy x-ray diffraction study of the structure of supercooled calcium aluminosilicate liquids**
James W. E. Drewitt, Aleksei Bytchkov, Jad Kozaily, Viviana Cristiglio, Henry E. Fischer, Sandro Jahn, Noël Jakse, Alain Pasturel, Louis Hennet

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P8.14 **Freezing of water: local structure detection using neural networks**
Philipp Geiger, Christoph Dellago

P8.15 **Mode coupling theory of the glass transition in fluids of hard particles: effect of the triplet correlation functions**
Philippe Germain, Abderrahime Ayadim, Saïd Amokrane

P8.16 **Connecting structural relaxation with the low frequency modes in a hard-sphere colloidal glass**
Antina Ghosh, Vijayakumar Chikkadi, Peter Schall, Daniel Bonn

P8.17 **Structural relaxation times in high-density amorphous ice (HDA)**
Philip H. Handle, Markus Seidl, Erwin Mayer, Thomas Loerting

P8.18 **Multi-scale micro-relaxation of the quenched dusty plasma liquid**
Lin I, Yen-Shuo Su, Chong-Wai Io

P8.19 **Higher order parameters for establishing transient crystals**
Masaharu Isobe, Berni Alder

P8.20 **Structure of coexisting liquid phases of supercooled water; analogy with ice polymorphs**
Pál Jedlovszky, Lívia Pártay, Albert Bartók, Giovanni Garberoglio, Renzo Vallauri

P8.21 **Simple scenario for ”fast sound” phenomena and liquid-liquid phase transition**
Yukio Kajihara, Masanori Inui, Kazuhiro Matsuda

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Amit Kumar Bhattacharjee, Jürgen Horbach, Thomas Voigtmann

P8.23 **Confocal microscopy of colloidal hard sphere and charged sphere fluids and crystals**
Achim Lederer, Hans Joachim Schöpe

P8.24 **Bond order in hard sphere colloidal systems tracked by coherent x-rays**
Felix Lehmkühler, Christian Gutt, Peter Wochner, Birgit Fischer, Heiko Conrad, Miguel Catro-Colin, Sooheyong Lee, Ingo Steinke, Michael Sprung, Diling Zhu, Henrik Lemke, Stephanie Bogle, Paul Fuoss, G. Brian Stephenson, Marco Cammarata

P8.25 **Enthalpy and heat capacity measurements by adiabatic scanning calorimetry of some pure alkanes: melting, solidification and supercooling**
Jan Leys, Christ Glorieux, Jan Thoen

P8.26 **Structure and dynamics of depletion-induced protein-polymer gels**
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P8.27 **Using the topological cluster classification to identify slow clusters within supercooled liquids**
Alex Malins, C. Patrick Royall, Jens Eggers, Stephen Williams, Hajime Tanaka

P8.28 **Connecting diffusion and dynamical heterogeneities in actively deformed amorphous systems**
Kirsten Martens, Lydéric Bocquet, Jean-Louis Barrat

P8.29 **Influence of pores on the polyamorphic transition in water**
Christian Mitterdorfer, Michael S. Elsaesser, Katrin Winkel, Erwin Mayer, Thomas Loerting

P8.30 **Vitrification and crystallization processes of a monatomic system**
Tomoko Mizuguchi, Takashi Odagaki

P8.31 **The transient response of supercooled colloidal fluids to external shear**
Kevin Mutch, Marco Laurati, Georgios Petekidis, Nikos Koumakis, Stefan Egelhaaf

P8.32 **Dynamic heterogeneities, boson peak and activation volume in glass-forming liquids**
Vladimir Novikov, Liang Hong, Alexei Sokolov

P8.33 **FEL formalism of non-equilibrium statistical mechanics and dielectric responses of a super cooled liquid**
Takashi Odagaki

P8.34 **A leading model to describe the secondary processes in glasses and glass formers**
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P8.35 **Gradient of glass transition in nanocomposites: evidence by NMR et scanning differential calorimetry**
Aurélie Papon, Helene Montes, Laurent Guy, Kay Saalwachter, Francois Lequeux

P8.36 **Factors contributing to the glass forming ability of a simulated molecular liquid**
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P8.37 **Adaptive resolution coupling of classical and quantum scale: the case of liquid parahydrogen**
Raffaello Potestio, Luigi Delle Site

P8.38 **Theoretical study of aging and instantaneous quenchings in attractive Yukawa systems**
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P8.39 **Competitive nucleation in the freezing of nanoparticle clusters**
Bowles Richard, Cletus Asuquo

