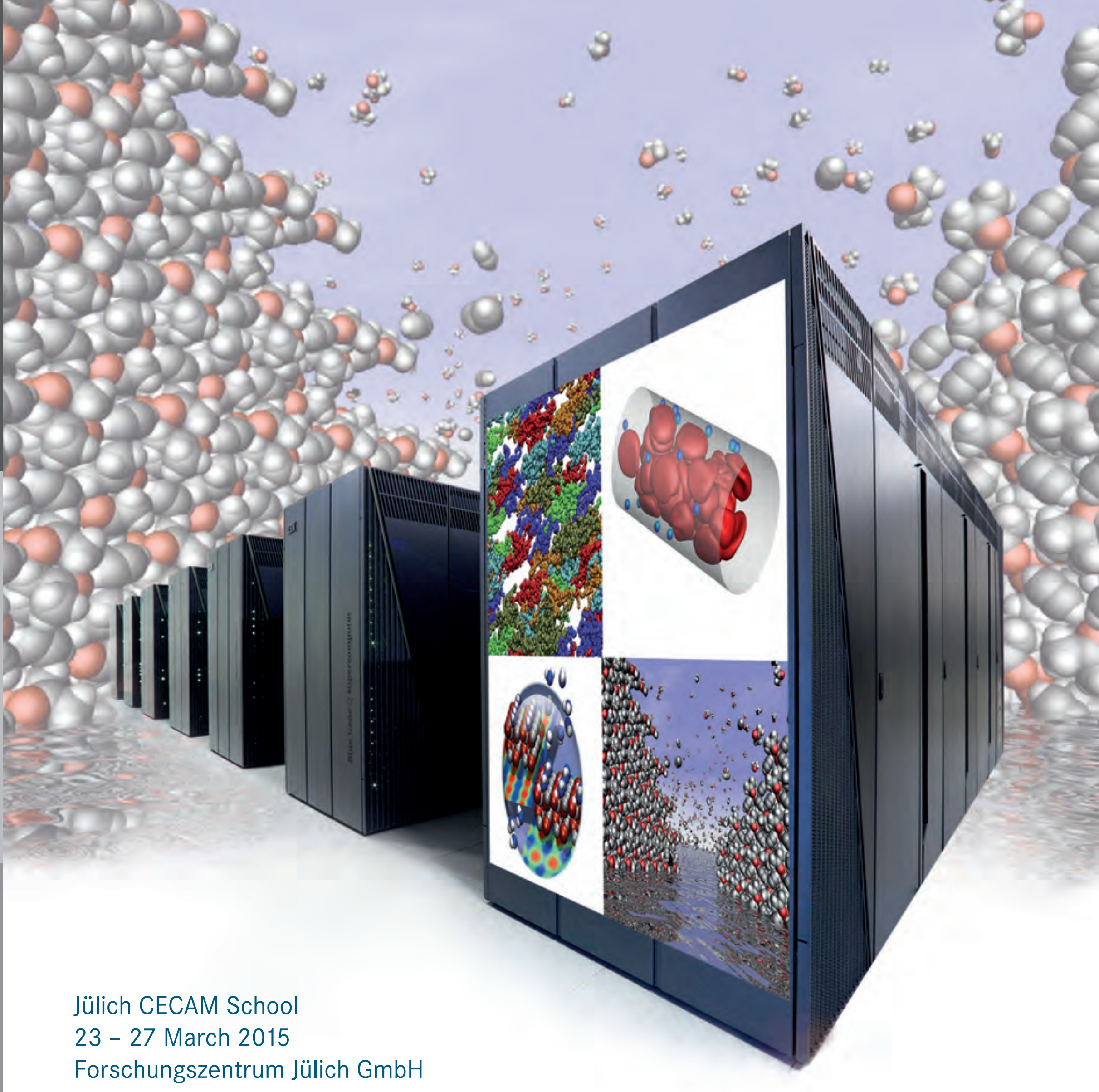

Jülich CECAM School
23 – 27 March 2015
Forschungszentrum Jülich GmbH

Computational Trends in Solvation and Transport in Liquids

Poster Presentations

Godehard Sutmann, Johannes Grotendorst, Gerhard Gompper, Dominik Marx

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Centre Européen de Calcul Atomique et Moléculaire

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Computational Trends in Solvation and Transport in Liquids

edited by
Godehard Sutmann
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Preface

