

Ulam Computer Simulations Workshop

Challenges & Opportunities in Molecular Simulations

21–24 June 2017, Lviv, Ukraine

*On the occasion of the 70th anniversary
of the invention of the Monte Carlo method*

PROGRAMME AND ABSTRACTS

Lviv – 2017

In 2017, 70 years will elapse from the invention of the Monte Carlo method — one of the greatest numerical algorithms to solve the problems in various fields of physical and life sciences, engineering, finance, statistics, mathematics, etc. One of the key figures in this invention was Stan (Stanislaw) Ulam (1909–1984). Stan Ulam was born in Lviv (Lemberg), at that time the capital city of province Galicia in Austro-Hungarian Empire, while when he graduated from the local Polytechnic University in 1930, the city of Lwow belonged to Poland. Nowadays, Lviv is an important educational and scientific center of Western Ukraine with its “Ensemble of the Historic Centre” enlisted among the UNESCO World Heritage sites.

On the occasion of this anniversary there will be held in Lviv the Ulam Computer Simulations (UCS) workshop on challenges and opportunities in molecular simulations. The aim of this first UCS Workshop is twofold. First of all, we are looking forward to paying tribute to the legacy of Ulam for his pioneering contribution to the development of the field of computer simulations. Secondly, we wish to bring together leading researchers on computer simulations of soft matter and to offer the young researchers and graduate students an in-depth review of the most recent developments in the field that poses many challenges nowadays.

The UCS workshop will take place from the 21st to 24th June, 2017 with the first day (June 21st) as the arrival day and opening in the late afternoon; the second and the third days will be fully working days (10 plenary lectures, 24 short communications and one poster session) with free evening on June 22nd, workshop banquet on June 23rd, and participant’s departure during the fourth day (June 24th). During the first and fourth days the City sightseeing tours will be organized by adjusting to the arrival and departure time of participants.

Main topics

- Historical aspects of computer simulations
- Multiscale molecular simulations
- *Ab initio* & quantum simulations
- The latest development of simulation algorithms
- Interfaces between hard & soft matter
- Biologically motivated systems
- Water, electrolytes & hydrogen bonding systems

Contacts

UCSW-2017

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Organizers

Andrij Trokhymchuk

(chairman; Institute for Condensed Matter Physics, Lviv)

Ivo Nezbeda (Czech Academy of Sciences & J.E. Purkinje University, Prague),

Carlos Vega (University Complutense of Madrid, Madrid)

Local organizing committee

Taras Bryk (chairman; Institute for Condensed Matter Physics),

Andriy Baumketner (Institute for Condensed Matter Physics),

Ioanna Beda (Institute for Condensed Matter Physics),

Taras Demchuk (Institute for Condensed Matter Physics),

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Roman Gladyshevskii (Ivan Franko National University of Lviv)

Organizing institutions

Institute for Condensed Matter Physics

of the National Academy of Sciences of Ukraine

Lviv Polytechnic National University

Ivan Franko National University of Lviv

Hugo Steinhaus Center of the Wroclaw University

of Science and Technology

Lviv City Government

Hi Tech Office Ukraine

Ulam Computer Simulations Workshop
Challenges & Opportunities in Molecular Simulations

Programme

21–24 June 2017, Lviv, Ukraine

Ulam Computer Simulations Workshop

Wednesday, 21 June, 2017

Lviv Polytechnic National University, main building, Mateyko hall

Chaired by A. ТROKHYMCHUK (*Lviv, Ukraine*)

- 14.00 – 18.00 Registration
- 18.00 – 18.20 Opening address
- 18.20 – 19.00 M. ZARICHNYI (*Lviv, Ukraine*)
Stanislaw Ulam: life, mathematics, and science
- 19.00 – 19.40 D. FRENKEL (*Cambridge, UK*)
Certainty from uncertainty and order from disorder: how the Monte Carlo method changed our understanding of entropy
- 20.00 – 22.00 Social Mixer

21–24 June 2017, Lviv, Ukraine

Thursday, 22 June, 2017

Ivan Franko National University, main building, Conference hall

Chaired by D. FRENKEL (*Cambridge, UK*)

- 9.00 – 9.40 G. CICCOTTI (*Rome, Italy*)
**Hydrodynamics from dynamical non-equilibrium
molecular dynamics**
- 9.40 – 10.00 R. VUILLEUMIER (*Paris, France*)
**Extracting random forces and Mori-Zwanzig kernels from
molecular dynamics simulations**
- 10.00 – 10.20 N. JAKSE (*Grenoble, France*)
Is diffusion in liquid metals universal?
- 10.20 – 10.40 A. WERON (*Wroclaw, Poland*)
**Algorithms for testing of fractional dynamics: A practical
guide for stochastic modelling**
- 10.40 – 11.10 Coffee Break

Chaired by G. KAHL (*Vienna, Austria*)

- 11.10 – 11.50 A. SEITSONEN (*Paris, France*)
**Liquid of Life in silico: Electronic structure-based
atomistic simulations of liquid water**
- 11.50 – 12.10 J.-F. WAX (*Metz, France*)
Dynamic structure of liquid water
- 12.10 – 12.30 E. SANZ (*Madrid, Spain*)
**What simulations can teach us about homogeneous ice
nucleation**
- 13.00 – 14.00 Lunch

Ulam Computer Simulations Workshop

Chaired by I. SIEPMANN (*Minneapolis, USA*)

- 14.30 – 15.10 E. SPOHR (*Essen, Germany*)
Electrostatic driving forces in molecular simulations of stochastic proton discharge reactions on electrodes. Beyond a 1D-Poisson-Boltzmann view
- 15.10 – 15.50 S. BONELLA (*Lausanne, Switzerland*)
Molecular dynamics simulation of charged systems in external magnetic field
- 15.50 – 16.20 Coffee Break

Chaired by J. GROSS (*Stuttgart, Germany*)

- 16.20 – 17.00 D. KOFKE (*Buffalo, USA*)
Mapped averaging methods for high-precision, high-efficiency calculation of properties by molecular simulation
- 17.00 – 17.20 R. DAVIDCHAK (*Leicester, UK*)
Langevin and gradient thermostats for rigid body dynamics
- 17.20 – 17.40 A. HENRICI (*Winterthur, Switzerland*)
Fermi-Pasta-Ulam chains: simulation and theory
- 17.40 – 18.00 A. HUERTA (*Xalapa, Mexico*)
Computer simulations of low-dimensional materials
- 18.00 – 19.00 POSTER SESSION
- 19.00 – 20.00 Walking Tour
- 20.00 – 22.00 Szkoocka Dinner

21–24 June 2017, Lviv, Ukraine

Friday, 23 June, 2017

Ivan Franko National University, main building, Conference hall

Chaired by G. CICCOTTI (*Rome, Italy*)

- 9.00 – 9.40 G. KAHL (*Vienna, Austria*)
Inverse patchy colloids: structure, dynamics, and self-assembly from Monte Carlo simulations
- 9.40 – 10.00 S. SOKOLOWSKI (*Lublin, Poland*)
Molecular Dynamics studies of hairy nanoparticles in confined systems
- 10.00 – 10.20 A. BAUMKETNER (*Lviv, Ukraine*)
Monte Carlo study of cluster crystals stabilized by hydrophobic and electrostatic interactions
- 10.20 – 10.40 S. PEREPELYTSA (*Kyiv, Ukraine*)
Dynamics of counterions in the ion-hydrate shell of DNA double helix: A molecular dynamics study
- 10.40 – 11.10 Coffee Break

Chaired by E. SPOHR (*Essen, Germany*)

- 11.10 – 11.50 I. SIEPMANN (*Minneapolis, USA*)
First principles Monte Carlo simulations of phase, sorption, and reaction equilibria
- 11.50 – 12.10 I. NEZBEDA (*Usti nad Labem, Czech Republic*)
Evaluation of the contact angle from molecular simulations
- 12.10 – 12.30 S. RAVIPATI (*London, UK*)
Contact angle of nanodroplets from molecular dynamics simulations
- 13.00 - 14.00 Lunch

Ulam Computer Simulations Workshop

Chaired by A. SEITSONEN (*Paris, France*)

- 14.30 – 15.10 N. QUIRKE (*London, UK*)
Excess electrons in polyethylene: molecular dynamics and ab initio studies
- 15.10 – 15.50 K. PROCHÁZKA (*Prague, Czech Republic*)
Coarse-grained simulations of polymer and polyelectrolyte self-assembly
- 15.50 – 16.20 Coffee Break

Chaired by D. KOFKE (*Buffalo, USA*)

- 16.20 – 17.00 J. GROSS (*Stuttgart, Germany*)
Molecular simulations of phase equilibrium properties and force field development supported by analytic fluid theories
- 17.00 – 17.20 M. HORSH (*Kaiserslautern, Germany*)
Multicriteria optimization of molecular force field models
- 17.20 – 17.40 T. ŻÓRAWIK (*Wrocław, Poland*)
Levy walks: theory and simulations
- 17.40 – 18.00 B. NOWAKOWSKI (*Warsaw, Poland*)
Monte Carlo simulation of stochastic effect in thermochemical system
- 18.00 – 18.20 Closing remarks
- 18.20 – 20.00 Walking Tour
- 20.00 – 22.00 Workshop Dinner