P8.40 **Computer simulation study of ionic liquids near the glass transition**
Alvaro Rodriguez-Rivas, Jose Manuel Romero-Enrique, Luis F. Rull

P8.41 **Non-monotonic temperature evolution of dynamic correlations in glass-forming liquids**
Sandalo Roldan-Vargas, Walter Kob, Ludovic Berthier

P8.42 **Clear structural and dynamical signatures for the difference between the glass and gel transitions in colloids**
Paddy Royall, Stephen R. Williams, Hajime Tanaka

P8.43 **Slow-dynamics of glass formers and soft matters observed by time domain interferometry using nuclear resonant scattering**
Makina Saito, Makoto Seto, Shiji Kitao, Yasuhiro Kobayashi, Masayuki Kurokuzu, Yoshitaka Yoda

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Thomas B. Schrøder, Nicoletta Gnan, Ulf R. Pedersen, Nicholas P. Bailey, Jeppe C. Dyre

P8.45 **Quantities affecting the glass transition temperature of amorphous ices in molecular dynamics**
Markus Seidl, Ferenc Karsai, Thomas Loerting, Gerhard Zifferer

P8.46 **Presence and absence of crystallization nuclei in high-density amorphous ice**
Markus Seidl, Katrin Winkel, Philip H. Handle, Gerhard Zifferer, Erwin Mayer, Thomas Loerting

P8.47 **Reorientational dynamics in a supercooled molecular liquid**
Gemma Sesé, Jordi Ortiz de Urbina, Ricardo Palomar

P8.48 **Glass transition and concentration fluctuation in polymer blends: DSC and viscoelastic measurements**
Peiluo Shi, Francois Lequeux, Hélène Montes

P8.49 **Quantitative analysis for inter-molecular correlation of radical Chlorine dioxide molecular liquid**
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P8.50 **Study of the kinetics of liquid-liquid transition in triphenyl phosphite**
Ryotaro Shimizu, Mika Kobayashi, Hajime Tanaka

P8.51 **Structure and phase diagram of self-assembling rigid rods on the cubic lattice**
Marcos Simoes, Noé Almarza, José Maria Tavares, Margarida Telo da Gama

P8.52 **Particle correlations, entropy and cooperative dynamics in supercooled liquids**
Murari Singh, Charusita Chakravarty

P8.53 **Dynamic arrest in ultrasoft systems**
Hernandez Sol Maria, Laura Yeomans-Reyna, Pedro E. Ramirez-Gonzalez, Magdaleno Medina-Noyola

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Thomas Speck

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Igor Stankovic, Aleksandar Belic, Milan Zezelj

P8.56 **Avalanche excitations in the quenched dusty plasma liquid**
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P8.57 **Crystallization mechanism of hard sphere glasses**
Chantal Valeriani, Eduardo Sanz, Emanuela Zaccarelli, Wilson Poon, Peter Pusey, Mike Cates

P8.58 **Effect of size polydispersity on the Yukawa melting transition**
Marjolein van der Linden, Alfons van Blaaderen, Marjolein Dijkstra

P8.59 **Compressing charged colloids by centrifugation: formation of soft glasses**
Marjolein van der Linden, Marjolein Dijkstra, Alfons van Blaaderen

P8.60 **Gauge theory of glass transition in frustrated system**
Mikhail Vasin

P8.61 **Liquid-liquid critical point in supercooled silicon**
Vishwas Vasisht

P8.62 **Phase-separation perspective on dynamic heterogeneities in glass-forming liquids**
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P8.63 **Effect of polydispersity on the dynamic arrest of colloidal systems**
Alejandro Vizcarra, Rigoberto Juarez, Magdaleno Medina

P8.64 **Quasi-equilibrium and the emergence of solid behaviour in amorphous materials**
Stephen Williams, Denis Evans

P8.65 **Hard-sphere percolation transitions and thermodynamic status of random close packing**
Les Woodcock

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Chi Yang, Lin I, Yen Shuo Su

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Oleksander Alekhin, Oksana Bilous, Alla Kulinich, Yuriy Ostapchuk, Evgenii Rudnikov

P9.2 **Thermodynamic theory for non-equilibrium pattern formation: measured wavelength variation of convective rolls for heat flow**
Phil Attard

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P9.4 **Rare events in non-stationary non-equilibrium**
Josh Berryman

P9.5 **Molecular dynamics simulation of the imbibition of surfactant solutions in nano-capillaries of varying roughness and wettability**
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P9.6 **Calculation of strain rate dependent shear viscosity of molecular liquids**
István Borzsák