The present Jülich CECAM School on Computational Science, which is co-supported by the Cluster of Excellence Ruhr Explores Solvation RESOLV, has a main focus on "Solvation Science", which is increasingly recognized as an interdisciplinary field akin to "Materials Science" or "Neuroscience". The School addresses a variety of different computational and simulation methods, appropriate for those hierarchies of time- and length-scales which are a challenge for modeling and simulation in Solvation Science. Therefore, the School is intended as a continuation of former Schools, organized in Jülich in 2009 and 2012, focusing on *Multiscale Simulation Methods in Molecular Sciences* and *Hierarchical Methods for Dynamics in Complex Molecular Systems*. The key of the present School is to introduce to a broad scientific audience modern computational methods which originate from a wide background but which can be applied to a variety of different scales, both in time and length, to describe solvation and transport phenomena on different levels of approximation. Problems associated with solvation and transport emerge in various distinct fields, ranging from fundamental questions in wet chemistry or soft matter physics to industrial applications in chemical engineering, which naturally induces a highly interdisciplinary character. Therefore, one aim of this School is to bring people together from diverse disciplines and various background in addition to triggering exchange of ideas between established experts and students - being the next generation of researchers.

More specifically, the Jülich CECAM School 2015 focuses on computational trends, multi-method approaches and modeling in the field of solvation and transport in liquids. It covers the field from large-scale coarse-grain modeling down to fully quantum-mechanical simulations of liquids at the level of electrons and nuclei. Not only bulk liquids and homogeneous solutions will be discussed, but also heterogeneous systems such as liquid/solid interfaces as well as solvated (bio)molecules. In particular, recent advances in adaptive resolution methods both in the realm of finite element modeling and of interfacing atomistic and coarse-grain descriptions of liquids are presented. Moreover, a variety of hybrid methods, such as QM/MM approaches for solvated biomolecules, continuum solvation and Lattice-Boltzmann techniques, will be part of the program. Coarse-graining in many distinct flavors is certainly an important approach to describe transport in liquids and solvation of increasingly complex systems. This includes methods such as Brownian dynamics for biomolecular recognition, mesoscale particle methods for hydrodynamics to model particle-fluid interactions or neural network potentials to describe water not just as an inert but as a potentially reactive solvent.

The recent revival of liquid-state integral equation methods in combination with molecular dynamics and electronic structure theory is acknowledged in the program as well as new developments in molecular density functional theory of aqueous solutions. Well-established techniques such as force field molecular dynamics for large-scale simulations and ab initio molecular dynamics for wet chemical reactions will be addressed as well in order to introduce the audience to these fields. Within molecular dynamics special attention will be given to methods that are tailored to unravel solvation effects. Presentation of most recent developments in path integral simulation techniques will complement the lectures to cover the smallest scales down to the nuclear level, which are relevant in the atomistic description of solvation.

The solution of large-scale complex problems needs a direct link to high performance computing, which today includes the use of GPUs in addition to massively parallel CPU based systems. Recent developments and trends will be addressed in the School not only by providing lectures but also by including a hands-on practical tutorial on elementary GPU programming.

The target group of this Jülich CECAM School on Computational Science are young scientists, especially PhD students and early postdocs.

Many individuals have significantly contributed to the success of the School and we are particularly grateful to all the lecturers who have prepared and contributed the lecture notes, which form the basis of the present book that will be made available at the School. Without their effort, compiling such an excellent reference book on *Computational Trends in Solvation and Transport in Liquids* would not have been possible.

We are greatly indebted to the School's secretaries Helga Offergeld and Britta Hoßfeld, who were indispensable for this School by taking care of logistics, transport, registration and catering. Very special thanks go to Monika Marx and Ilona Lütje, who realized technically the present Lecture Notes as well as the poster booklet by not only collecting but also carefully editing the written contributions. Last but not least, technical support during the lectures and hands-on sessions by Oliver Bücker and René Halver is greatfully acknowledged.

Jülich and Bochum
March 2015

Godehard Sutmann
Johannes Grotendorst
Gerhard Gompper
Dominik Marx

Jülich CECAM School 2015
Computational Trends in Solvation and Transport in Liquids