List of posters

1. M. BALCEREK (*Wrocław, Poland*)
Calibration surface approach to the real data
2. M. BORÓWKO (*Lublin, Poland*)
Self-organisation of disks with attached short chains
3. T. DEMCHUK (*Lviv, Ukraine*)
Structural and dynamical properties of liquid silicon at high pressures via *ab initio* molecular dynamics
4. D. DUQUE (*Madrid, Spain*)
Nanoscale heat transport in fluids near solids
5. J.R. ESPINOSA (*Madrid, Spain*)
Interfacial free energy as the key to the pressure-induced deceleration of ice nucleation
6. S. FIGUEROA-GERSTENMAIER (*León, Mexico*)
Fullerene inhibit β -amyloid peptide aggregation: a molecular simulation study
7. J. GORECKI (*Warsaw, Poland*)
Chemical classifiers based on oscillatory chemical reactions
8. K. HAYDUKIVSKA (*Lviv, Ukraine*)
Partially directed polymers in anisotropic environment
9. V. HORDIICHUK (*Lviv, Ukraine*)
Application of the van der Waals concept towards computer simulations of Lennard-Jones fluid
10. T. HVOZD (*Lviv, Ukraine*)
Phase equilibria of polydisperse fluids confined in random porous media
11. O. KALYUZHNYI (*Lviv, Ukraine*)
Universal shape properties of mesoscopic polymer chains, polymer stars and their aggregates

12. YU. KALYUZHNYI (*Lviv, Ukraine*)
Melting upon cooling and freezing upon heating: Fluid-solid phase diagram for Švejč-Hašek model of dimerizing hard spheres
13. I. KIRIAN (*Kyiv, Ukraine*)
The simulation of structure transformations in ball-milled graphite by reverse Monte-Carlo method
14. M. LITNIEWSKI (*Warsaw, Poland*)
On simulation of evaporation of liquid
15. H. LOCH-OLSZEWSKA (*Wroclaw, Poland*)
Anomalous diffusion — epsilon-ergodicity testing simulations
16. B. MARKOVYCH (*Lviv, Ukraine*)
Effect of Coulomb interaction on chemical potential of metal film
17. I. MELNYK (*Lviv, Ukraine*)
On application of the effective LGW Hamiltonian to analyze impact of the finite-size effects in computer simulation studies of the gas-liquid criticality
18. N. MEYER (*Metz, France*)
Influence of the interaction model on the shear viscosity of liquid water
19. B. NOWAKOWSKI (*Warsaw, Poland*)
Master equation simulation of FKPP front: effect of perturbed particle velocity distribution
20. I. OMELIAN (*Lviv, Ukraine*)
Speeding up molecular dynamics of biochemical liquids by advanced solvation force extrapolation
21. W. RŻYSKO (*Lublin, Poland*)
Monte Carlo study of Janus particles in solvents
22. I. SHTABLAVYI (*Lviv, Ukraine*)
Atomic scale features of the free volume variations in liquid Sn, Bi, and Sn-Bi eutectic alloy by reverse Monte Carlo simulation

23. K. ŠINDELKA (*Prague, Czech Republic*)
Dissipative particle dynamics study of poly(N-isopropylamide) with carboxylic and dodecyl terminal groups (PNIPAm-C12) in aqueous solutions
24. J. ŠKVÁRA (*Ústí nad Labem, Czech Republic*)
Identification of molecular interfaces and layers
25. A. SLYUSARCHUK (*Lviv, Ukraine*)
Photocontrollable self-assembly and aggregation of decorated nanoparticles by molecular dynamics simulations
26. A. STELMAKH (*Lviv, Ukraine*)
Effective attraction between like-charged macroions in aqueous medium
27. X. WANG (*Prague, Czech Republic*)
Computer study of chromatographic separation of functionalized polymers

Ulam Computer Simulations Workshop
Challenges & Opportunities in Molecular Simulations

Invited Lectures

Abstracts

21–24 June 2017, Lviv, Ukraine

Stanisław Ulam: life, mathematics, and science

M. Zarichnyi

*Department of Mechanics and Mathematics, Ivan Franko Lviv University,
Universytetska Str. 1, Lviv 79000, Ukraine E-mail: mzar@litech.lviv.ua*

The talk is devoted to a (mathematical and scientific) biography of Stanisław Ulam. A special attention will be paid to Ulam's mathematical achievements.

Certainty from uncertainty and order from disorder: how the Monte Carlo method changed our understanding of entropy

D. Frenkel

University of Cambridge, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW, UK

Ulam's ideas about "random sampling" lie at the basis of all Markov-Chain Monte Carlo methods from Metropolis onwards. I will describe part of this story (including some very recent developments) and illustrate the power of the method by discussing what we have learned about the entropy of crystals and granular materials.

Hydrodynamics from dynamical non-equilibrium molecular dynamics

G. Ciccotti^{a,b,c}

^a*Istituto di Applicazioni del Calcolo “Mauro Picone” (IAC), CNR, Roma, Italia*

^b*Università di Roma “La Sapienza”, Roma, Italia*

^c*School of Physics, University College of Dublin, Dublin, Ireland*

Our starting point will be the relationship between hydrodynamics from the macroscopic continuum point of view and its atomistic interpretation in statistical mechanical terms. Then we extend stationary state (equilibrium and nonequilibrium) Molecular Dynamics to time dependent situations, including response and relaxation. We call the procedure Dynamical Non-Equilibrium Molecular Dynamics (D-NEMD), to distinguish it from standard NEMD, rigorously useful only to simulate stationary nonequilibrium states. It is, in essence, a generalization of linear response theory. The idea, formulated by Onsager in the thirties in metaphysical language, has received a solid foundation in the fifties by the work of Kubo (in the linear and nonlinear regimes). Adapted to MD simulations by G.Jacucci , I.R.Mac Donald and myself in the seventies, it has been baptized as the (nonlinear) Kubo-Onsager relation, connecting dynamical nonequilibrium averages or dynamical relaxations to initial distribution which can be sampled in MD by stationary processes. Finally we go back to hydrodynamics, to illustrate the method, by studying the hydrodynamic relaxation of an interface between two immiscible liquids.

Liquid of Life *in silico*: Electronic structure-based atomistic simulations of liquid water

A.P. Seitsonen

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Water, due to its involvement in various of our every day life events, practical applications and scientific research disciplines, serves as an important test case for atomistic computer simulations. As parametrised or polarisable force fields yield overall reasonably good an accuracy in comparison with experimental findings, the methods where the electronic structure is explicitly solved at every time step in order to obtain the total energy of the system and/or forces acting on the ionic nuclei need to demonstrate a superior accuracy in order to justify the vast additional computing time required. Progress has been achieved in recent years, but improvement is still necessary to achieve a satisfying level of quality in the results, and that we can rely on the *predictive* capabilities of the simulations.

In this Presentation we review the recent literature on the simulation of liquid water using the electronic structure-based methods. We concentrate on the results obtained with the Density Functional Theory-based Molecular Dynamics (DFTbMD) approach, but we shortly demonstrate related approaches as well. We enlist various properties, from the geometric structure, to dynamical, vibrational and electronic quantities. In particular we demonstrate the recent evaluation of the melting temperature of water using such simulations. Within the DFTbMD scheme we discuss the influence of the choice of the approximation of the exchange-correlation term to the results obtained. We also mention the recent progress in describing the nuclear quantum effects in liquid water, yielding ever-improving degree of reality in the computer simulations.

Electrostatic driving forces in molecular simulations of stochastic proton discharge reactions on electrodes. Beyond a 1D-Poisson-Boltzmann view

E. Spohr

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Approximately 20,000 proton discharge events from aqueous NaCl solutions to charged electrodes [1, 2], obtained from classical Molecular Dynamics trajectories with an empirical valence bond reactive force field for varying surface charge densities of the electrode and varying electrolyte solution compositions (sets with different numbers of cations and anions) are analysed. Individual trajectories are started randomly from equilibrated snapshots of a non-reactive system. We calculate static and dynamic average electric fields acting on the proton transfer complex in directions perpendicular and parallel to the electrode surface. The time evolution of electric fields and of hydrogen bonding just before the discharge events provide insight into the discharge mechanism. Since the description of hydrogen bonding in force field models of water and aqueous solutions is an electrostatic one, the relative importance of global ('electrochemical') and local ('hydrogen bonding') electric fields on the reaction mechanism will be assessed in a stochastic manner.

1. J. Wiebe and E. Spohr. "Double layer effects in a model of proton discharge on charged electrodes". In: Beilstein J. Nanotech. 5 (2014), pp. 973-982. doi: 10.3762/bjnano.5.111.
2. J. Wiebe, K. Kravchenko, and E. Spohr. "Electrolyte effects in a model of proton discharge on charged electrodes". In: Surf. Sci. 631 (2015), pp. 35-41. doi: 10.1016/j.susc.2014.06.016.

Mapped averaging methods for high-precision, high-efficiency calculation of properties by molecular simulation

A.J. Schultsand, D.A. Kofke

Department of Chemical and Biological Engineering, University at Buffalo — SUNY, Buffalo, NY, USA

We present a general framework for reformulation of the ensemble averages commonly encountered in statistical mechanics. This “mapped-averaging” scheme allows approximate theoretical results that have been derived from statistical mechanics to be reintroduced into the underlying formalism, yielding new ensemble averages that represent exactly the error in the theory. The result represents a distinct alternative to perturbation theory for methodically employing tractable systems as a starting point for describing complex systems. Calculation of the reformulated averages by molecular simulation can proceed without contamination by noise produced by behavior that has already been captured by the approximate theory. Consequently, accurate and precise values of properties can be obtained while using less computational effort, in favorable cases, many orders of magnitude less. The framework opens many avenues for further development, both as a means to improve simulation methodology and as a new basis to develop theories for thermophysical properties.

