Scientific report on the SIMBIOMA-conference:
"SIMBIOMA 2011"
28.9.-1.10.2011 in Konstanz (Germany)
www.uni-konstanz.de/simbioma2011

In this conference computational scientists have been brought together who are involved in the challenges that are faced in the fundamental modeling of matter on time and spatial scales which are relevant in biosystems and material science at the nanometer length scale. The conference has focused on new techniques as well as on current applications for bridging the gap between ab-initio- and meso- and macroscopic levels.

The conference has been a big success:
The invited speakers in general had a very high international reputation, and the scientific quality of most of the 25 invited and 8 contributed talks has been very good as well as the quality of the majority of the 99 poster contributions. In total we had 150 registrations at the conference. The organization of the conference in plenary talks and few parallel sessions and short oral summaries of the poster contributions as well as well chosen times for breaks allowed vital discussions among the groups participating in the SIMBIOMA ESF programme and others (e.g. invited speakers from the USA). The production of a book with the most important contributions is planned.

A summary of the content of invited talks as well as of the oral and poster contributions is given in the abstract booklet (www.uni-konstanz.de/simbioma2011/start/program).

By this conference the SIMBIOMA-community got the chance to exchange novel results and discuss their relevance for future studies such that the cooperations in the SIMBIOMA-programme most probably will result in very valuable scientific results on molecular simulations in biosystems and material science in the future.

The international advisory committee consisted of 21 scientists (W. Andreoni (CH), M. Athenes (FR), K. Binder (DE), I. Economou (GR), P. Faisca (PT), D. Frenkel (UK), B. Hafskjold (NO), K. Kremer (DE),B. Lesyng (PL), H. Jonsson (IS), D. Galli (IT), E. Leontidis (CY), D. MacKernan (IE), V. Mohacek-Grosev (HR), O.G. Mouritsen (DK), L. Nilsson (SE), M. Rodger (UK), J.P. Ryckaert (BE), J. Ulicny (SI), I. Vattulainen (FI), M. Waroquier (BE)), the organizing committee was: G. Ciccotti (IT), C. Dellago (AT), M. Dijkstra (NL) and P. Nielaba (DE). The conference was organized with 6 plenary sessions with 50-minutes invited talks and a plenary discussion round (2 hours). Those were selected by the scientific committee to provide large overviews of recent advances in particular fields. The titles and abstracts of those invited talks (as can be seen from the attached excerpt from the book of abstracts) speak by themselves. The first talk by Bolhuis gave the perspectives of the computation of proteins in action. Then Alavi made a presentation on the Quantum Monte Carlo approach to the full CI problem, and Garrahan explained the large deviation methods and thermodynamics of trajectories in non-equilibrium systems. Delle Site focused on the coupling of different levels of resolution in molecular simulations, and Schütte discussed the analysis of complexity of molecular kinetics in Markov Chain models. Roux presented simulation methods, force fields and applications in computational studies of biomolecular systems. It was a general feeling that those plenary talks were of a very high quality and addressed questions at the heart of the problem faced in molecular simulations in biosystems and material science at the nanometer length scale. The plenary discussion round (with J.L. Barrat, K. Binder, M. Mareschal, M. Sprik and others) was devoted to the future problems in our science and found great resonance as well.

The other talks were grouped into 8 sessions run in two parallel sessions. Each session would start with two 30-minutes invited talks devoted to a presentation of the session subject, followed by one shorter more focused presentation on recent advances. Then at the end of the session, all participants presenting a poster in that session have been given the opportunity to state very briefly (three minutes) what the research reported was about, before the poster session eventually takes place.

The following sessions have been organized:

- Glasses and Granular Systems
- Transport in Classical and Quantum Systems
- Quantum Systems
- Proteins, Peptides and Bio-Informatics
- Soft Matter
- Interfaces
- Methods
- Multiscale Methods

The list of invited speakers and discussion round members:

- A. Alavi (UK)
- W. Andreoni (Switzerland)
- J.-L. Barrat (France)
- K. Binder (Germany)
- P. Bolhuis (Netherlands)
- C. Cuevas (Spain)
- R.L. Davidchack (UK)
- L. Delle Site (Germany)
- D. Donadio (Germany)
- R. Everaers (France)
- J. Garrahan (UK)
- W. Krauth (France)
- M. Mareschal (Belgium)
- B. Roux (USA)
- M. Schoen (Germany)
- C. Schütte (Germany)
- S. Sengupta (India)
- M. Sprik (UK)
- H. Tanaka (Japan)
- I. Tavernelli (Switzerland)
- M. Troyer (Switzerland)
- I. Vattulainen (Finland)

From the point of view of participation, the most successful were the sessions devoted to proteins, peptides and bioinformatics, to soft matter, and to methods. Most of the presentations were dealing with atomistic classical modeling and some tried to connect to macroscopic scales. Abstracts can be found in the conference booklet (see conference web-site, excerpt attached), but a general impression was really that the scientific simulation community starts now is in a position to model time and space scales which will be comparable with those of some experiments in biosystems and material science at the nanometer length scale. This will certainly be more and more so in the near future. It is also worth to point out that the level of complexity of the fluids under investigation was much higher than just a few years ago. Several sessions revealed the difficulty faced in an atomistic modeling of materials. Simulations have to involve various levels of descriptions: quantum, ab-initio, fully classical, mesoscopic and macroscopic and, of course, multiscale approaches are most of the time necessary to be predictive. Several methodological developments were also presented at the conference.

There was also a part dedicated to the organization of the programme itself. The SIMBIOMA steering committee was very happy on the success of the programme in the last years. The science political decisions for the winding down of the ESF, however, was identified as a science political mistake, and the steering committee expressed the hope, that future programmes like SIMBIOMA will again be supported in the future.

Organizing Committee:

G. Ciccotti (IT), C. Dellago (AT), M. Dijkstra (NL), P. Nielaba (DE)

The Conference

Similar to the SIMBIOMA-conference in 2008 (www.uni-konstanz.de/simbioma), the conference in 2011 has been organized with 6 plenary talks (50 minutes), a session on "Challenges beyond SIMBIOMA" (2 hours), 8 sessions with three speakers (invited talks with 30 minutes talks and contributing talks with 20 minutes) and short poster presentation talks (3 minutes) each, and in addition a general poster session.
The titles of the sessions are:

- Glasses and Granular Systems
- Transport in Classical and Quantum Systems
- Quantum Systems
- Proteins, Peptides and Bio-Informatics
- Soft Matter
- Interfaces
- Methods
- Multiscale Methods

In this conference we conveyed computational scientists involved in the challenges that are faced in the fundamental modeling of matter on time and spatial scales which are relevant for materials and biosystems. We focused the subject of this conference on new techniques as well as on current applications for bridging the gap between ab-initio and meso and macroscopic levels.

The conference aimed at developing cooperations among the groups participating in the SIMBIOMA ESF programme. It has been open to participants who are not members of the programme.