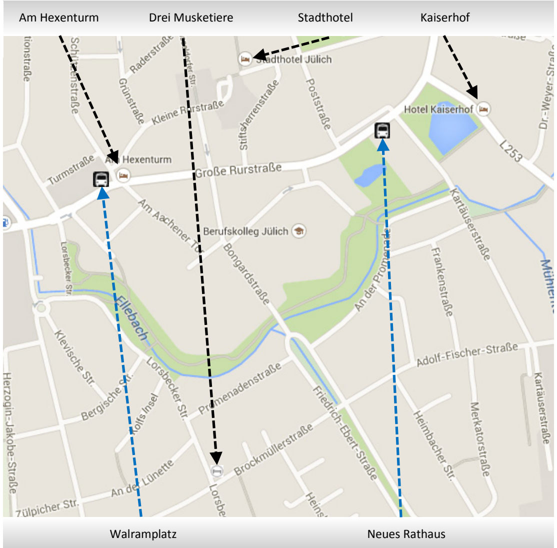
	Monday 23 March	Tuesday 24 March	Wednesday 25 March	Thursday 26 March	Friday 27 March
9:00-10:00	9:45-10:00 Opening	*Gerald Mathias* QM/MM-MD	*Christian Holm* Transport in Electrolyte Solutions	*Rodolphe Vuilleumier* Ab initio Molecular Dynamics Approach to Solvation and Chemical Reactions	*Dmitri Fedosov* Smooth Dissipative Particle Dynamics for Complex Flow
10:00-11:00	*Kurt Kremer* Adaptive Resolution MD	*Robert Franke* Continuum Solvation Modeling of Solute/Solvent Interactions	*Rebecca Wade* Brownian Dynamics for Biomolecular Recognition	*Daniel Potts* Advances in Parallel (N)FFT for Fast Molecular Simulations	*Matthias Heyden* Biomolecular Solvation
11:00-11:30	**Coffee Break**				
11:30-12:30	*Daniel Borgis* Classical Density Functional Theory for Complex Solutions	*Marisol Ripoll* Multi-Particle Collision Dynamics: Methods and Applications	*Andrij Kovalenko* RISM-3D Integral Equation Theory Combined with MD for Molecular Solvation	*Roland Netz* Simulation Techniques for Solvation-Induced Surface-Interactions at Prescribed Water Chemical Potential	*Michele Ceriotti* Path Integral MD for Quantum Solvents
12:30-14:00	**Lunch Break**				
14:00-15:00	*Dominik Horinek* Force Field Molecular Dynamics for Solvation	*Jens Harting* Lattice Boltzmann: Colloids at Interfaces	*Thorsten Hater / Peter Philippen* Introduction to GPU Programming	*Stefan Kast* Solvation from Liquid-State Integral Equation Theory	
15:00-16:00	*Wim Briels* Responsive Particle Dynamics	*Lars Schäfer* Coarse-Grain Water and Solutions: Hybrid AA/CG with MARTINI	Practical Session GPU	*Jörg Behler* High-Dimensional Neural Network Potentials as a Tool to Study Solvation	
16:00-16:30	**Coffee Break**				
16:30-17:30	*Maxim Fedorov* Advanced Atomistic Methods for Molecular Solvation	*Dirk Pleiter* Modern Trends in Hardware Developments Especially GPU	Practical Session GPU	*Christos Likos* Phenomenological Coarse-Grained Potentials for Soft Matter Systems	
Evening	**Reception and Get-Together**	**Poster-Session I**	**Poster-Session II**	**Excusion and Conference Dinner**	

Bus Schedule

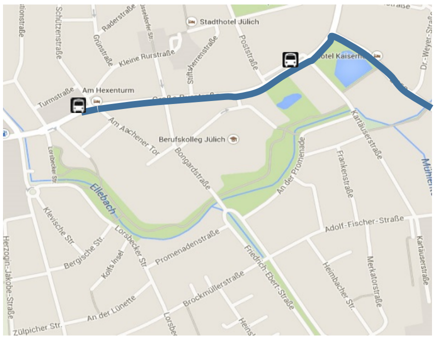
Bus is free of charge for participants.

Date	Departure Time	Meeting Point	Destination
23 March	8:15	Walramplatz	Research Centre Jülich
	8:20	Neues Rathaus	
	8:30	Gut Alte Burg	
	19:00	ForschungszentrumJülich	Hotels in Jülich, Gut Alte Burg
24 March	8:30	Walramplatz	Research Centre Jülich
	8:35	Neues Rathaus	
	8:45	Gut Alte Burg	
	19:00	Forschungszentrum Jülich	Hotels in Jülich, Gut Alte Burg
25 March	8:30	Walramplatz	Research Centre Jülich
	8:35	Neues Rathaus	
	8:45	Gut Alte Burg	
	19:00	Forschungszentrum Jülich	Hotels in Jülich, Gut Alte Burg
26 March	8:30	Walramplatz	Research Centre Jülich
	8:35	Neues Rathaus	
	8:45	Gut Alte Burg	
	17:45	Forschungszentrum Jülich	Conference Dinner, Indemann
	ca 22:00	Indemann	Gut Alte Burg, Hotels in Jülich
27 March	8:30	Walramplatz	Research Centre Jülich
	8:35	Neues Rathaus	
	8:45	Gut Alte Burg	
	13:30	Forschungszentrum Jülich	Düren Train Station

City



Bus Route



Contents

Poster Session A

Poster Session B

Computational Study of Copper (II) Binding to the Physiological Form of α-Synuclein.