**Inverse patchy colloids:
structure, dynamics, and self-assembly from Monte Carlo simulations**

G. Kahl, E. Bianchi, and S. Ferrari

*Institute for Theoretical Physics, TU Wien, Vienna, Austria,
E-mail: gerhard.kahl@tuwien.ac.at*

Anisotropy – be it in shape or in the interactions – has turned out to be an essential feature of colloidal particles that triggers their self-assembly strategies into mesoscopic target structures with desired properties. A relatively novel class of colloids that feature anisotropy in their interactions are colloidal particles whose surface is decorated by a heterogeneous charge distribution. As the particles are charged themselves, the interplay of attraction and repulsion between oppositely and likely charged surface regions guarantees that these colloids are able to form highly directional and, at the same time, strongly selective bonds with other particles. This particular bonding mechanism is the reason why such particles are ideally suited to self-assemble into highly stable ordered structures which are otherwise inaccessible to conventional colloidal particles with surface decoration (commonly termed patchy particles) [1, 2]. The fact that, in addition, the differently charged regions are susceptible to external stimuli (such as electric fields) make such particles ideal building entities in targeted bottom-up assembly processes.

Quite a few theoretical models for such particles have been put forward in literature; this contribution will focus on Monte Carlo simulation based investigations on the physics of charged particles, decorated on their polar regions by oppositely charged patches. These colloids show an unexpected rich variety of self-assembly scenarios, which can be triggered by confinement and/or external electric fields. One of the preferred ordered structures of these colloids are lamellar phases: they can emerge as hybrid crystal-liquid structures where transport of particles takes place through an otherwise stable layered structure [3].

1. E. Bianchi, C.N. Likos, and G. Kahl, *ACS Nano* **7**, 4657 (2013).
2. E. Bianchi, C.N. Likos, and G. Kahl, *Nano Letters* **14**, 3412 (2014).
3. S. Ferrari, E. Bianchi, and G. Kahl, *Nanoscale* (in press; 10.1039/C6NR07987C).

First principles Monte Carlo simulations of phase, sorption, and reaction equilibria

I. Siepmann

University of Minnesota, Department of Chemistry, B-8, 139 Smith Hall, 207 Pleasant St. SE, Minneapolis, MN 55455, USA

This talk will highlight recent developments enabling first principles Monte Carlo (FPMC) simulations for which energies are calculated on the fly using Kohn-Sham density functional theory. Applications of FPMC to the prediction of vapor-liquid equilibria for water, adsorption isotherms for gas molecules in metal-organic frameworks, and reaction equilibria in compressed vapors and in porous materials will be discussed.

Excess electrons in polyethylene: molecular dynamics and ab initio studies

N. Quirke

Department of Chemistry, Imperial College, London, SW7 2AZ, United Kingdom

The behaviour of an excess electron in ordered and amorphous polymer materials is both a practical problem of immense commercial importance and a fundamental problem involving electron localisation in disordered materials. Breakdown of high tension cables used to transmit power over long distances has been linked to electron trapping while, although it has been known for 50 years, that disorder localises electrons, it has not been obvious how the localisation is linked to local structure and chemistry in real materials. We have employed classical molecular dynamics and various ab initio methods to study this problem in polyethylene. We will discuss computer simulations of an excess electron in various structural motifs of polyethylene at room temperature, including lamellar and interfacial regions between amorphous and lamellae, as well as nanometre-sized voids. Electronic properties such as density of states (DoS), mobility edges, and mobilities are computed on the different phases using a block Lanczos algorithm. Our results suggest that the electronic density of states for a heterogeneous material can be approximated by summing the single phase density of states weighted by their corresponding volume fractions. Additionally, a quantitative connection between the localized states of the excess electron and the local atomic structure is presented. For more complicated chemistries we would like to use all electron DFT as it avoids the necessity of creating pseudopotentials for systems with many different interactions. It is not obvious how to calculate the excess electron properties within DFT. We have tested all electron DFT against one electron methods for methane and for polyethylene including polyethylene/vacuum interfaces. Finally we will show results for various interfacial systems that would be found in polymer nanocomposites. Reference will be made to the use of the one electron DoS in Monte Carlo methods to predict conductivity of bulk materials.

Coarse-grained simulations of polymer and polyelectrolyte self-assembly

K. Procházka^a, Z. Limpouchová^a, K. Šindelka^a, and M. Lísal^b

^a*Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, Albertov 6, CZ-12843 Prague 2, Czech Republic*

^b*Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, Rozvojová 135/1, Prague 6 — Suchbátka, Czech Republic*

The behavior of high-molar-mass compounds and the most important differences between systems of small molecules and long polymer chains will be briefly outlined in the short introduction.

The first part of the lecture will be devoted to the explanation of principles of dissipative particle dynamics (DPD) simulations and to their applications for studies of polymer systems. DPD is a coarse-grained molecular dynamics, which employs three types of forces acting between the DPD beads: (a) conservative force (derived from interaction potentials), (b) dissipative force (emulating friction) and (c) random force (emulating thermal motion and random collisions). The last two forces have to be well set with respect to each other to secure constant temperature. In DPD studies of polyelectrolyte systems, several types of conservative forces have to be considered: (a) soft repulsion between DPD beads, (b) spring force connecting the beads that form polymer chain and (c) electrostatic forces acting between charged polyelectrolyte beads, counterions and co-ions. We will describe how the parameters of soft repulsion forces emulating the coarse-grained effect of the excluded volume of solvent molecules and building units of the polymer chain can be recalculated from the dependence of the solvent compressibility on the density and from the Flory interaction parameters.

The implementation of electrostatic forces into DPD machinery generates several serious problems that have to be solved before DPD simulations can be applied to polyelectrolyte systems. A considerable part of the presentation will focus on the solution of this problem and on the second related issue which is the calibration of repulsion and electrostatic forces with respect to each other.

In the second (main) part of the lecture, we will present several examples of DPD studies of the electrostatic self-assembly of polyelectrolytes and show how the coarse-grained simulations help to improve the understanding and interpretation of experimental data. We will discuss both the behavior of stoichiometric and non-stoichiometric polyelectrolyte mixtures.

Molecular simulations of phase equilibrium properties and force field development supported by analytic fluid theories

J. Gross

University of Stuttgart, Institute of Thermodynamics and Thermal Process Engineering, Stuttgart, Germany,

The development of fluid theories is long since facilitated by molecular simulations. This contribution emphasizes that molecular simulations can in turn also be facilitated by analytic fluid theories. It is shown how an analytic equation of state can be used to significantly enhance the convergence characteristics of the multidimensional force field optimization. The procedure is iterative, due to imperfect approximations of the model, but convergence is swift and the final result is not biased by the analytic model. We show results for the development of a transferable force field for pure substances and for mixtures. It is further emphasized how the analytic model can be used to estimate properties that are otherwise unknown a priori. Monte Carlo simulations in the grand canonical ensemble for example require as input values of the chemical potential for a series of temperatures approximately corresponding to coexistence conditions.

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Contributed Talks

Abstracts

21–24 June 2017, Lviv, Ukraine

Extracting random forces and Mori-Zwanzig kernels from molecular dynamics simulations

R. Vuilleumier^a, D. Lesnicki^a, A. Carof^b, and B. Rotenberg^b

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The influence of the environment on the dynamics of a subsystems has two components: a random force and a friction force. This friction, which describes the feedback of the environment on the subsystem dynamics, is in general retarded and the environment keeps a memory of the past dynamics of the subsystem. This was formalized by Mori and Zwanzig, who introduced for this purpose projection operators, which single-out the degrees of freedom of interest. In this formalism, the dynamics of the subsystem is described by a generalized Langevin equation. The memory kernel for this evolution, that describe the retardation of the friction force, is the correlation function of the random force. This correlation function however is unusual as the force is not propagated along the normal dynamics but along an orthogonal dynamics. Here we will describe how, using an explicit representation of the orthogonal dynamics, the Mori-Zwanzig memory kernel can be computed from standard molecular dynamics simulations.

We will then apply this algorithm to the computation of the Mori-Zwanzig memory kernel of a Lennard-Jones particle immersed in a fluid of identical Lennard-Jones particles. We will show that this Mori-Zwanzig memory kernel decays algebraically. We will relate this algebraic decay to the hydrodynamic response of the bath and identify it with the Basset-Boussinesq force. Finally, an added mass to the particle mass will be extracted from the Mori-Zwanzig memory kernel. At odds with incompressible hydrodynamics predictions, this mass term is negative in the present case.

Is diffusion in liquid metals universal?

N. Jakse

*Science et ingénierie des matériaux et procédés (SIMAP), UMR CNRS 5266,
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Understanding how dynamic properties depend on the structure and thermodynamics in liquids is a long-standing open problem in condensed matter physics. Our current knowledge is based on two different contributions developed for model fluids in which universal scaling relationships between the excess entropy of the fluid and its reduced diffusion coefficient is considered. Difference holds in the way to obtain reduction parameters, using either macroscopic arguments as proposed by Rosenfeld [1] or microscopic ones as in the Dzugutov scheme [2]. However their applications to “real” liquids still remains elusive due to the ability of model reference fluids to describe more complex interactions that may occur in the real systems. The purpose of this contribution is use ab initio molecular dynamics simulations to calculate both structural and dynamic properties at different temperatures for a wide series of liquid metals including Al, Au, Cu, Li, Ni, Ta, Ti, Zn as well as liquid Si and B [3-5], as well as Aluminum-based liquid alloys [6] From this analysis, we demonstrate that the Dzugutov scheme remains successful only if a self-consistent method to determine the packing fraction of the hard sphere reference fluid as well as an appropriate approach to express the excess entropy are used. We compare our results with original Rosenfeld’s scaling law [1] as well as with its generalized version proposed very recently [7] for pure metals.