Conference Advisory Committee:

W. Andreoni (CH), M. Athenes (FR), K. Binder (DE), I. Economou (GR), P. Faisca (PT), D. Frenkel (UK), B. Hafskjold (NO), K. Kremer (DE),B. Lesyng (PL), H. Jonsson (IS), D. Galli (IT), E. Leontidis (CY), D. MacKernan (IE), V. Mohacek-Grosev (HR), O.G. Mouritsen (DK), L. Nilsson (SE), M. Rodger (UK), J.P. Ryckaert (BE), J. Ulicny (SI), I. Vattulainen (FI), M. Waroquier (BE)

Local Organizing Committee:

P. Nielaba, Y. Fischer (Conference Secretary), M. Beck, A. Geng

Program SimBioMa 2011

Conference on Molecular Simulations in Biosystems and Material Science
September 28 - October 1, 2011
University of Konstanz, Germany

Session	Topics
1	Glasses and Granular Materials
2	Transport in Quantum and Classical Systems
3	Quantum Systems
4	Proteins, Peptides and Bioinformatics
5	Soft Matter
6	Interfaces
7	Methods
8	Multiscale Methods

Time	Wednesday, 28.09.2011	
14:00	**Opening / Welcome** Rector / SimBioMa Audimax (Room: A600)	
14:30	**Plenary Talk** P. Bolhuis Audimax (Room: A600)	
15:20	Break	
	Parallel Sessions	
	Session 1 Room: A701	Session 6 Room: A703
15:50	W. Krauth	R.L. Davidchack
16:20	H. Tanaka	M. Schoen
16:50	D. Winter	S. Gekle
17:10	Poster Talks	Poster Talks
18:00	**Welcome Reception** (Room: K7)	

Time	Thursday, 29.09.2011	
09:00	**Plenary Talk** A. Alavi Audimax (Room: A600)	
09:50	Break	
	Parallel Sessions	
	Session 4 Room: A701	Session 5 Room: A703
10:20	R. Everaers	S. Sengupta
10:50	C. Oostenbrink	I. Vattulainen
11:20	H. Krobath	A. Milchev
11:40	Poster Talks	Poster Talks
12:20	Lunch Break	
14:00	**Plenary Talk** J.P. Garrahan Audimax (Room: A600)	
14:50	Break	
15:20	**Poster Session**	
17:20		
17:30	**Meetings** (SIMBIOMA)	
19:00	**Guided City Tour**	

Time	Friday, 30.09.2011	
09:00	**Plenary Talk** L. Delle Site Audimax (Room: A600)	
09:50	Break	
	Plenary Discussion Round Audimax (Room: A600)	
10:20	**W. Andreoni, J.L. Barrat, K. Binder, G. Ciccotti, D. Frenkel*, M. Mareschal, M. Sprik, and others …** **(*: to be confirmed)**	
12:20	Lunch Break	
14:00	**Plenary Talk** C. Schütte Audimax (Room: A600)	
14:50	Break	
	Parallel Sessions	
	Session 8 Room: A701	Session 3 Room: A703
15:20	P. Koumoutsakos	I. Tavernelli
15:50	I. Pagonabarraga	M. Troyer
16:20	P. Ballone	J. Prior
16:40	Poster Talks	Poster Talks
19:00	**Banquet** Evening talk: D. Coker (Konzil)	

Time	Saturday, 1.10.2011	
	Parallel Sessions	
	Session 7 Room: A701	Session 2 Room: A703
09:00	C. Hartmann	F. Pauly
09:30	C. Peter	D. Donadio
10:00	S. Meloni	P. Malgaretti
10:20	Poster Talks	Poster Talks
11:00	Break	
11:30	**Plenary Talk** B. Roux Audimax (Room: A600)	
12:20	**Closing at the University**	
12:30	Lunch Break	
13:00	**Excursion**	

Contents

PT-1: Understanding proteins in action

Peter Bolhuis
Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands

Molecular dynamics simulations can in principle provide useful predictions of cellular processes on an atomistic level, that are complementary to experiment. However, in practice, molecular dynamics is far from fulfilling this promise due to the large size of a cellular system (10^{10} atoms) and the long times involved (at least on the order of seconds). The multiscale modeling framework aims to circumvent this problem by envisioning hierarchical levels of description, each appropriate for certain length and time scales of a biophysical system. The challenge for the computer simulator is to develop the right description for each length or time scales, to link different scales together and to develop efficient sampling algorithms.

One approach is to start with the atomistic level molecular dynamics description and use this to define a coarser grained description. Another approach is to realize that many processes such as (un)folding and other conformational changes in proteins in fact are rare events caused by high free energy barriers between stable states. To overcome such barriers, many techniques have been developed, e.g. replica exchange, metadynamics, and transition path sampling.

In this presentation I will discuss several simulation methods within the multiscale modeling framework. In addition, I will exemplify these methods with applications such as conformational changes in (signalling) proteins, protein fiber self-assembly, and co-operativity in G-coupled receptors. In each case we can gain novel insight from these simulations. In the first case, about the mechanism and reaction coordinate of protein conformational changes. In the second case, about possible fiber structures and assembly mechanisms. And in the last case, about a possibly novel physical origin for cooperativity in protein receptors.

PT-2: Quantum Monte Carlo approach to the Full CI problem

Ali Alavi
Department of Chemistry, University of Cambridge, UK

The Full CI problem of quantum chemistry can be cast as a stochastic process involving an annihilating population of positive and negative walkers that inhabit Slater determinant space [1]. The population of walkers evolve according to a simple set of rules (akin to a "game of life"), which are derived from the underlying imaginary-time Schrödinger equation, such that the long-time distribution of the walkers matches the exact ground-state eigenvector. We show that this algorithm has a remarkable emergence characteristic, akin to symmetry-breaking phase transitions in classical statistical mechanical systems.

The sign problem posed by Hamiltonian matrix elements of positive and negative sign is solved through a combination of walker annihilation and a "survival of the fittest" criterion [2] (the latter greatly reducing the dependence of the algorithm on walker annihilation).

We will give examples of the algorithm at work in real systems in sizeable basis sets, ranging from atoms, anions and diatomic molecules (C_2, N_2, O_2, F_2, CN and NO), and to the uniform electron gas.

I hope also to show some preliminary applications to solids (with periodic boundaries).

Finally, we discuss the scaling of the algorithm with the number of electrons and orbitals [3], and future perspectives.

[1] G.H. Booth, A.J.W. Thom and Ali Alavi, J. Chem. Phys., 131 , 054106, (2009)
[2] Deidre Cleland, G.H. Booth, and Ali Alavi, J. Chem. Phys., 132 , 041103, (2010)
[3] Deidre Cleland, George Booth, and Ali Alavi, J. Chem. Phys., 134 , 024112, (2011)

PT-3: Large deviation methods and the thermodynamics of trajectories in non-equilibrium systems

Juan Garrahan
School of Physics and Astronomy, The University of Nottingham, UK

Large deviation theory provides a natural framework for studying many-body systems that display complex dynamics by treating ensembles of trajectories in a way analogous to what is done in equilibrium statistical mechanics with ensembles of configurations. This leads to an understanding of dynamical behaviour in terms of concepts such as dynamical (rather than thermodynamical) phases and consequent crossovers and "space-time" phase transitions between them. A notable example is that of glass forming liquids, which I will discuss in some detail. I will also describe how these ideas can be extended to the study of quantum jump trajectories in open quantum systems.

PT-4: Coupling different levels of resolution in molecular simulations

Luigi Delle Site
Institute of Mathematics, Freie Universität Berlin, Germany

I will discuss multiscale approaches to study complex molecular systems via computer simulation. In particular, it will be treated the case of concurrent coupling of scales via an adaptive resolution approach as implemented in the AdResS method. This allows to change molecular resolution on-the-fly during a simulation by changing the number of degrees of freedom in the specific regions of space where the desired resolution must be higher than the rest of the system. I will discuss its basic conceptual and algorithmic principles and show the latest applications with a particular attention to the problem of adaptive coupling between a quantum and a classical representation.