Enrique Abad[1], **Francesco Musiani**[2], **Giulia Rossetti**[1,3], **and Paolo Carloni**[1]

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Intrinsically disorder proteins (IDPs) defy the classic structure-function paradigm. They are important for a wide variety of processes in eukaryotes, from signaling to protein biosynthesis. Some prevalent diseases, such as Alzheimer and Parkinson's disease are related to IDP malfunctioning; and others, such as Creutzfeldt-Jakob disease, involve proteins with unstructured regions. α-synuclein (AS) is an IDP expressed in the nervous system, that is thought to be a modulator of synaptic transmission, and it is the primary component of amyloid fibrils (Lewis bodies) found in patients with Parkinson's disease[1]. Recently it has been discovered that it is acetylated in vivo[2].

Copper ions have shown to be important aggregation modulators. Cu(II) binding to the acetylated physiological form of AS (AcAS) has been shown to be different from its non-acetylated counterpart[3,4]. In particular, experiments show that the highest affinity binding site of AcAS is at the ^{48}VVHGV^{52} sequence[3]; while it is on ^{1}MD^{2} in non-acetylated AS[4]. In the present study, we use computational methods to investigate Cu(II)-binding to AcAS, and its effect on structural determinants. Three possible Cu(II) binding geometries, suggested by experimental evidence[5,6] are being considered. Due to the lack of permanent secondary structure of IDPs, we are using computational techniques designed to accelerate the exploration of the conformational space such as replica exchange molecular dynamics in its most recent implementation (REST2)[7]. Force field parameters for the Cu(II) ion are being developed using the so-called Force Matching procedure.

The work is in collaboration with the group of Prof. Fernandez at the Max Planck Institute for Biophysical Chemistry (Göttingen, Germany) and Consejo Nacional de Investigaciones Científicas y Técnicas (Rosario, Argentina) and it is funded by the German DFG under the grant CA 973/14-1.

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Direct Path Integral Estimators for Isotope Fractionation Ratios

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Most notably for the lighter elements, the quantum nature of the nuclei gives rise to significant physical effects even at room temperature or above. One of the most evident signs of the quantum nature of light nuclei is the fractionation of two isotopes between two environments. The isotope fractionation ratio can be determined experimentally with exquisite precision, and is used routinely to gain insight into reactions and phase transformations in geochemistry, biology, astrophysics, and atmospheric sciences.

Molecular dynamics combined with a path integral formalism[1] provides an accurate but computationally demanding approach to fully account for the quantum nature of the nuclei. The conventional approach to compute the exact fractionation ratio in path integral molecular dynamics (PIMD) simulations involves performing a thermodynamic integration with respect to the isotope mass.[2] Here, we demonstrate that it is possible to evaluate the isotope fractionation ratios directly, without the need for a thermodynamic integration. The corresponding estimators are derived from the ratio of the partition functions of the isotope substituted systems, which is obtained by a virtual substitution of the isotopes of the tagged atom. Since it avoids the mass integration altogether it is more convenient, computationally advantageous, and immune to errors in the integral for the isotope mass.[3] Finally, we demonstrate the efficiency of these estimators by applying them to investigate the isotope fractionation ratios in the gas-phase Zundel cation, and in a few simple hydrocarbons.

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Understanding the THz Spectra of Biomolecular Building Blocks in Aqueous Solutions

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The question of how a solute is affected during solvation is the question of how the dynamics of the solute and the dynamics of the solvent change upon solvation. From the experimental point of view THz spectroscopy has proven to be very sensitive in measuring these changes, thus allowing the study of those the solvent effects.

But in order to fully understand an experimental THz spectrum, the assignment of the spectroscopic bands is needed, which must be provided on a theoretical basis[1–3].

We computed the THz spectra of glycine[4] and valine solvated in water based on dipole auto-correlation function data obtained from ab inito molecular dynamics simulations.