1. Y. Rosenfeld, J. Phys. Condens. Mat, 11, 5415 (1999).
2. M. Dzugutov, Nature 381, 137 (1996).
3. N. Jakse and A. Pasturel, Sci. Rep. (Nature) 3, 3135 (2013).
4. N. Jakse and A. Pasturel, Cond. Mat. Phys. 18, 43603 (2015).
5. N. Jakse and A. Pasturel, Sci. Rep. (Nature) 6, 206689 (2016).
6. N. Jakse and A. Pasturel, J. Chem. Phys. 144, 244502 (2016).
7. W.P. Krekelberg et al., Phys. Rev. E, 80, 061205 (2009).

Algorithms for testing of fractional dynamics: a practical guide for stochastic modelling

A. Weron

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In this talk we present a systematic methodology which demonstrates how to identify the origins of fractional dynamics. We consider three mechanisms which lead to it, namely fractional Brownian motion, fractional Levy stable motion and an autoregressive fractionally integrated moving average (ARFIMA) process. The methodology is based on statistical tools for identification and validation of the fractional dynamics, in particular on an ARFIMA parameter estimator, an ergodicity test, a self-similarity index estimator based on sample p-variation and a memory parameter estimator based on sample mean-squared displacement. Finally, we illustrate the methodology on biological SPT data and show that ARFIMA can be considered as a universal model for fractional dynamics. Thus, we provide a practical guide for experimentalists on how to efficiently use ARFIMA modelling for a large class of anomalous diffusion data.

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Dynamic structure of liquid water

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In this work, we study the dynamic structure of liquid water by classical molecular dynamics simulations. We compare the collective excitations spectra predicted by two rigid models of interactions, non-polarizable SPC/E (J. Phys. Chem. 91, 6269 (1987)) and polarizable BK3 (J. Chem. Phys. 138, 204507 (2013)) models. After having discussed the influence of the polarizability of the molecule on this property, we investigate its density and temperature dependence.

What simulations can teach us about homogeneous ice nucleation

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In the last 5 years we have been using computer simulations with the aim of shedding light in the process of ice nucleation. Such process is the first step of water freezing, arguably the liquid-to-solid transition with the greatest relevance on Earth. In particular, the extent of freezing in atmospheric clouds has a great impact on the Earth's albedo and, therefore, on climate change. Simulations is a particularly suitable tool to study ice nucleation because it enables access to the time and length scales relevant to this process, ns and nm, complementing the information obtained in experiments where such small scales can not be probed.

Using simple models for simulating water we have been able to reach a nearly quantitative agreement with experimental ice nucleation rates. We have used the information drawn in our simulations to gain a better understanding of the ice nucleation process in terms of molecular mechanism and thermodynamic parameters affecting the nucleation rate. With this information we propose a tentative explanation for the decelerating effect of pressure on ice nucleation as well as for current discrepancies in measurements of the nucleation rate between different experimental groups.

Molecular dynamics simulation of charged systems in external magnetic field

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The current statistical mechanics description of charged systems subject to external magnetic field, dating back to the work of Kubo in the 1950s and commonly upheld today [1], states, in particular, that the parity properties of time-correlation functions cannot be established because the direct coupling of momenta and coordinates in the Hamiltonian hinders standard time reversal symmetry for these systems. In fact, this and other related results, such as the Onsager relations, refer to relationships between systems in two oppositely oriented magnetic fields, an unsatisfactory situation given that experiments and simulations usually occur in a single field.

In this Presentation, two new generalized time reversal symmetries are introduced [2, 3]. These symmetries enable to determine parity of time correlation functions for a single field and, more in general, make it possible to recast several aspects of the theory for these systems on the same formal footings as for those with Hamiltonians of standard form. They also allow predicting zero cross correlation between specific pairs of observables and thus establish analytically the behavior of some elements of the diffusion and conductivity tensors difficult to access experimentally or numerically.

Employing a recently developed algorithm based on the Liouvillian formalism [4], it will be shown that these theoretical findings are indeed verified in molecular dynamics simulations of superionic conductors. Furthermore, it will be shown that, using these new formal and algorithmic tools, the on-set of the ionic Hall effect and ionic magnetoresistance in AgI [5] and CaF₂ can be characterised via simulation, with results in very good agreement with experiments, when available.

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Langevin and gradient thermostats for rigid body dynamicsR.L. Davidchack^a, T.E. Ouldridge^b, and M.V. Tretyakov^c

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We introduce new Langevin and gradient (Brownian) thermostats for rigid body dynamics, which can be used in molecular dynamics simulations of systems with rigid body components. Rotations are represented by unit quaternions and the proposed numerical integrators for these thermostats automatically preserve the unit length of quaternions. In addition, the Langevin integrators also ensure that the conjugate quaternion momenta remain tangent to the quaternion coordinates. The Langevin integrators are quasi-symplectic and of weak order two. The integrator for the gradient thermostat is of weak order one. We numerically compare the discretization errors of the Langevin integrators, as well as the efficiency of the gradient integrator compared to the Langevin ones when used in the simulation of rigid TIP4P water model with smoothly truncated electrostatic interactions. Finally, we present a new rigid body Langevin thermostat and numerical integrator for the simulation of systems with hydrodynamic interactions, which can be used for modelling the dynamics of colloids, DNA, proteins and other macromolecules in solutions. The performance of this thermostat and integrator is demonstrated in numerical experiments of several model systems.

Fermi-Pasta-Ulam chains: simulation and theory

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In the early 1950s, Enrico Fermi, John Pasta, and Stanislaw Ulam (FPU) numerically simulated a one-dimensional chain of mass points connected by weakly nonlinear forces (FPU chains); it was one of the first computer simulations for purely scientific purposes. The intention was to test some simple assumptions of equilibrium statistical mechanics such as ergodicity or the equipartition of energy; Fermi predicted that the energy of the chain would asymptotically be distributed equally among the different harmonic modes. However, the experiments showed that this was not the case. The assumed thermalization did not occur, the energy seemed to oscillate between the first few harmonic modes in a quasi-periodic way, a phenomenon which was henceforth known as the “FPU paradox”.

Since then, the quest for an explanation of this unexpected stability has been going on, and various possible explanations have been proposed; most of these explanations are either soliton-based or use perturbative approaches. Here, we discuss one of the possible perturbative explanations, namely the Kolmogorov-Arnold-Moser (KAM) theorem and related results, together with their applicability to FPU chains.

Precisely, we formulate a model of FPU chains, give an overview of the KAM theorem and related results of perturbation theory, and show how these abstract results can be applied to FPU chains; we also make some remarks on some special case of FPU chains, the so-called Toda lattice, which has especially strong integrability properties.

Besides its practical significance as a model for various phenomena in areas such as solid state physics, the research on FPU chains is one of the first examples of research in mathematical and theoretical physics which is driven by experiments of computer simulations and not by laboratory experiments; Fermi, Pasta, and Ulam thus initiated the use of computer not just as tools for doing computations, but as electronic laboratories.

Computer simulations of low-dimensional materials

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The caging mechanism, introduced by Huerta, Henderson, Trokhymchuk in 2006 to describe the freezing of two dimensional hard disks, is applied here to contrast the frustration of freezing of a binary mixture of hard disks and overlapped hard dumbbells, both by using Monte Carlo simulations. In both cases the caging mechanism is frustrated but, meanwhile the binary mixture shows an extension of the fluid-like branch avoiding the solidification, the hard dumbbells shows a KTHNY-like transition. Extensions to study other low-dimensional systems are discussed.

Molecular Dynamics studies of hairy nanoparticles in confined systems

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Molecular Dynamics simulations are used to study the structure of hairy nanoparticles at a hard wall. Two models of hairy particles are considered. In the first case the chains are tethered at fixed points of the core molecule, while in the second case they can slide over the core surface. In both models the chains have been built of tangentially jointed spherical segments. We have determined local densities of core molecules and of segments of chains, radial distribution function for pairs molecules located in some selected slabs parallel to the wall, the end-to-end distances for tethered segments. Moreover, we have employed the concept of mass dipole to characterize how the distribution of the segments of chains around the cores changes with the distance to the surface.

Monte Carlo study of cluster crystals stabilized by hydrophobic and electrostatic interactions

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The term “cluster crystal” refers to crystalline materials in which each site is occupied by multiple entities of the same sort, atoms, colloids or polymers that, collectively, are known as clusters. There are two types of systems that are able to make cluster crystals: a) those that interact via potentials that are bound at the origin and thus allow inter-penetration of constituent particles and b) those that are represented by particles of finite size and, possibly, hard cores. Systems of the first class, polymers, dendrimers and other soft materials, have received much attention over the last several years. In this presentation we will focus on systems of the second class, such as colloids.

First we will establish conditions required for the cluster crystal assembly using a simple model potential and Monte Carlo simulations. Next we will show how potentials with the required properties can be generated by combining hydrophobic attraction at short distances and electrostatic repulsion at long distances. For that purpose, colloidal particles that consist of a hard-sphere core and a repulsive wall will be introduced as a model of hydrophobic interaction. Charge will be added to the colloids to induce the long-range repulsion. Effective interactions between colloids in explicit solvent will be computed as potentials of mean force in umbrella sampling simulations. For select models molecular dynamics simulations will establish the stability of the cluster crystal conformations at room temperature. Finally we will comment on how finite-size systems making cluster crystals can be realized in practice.