PT-5: Unravelling the Complexity of Molecular Kinetics by Markov State Models

Christof Schütte
Institute of Mathematics, Freie Universität Berlin, Germany

Simulations of biomolecular systems often exhibit complex multistate behavior. Markov State Models (MSMs) allow to reduce this complexity and to model and understand the essential kinetic behavior. We will review the theoretical foundations of MSMs, discuss how to efficiently build MSMs from molecular simulations, and illustrate their application to peptide and protein folding kinetics.

PT-6: Computational Studies of Biomolecular Systems: Simulation Methods, Force Fields, and Applications

Benoit Roux
Dept. of Biochemistry & Molecular Biology, University of Chicago, USA

Classical simulations based on atomic models play an increasingly important role in a wide range of applications in physics, biology and chemistry. They are particularly valuable for the study of soft matter systems involving liquids, polymers, membranes, microemulsions and surfactants, as well as complex biomolecules like proteins and nucleic acids. Subjects of great interest in biophysics include, for example, the development and applications of effective methods for the computation of binding free energy, the determination of experimental structure using low-resolution information, and the simulation of slow conformational transitions. Another subject of great interest is the development of advanced force fields taking induced electronic polarization into account explicitly. Recent applications to tyrosine kinases, the sodium-potassium pump, the voltage-gated potassium channel will be discussed.

S1-T1: Melting transitions and glass transitions of hard disks

Werner Krauth
Laboratoire de Physique Statistique, École normale supérieure, Paris, France

The hard-disk model has exerted outstanding influence on computational physics and statistical mechanics. Decades ago, hard disks were the first system to be studied by Markov-chain Monte Carlo methods and by molecular dynamics. It was in hard disks, through numerical simulations, that a two-dimensional melting transition was first seen to occur even though such systems cannot develop long-range crystalline order. Hard disks have also played a key role in our understanding of the glass transiton. Analysis of the system was made difficult by the absence of powerful simulation methods.

In recent years, we have developed a number of powerful Monte Carlo algorithms for hard disks and related systems. I will in particular show how the powerful event-chain Monte Carlo algorithm which has allowed us to prove that hard disks melt with a first-order transition from the liquid to the hexatic and a continuous transition from the hexatic to the solid.

S1-T2: An intimate link between glass transition and crystallization

Hajime Tanaka
Institute of Industrial Science, The University of Tokyo, Meguro-ku, Tokyo 153-8505, Japan

Recently it has been revealed that when approaching the glass transition temperature Tg, liquid dynamics not only drastically slow, but also become progressively more heterogeneous. From our simulations and experiments of several different glass-forming liquids, we find that the heterogeneous dynamics is a result of critical-like fluctuations of static structural order, contrary to a common belief that it is purely of dynamic origin: The 'static' correlation length and susceptibility of a structural order parameter exhibit Ising-like power-law divergence towards the ideal glass-transition point. However, this structural ordering accompanies little density change over a long range, which explains why it has not been detected by the static structure factor so far. Our results suggest a far more direct link than thought before, between glass transition and critical phenomena: Glass transition may be a novel type of critical phenomena, where a structural order parameter is directly linked to slowness.

This critical-like structural ordering also has an important implication on crystallization, which intrinsically takes place in a supercooled liquid state. For hard-sphere-like colloidal liquids, for example, we reveal that in a supercooled liquid state, medium-range fcc-like crystalline bond orientational order grows in its size and lifetime with increasing the packing fraction. We reveal that nucleation of crystals preferentially occurs in regions of high medium-range order, reflecting the low crystal-liquid interfacial energy there. These findings may shed new light not only on the fundamental nature of glass transition, but also the mechanism of crystal nucleation.

I thank Takeshi Kawasaki, Mathieu Leocmach, John Russo, Hiroshi Shintani, and Keiji Watanabe for their collaboration in this study. This work was partially supported by a grant-in-aid from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

S1-T3: Non-linear single-particle-response of glassforming systems to external fields

Speaker: David Winter

David Winter[1], Peter Virnau[1], Kurt Binder[1], Jürgen Horbach[2]
[1] *Johannes-Gutenberg-Universität Mainz, Germany*
[2] *Heinrich-Heine-Universität Düsseldorf, Germany*

Glassy dynamics of viscous liquids are characterized by a drastic slowing down of dynamical properties, while structural and thermodynamic quantities only show a weak gradual change. Recently, various independent studies have revealed that the interplay of the glass transition with external fields provides a wealth of new phenomena yet to be explored. There is hope that the understanding of the non-linear response of glassforming systems to external fields leads to new insight into the nature of the glass transition. In this work, we study the behavior of single particles in a supercooled liquid under the influence of an external force. Our model system is a 50:50 binary mixture whose particles interact via a Yukawa potential.

$$V_{\alpha\beta}(r) = \varepsilon_{\alpha\beta} d_{\alpha\beta} \exp[-\kappa(r - d_{\alpha\beta})]/r$$

By choosing slightly different potentials between A and B particles we prevent the system from crystallizing. In the equilibrated system, we add a constant force field to one of these particles which as a consequence will be accelerated. After some time, this particle reaches a steady state. In this state we measure characteristic properties of the particle and the surrounding like the steady state velocity, the friction coefficient, mean square displacements and correlation functions in dependence of the external force and system temperature. We observe that for low temperatures and high enough force fields the particle leaves the linear response regime and enters the non-linear regime. Here, the friction coefficient is not constant any more. For even higher forces all curves reach a second plateau and fall on top of each other. This work also allows to check new theoretical approaches for the micro-rheology of glassforming systems in the framework of mode coupling theory.

S2-T1: Mechanical and transport properties of metallic atomic-size contacts

J.C. Cuevas
Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

The appearance of the scanning tunneling microscope (STM) and the development of techniques such as the break-junctions or electromigration has allowed exploring the electronic transport through metallic wires at the atomic scale. Metallic atomic-size contacts have turned out to be an amazing playground where many theories of electronic transport in nanoscale systems have been tested [1]. Moreover, the study of these metallic nanowires has paved the way for the emergence of the field of molecular electronics [2]. Over the years, it has been understood that there is an intimate relation between the transport properties of these nanowires and their mechanical properties. These latter properties determine, in particular, the geometries of the nanowires, which has a strong impact in their electrical and thermal conduction. In spite of the great progress made in the last 15 years in the understanding of the conduction properties of metallic atomic-size contacts, the theoretical investigations of the interplay between their mechanical and transport properties are rather scarce.

In this talk, I will review our efforts in the last years to elucidate the physics of metallic atomic-size contacts. I will show that the combination of classical molecular dynamics simulations and quantum-mechanical methods based on non-equilibrium Green's function techniques allows us to understand many basic transport properties of these systems. As an illustration, I will discuss in this talk the following three fundamental issues concerning the conduction properties of these metallic nanowires: (i) Origin of the peaks in the so-called conductance histograms of a variety of metals [3-5], (ii) the anisotropic magnetoresistance in ferromagnetic atomic-size contacts [6], and (iii) the thermopower of atomic contacts made of both noble and transition metals [7]. In all these examples, it will become clear that a correct theoretical description of the transport properties of metallic atomic-size contacts requires realistic methods for the determination of the contact geometries realized in the experiments.