The bands in the spectra were then assigned based on an extended version of a mode-specific decomposition method[5,6] allowing us to classify the modes into three categories. In particular, we obtained intramolecular modes of the glycine[7] and valine molecule itself, librational and rattling motion of glycine and valine in the presence of water, and intermolecular coupling modes of the glycine and valine molecule with water.

The rattling/librational modes show that the solute molecule moves within the water environment and the intramolecular modes of the solute are very well decoupled from the water motion. The information of the interaction of the solute with the solvent is carried in the intermolecular modes that reveal the coupled movement of the solute and the solvent molecules.

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Fast and Accurate Calculation of Solvation Free Energies in Supercritical Fluids Using Fully Atomistic Simulations: Probing the Theory of Solutions in Energy Representation

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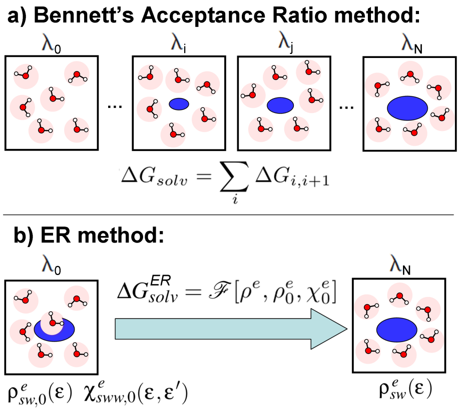
Conventional way to calculate SFEs requires performing a series of independent molecular simulations (usually 10 - 20) where a solute molecule is continuously coupled to the solvent - the so-called free energy perturbation calculations (see Figure 1a). These methods require large computational resources which limits its applicability for fast exploration of the phase diagram for supercritical fluids. Recently, we found that the theory of solutions in energy representation (ER method)[1] works surprisingly well for SFE calculations of organic molecules in sc-CO2 with addition of cosolvents: the theoretical error of the ER predictions is 0.1 kcal/mol[2]. ER method allows avoiding the artificial alchemical perturbation path in free energy calculations and thus reduces the computational consumption by 10 - 20 times (see Figure 1b). Therefore, ER method can be used instead of the computationally demanding free energy perturbation calculations for supercritical solvents.



a) Schematic illustration of the free energy perturbation path of the gradual growth of the solute molecule in the solvent controlled by the λ coupling parameter. The free energy difference between the neighboring stages can be estimated by the Bennett Acceptance Ratio (BAR) method.
b) Schematic illustration of the idea behind the ER method. The free energy difference between the final and initial stages is approximated by a functional of distribution functions in energy representation.

ER method can be seen as a bridge between molecular simulations and the classical DFT for liquids. In ER method, a new collective coordinate is introduced - the interaction energy of a solute and a solvent molecule (see Ref.[3] for derivation details). The distribution functions over this coordinate are calculated from molecular dynamics (MD) simulations

both at full and zero solute-solvent coupling. Additionally, at zero coupling the density-density correlation matrix is calculated. Secondly, these functions enter an approximate free energy functional in energy representation, which is obtained by the Percus's method of functional expansion (see Figure 1b).
In this poster we discuss how molecular simulations can help in prediction of cosolvent effect on solubilities of organic compounds in supercritical carbon dioxide[4] and show that ER method allows to dramatically speed up the calculations without loosing accuracy.

The work is supported by the Russian Foundation for Basic Research (Grant No. 12-03-31354) and the REA-Research Executive Agency, Grant No. 247500 "BioSol", Programme FP7-PEOPLE-2009-IRSES.

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A New Force Field Parametrization of Trimethylamine-N-Oxide for Simulations at High Pressure

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Osmolytes are a class of molecules that, in addition to adjusting the osmotic pressure in cells, also influence the stability of proteins[1]. As an example of a protecting osmolyte, trimethylamine-N-oxide (TMAO) has been shown to stabilize proteins against chemical, thermal, and pressure denaturation[1,2].

For quite some time it has been of interest to create a classical model of TMAO in order to be able to investigate these effects using force field molecular dynamics: After the first flexible model was developed by Kast et al. using *ab initio* calculations and experimental data[3], it was modified by scaling the contact distance of carbon and the partial charges of oxygen and nitrogen[4]. This model by Schneck et al. was optimized with respect to activity coefficients in aqueous solutions and the transfer free energy of a polyglycine model peptide. However, none of the existing models give a good description of the density of aqueous solutions, a quantity that is very important when investigating the effects of pressure on these systems.