Dynamics of counterions in the ion-hydrate shell of DNA double helix: A molecular dynamics study

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Starting with the early works by Rosalind Franklin, James Watson and Francis Crick, water molecules and metal counterions revealed the essential role in organization of the structure of DNA macromolecule. Now it is well known that water molecules are indispensable for the formation of stacked base pairs in the double helix, while the counterions neutralize the negatively charged phosphate groups of the macromolecule backbone, reducing the electrostatic repulsion between different strands of the macromolecule. Due to the regular structure of the double helix the counterions tethered to DNA may form an ordered system of charges around macromolecule. Considering such system as the lattice of ionic type it has been shown that the dynamics of DNA is characterized by ion-phosphate vibrations that are prominent in the low-frequency spectra range ($<200 \text{ cm}^{-1}$) [Perepelytsya S.M., Volkov S.N. *Eur. Phys. J. E.* 24, 261 (2007); *Eur. Phys. J. E.* 31, 201 (2010); *J. Molec. Liq.* 164, 113 (2011); *J. Phys.: Conf. Ser.* 438, 012013 (2013)]. To study the dynamics of ordered counterions around the double helix the molecular dynamics simulation of DNA fragment d(CGCGAATTCGCG) in water solution with different ions (Na^+ , K^+ , Cs^+ and Mg^{2+}) have been performed. The results of preliminary study [Liubysch O.O., Vlasiuk A.O., Perepelytsya S.M. *Ukr. J. Phys.* 60, 433 (2015)] have been also used. The obtained results show that the Na^+ counterions interact with the phosphate groups directly from outside of the double helix and via water molecules at the top edge of DNA minor groove. K^+ ions interact with the phosphate groups (directly and via water molecules) and with the atoms of nucleic bases from the minor groove of the double helix. The cesium ions penetrate deeply inside the minor groove and interact directly with the atoms of nucleic bases. Cs^+ counterions form a structured system of charges in the DNA minor groove that may be considered as a specific case of ionic lattice. The magnesium ions interact with the atoms of DNA only via water molecules of the hydration shell. The considered ions in the major groove of the double helix do not have a defined interaction site.

Simulations of supersaturated steam

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An alternative method for determination of the contact angle of droplets at a solid underlay from molecular simulations is proposed. The method is based on a recently developed general method of identification the surface molecules of a molecular system with the interface of an arbitrary shape and on a subsequent parametrization of the surface of the droplet by a smooth function. The method has been verified first by considering two artificial systems with the exactly known contact angles and then by comparison with literature data for two realistic systems.

Contact angles of nanodrops from molecular dynamics simulations

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With the computational tools available today it is straightforward to simulate a sessile drop on a substrate, but analysis of the droplet to estimate the contact angle is still ambiguous. Most commonly employed methods either use diverse choices of parameters in the analysis, different interface profile fitting functions or require a large number of particles. To address this problem, we propose a methodology that does not presume any shape of the interface and consider an appropriate coarse-grained density field from discrete particles. We calculate the contact angle values of sessile drops using the proposed method for three different systems: (i) Lennard Jones (LJ) drop on LJ 9–3 surface, (ii) SPC/E water drop on LJ 9–3 surface and (iii) SPC/E water drop on graphite surface. We compare the sessile drop contact angles with Young contact angle values for the first two systems and observe a very good agreement.

Multicriteria optimization of molecular force field models

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To reach the precision required by engineering applications, molecular models need to be adjusted to a variety of thermodynamic properties. This implies the presence of multiple conflicting objectives. In the present work, the two-centre Lennard-Jones plus point quadrupole (2CLJQ) model class is considered, and the multicriteria optimization problem is addressed by constructing the Pareto front, i.e., the set of rational compromises, from which models tailored to special needs can subsequently be chosen consciously by individual users or automatically, e.g., by thermodynamic property databases and simulation software.

Ten real quadrupolar fluids are considered here by multicriteria optimization: Nitrogen, oxygen, fluorine, chlorine, bromine, ethane, ethylene, acetylene, perfluoroethylene, and perchloroethylene [1]. Three optimization criteria are defined by the normalized root mean square deviation for the saturated liquid density, the saturated vapour pressure, and the vapour-liquid surface tension. A recently developed efficient long-range correction scheme is used to determine the surface tension by molecular dynamics simulation with a high precision [2]. An approach based on self-organizing patch plots is introduced for visualizing the Pareto front. The Pareto knee region is investigated, and model parameterizations are identified which constitute an overall compromise between interfacial and bulk properties [1].

From previous work, 2CLJQ models are available for 29 low-molecular fluids [3]. These models are validated against the vapour-liquid surface tension, to which they were not adjusted. It is found that on average, the vapour-liquid surface tension is overestimated by about 20% [4], and that a significant improvement can be achieved by multicriteria optimization.

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Lévy walks: theory and simulations

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Lévy walks are useful models of anomalous diffusion and have found a number of applications in physics and biology. We present some newest key results regarding their probability distributions and aging property in ballistic regime. In particular we show that despite a complicated memory structure and the appearance of α -stable processes in the definition of 3D isotropic Lévy walks their probability density functions are given by elementary functions. In 2D the result for PDF is more complicated and it requires a fractional derivative and hypergeometric functions.

We also discuss a simulation algorithm for these processes. It turns out that there is a perfect agreement between statistics obtained via Monte Carlo simulations and our theoretical findings.

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Monte Carlo simulations of stochastic effects in thermochemical systemB. Nowakowski^{a,b}

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The studied thermochemical system is governed by two dynamical equations describing chemical and energy balance. Despite simplicity of the chemical scheme, it exhibits quite rich behaviour and all features possible for dynamics of 2-variable nonlinear system: multistability, excitability, and limit cycles appearing due to Hopf (regular or subcritical) or homoclinic-orbit bifurcations. Effect of intrinsic fluctuations is included in the stochastic dynamics; for its description we develop the specific master equation, employing discrete variable describing population of chemical species and a continuous variable for temperature. The stochastic evolution of the system is studied by means of kinetic Monte Carlo simulations, appropriately adopted to the integro-differential form of the master equation.

Calculations show important effects of fluctuations on dynamics of the system: (1) coherence resonance in excitable[1] and oscillating[2] systems, (2) stochastic resonance due to thermostat temperature variations[3], (3) fluctuation-induced shift of bifurcation parameters[4]. The results once more indicate that systems described by nonlinear dynamics are highly sensitive to fluctuations, which can induce qualitative changes in their macroscopic evolution.

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Ulam Computer Simulations Workshop
Challenges & Opportunities in Molecular Simulations

Posters

Abstracts

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Calibration surface approach to the real data

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Precise characterization of the anomalous diffusion for SPT experiments has become a central issue in biophysics. However, measurement errors raise difficulty in the analysis of single trajectories. In this poster, we present a novel surface calibration method based on fractionally integrated moving average (FIMA) process as an effective tool for extracting both the anomalous exponent and the magnitude of the measurement error for autocorrelated processes of various origins. This method is developed using a toy model – fractional Brownian motion disturbed by independent Gaussian white noise – and is illustrated on both simulated and experimental data. We also compare this new method with the mean-squared displacement (MSD) technique, extended to capture the measurement noise in the toy model, which shows inferior results. The introduced procedure is expected to allow for more accurate analysis of trajectories with measurement errors across different experimental fields and without the need for any calibration measurements.

Self-organisation of disks with attached short chains

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We use the large scale molecular dynamics simulations to study the self-organisation of hairy disks in monolayer films. The particles are circular cores with attached three oligomeric chains. The chains are modelled as freely joined soft disks. All entities interact via Lennard-Jones (12-6) potential. The core-core and ligand-ligand interactions are assumed to be attractive, whereas core-ligand interactions are repulsive. Two models of hairy particles are considered. The first one corresponds to cores with symmetrically distributed and permanently fixed ligands. In the second one the chains are mobile and can slide over the core. We show that the mobility of ligands affects considerably the self-assembly. The disks with rigid geometry form a hexagonal-like structure for tethered trimers and a "spaghetti-like" structure built of strings of cores for longer chains. The disks with mobile ligands always aggregate into the "wires" composing of double strings of cores with the ligands facing outwards. These wires gradually assemble into the lamellar phase. Our results indicate that ligand mobility plays a considerable role in the aggregation. The distributions of cluster sizes calculated for fixed and mobile ligands are considerably different. The average cluster size is greater for disks with fixed ligands.

Structural and dynamical properties of liquid silicon at high pressures via *ab initio* molecular dynamics

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We report an *ab initio* study of changes in structure and dynamics of molten silicon along the isothermal line at 1150 K, above the minimum of melting curve of Si. The pressure in the system was changing in the range 10.2-27.5 GPa. There are 4 different phases in the crystalline Si in this range of pressures. One of the aims of this study was to explore the issue whether the liquid above the melting line reflects specific features of the crystalline state at corresponding pressure. The *ab initio* simulations were carried out for 7 pressures on a system of 300 Si atoms with electron-ion interaction represented by PAW potentials (VASP package). The gradient approximation in the form of PBE (Perdew-Burke-Ernzerhof) was used for exchange-correlation interaction functional. Pair distribution functions $g(r)$ for different pressures showed almost the same position of the first maximum, that can be explained existing covalent bonds in liquid Si. The angular three-particle distribution function gives evidence that at lower pressure (10.2 GPa) the maximum is about 109 degrees which is typical for tetrahedral structure but with increasing pressure in the system the peak at 60 degrees becomes more pronounced, that is a consequence of breaking the covalent bonds and emergence of typical for dense liquids close packed structures of nearest neighbors.

Dynamic properties are represented by analysis of diffusion coefficients, spectral functions of velocity autocorrelations and dispersions of collective excitations vs pressure in liquid Si. Both longitudinal and transverse dispersion curves of collective excitations are reported at different pressures. We found, that for pressures above 16.6 GPa are two peaks observed on transverse spectral current function that gives evidence of increasing L-T coupled dynamics with pressure.