[1] For a review see N. Agrait, A. Levy Yeyati, and J.M. van Ruitenbeek, Phys. Rep. 377, 81 (2003)

[2] J.C. Cuevas and E. Scheer, Molecular Electronics: An Introduction to Theory and Experiment, World Scientific, Singapore (2010)

[3] M. Dreher, F. Pauly, J. Heurich, J.C. Cuevas, E. Scheer, P. Nielaba, Phys. Rev. B 72, 075435 (2005)

[4] F. Pauly, M. Dreher, J.K. Viljas, M. Häfner, J.C. Cuevas, and P. Nielaba, Phys. Rev. B 74, 235106 (2006)

[5] M. Häfner, J.K. Viljas, D. Frustaglia, F. Pauly, M. Dreher, P. Nielaba, and J.C. Cuevas, Phys. Rev. B 77, 104409 (2008)

[6] M. Häfner, J.K. Viljas and J.C. Cuevas, Phys. Rev. B (RC) 79, 140410 (2009)

[7] F. Pauly, J.K. Viljas, M. Bürkle, M. Dreher, P. Nielaba, and J.C. Cuevas, arXiv:1107.1361.

S2-T2: Atomistic simulations of heat transport in real scale nanodevices

Davide Donadio
MPI for Polymer Research, Mainz, Germany

We have developed a stable and efficient kernel method to compute thermal transport in open systems, based on the scattering matrix-approach. This method is applied to compute the thermal conductance of a junction between bulk silicon and silicon nanowires with diameter up to 10 nm. We have found that beyond a threshold diameter of 7 nm transmission spectra and contact conductances scale with the cross section of the contact surface, whereas deviations from this general trend are observed in thinner wires. This result allows us to predict the thermal resistance of bulk-nanowire interfaces with larger cross sections than those tractable with atomistic simulations, and indicate the characteristic size beyond which atomistic systems can in principle be treated accurately by mean-field theories. Our calculations also clarify how dimensionality reduction and shape affect interfacial heat transport. We also elucidated the physical principles that determine the heat conduction properties of SiNWs of finite length clamped between bulk semi-infinite contacts. Thermal transport in such devices stems from the combination of quantum tunneling, interference, and contact resistance. We show that in this context the effect of surface roughness is attenuated with respect to the case of infinitely long wires.

S2-T3: Running faster, running together: hydrodynamic coupling of molecular motors

Speaker: Paolo Malgaretti

Paolo Malgaretti[1], Ignacio Pagonabarraga[1], Daan Frenkel[2]
[1]*Department de Fisica Fonamental, Universitat de Barcelona, Spain*
[2]*Department of Chemistry, University of Cambridge, UK*

Molecular motors are proteins that are able to transform the chemical energy gained by the hydrolyzation of ATP into mechanical work. Due to this characteristic molecular motors are involved in many cellular processes ranging from cellular signalling to cellular locomotion. Even though a single motor can perform mechanical work by itself molecular motors generally work in teams whose typical size can vary from some units, as in intracellular transport, up to millions and even more in muscular fibers. A, nowadays, open question is to understand whether ensembles of motors show different dynamics than the one expected for an isolated one.

Here we focus our attention on the coupling between processive motors generated by the fluid they are embedded in. In fact due to their small size and to the high viscosity of the cytoplasm surrounding them molecular motors move in the "low Reynolds" regime in which hydrodynamic coupling can play a crucial role. We have developed a mesoscopic approach, that ensure local momentum conservation, capable to couple the step like motion of molecular motors to the fluid they are embedded in. Such model permits us to study the genuine hydrodynamic interactions between processive motors walking on the same biofilament. Our simulations show a more than 10-fold fluid-mediated enhancement of the velocity of ensembles of motors due to the reduction of the waiting time between subsequent steps. Such a reduction also increases the motor efficiency and leads to the formation of a net fluid-flux that leads to the transport of suspended and/or passive particles. Moreover the non-monotonic behaviour of the motor-ensemble velocity respect to the occupancy of the filament leads to the formation of aggregates that results to be stable for long times. Such results might be extended to the case of the transport of colloids optically-trapped in ratchet potentials.

S3-T1: Nonadiabatic Molecular Dynamics: a TDDFT-based approach

Speaker: I. Tavernelli

I. Tavernelli, B. F. E. Curchod, U. Rothlisberger
Laboratory of Computational Chemistry and Biochemistry, Ecole Polytechnique Fédérale de Lausanne, Lausanne, 1015, Switzerland

In the mixed quantum-classical description of molecular systems, only the quantum character of the electronic degrees of freedom is considered while the nuclear motion is treated at a classical level. In the adiabatic case, this picture corresponds to the Born-Oppenheimer limit where the nuclei move as point charges on the potential energy surface (PES) associated with a given electronic state. Despite the success of this approximation, many physical and chemical processes do not fall in the regime where nuclei and electrons can be considered decoupled. In particular, most photoreactions pass through regions of the PES in which electron-nuclear quantum interference effects are sizeable and often crucial for a correct description of the phenomena.

Recently, we have developed a trajectory-based nonadiabatic molecular dynamics scheme that describes the nuclear wavepacket as an ensemble of particles following classical trajectories on PESs derived from time-dependent density functional theory (TDDFT) [1]. The method is based on Tully's fewest switches trajectories surface hopping (TSH) where the nonadiabatic coupling elements between the different potential energy surfaces are computed on-thefly as functionals of the ground state electron density or, equivalently, of the corresponding Kohn-Sham orbitals [2-4].

Here, we present an extension of this approach that allows for the direct coupling of the system dynamics to an external electromagnetic field [5-6] as well as to the external potential generated by the environment (solvent effects). The method is applied to the study of the photodissociation dynamics of simple molecules in gas phase and to the description of the fast excited state dynamics of ruthenium (II) tris(bipyridine) in water.

[1] E. Tapavicza, I. Tavernelli and U. Rothlisberger, Phys. Rev. Lett., 98, (2007) 023001

[2] Tavernelli I.; Tapavicza E. and Rothlisberger U., J. Chem. Phys., 130, (2009) 124107

[3] Tavernelli I., Curchod B.F.E. and Rothlisberger U., J. Chem. Phys., 131, (2009) 196101

[4] Tavernelli I., Curchod B.F.E., Laktionov A. and Rothlisberger U., J. Chem. Phys., 133, (2010) 194104

[5] Tavernelli I., Curchod B.F.E. and Rothlisberger U., Phys. Rev. A, 81, (2010) 052508

[6] Tavernelli I., Curchod B.F.E. and Rothlisberger U., Phys. Chem., accepted 2011.

S3-T2: Ultracold atoms and fermionic simulations

Matthias Troyer
Institute for Theoretical Physics, ETH Zürich, Switzerland

The accurate simulation of fermionic quantum many body problems is one of the most important challenges in theoretical physics, with huge impact especially on the understanding and design of materials. However, the exponential scaling of the Hilbert space makes direct simulations impossible for all but the smallest systems and Monte Carlo simulations suffer from the negative sign problem. The goal thus has to be to develop efficient approximate methods for fermionic systems. I will report on recent progress in the simulation of fermionic systems, especially in the context of ultracold atomic gases in optical lattices. In deep optical lattice fermionic gases are well described by the Hubbard model, which we can now accurately simulate down to the Néel temperature, substantially lower than the lowest temperature achieved in experiments so far. In shallow optical lattices the simulation and the physics become more complex, as band mixing and orbital effects become important, and multi-band models are hard to derive and simulate. Here we propose to use density functional theory for such systems, using a new exchange correlation functional for ultracold atomic gases instead of electrons. This lets us use all the tools developed for materials simulations also for the simulation of atomic gases. In the future, comparison to controlled experiments will allow to test and improve density functionals for strongly correlated fermionic systems, and thus in return also improve simulation methods for materials.