P9.7 **A microscopic derivation of the constitutive equation describing the rheology of complex polymer liquids**
Wim Briels, Jan Dhont

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Stefano Buzzaccaro, Eleonora Secchi, Roberto Piazza

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Peilong Chen

P9.10 **Entropy production and Onsager's coefficients evaluation in the drop evaporation process**
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P9.11 **A novel optical approach to the Ludwig-Soret effect: validating data close to the critical point of a binary mixture**
Fabrizio Croccolo, Frank Scheffold

P9.12 **Complex fluids flows in sub-microchannels**
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P9.13 **Evolution of dynamics and structure formation in resorcinol - formaldehyde polymer gel**
Orsolya Czakkel, Anders Madsen
Beatrice Ruta, Yuriy Chushkin

P9.14 **Shear-driven solidification of dilute colloidal suspensions**
Emanuela Del Gado, Alessio Zaccone, Daniele Gentili, Hua Wu, Massimo Morbidelli

P9.15 **Stress overshoot in a simple yield stress fluid: an extensive study combining rheology and velocimetry**
Thibaut Divoux, Catherine Barentin, Sebastien Manneville

P9.16 **From stress induced fluidization processes to Herschel-Bulkley behavior in simple yield stress fluids**
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P9.17 **Effects of a nonuniform density profile upon the velocity flow and the viscosity of a shear thinning colloidal dispersion**
Thomas Farage, Joseph Brader

P9.18 **Computer simulations of colloidal transport on a patterned magnetic substrate**
Andrea Fortini, Matthias Schmidt

P9.19 **Modifying deformation properties of droplets - particles versus surfactants**
Stefan Frijters, Jens Harting, Florian Günther

P9.20 **Variational principles for perfect and viscous fluids**
Hiroki Fukagawa, Youhei Fujitani

P9.21 **Efficiently accounting for ion correlations in electrokinetic nanofluidic devices using density functional theory**
Dirk Gillespie

P9.22 **A non-Brownian suspension with switchable attractive interactions**
Christoph Goegelein

P9.23 **Soft matter in hard confinement: how molecular fluids arrange in and huddle through mesoporous solids**
Simon Gruener, Anke Henschel, Sebastian Mörz, Andre Kusmin, Andriy Kityk, Klaus Knorr, Dieter Richter, Patrick Huber

P9.24 **Bubbles dynamics in complex fluids**
Florence Haudin, Christophe Raufaste, Xavier Noblin

P9.25 **Droplet mobility on heterogeneous substrates**
Daniel Herde, Stephan Herminghaus, Martin Brinkmann

P9.26 **Rheology close to a jamming transition**
Claus Heussinger

P9.27 **Cell-level canonical sampling by velocity scaling for multiparticle collision dynamics simulations**
Chien-Cheng Huang

P9.28 **Transient cage formation around laser-heated gold colloids in polymer solutions**
Werner Köhler, Florian Schwaiger

P9.29 **Active microrheology to probe directional viscoelasticity : applicability and limitations**
Manas Khan, A. K. Sood

P9.30 **Breach of equilibrium of double electric layer. Surfactants in tribology**
Natalia Kochurova, N. Abdulin

P9.31 **Subdiffusive in a membrane system**
Tadeusz Kosztolowicz, Katarzyna Lewandowska

P9.32 **Stresses and structure of colloidal gels under shear**
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P9.33 **Dynamics and rheology of vesicle suspension in shear flow**
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P9.34 **Reverse osmosis in non-equilibrium simulations with active solute particles**
Thomas Lion, Rosalind Allen

P9.35 **Single file diffusion of colloids: experimental and theoretical aspects**
Emanuele Locatelli, Davide Ferraro, Fulvio Baldovin, Enzo Orlandini, Giampaolo Mistura, Matteo Pierno

P9.36 **Electric field-assisted dynamics of contact lines**
Dieter Mannetje, Chandrashekhar Murade, Dirk van den Ende, Frieder Mugele

P9.37 **Complex dynamics of knotted filaments in shear flow**
Richard Matthews, Ard Louis, Julia Yeomans

P9.38 **A non-equilibrium molecular dynamic simulation of flow of liquids in nanochannels using Laplacian smoothing method**
Mohammad Mehdi Maneshi

P9.39 **Dynamic approach to flowing liquids in confined systems**
Simone Melchionna

P9.40 **Hydrodynamics from statistical mechanics: combined dynamical-NEMD and conditional sampling to relax an interface between two immiscible liquids**
Simone Meloni, Sergio Orlandini, Giovanni Ciccotti