Nanoscale heat transport in fluids near solids

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Boundary conditions are an idealized way to deal with the interaction of a fluid of interest with solid objects (or other fluids). Microscopically, the forces that the solid exerts on the fluid are confined to a thin region of molecular size. At these nanoscales, the local fluid structure and molecular correlations become important issues that are usually disregarded in usual derivations of the hydrodynamics from microscopic first principles.

We present a first principles theory for thermal transport that takes into account the microscopic interactions between fluid and solid. The fluid is described with the local conserved quantities of mass and energy density fields while the solid is described with the total energy. The interactions of the fluid with the solid appear directly in the equations of hydrodynamics governing the fluid variables, as “external forces” of reversible and irreversible nature.

Under a number of approximations we can predict the evolution of a sudden increase of the temperature of the crystalline wall in contact with a fluid.

We also present a Galerkin discretization of the continuum theory that allows us to compare MD simulations with the theoretical predictions. In particular we describe with MD simulations the thermal transport behaviour of the fluid when the crystalline slab is suddenly heated. The microscopic as well as coarse-grained evolution of the system is monitored.

The model predicts the late stages of evolution of the selected variables. However, the initial stages of the heating process show a substantial motion of the fluid. For a successful treatment of this effect is necessary to include to the list of variables also the momentum of the fluid. This is work underway.

Interfacial free energy as the key to the pressure-induced deceleration of ice nucleation

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The avoidance of water freezing is the holy grail in the cryopreservation of biological samples, food, and organs. Fast cooling rates are used to beat ice nucleation and avoid cell damage. This strategy can be enhanced by applying high pressures to decrease the nucleation rate, but the physics behind this procedure has not been fully understood yet. We perform computer experiments to investigate ice nucleation at high pressures consisting in embedding ice seeds in supercooled water. We find that the slowing down of the nucleation rate is mainly due to an increase of the ice I-water interfacial free energy with pressure. Our work also clarifies the molecular mechanism of ice nucleation for a wide pressure range. This study is not only relevant to cryopreservation, but also to water amorphization and climate change modeling.

Fullerene inhibit β -amyloid peptide aggregation: a molecular simulation study

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Alzheimer's disease (AD) is a degenerative, and irreversible neurological disease with no cure. The neuropathological hallmarks of AD are both the neurofibrillary tangles and senile plaques composed by τ protein and β -amyloid (β A) peptide deposits respectively. This peptide is derived from a transmembrane protein called amyloid precursor protein, cleaved by proteolytic enzymes highly active during AD. Fullerenes, such as C_{60} or C_{70} are small carbon nanostructures with spherical cage shape and diameter of 1 nm. Increasing experimental studies indicate that fullerene derivatives (F) have remarkable anti-amyloid aggregation properties for AD. The cyclopropanation of C_{60} has been shown to provide precursors from which it is possible to synthesize amphipathic adducts, increasing both their solubility in water and biological activity. We have synthesized adducts of C_{60} , specifically ethyl fullerenmalonates and the corresponding fullerenmalonic acid sodium and demonstrated in vitro their properties as inhibitors of peptide aggregation. In this work, we have analyzed the interaction of different fullerenes with β A in water by means of molecular dynamics simulation using an atomistic force field. We used the NPT ensemble at atmospheric pressure and body temperature. Through the simulations we will be able to learn the specific sites where the F are binding to β A giving a new insight for the design of very specific drugs against AD.

Chemical classifiers based on oscillatory chemical reactions

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Unconventional computing devices using nonlinear chemical media to process information offer an interesting alternative to standard semiconductor-based computers. We illustrate chemical information processing considering database classifiers formed by a network of interacting droplets in which a photosensitive variant of Belousov-Zhabotinsky (BZ) reaction proceeds. In such system information is introduced by illumination of droplets selected as the input ones. Using optical control we can adjust the time evolution of individual droplets and teach the system to perform a specific computational task. We demonstrate that chemical classifiers made of droplets can be designed in computer simulations based of evolutionary algorithms. Such algorithms maximize the mutual information between the database and the observed time evolution of droplets. In the paper we show that for the CANCER database (the Wisconsin Breast Cancer Dataset) even a classifier build with a relatively small number of droplets can perform classification tasks with accuracy exceeding 90%. The reliability of optimized chemical classifiers of this database is discussed for different numbers of droplets involved in data processing.

Partially directed polymers in anisotropic environment

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We analyze conformational properties of partially directed polymers in anisotropic environment, when anisotropy is caused by presence of columnar disorder. We analyze two cases, when polymers are considered to be oriented in direction perpendicular as well as at the 45 degree angle to the direction of the columnar defects. We consider a lattice model of a self-avoiding walks on the simple cubic lattice and we apply the Pruned-Enriched Rosenbluth method in order to analyze conformational properties of polymers, which include both scaling exponents and shape characteristics.

For the case of perpendicular orientation of the stretching field and columnar defects, we observe a reorientation transition of polymers, while in the other case this transition is absent.

Application of the van der Waals concept towards computer simulations of Lennard-Jones fluid

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Recently it has been shown that thermodynamics as well as vapour-liquid equilibrium in the Lennard-Jones-like hard-core attractive Yukawa fluid can be rather accurately described within the augmented van der Waals theory. Within this theory the original pair interaction is represented as a sum of the short-ranged and long-ranged contributions where the former consists of both the hard-core repulsive and short-range attractive interactions and can be identified as the interaction energy of a target molecule with its nearest neighbour counterpart. The nearest neighbour molecules and corresponding interaction energy are identified by means of the range (distance) criterion. According to this criterion the short-range interaction energy includes the full repulsion energy and the short-range part only of the full attraction energy, namely, the part that is responsible for the interaction of target molecule with its nearest neighbour molecule. The long-range interaction energy corresponds to the interaction energy of the target molecule with any other molecule but from outside the first coordination shell. Then properties of the system as whole are the sum of two terms: (i) the corresponding properties of the system with short-ranged interaction, that is well suited to be evaluated from computer simulations, and (ii) the van der Waals correction term, that can be evaluated analytically. In present study this idea is discussed with respect to Lennard-Jones interaction model that is most popular to describe the real systems.

Phase equilibria of polydisperse fluids confined in random porous media

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We have studied the phase behavior of polydisperse square-well (SW) chain fluid with chain length polydispersity and polydisperse Yukawa hard-sphere (HS) fluid with energy polydispersity confined in random porous media using extension and combination of second-order Barker-Henderson perturbation theory, SAFT-VR [1], high temperature approximation [2] and scaled particle theory [3]. The porous media are represented by the matrix of randomly placed hard-sphere obstacles. We also propose the original method to calculate analytically the radial distribution function for the hard-sphere fluid confined in the hard-sphere matrix [4]. Due to the confinement, polydispersity effects are substantially enhanced. For polydisperse SW chain fluid we obtain two-phase coexistence, and cloud and shadow curves. For polydisperse Yukawa HS fluid at an intermediate degree of fluid polydispersity and low density of the matrix, we observe two-phase coexistence with two critical points, and cloud and shadow curves forming closed loops of ellipsoidal shape. With the increase of the matrix density and the constant degree of polydispersity, these two critical points merge and disappear, and at lower temperatures the system fractionates into three coexisting phases [4].

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Universal shape properties of mesoscopic polymer chains, polymer stars and their aggregates

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We analyse the shape characteristics of various macromolecules dissolved in a solvent. Both solute and solvent are considered on a coarse-grained level via the dissipative particle dynamics simulations, thus reducing the effects of chemical content down to the level of solvophobicity of the individual polymer fragments. In the **case study A** we discuss a linear chain in a good solvent in the infinite dilution regime. At this level of detailisation, its properties depend exclusively on the space dimension d . The results obtained for the mean prolateness, asphericity and size ratio at $d = 3$ are in a good agreement with available analytic and MC simulation data and give an evidence of the universality of the shape of the coarse-grained polymer coil in a good solvent. We also discuss the probability distributions for the same set of shape characteristics. In the **case study B** we extend our analysis to the cases of homo-star (has been considered earlier) and hetero-star (considered for the first time here) polymers and to the case of a solvent of variable quality. The hetero-star molecule is characterised by different solvophobicity of its individual arms. We found an interesting effect that, upon the change of the solvent properties, the asphericity of a homo-star reaches its maximum value when the solvent is at the θ -point condition. The effect is explained by the interplay of the enthalpic and entropic contributions to the free energy. In the **case study C** we consider aggregation of the amphiphilic stars in a solvent. Four different architectures of the same molecular weight and composition are examined, namely: the miktoarm star, two different diblock stars and a set of four disjoint linear diblock copolymers. The shape of the aggregate is examined depending on the aggregation number N_a . In total, four different shape types are observed: spherical, rod-like and disc-like micelle and a spherical vesicle. Upon the increase of N_a , a continuous transition from the spherical to a non-spherical micelle is observed first, followed by a discontinuous transition of a non-spherical micelle into a spherical vesicle. Both transitions are discussed in terms of various free-energy contributions.

Melting upon cooling and freezing upon heating: Fluid-solid phase diagram for Švejk-Hašek model of dimerizing hard spheres

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Resummed thermodynamic perturbation theory for central force associating potential is extended and applied to study the properties of shielded attractive shell model of polymerizing hard spheres [1–3]. The model is represented by the two-component mixture of hard spheres with additional square-well interaction treated in the sticky limit and located inside the hard-core region and acting only between particles of different species. The theory self-consistently takes into account the changes in the excluded volume of the system due to bonding of the particles. Theoretical predictions for the pressure and fraction of the particles in different bonding states at different temperatures and densities are compared against computer simulation predictions.