S3-T3: Non-perturbative simulations of exciton dynamics in complex biological environments

Speaker: Javier Prior

Javier Prior[1,2]
[1] *Departamento de física aplicada, Universidad Politécnica de Cartagena, Cartagena, Spain*
[2] *Institute of Theoretical Physics, Ulm University, Ulm, Germany*

Multi-component quantum systems in strong interaction with their environment are getting more and more relevance for their importance in processes like the quantum dynamics of bio-molecular aggregates. Unfortunately, these systems are difficult to simulate as the system-bath interactions cannot be treated perturbatively and standard approaches are not valid or inefficient. Here we combine the Time-Evolving Block Decimation (TEBD) methods with techniques from the theory of orthogonal polynomials (OP) to provide an efficient method for simulating open quantum systems, including spin-boson models and their generalizations to multi-component systems. TEBD is an efficient algorithm to simulate time evolution in systems in with the entanglement doesn't increase rapidly. The OP theory will map a Hamiltonian representing a quantum system coupled linearly to a continuum of bosonic or fermionic modes to a Hamiltonian that describes a one-dimensional chain with only nearest neighbor interaction.

S4-T1: Bubble statistics and positioning in superhelically stressed DNA

Ralf Everaers
Laboratoire de Physique and Centre Blaise Pascal of the École Normale Supérieure de Lyon, Université de Lyon, CNRS UMR5672, Lyon, France

We report calculations of position- and size-dependent opening probabilities for bubbles in double- stranded DNA. Our results are obtained from transfer-matrix solutions of (i) the Zimm-Bragg model for unconstrained DNA and of (ii) a self-consistent linearization of the Benham model for DNA under a superhelical constraint. The numerical efficiency of our method allows for the analysis of entire genomes and of random sequences of corresponding length (10^6 – 10^9 bp). At physiological temperatures and superhelical densities, opening is strongly cooperative with average bubble sizes of $O(100 - 1000)$ bp. In general, the statistics and location of bubbles is dominated by sequence heterogeneity. For genomic DNA, bubbles are frequently located directly upstream of transcription start sites.

S4-T2: Barriers in binding – biomolecular free energy differences

Chris Oostenbrink
Institute of Molecular Modeling and Simulation, University of Natural Resources and Life Sciences, Vienna, Austria

All chemical equilibria are governed by the difference in free energy between various states. Examples are free energy differences between different conformations of a biomolecule or the free energy difference between the bound and unbound state of a ligand and its pharmaceutical target. We try to develop methods to efficiently and accurately calculate free energy differences for such processes, using statistical mechanics and molecular simulation. As the free energy is made up of enthalpic and entropic contributions, both sampling and scoring issues are crucial for accurate calculations. Molecular systems that are characterized by energy landscapes with high barriers between relevant conformations form a particular challenge, which we address by combining modern simulation techniques and free energy methods. In this presentation, I will discuss some of our recent research on these topics.

S4-T3: Identification of aggregation-prone intermediate states in the folding pathways of spc-SH3 amyloidogenic variants via Discrete Molecular Dynamics simulations

Speaker: Heinrich Krobath

H. Krobath [1], S. G. Estácio [1,2], P.F.N. Faísca[1], E.I. Shakhnovich [3]
[1]*Centro de Física da Matéria Condensada and Departamento de Física, Universidade de Lisboa, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal*
[2]*Research Institute for Medicines and Pharmaceutical Sciences (iMed.UL), Faculdade de Farmácia, Universidade de Lisboa,Av. Prof. Gama Pinto 1, 1649-003 Lisboa, Portugal*
[3]*Departmentof Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, MA 02138, USA*

There is accumulating evidence that under appropriate physicochemical conditions (e.g., temperature, pH and protein concentration) many different protein sequences can form amyloids. Here we use a continuum, off-lattice model that combines a full atomistic protein representation with the Gi$\bar{o}$ interaction potential to investigate the folding pathways of selected variants of the spc-SH3 protein domain. Our model suggests the formation of an aggregation-prone intermediate species in which more than half of the major hydrophobic core residues are highly solvent exposed. In agreement with the experimental results for the amyloidogenic propensities of the spc-SH3 variants, we have found that the intermediate is not present in the folding pathway of the WT protein, is only scarcely populated by the N47G mutant, is transiently populated in the case of the N47A mutant and low populated in the D48G(2Y) mutant. However, it is clearly more ubiquitous in the folding pathway of the more aggressive D48G(2Y) mutant. Interestingly, the triple mutant significantly populates an additional intermediate state that is less native-like and even more aggregation-prone than the common intermediate species. The common intermediate found here shows striking structural similarities with the intermediate identified for fyn-SH3 mutated at position 48.

S5-T1: Non-affine droplet fluctuations in sheared solids and hidden mechanical critical points.

Surajit Sengupta
Centre for Advanced Materials, Indian Association for the Cultivation of Science,
Jadavpur, Kolkata 700032, India

It is now rather well established that deformation in many kinds of non-crystalline matter such as bubble rafts, bulk metallic glasses, sheared granular matter and colloids is mediated by droplet fluctuations known as shear transformation zones or STZs with large non-affine displacements which tend to change local coordination. Under shear, STZs are easily produced on expending only a few k_BT of energy, undergo shape and size transformations and disappear as readily as they are formed. While STZs may be defined and identified easily during shear deformation, the identity of these regions is ambiguous for an amorphous solid under zero strain because of the lack of a well defined reference configuration with respect to which deformation can be readily defined. In contrast, the situation in a crystalline material is much clearer. An ideal reference configuration exists in this case against which non-affineness can be measured in a straight-forward way. However, do STZ exist in a crystalline solid? Molecular dynamics simulations of a two-dimensional Lennard-Jones crystal under pure shear shows finite size droplet fluctuations characterized by non-affine deviations from local crystallinity. The excess pressure of the droplets plotted vs local density shows a prominent van-der Waals loop which disappears above a certain temperature and strain value (below the yield strain) - showing a novel metastable critical point. We argue that these droplet fluctuations are analogues of STZs for crystalline solids and determine an-elastic behaviour.

S5-T2: Cholesterol in motion: how it travels and modulates membrane receptors and proteins

Ilpo Vattulainen
Biological Physics and Soft Matter Group, Institute of Physics, Tampere University of Technology, Finland

Cholesterol is one of the essential structural components of eukaryotic cell membranes and plays a role in quite a few cellular functions. It is tempting to think that cholesterol participates in the cellular functions by controlling the conformational changes of membrane proteins and receptors through specific interactions. However, while quite a few proteins have been shown to partition into highly ordered lipid rafts rich in cholesterol, clear-cut evidence for this view is limited.

Meanwhile, cholesterol can also cause problems. Increasing levels of low density lipoproteins (LDL) that carry cholesterol to the cells have been clinically linked to an increasing risk of cardiovascular disease (CVD). High density lipoproteins (HDL) in turn carry excess cholesterol back to liver for recirculation, and it has been shown that increasing levels of HDL correlate with a reduced risk of being exposed to CVD. As CVD is one of the greatest causes of death in the Western countries, there is some interest to understand how its emergence could be avoided. Very recently clinical studies have shown [1] very promising data in this regard: a sound strategy to increase HDL and decrease LDL level is to interfere with the transfer of cholesteryl esters by inhibiting the function of CETP (cholesteryl ester transfer protein). However, again there is a problem, as the molecular scale insight of the transfer mechanisms associated with cholesterol and CETP is limited.

Here, we discuss how atomistic and coarse grained simulations can be exploited to shed light on these issues. We use atomistic simulations to show how cholesterol interacts specifically with membrane-associated receptors, and how cholesterol uses these specific interactions to control the function of the receptor [2]. Further, atomistic simulations together with coarse grained models are used to consider the transfer of cholesterol from membranes and lipoproteins to CETP, and vice versa, and thereby to unravel the atomic-scale mechanisms that control the transfer process [3]. Through these case studies we discuss how computer simulations can complement experiments and provide added value for understanding the biological significance of cholesterol.