P9.41 **On mechanism of the nonmonotonic relaxation processes in nonequilibrium AL-TM-REM melts**
Svetlana Menshikova, Vladimir Ladyanov, Anatolii Beltyukov, Mikhail Vasin

P9.42 **Anisotropic microrheological properties of chain-forming magnetic fluid**
Alenka Mertelj, Andraz Resetic, Saso Gyergyek, Darko Makovec, Martin Copic

P9.43 **Peclet number effects on colloidal sedimentation with interparticle attractions**
Arturo Moncho, Ard Louis, Johan T. Padding

P9.44 **Transient shear banding in complex fluids**
Robyn Moorcroft, Suzanne Fielding

P9.45 **Heat transport in liquid water and amorphous ices**
Jordan Muscatello

P9.46 **A perturbation theory for friction of a large particle immersed in a binary solvent**
Yuka Nakamura, Akira Yoshimori, Ryo Akiyama

P9.47 **Rheology of dilatant fluid**
Hiizu Nakanishi

P9.48 **Cluster crystals under shear**
Arash Nikoubashman, Gerhard Kahl, Christos Likos

P9.49 **Oscillatory flow of viscoelastic fluids: theory and experiments**
Jordi Ortin, Laura Casanellas

P9.50 **Amplification of thermal fluctuations by planar Couette flow**
José Ortiz de Zárate, Jan Sengers

P9.51 **Scaling equation of non-equilibrium liquid system at critical state**
Yuriy Ostapchuk, Oleksander Alekhin, Bakhyt Abdikarimov, Leonid Bulavin, Evgen Rudnikov

P9.52 **Understanding yield stress fluids**
José Francisco Paredes Rojas, Noushine Shahidzadeh-Bonn, Daniel Bonn

P9.53 **Transport properties of polymeric fluids in 2D and 3D**
Tarak Patra, Jayant Singh

P9.54 **Molecular alignment under thermal gradients: a non-equilibrium molecular dynamics study**
Frank Römer, Fernando Bresme

P9.55 **Simulation studies of hard sphere suspensions exposed to various flow dynamics**
Marc Radu, Tanja Schilling

P9.56 **Structural signature of a brittle-to-ductile transition in self-assembled networks**
Laurence Ramos, Arnaud Laperrousaz, Philippe Dieudonné, Christian Ligoure

P9.57 **A rheological study (thixotropy) of some filled polymers**
F. J. Rubio-Hernández, N. M. Páez-Flor

P9.58 **Effect of HMPNa dispersant on the rheological behavior of kaolin aqueous suspensions**
F. J. Rubio-Hernández, F. J. Sánchez-Luque

P9.59 **Limestone filler / cement ratio effect on the rheological behavior of a fresh SCC cement paste**
F. J. Rubio-Hernández, J. M. Morales-Alcalde

P9.60 **Signature of the presence of long chain branches on the flow kinematics and stress field in a cross-slot channel**
Monirosadat Sadati, Clarisse Luap, Martin Kröger, Hans Christian Öttinger

P9.61 **Incomplete equilibration of dense hard-sphere fluids**
Luis Enrique Sanchez Diaz, Pedro Ezequiel Ramirez Gonzalez, Magdaleno Medina Noyola

P9.62 **Adsorption of polydisperse soft shell nanoparticles on liquid interfaces: a numerical study**
Konrad Schwenke, Emanuela Del Gado, Lucio Isa

P9.63 **Transition mechanism of melting and freezing of gold nanoclusters**
Andreas Singraber, Christoph Dellago

P9.64 **Liquid transport through a single nanotube**
Alessandro Siria, Anne-Laure Biance, Christophe Ybert, Cecile Cottin-Bizonne, Steve Purcell, Philippe Poncharal, Lyderic Bocquet

P9.65 **Nonequilibrium dynamics of sheared liquid crystals above the nematic transition**
David Alexander Strehober, Sabine H. L. Klapp

P9.66 **Study of fullurene (C_{60}) aggregation in aromatic solvents**
Telyaev Sukhrob, Akhmedov Tursunboy, Mirzaev Sirojiddin

P9.67 **Phase-field model of solid-liquid phase transition with density difference and latent heat in velocity and elastic fields**
Kyohei Takae, Akira Onuki

P9.68 **Optical tweezers: wideband microrheology**
Manlio Tassieri

P9.69 **Enhanced shear separation for chiral magnetic colloidal aggregates**
Fabrice Thalmann, Carlos Mendoza, Carlos M. Marques

P9.70 **Nanoscopic modelling: a fractal concept for protein form and structures**
Rupert Tscheliessnig

P9.71 **Dynamics of the 2D airbed granular system**
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