In the limiting case of the model with zero bonding length (Švejk-Hašek model of dimerizing hard spheres) highly nontrivial fluid-solid phase behavior is observed. The phase diagram has the fluid branch of the fluid-solid coexistence curve located at temperatures lower than those of the solid branch. This unusual behavior is related to the strong dependence of the system excluded volume on the temperature, which for the model at hand decreases with increasing temperature. This effect can be also seen for a wide family of fluid models with an effective interaction that combines short range attraction and repulsion at a larger distance. We expect that for sufficiently high repulsive barrier, such systems may show similar phase behavior.

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The simulation of structure transformations in ball-milled graphite by reverse Monte-Carlo method

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The goal of this work is the systematic study of the evolution of local atomic arrangements during the quasi-continuous crystalline-amorphous transition under the graphite ball-milling. Crystalline spectrally pure graphite powder was used as the starting material. Graphite was milled in argon gas atmosphere in the laboratory planetary ball mill Fritsch Pulverisette P-6. The quantitative characteristics of a short- and a medium-range order in carbon nanomaterials structure are determined by a combined application of X-ray diffraction analysis, reverse Monte Carlo modeling and Voronoi diagram method. The simulated atomic configurations are reconstructed from experimental curves of the structure factors by RMC method using RMCPow v.2.4 software package [1]. All configurations consist of 4000 carbon atoms placed into a configuration cell. Quasi-continuous structural transformation from the crystalline to amorphous state takes place in graphite during ball-milling. The Voronoi polyhedra constructed for simulated atomic configurations of the ball-milled graphite have an extraordinary variety in their topological and metric characteristics and contain a lot of 5-fold faces [2]. It should be indicated, that regular configuration polyhedra (clusters) are virtually absent in the synthesized carbon nanomaterials. The analysis of VP sphericity coefficient K_{sph} enables a conclusion about changing local atomic arrangement in a structure of ball-milled carbon from graphite-like to typical for disordered tetrahedral network and random systems of points (atoms), proper for amorphous state. The sphericity coefficient is proposed to be as a parameter of the topological order to quantitative estimation of disordering degree in amorphous structures [3].

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On simulation of evaporation of liquid

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Intensive computer simulations of evaporation of Lennard-Jones liquid droplet have been performed [1–3]. The poster presents two problems appearing during the simulations and discuss the solution. The first is a consequence of the step error [4] that may lead to nonphysical artefact e.g. decreasing the liquid pressure when compared to the gas one. The second is the boundary condition for the gas phase. The boundary condition may be very important if we want to compare the simulation results with real experiment in which the gas container can be treated as infinite one.

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Anomalous diffusion — epsilon-ergodicity testing simulations

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The problem of ergodicity of the process is an essential issue for the real-life processes. In the ergodic system the Boltzmann hypothesis is satisfied, i.e. the time and ensemble averages are asymptotically equal. Lately, in various fields of physics, biology and related sciences, the non-ergodic systems that show the anomalous behaviour have been noted.

A crucial practical question is how long trajectories one needs to observe in an experiment in order to claim the ergodicity breaking of the sample. Based on the empirical estimator $F(n)$ for the dynamical functional $D(n)$, defined as a Fourier transform of the n -lag increments of the process, one can verify so-called ε -ergodicity - convergence of the estimator to some pre-defined interval $(-\varepsilon, \varepsilon)$.

The current work is based on α -stable autoregressive fractionally integrated moving average (ARFIMA) processes which form a large class of anomalous diffusions, observing both empirical simulation of the functional and the computations of theoretical formula for different values of parameters of the process. Simulations have been carried out using resources provided by Wroclaw Centre for Networking and Supercomputing, that is High Performance Computer within the Supernova cluster.

Effect of Coulomb interaction on chemical potential of metal film

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The rapid development of nanotechnology involving processes of metal deposition on various substrates requires a theoretical analysis and understanding of electronic effects in nanoclusters and nanofilms. If the size of nanostructure is comparable with the corresponding Fermi wavelength of electrons in the nanostructure, various physical properties may strongly depend on the size of this nanostructure. This phenomenon is called the quantum size effect and is typical for many physical quantities of metal nanofilms, such as thermodynamic stability, electrical resistivity, work function, surface energy, etc. Due to possible differences in properties of metal nanostructures from properties of the bulk metal, the research of such properties has considerable theoretical and experimental interests.

In the present work, the metal film within the jellium model taking into account the Coulomb interactions between electrons is studied. The surface potential is modeled by the infinite rectangular potential well. In the limit of low temperatures, calculations of the chemical potential and the distance between the side of the film and the potential wall of infinite height are performed for different values of the Wigner-Seitz radius. The chemical potential is found as a solution of the nonlinear equation. The dependences of the calculated quantities on the film thickness are studied, it is shown that taking into account the Coulomb interaction between electrons leads to a significant decrease in the chemical potential and increase in the distance between a side of the film and the infinite potential wall, and to an increase of the amplitudes of its oscillations, i.e. to an enhancement of the quantum size effect. It is shown that if the film thickness increases, the chemical potential of the film tends to the bulk chemical potential, i.e. to the chemical potential of unbounded metal within the jellium model, and the distance tends to magnitude, which is obtained earlier for the semi-infinite jellium.

On application of the effective LGW Hamiltonian to analyze impact of the finite-size effects in computer simulation studies of the gas-liquid criticality

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The effective Landau-Ginzburg-Wilson (LGW) Hamiltonian approach is used to analyze the finite-size effects in computer simulations of the critical parameters of the Sutherland fluid. In order to do this, the microscopic equations for the coefficients of the effective Landau-Ginzburg-Wilson (LGW) fluid Hamiltonian are presented in the case of the reference system that consists of hard spheres with a short-range Yukawa attraction. The mean-field level analysis of the critical parameters of the Sutherland fluid is performed and comparison against Monte Carlo simulation data is discussed.

To analyze the impact of the finite-size effects on the results of computer simulation studies, an estimate of the correlation length ξ near the critical point is calculated based on the Gaussian approximation for the effective LGW Hamiltonian and condition that correlation length must not exceed half the length L of the computational cell is used. Since correlation length diverges at the critical point, its calculated value will increase upon approaching the critical temperature. Based on the requirement $\xi \leq L/2$, the condition on the temperature T used in computer simulations, that is closest to the critical temperature T_c , and the size (number N of particles used in computer simulations) is verified for set of Monte Carlo data on Sutherland fluid criticality already reported in literature. The comparison against similar results that were obtained with the reference system composed of purely repulsive hard spheres is discussed.

Influence of the interaction model on the shear viscosity of liquid water

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In this work, we study self-diffusion coefficient and viscosity of liquid water by classical molecular dynamics simulations. We compare the predictions of two rigid models of interactions, non-polarizable SPC/E (J. Phys. Chem. 91, 6269 (1987)) and polarizable BK3 (J. Chem. Phys. 138, 204507 (2013)) models. After having discussed their respective ability to predict experimental results, we focus on the density and temperature dependence of these two properties. The validity of Stokes-Einstein relation is finally investigated.

Master equation simulation of FKPP front: effect of perturbed particle velocity distribution

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We develop a master equation for reaction-diffusion processes including the corrections due to the perturbation of the particle velocity distribution by the chemical reaction. Simulations of the mesoscopic dynamics for the FKPP chemical wavefront [1] are based on the modified master equation [2,3]. Significant deviations are observed for the speed and width of the front with respect to the results of the macroscopic reaction-diffusion equation without nonequilibrium corrections. The results at the mesoscopic level agree with microscopic simulations obtained by means of the direct simulation Monte Carlo method for dilute gases.

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Speeding up molecular dynamics of biochemical liquids by advanced solvation force extrapolation

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We propose an advanced algorithm for accurate and fast extrapolation of time-consuming mean solvation forces obtained from the 3D-RISM integral equations theory to accelerate molecular dynamics (MD) of biochemical liquids. The algorithm introduces distance and rotational transformations of coordinate space for each solute atom of the macromolecule to smooth the solvation forces. In addition, the basic coordinate-force pair set is extended to select the best subset for the normal equations to minimize the deviations by modified least-squares with dynamical balancing between the coordinate and force extrapolations. The mean solute-solvent interactions for the current inner configuration are then readily evaluated involving a relatively small number of the top outer previous coordinates in which the already known solvation forces were computed directly by 3D-RISM. The resulting equations of motion are solved analytically using the multiple time step exponential decompositions of the evolution operator within our optimized isokinetic Nosé-Hoover (OIN) chain thermostat to stabilize the propagation. The new method has been validated in MD/3D-RISM simulations of various systems including the hydrated alanine dipeptide, asphaltene in toluene, as well as the miniprotein 1L2Y and protein G, both dissolved in water. For all these cases it has been shown that, without affecting conformational properties, the size of the outer time step can be enlarged up to huge values of order of several picoseconds or even bigger, significantly accelerating the simulations. Moreover, the MD/3D-RISM/OIN quasidynamics provides time scale compression of solute configurational changes coupled with solvent exchange, leading to further substantial speedup of conformational sampling with respect to real time MD. Overall, a 50- to 1000-fold effective acceleration has been reached, compared to conventional MD with explicit solvent. As a consequence, we have been able to quickly fold the miniprotein from a fully extended state spending only 60 nanoseconds of the MD/3D-RISM/OIN quasidynamics, while the average physical folding time in MD and experiment is about 6 milliseconds.

Monte Carlo study of Janus particles in solvents

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We investigate self-organization of amphiphilic Janus disks and small isotropic molecules using Monte Carlo method. During simulations A number of Janus particles remains fixed while solvent molecules can be exchanged with a reservoir. A Janus particle is composed of two parts with dissimilar properties. As interactions between Janus particles are considered these parts are attractive (*A*) and repulsive (*R*). Solvent molecules are strongly attracted by the *R*-sides and repelled by the *A*-sides. To describe the interactions between particles we apply the method used in our previous work (J. Phys. Chem. B 117 (2013) 1166). The interactions between Janus particles switches from an extreme of attraction as the *A*-sides point toward one another to an extreme repulsion as the *R*-sides point toward one another, and takes intermediate values in between.