[1] C.P. Cannon et al., N. Engl. J. Med. 363, 2406 (2010)

[2] D. Lingwood et al., Nature Chem. Biol. 7, 260 (2011)

[3] A. Koivuniemi et al., submitted (2011).

S5-T3: Ejection Mechanism of a Polymer Chain from a Nanopore: Theory & Computer Experiment

Speaker: Andrey Milchev

Andrey Milchev[1,2], Leonid Klushin[3], Alexander Skvortsov[4], Kurt Binder[2]
[1] *Institute for Physical Chemistry, Bulgarian Academy of Science, 1113 Sofia, Bulgaria*
[2] *Institut fuer Physik, Johannes Gutenberg Universitaet Mainz, Staudinger Weg 7, 55099 Mainz, Germany*
[3] *American University of Beirut, Department of Physics, Beirut, Lebanon*
[4] *Chemical-Pharmaceutical Academy, Prof. Popova 14, 197022 St. Petersburg, Russia*

We consider the ejection dynamics of a flexible polymer chain out of confined environment. This situation arises in different physical contexts, including a flexible synthetic polymer partially confined in a nanopore and a viral genome partially ejected from its capsid. The chain release from confinement is described both analytically and by means of dynamic Monte Carlo simulation. One finds two distinct regimes of ejection dynamics depending on whether the chain is fully or partially confined:

(i) Partially confined chains are ejected from a pore of length L and diameter D after a typical time $\tau \propto L^2 D^{5/3}$, *regardless* of their contour length N. The process is driven by a *constant* force $f \approx 5k_BT/D$ and follows a "capillary" law. The force value is model-independent as long as the pore diameter exceeds the persistence length of the polymer chain and for pore walls that do not attract the segments of the polymer.

(ii) In contrast, the ejection of fully confined chains is largely diffusive, the residence time being a non-monotonic function of N. The drift-dominated ejection of long chains is characterized by narrow distribution of exit times whereas for diffusive-dominated ejection the exit times are described by a broad distribution.

One finds good agreement with recent nanofluidic experiments with DNA.

[1] A. Milchev, L. Klushin, A. Skvortsov, K. Binder, Macromolecules, **43**, 6877 (2010).

S6-T1: Cleaving method for determining solid-liquid interfacial free energy in molecular systems: Results for simple models of water

Ruslan L. Davidchack
Department of Mathematics, University of Leicester, UK

The cleaving method for computing solid-liquid interfacial free energy has been very successful in atomic systems (hard and soft spheres, Lennard-Jones). The challenge for molecular systems is to take into account the rotational degrees of freedom of a molecule. I will present an extension of the cleaving method to molecular systems [1] and results for several simple models of water, TIP4P, TIP4P-Ew, TIP5P-Ew, also elucidating the effect of including full electrostatic interactions.

[1] R. Handel, R. L. Davidchack, J. Anwar and A. Brukhno, Phys. Rev. Lett. 100, Art. No. 036104 (2008).

S6-T2: Sorption-induced deformation of compliant solids

Martin Schoen[1,2]
[1]*Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Germany*
[2]*Department of Chemical and Biomolecular Engineering, North Carolina State University, USA*

We employ grand canonical ensemble Monte Carlo simulations to investigate the strain experienced by a nanoscopic slit pore when this pore fills with fluid material. Both solid substrates of our model system consist of a single layer of solid atoms bound to their equilibrium lattice sites by a harmonic potential such that these atoms are thermally coupled to molecules of a fluid phase confined between them. Parameters are tuned such that they represent an experimental situation in which pentane is adsorbed by mesoporous silica. Our focus is on strain isotherms, that is the net deformation of the solid as fluid material is imbibed by the pore. At low pressures prior to pore filling strain isotherms are dominated by wetting characteristics of the fluid-solid interface whereas nanomechanical properties of the pore may be deduced quantitatively from high-pressure portions of the strain isotherm after the pore is completely filled with fluid. To that end we introduce a thermodynamic analysis of the high-pressure portion of the sorption isotherm that permits us to determine the elasticity of the confining solid material in terms of a so-called pore-load modulus which is also accessible experimentally.

S6-T3: Dielectric spectrum of interfacial water

Speaker: Stephan Gekle

Stephan Gekle[1], Roland Netz[2]
[1]*Physik Department, TU München, Germany*
[2]*Fachbereich Physik, Freie Universität Berlin, Germany*

Dissolving small particles in water leads to the formation of a nanometer-sized hydration layer in which the water properties are often very different from bulk water. Here we use molecular dynamics computer simulations to study the behavior of such hydration water when it is subjected to electromagnetic fields. We find that the absorption characteristics depend strongly on the direction of the applied field: for fields parallel to the surface the absorption peak is shifted slightly towards lower frequencies while for perpendicular fields the peak position is found at much higher frequencies than in bulk water. This strongly anisotropic behavior is generic for hydrophobic, hydrophilic, and even water/vapor interfaces. Contrary to intuition, the blue-shift of the absorption peak is not connected to an accelerated decay of the molecular correlations in the time domain but instead is caused by a strong reduction in their spatial correlations. The isotropic frequency-dependent dielectric function (averaged over both directions) is found to be attenuated and its absorption peak shifted towards lower frequencies in agreement with previous experiments.

S7-T1: Bilinear systems and optimal control: applications to light-induced control of open quantum systems and single-molecule pulling experiments

Carsten Hartmann
Institut für Mathematik, Freie Universität Berlin, Germany

The talk reviews recent development in the theory of bilinear control systems that appear in a variety of context (e.g., molecular dynamics, mathematical finance etc.). A particular focus is on low-rank approximation techniques that make the calculation of an optimal control numerically feasible. We illustrate this with simple numerical examples from stochastic and quantum control.

S7-T2: Transferability of coarse grained potentials for biomolecular systems

Christine Peter
Max Planck Institute for Polymer Research, Mainz, Germany

Coarse grained models have become increasingly popular in the simulation of biomolecular systems. In multiscale simulation approaches, coarse grained models are frequently devised in such a way that they are intimately linked to a higher-resolution (e.g. atomistic) model. In this case much attention is paid to the thermodynamic and structural consistency of the models at different resolution levels. One important aspect in the development of coarse grained models is the question of transferability, where transferability may refer to a variation in state point or system, e.g. temperature, concentration, chemical environment, but also to a different molecular environment of coarse grained beads in a chain molecule etc. Coarse grained models are by construction state point dependent and can strictly speaking only be applied to the state point(s)/systems they were parameterized for. This however puts a severe limitation to their applicability and predictive power since one would like to use them for precisely those systems (large macromolecules, complex biomaterials) and processes (aggregation, phase separation etc.) where one cannot easily obtain atomistic reference simulations. Therefore, we investigate the transferability of coarse grained potentials in order to understand the limitations and – based on this understanding – to devise new coarse graining strategies.

S7-T3: Vacancy dynamics by rare events simulation techniques.

Speaker: Simone Meloni

Simone Meloni[1,2], Pierre Antoine Geslin[3], Giovanni Ciccotti[1,4]
[1] *School of Physics, University College Dublin, Dublin, Ireland*
[2] *CASPUR Supercomputing Centre, Rome, Italy*
[3] *Laboratoire d'Etudes des Microstructures, CNRS-ONERA, France*
[4] *Dept. of Physics and CINSM, University "La Sapienza", Roma, Italy*

We describe a single vacancy in a crystal in terms of a quantum particle subject to the field generated by the atoms in the sample. On the basis of this model, we derive a set of collective variables that can be used to study the vacancy diffusion dynamics. As an illustration of the method, we run Temperature Accelerated Monte Carlo simulations [G. Ciccotti and S. Meloni, Phys. Chem. Chem. Phys. 13 (2011), 5952] based on these collective variables to study the vacancy diffusion patterns in a 2D crystal of Lennard-Jones particles. Our simulations reveal that, in addition to the simple nearest neighbor vacancy hopping mechanism, the vacancy can migrate over a longer space scale via a collective process involving several lattice sites. Finally, in our simulations we observe the formation of a displocation-like defect.

S8-T1: Nanoparticle, fluid, lipid bilayer interactions

Petros Koumoutsakos
Chair of Computational Science, ETH Zürich, Switzerland

We study the interaction of pristine and coated nanoparticles with lipid bilayers in the presence of fluid flow. We investigate coating patterns for effective membrane penetration and the role of flow shear in the structure of the membrane and its interaction with the nanoparticles.

S8-T2: Mesoscale modeling of electrolyte transport in heterogeneous media

Ignacio Pagonabarraga
Department of Fundamental Physics, University of Barcelona, Spain

The dynamics of electrolytes poses a number of challenges because of the diversity of lengths class involved and the need to treat the motion of the solvent, ions and suspended macroions on the same footing.

I will describe a mesoscopic approach which focuses on the macroin dynamics by appropriately coarse graining the description f the fluid solvent and suspended ions. Such a flexible hybrid scheme is exploited to characterize the dynamics of electrolytes in porous media and also the electrokinetics of colloidal suspensions. The underlying description of the fluid solvent, based on a kinetic description, allows to exploit the probabilistic interpretation to analyze efficiently the kinetics of charged tracers.

I will analyze the motion of charged tracers in porous medias and will discuss the different kinetic regimes which determines the electrophoresis of colloids. I will also consider how the approach can be extended to describe the dynamics of electrolytes in complex fluids.

[1] B. Rotenberg, I. Pagonabarraga and D. Frenkel, *Coarse-grained simulations of charge, current and flow in heterogeneous media*, Faraday Discussions **144**, 223 (2010)

[2] G. Giupponi and I. Pagonabarraga, *Colloidal electrophoresis for strong and weak ion diffusivity*, Phys. Rev. Lett. **106**, 248304 (2011)

S8-T3: Entropy scaling of dynamical properties: a route to predict time acceleration in coarse graining models

Speaker: Pietro Ballone

P. Ballone, J. A. Armstrong
School of Mathematics and Physics, Queen's University Belfast, Northern Ireland, UK

Simple scaling relations proposed by Rosenfeld [Phys. Rev. A 15, 2545 (1977)] and Dzugutov [Nature 381, 137 (1996)] to predict diffusion coefficients on the basis of excess entropy have been verified by an extensive series of molecular dynamics simulations for atomic and molecular fluids.

Results for simple ionic fluids confirm the validity of these relations for systems with long range interactions. The extension of entropy scaling relations to cover viscosity and electrical conductivity has also been investigated.

Simulations for water and liquid nitrogen quantify the relative role of translational and orientational entropy in determining dynamical properties, and suggest an a-priori route to predict the scaling of time connecting atomistic and coarse grained molecular dynamics simulations of complex systems.

List of authors

Invited speakers and participants

Plenary Speakers

Alavi, Ali	Department of Chemistry, University of Cambridge (UK)
Barrat, Jean-Louis	Universite Joseph Fourier, Grenoble (France)
Binder, Kurt	Institute of Physics, Johannes Gutenberg University, Mainz (Germany)
Bolhuis, Peter	Van't Hoff Institute for Molecular Sciences, University of Amsterdam (Netherlands)
Delle Site, Luigi	Institute of Mathematics, Free University Berlin (Germany)
Garrahan, Juan	School of Physics and Astronomy, The University of Nottingham (UK)
Mareschal, Michel	University Libre de Bruxelles (Belgium)
Roux, Benoit	Dept. of Biochemistry & Molecular Biology, University of Chicago (USA)
Schuette, Christof	Free University of Berlin (Germany)

Invited Speakers

Cuevas, Juan Carlos	Universidad Autonoma de Madrid (Spain)
Davidchack, Ruslan L.	Department of Mathematics, University of Leicester (UK)
Donadio, Davide	MPI for Polymer Research, Mainz (Germany)
Everaers, Ralf	Universite de Lyon (France)
Hartmann, Carsten	Free University Berlin (Germany)
Koumoutsakos, Petros	Chair of Computational Science, ETH Zuerich, (Switzerland)
Krauth, Werner	Laboratoire de Physique Statistique, Ecole Normale Superieure Paris (France)
Oostenbrink, Chris	University of Natural Resources and Life Sciences, Vienna (Austria)
Pagonabarraga, Ignacio	Department of Fundamental Physics, University of Barcelona (Spain)
Peter, Christine	Max Planck Institute for Polymer Research Mainz (Germany)
Schoen, Martin	Technische Universitaet Berlin and North Carolina State University (Germany) and (USA)
Sengupta, Surajit	IACS, Jadvapur, Kolcata (India)
Tanaka, Hajime	Institute of Industrial Science, The University of Tokyo (Japan)
Tavernelli, Ivano	Ecole Polytechnique Federale de Lausanne (Switzerland)
Troyer, Matthias	Institute for Theoretical Physics, ETH Zuerich (Switzerland)
Vattulainen, Ilpo	Tampere University of Technology (Finland)

Registered Participants

Athenes, Manuel	CEA (France)
Ballone, Pietro	School of Mathematics and Physics, Queen's University Belfast (United Kingdom)
Bartok-Partay, Albert	University of Cambridge (United Kingdom)
Bauer, Sebastian	Lehrstuhl fuer BioMolekulare Optik LMU Muenchen (Germany)
Beck, Marcus	University of Konstanz (Germany)
Behringer, Hans	Johannes Gutenberg-Universitaet Mainz, Institut fuer Physik (Germany)
Belzig, Wolfgang	Department of Physics, University of Konstanz (Germany)
Benet, Jorge	Universidad Complutense, Dpto. de Quimica Fisica, Facultad de Quimica (Spain)
Bhattacharjee, Amit Kumar	Institut fuer Materialphysik im Weltraum (Germany)
Block, Benjamin	University Of Mainz (Germany)
Blumberger, Jochen	University College London (UK)
Borgis, Daniel	Ecole Normale Superieure (France)
Brokamp, Theda	University of Konstanz (Germany)
Buerzle, Florian	University of Konstanz (Germany)
Catak, Saron	Center for Molecular Modeling-Ghent University (Belgium)
Ciccotti, Giovanni	Dipartimento di Fisica, Universita' di Roma "La Sapienza" (Italy)
Coelfen, Helmut	University of Konstanz (Germany)
Cottone, Grazia	School of Physics, UCD Dublin (Ireland)
D'Adamo, Giuseppe	Physics Department, L'Aquila University (Italy)
Dellago, Christoph	University of Vienna (Austria)
Dieterich, Wolfgang	Universitaet Konstanz (Germany)
Dijkstra, Marjolein	Utrecht University (The Netherlands)
Dr. Smiatek, Jens	Institute of Physical Chemistry (Germany)
Enciso, Marta	Complutense University (Spain)
Everaers, Ralf	Laboratoire de Physique, ENS Lyon (France)
Farnoush, Farahpour	Sharif University of Technology (Iran)
Galli, Davide Emilio	Universita' degli Studi di Milan (Italy)