We show that the amphiphilic Janus disks and small fluid molecules assemble in different mixed structures at temperatures when the both components are supercritical fluids, if considered separately. The structure of the system depends strongly on a fluid density. The addition of a trace amount of fluid molecules to the Janus particles leads to the formation of the highly ordered, solid-like structure. At moderate densities, fluid molecules are encapsulated between long strings of Janus particles. Such “mixed wires” form the gel-like structure. For high fluid densities Janus particles aggregate in small clusters. The evolution of the system structure is continuous.

The strong interactions between Janus particles and fluid molecules cause “adsorption” of fluid molecules on *R*-parts of nanoparticles. This plays a key role in the process. The bond-switching between Janus particles is observed as a fluid density varies. Solvent molecules act as linkers between Janus particles leading to *SRS*-bonded clusters for moderate densities. In dense solvents, however, Janus particles are always joined by *A*-sides. The similar bond-switching caused by changes in temperature was experimentally observed (Angew. Chem. Int. Ed. 53 (2014) 4364).

Atomic scale features of the free volume variations in liquid Sn, Bi, and Sn-Bi eutectic alloy by reverse Monte Carlo simulation

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The free volume model has been widely accepted by researchers to interpret the diffusion processes and viscosity of metallic liquids. Unlike the point defects in crystals, free volume in disordered systems is usually of subatomic scale without fixed shape or characteristic size. According to Turnbull and Cohen, the free volume can be defined as follows: (1) it is possible to assign a local volume v of atomic scale to each atom in the glass (e.g. by Voronoi tessellation); (2) when v exceeds a critical value v_c , the excess ($v - v_c$) can be regarded as free volume. Many efforts have been devoted to characterizing the free volume in disordered systems experimentally, such as density measurements, positron annihilation spectroscopy, XRD and differential scanning calorimetry. However, none of these methods does not provide information about the distribution of free volume on atomic level.

The present study is dedicated to characterizing the content of free volume in liquid Sn, Bi, and Sn-Bi eutectic alloy by reverse Monte Carlo simulation. For the modeling process, an initial cubic cell was arranged with 8000 atoms. The sizes of the model cube were adapted with the melt density at the experiment temperature. The minimum distances between atoms r_{ij} was taken as a point of intersection of the left branch of the first maximum in an experimental pair correlation function curve with the abscissa axis. By means of an analysis of the RMC simulated local structure, the distribution of coordination numbers in the first coordination sphere of melts, temperature dependence of the most probable interatomic distances and coordination numbers as well as free volume distribution have been analyzed.

Dissipative particle dynamics study of poly(N-isopropylamide) with carboxylic and dodecyl terminal groups (PNIPAm-C12) in aqueous solutions

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We performed a parametric study of self-assembly of diblock copolymer imitating PNIPAm-C12 [1] which was proposed as a component of various thermoresponsive drug delivery systems [2]. The focus was placed on the effect of the length of the soluble poly(N-isopropylamide) block and the charge of the carboxylic group (i.e. different pH). We also studied associative behaviour of PNIPAm-C12 in solutions containing surfactant carrying either the same or opposite charge.

The simulations were performed using the computational simulation method known as the dissipative particle dynamics [3] with explicit electrostatics [4]. This highly coarse-grained method is similar to molecular dynamics and is well suited for investigation of complex systems.

We compared the simulation results with experimental measurements of light and X-ray scattering and found a satisfactory agreement at the qualitative and semi-quantitative level.

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Identification of molecular interfaces and layers

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The investigation of molecular layers behavior can be important to obtain a complex information about studied system. Change of the properties of liquids can be seen in individual layers. The interface of the structure belongs to the group of molecular layers. It provides information about shape characteristics of the system but it can also have the meaning of the phase boundary. This boundary combines the properties of both phases of fluid. This fact is an important feature for predicting the behavior of the system under different circumstances. For this reason, there is need to know these features for scientific purposes and the industrial usage. This is why Usti Software for Triangulated Interfaces (USTI) was developed to identify surface, interface and layers in systems which are described by coordinates of points in three-dimensional space (eg. centers of molecules). This software employs several types of triangulations for a suitable description of a wide range of physical systems (for example molecular systems with mixture of molecules with very different Van der Waals radii). This software is presented of several different systems. At first the whole methodology is illustrate on the simple artificial 2D system. Second system describes behavior of primitive model of water near to the solid wall. In this case orientation of molecules in the individual molecular layers was monitored. The last sort of physical relevant systems consists of water bulk in electric field of varying intensity, where the orientation of dipole moment of molecules and average charge density are observed in the individual molecular layers.

Photocontrollable self-assembly and aggregation of decorated nanoparticles by molecular dynamics simulations

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We study the photocontrollable self-assembly and aggregation of the azobenzene-functionalized nanoparticles using coarse-grained molecular dynamics simulations. Two case studies are considered: (i) bulk self-assembly of nanoparticles into lamellar smectic morphology and (ii) their aggregation in the pore with decorated walls filled by a solvent. In the case study (i) we demonstrate that illumination is able to reduce the interdomain physical crosslinks and promote faster polydomain-monodomain transition. In the case study (ii) we focus on the conditions for formation of the nanoparticles bridging path between two walls aimed on organic electronics and nanoconductors applications

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Effective attraction between like-charged macroions in aqueous medium

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Interactions between charged macroions in aqueous medium are of particular importance for the correct understanding of a multitude of biochemical processes, including protein aggregation, stability of colloidal dispersions or self-assembly of macroions and charged nanoparticles. In an effort to provide mechanistic insights into the phenomenon of attraction between like-charged macroions we use MD simulations to analyze pair potential of mean force (PMF) generated for macroions immersed in monovalent salt solutions. We find that for macroions carrying a high charge ($3e$ and more), attraction is caused by particularly stable configurations of counterions bound to the surface of the macroions. These configurations are very sensitive to the geometrical parameters and charge of the macroions and the counterions. In addition to the main minimum in the PMF profile, that corresponds to the bound state, a number of secondary minima are also present. In general, the shape of the PMF is determined by a delicate balance between various components of the internal energy and entropy. Our results will be useful for a better understanding of the aggregation and structure formation processes in highly asymmetric electrolyte solutions and in the design of molecules that can self-assemble through the mechanism of counterion-mediated binding.

Computer study of chromatographic separation of functionalized polymers

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Linear, two-arm and four-arm star polymers synthesized by the chain-growth polymerization, where the functionalities at the central and end positions are used for initiation and termination, can be separated by both normal-phase liquid chromatography (NPLC) and reversed-phase liquid chromatography (RPLC) at critical conditions. However, different retention behaviors have been experimentally observed in these two chromatographic processes caused by the difference in hydrophobicity. To confirm it, we study the partitioning of the three types of polymer chains between a bulk solution (mobile phase) and a pore (stationary phase) by Monte Carlo (MC) simulations using the model of self-avoiding walks (SAW) on a simple cubic lattice. A strongly attractive interaction between the functional groups and the pore wall is employed to emulate the favorable interaction of hydrophobic groups with the stationary phase in a RPLC column. We investigate the effects of functional groups at the critical adsorption point (CAP). The simulations yield inverse elution sequence of studied polymers in NPLC and RPLC. Our computer study contributes to a better understanding of the NPLC and RPLC separation mechanisms and helps to interpret experimental data obtained in different chromatography regimes.

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For notes

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Day	WEDNESDAY June 21	THURSDAY June 22	FRIDAY June 23
Time			
	Arrival	<i>Chaired by:</i> <i>D. Frenkel</i>	<i>Chaired by:</i> <i>G. Ciccotti</i>
9:00 – 9:40		G. CICCOTTI	G. KAHL
9:40 – 10:00		R. Vuilleumier	S. Sokolowski
10:00 – 10:20		N. Jakse	A. Baumketner
10:20 – 10:40		A. Weron	S. Perepelytsa
10:40 – 11:10		Coffee Break	Coffee Break
		<i>Chaired by:</i> <i>G. Kahl</i>	<i>Chaired by:</i> <i>E. Spohr</i>
11:10 – 11:50		A. SEITSONEN	I. SIEPMANN
11:50 – 12:10		J.-F. Wax	I. Nezbeda
12:10 – 12:30		E. Sanz	S. Ravipati
13:00 – 14:00	Registration	Lunch	Lunch
		<i>Chaired by:</i> <i>I. Siepmann</i>	<i>Chaired by:</i> <i>A. Seitsonen</i>
14:30 – 15:10		E. SPOHR	N. QUIRKE
15:10 – 15:50		S. BONELLA	K. PROCHAZKA
15:50 – 16:20		Coffee Break	Coffee Break
		<i>Chaired by:</i> <i>J. Gross</i>	<i>Chaired by:</i> <i>D. Kofke</i>
16:20 – 17:00		D. KOFKE	J. GROSS
17:00 – 17:20		R. Davidchak	M. Horsh
17:20 – 17:40		A. Henrici	T. Zorawik
17:40 – 18:00		A. Huerta	B. Nowakowski
18:00 – 18:20	Opening address	Poster session	Closing remarks
	<i>Chaired by:</i> <i>A. Trokhymchuk</i>		Walking Tour
18:20	M. ZARICHNYI		
19:00	D. FRENKEL	Walking Tour	
20:00 – 22:00	Social Mixer	Szkocka Dinner	Workshop Dinner