Gaspari, Roberto	Empa, Swiss Federal Laboratories for Materials Science and Technology (Switzerland)
Gekle, Stephan	Physik Department, TU Muenchen (Germany)
Geng, Annette	University of Konstanz (Germany)
Grisell Diaz Leines, Grisell	Van 't Hoff Institute for Molecular Sciences/ University of Amsterdam (Netherlands)
Hector, Martinez-Seara Monne	Tampere University of Technology (Finland)
Hinzke, Denise	University of Konstanz (Germany)
Holm, Christian	Institute for Computational Physics (Germany)
Horvat, Gordan	Department of Chemistry, Faculty of Science (Croatia)
Hug, Susanna	University of Western Ontario (Canada)
Ilg, Patrick	ETH Zuerich (Switzerland)
Ioannou, Filippos	University of Cyprus (Cyprus)
Jaeger, Sebastian	Technische Universitaet Berlin (Germany)
Jeanmairet, Guillaume	Departement de Chimie, Ecole Normale Superieure (France)
Jochum, Mara Nikola	Max Planck Institute for Polymer Research (Germany)
Jogi, Jakob	Institute of Physics, Univ. of Tartu (Estonia)
Kacar, Gokhan	Eindhoven University of Technology (The Netherlands)
Kilic, Murat	Van 't Hoff Institute for Molecular Sciences, University of Amsterdam (The Netherlands)
Krobath, Heinrich	Centro de Fisisca da Materia Condensada, Uni Lisboa (Portugal)
Kuehne, Thomas	Johannes Gutenberg University (Germany)
Kumar, Aatish	Van 't Hoff Institute for Molecular Sciences (HIMS) (The Netherlands)
Lasoroski, Aurelie	UMR 8640 ENS-CNRS-UPMC PASTEUR (France)
Lattanzi, Gianluca	School of Physics, University College Dublin (Ireland)
Leitold, Christian	University of Vienna (Austria)
Lesyng, Bogdan	University of Warsaw (Poland)
Levesque, Maximilien	Ecole Normale Superieure (France)
Liberatore, Elisa	Physics Department - University of Rome (Italy)
Lobaskin, Vladimir	University College Dublin (Ireland)
Luca, Bellucci	Centro S3, CNRS Istituto di Nanoscienze (Italy)
Luiken, Jurriaan	HIMS (University of Amsterdam) (Netherlands)
Lyakhova, Kateryna	Eindhoven University of Technology (The Netherlands)
Lyulin, Alexey	Technische Universiteit Eindhoven (The Netherlands)
MacKernan, Donal	ACAM, University College Dublin (Ireland)
Malgaretti, Paolo	Universitat de Barcelona, facultat de fisica (Spain)
Mani, Ethayaraja	University of Amsterdam (Netherlands)
Marco, Micciarelli	Universite degli studi di Napoli Federico II (Italy)
Marino, Kristen	University of Amsterdam (The Netherlands)
Mathias, Gerald	Lehrstuhl f. BioMolekulare Optik, LMU Muenchen (Germany)
Matt, Manuel	University of Konstanz (Germany)
Mauro, Ferrario	Universiti di Modena e Reggio Emilia (Italy)
Medina Hernando, Stefan	University of Mainz (Germany)
Meloni, Simone	University College Dublin (Ireland)
Menzl, Georg	Universitaet Wien (Austria)
Miguel Angel, Gonzalez	Universidad Complutense de Madrid, Facultad de Ciencias Quimicas (Spain)
Milchev, Andrey	Bulgarian Academy of Sciences, Institute of Physical Chemistry (Bulgaria)
Modi, Niraj	Jacobs University Bremen (Germany)
Mohacek Grosev, Vlasta	Rudjer Boskovic Institute (Croatia)
Mohammadkarim, Saeedghalati	IPM (Iran)
Mones, Letif	University of Cambridge (United Kingdom)
Muntean, Stela Andrea	Eindhoven University of Technology (The Netherlands)
Mutter, Daniel	Universitaet Konstanz, Fachbereich Physik (Germany)
Nair, Nisanth N	Departmet of Chemistry, Indian Institute of Technology Kanpur (India)
Naome, Aymeric	University of Namur (Belgium)
Nielaba, Peter	Physics Department, University of Konstanz (Germany)
Neratova, Irina	Ulm University (Germany)
Nilsson, Lennart	Karolinska Institutet (Sweden)
Nowosielski, Marcin	Van 't Hoff Institute for Molecular Sciences, University van Amsterdam (The Netherlands)
Oliviero, Andreussi	University of Oxford (United Kingdom)
Pacholczyk, Marcin	Silesian University of Technology (Poland)
Paillusson, Fabien	University of Cambridge (UK)

Peters, Frank	Eindhoven University of Technology (Netherlands)
PICCIANI, MASSIMILIANO	CEA Saclay, DEN/DMN/SRMP (France)
Picker, Andreas	University of Konstanz (Germany)
Pignedoli, Carlo	Empa, Swiss Federal Laboratories for Materials Science and Technology (Switzerland)
Praprotnik, Matej	National Institute of Chemistry (Slovenia)
Prior, Javier	Ulm university, Institute of Theoretical Physics (Germany)
Ronald Benjamin, Ronald	Instutute for Materials Physics in Space/German Aerospace Center (Germany)
Rossi, Maurizio	Dipartimento di Matematica, Politecnico di Milano (Italy)
Rovigatti, Lorenzo	Dipartimento di Fisica, Universita di Roma La Sapienza (Italy)
Rueter, Julien	LMU Muenchen (Germany)
RYCKAERT, JEAN-PAUIL	Universite Libre de Bruxelles (Belgium)
Sara, Bonella	Universita' di Roma La Sapienza Dipartimento di Fisica (Italy)
Scholz, Kristian	University of Konstanz (Germany)
Schubert, Franziska	Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)
Siems, Ullrich	University of Konstanz (Germany)
Sprik, Michiel	University of Cambridge (United Kingdom)
Starostin, Eugene	University College London (UK)
Stecher, Thomas	University of Cambridge (UK)
Strehober, David Alexander	Institut fuer Theoretische Physik, TU Berlin (Germany)
Suffritti, Giuseppe Baldovino	Dipartimento di Chimica/University of Sassari (Italy)
Sutton, Daniel	The University of Bath (UK)
Svaneborg, Carsten	Center for Fundamental Living Techology, Dept. of Physics and Chemistry (Denmark)
Tomic, Antonija	Institute Rudjer Boskovic (Croatia)
Tomic, Sanja	Rudjer Boskovic Institute (Croatia)
Tritschler, Ulrich	University of Konstanz (Germany)
Troester, Philipp	Institut fuer BioMolekulare Optik , LMU Muenchen (Germany)
Ulicny, Jozef	University of P.J.Safarik (Slovakia)
van Dijk, Erik	University of Cambridge (UK)
Vercauteren, Daniel	University of Namur (Belgium)
Vila Verde, Ana Celia	University of Amsterdam (The Netherlands)
Vila Verde, Ana Sofia A.	University College London (United Kingdom)
Villanueva, Jorge Bent	Universidad Complutense (Spain)
Vlad, Camelia	University of Konstanz (Germany)
Voigtmann, Thomas	University of Konstanz (Germany)
Weina, Du	Van 't Hoff Institute for Molecular Science (Netherlands)
Wichmann, Christoph	Institut fuer BioMolekulare Optik , LMU Muenchen (Germany)
Winter, David	Institute of Physics Johannes Gutenberg-University (Germany)
YADAV, VIVEK KUMAR	INDIAN INSTITUTE OF TECHNOLOGY KANPUR (India)
Zeiler, Rosanne	University of Amsterdam (The Netherlands)