We present a new set of force field parameters for TMAO that reproduces the experimental densities of aqueous solutions (using the TIP4P/2005 water model[5]) up to 700 bar, activity coefficients at normal pressure, and surface tension changes at the liquid-vapor interface. Furthermore the new model was applied to determine the free energies of transfer of a periodic polyglycine into TMAO solutions.

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On the Role of Interfacial Hydrogen Bonds in “On-Water” Catalysis

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It has been demonstrated that many classes of organic reactions exhibit increased reaction rates when performed in heterogeneous water emulsions[1]. This so-called “on-water” catalytic effect offers a highly promising perspective to improve reactions in organic chemistry. This is partly due to the widespread use of the catalyzed cycloaddition reaction in organic synthesis and partly due to the availability and environmental friendliness of the catalyst. Despite enormous practical importance of the observed “on-water” catalytic effect and numerous mechanistic studies[2,3] its microscopic origins remain unclear.

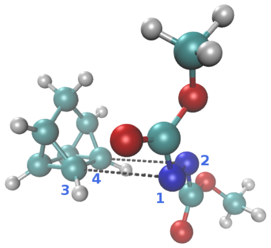

Figure 1. Schematic of the Diels-Alder reaction between Q (left) and DMAD (right). C, N, O and H atoms are represented with green, blue, red and white spheres, respectively.

In this work[4], we applied a second generation Car-Parrinello molecular dynamics algorithm[5] adapted for use with self-consistent density functional tight-binding[6] to perform a fully quantum mechanical calculation of the free energy barriers for Diels-Alder reaction between dimethyl-azodicarboxylate and quadricyclane – see Fig. 1 for a representation. Although experimentally measured reaction rate is $\sim$24 times higher under the heterogeneous conditions than in the homogeneous aqueous environment[1] our simulations predict the opposite trend: the calculated free energy activation barrier at the water-vacuum or water-organic interface is $\sim$10 kJ/mol higher than that in bulk water. Our results imply that the stabilization of the transition state by dangling hydrogen bonds exposed at aqueous interfaces plays a significantly lesser role in “on-water” catalysis than has been suggested before.

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First Principles Studies of Noncovalent Functionalization of Single-Walled Carbon Nanotubes with Small Polyethylene Glycol Molecules

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Due to their unique structure and length-to-diameter ratio, carbon nanotubes (CNTs) are among the most frequently examined novel materials. There is an increasing interest for CNTs applications ranging from (bio)sensors, field-emission transistors, nanofluids to drug-delivery systems[1–3]. CNTs bioconjugates have been reported also to be a promising nanomaterials for biomedical applications, such as the novel multifunctional nanodrugs, cancer treating or as substrates for the growth of cells for tissue regeneration[4]. Owing the structure of CNTs and the π–π stacking interactions between them, the pristine CNTs are very hydrophobic and have the tendency to form aggregates. To conquer this problem the covalent or noncovalent functionalization should be applied.

The functionalized CNTs with water solubility and biocompatibility are able to enter cells, delivering biologically active molecules, including drugs, genes, DNA, and proteins[5]. Polyethylene glycol (PEG) is a hydrophilic polymer with 4 to 120 subunits. It is often used as conjugated to drugs or drug carriers to increase their solubility and circulating lifetime, reducing their toxicity[5]. Also, PEG chains are able to wrap antimicrobial peptides, decreasing their interactions with the lipid bilayers[6]. PEG was used to functionalize CNTs either covalently or noncovalently, significantly increasing the solubility of CNTs[6]. PEG-modified carbon nanotubes have been used as a delivery system for anticancer and antifungal drugs, and for macromolecules such as peptides, proteins or DNA[5].

In the present work we use the DFT static calculations to obtain the noncovalent functionalization of single-walled CNT (SWCNT) (10,0) by the small PEG molecules with the 2-5 subunits. We focus on the description of the interactions between PEG and SWCNT with the help of the electron density analysis. Taking into account the existence of H-bonds in PEG molecule and the possibility to interact PEG with CNT via C-H$\cdots\pi$ H-bonds, we analyze structural and topological parameters of these H-bonds. Additionally, we estimate the influence of SWCNT on the stability of H-bonds in PEG.

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Molecular Density Functional Theory for Water with Liquid-Gas Coexistence and Correct Pressure

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When one solvates a hydrophobic solute in water, liquid and gas phase of water are close to coexistence. Nevertheless, in the common hypernetted chain approximation to integral equations, or equivalently in the homogenous reference fluid approximation of molecular density functional theory, coexistence is not taken into account. Hydration structures and solvation free energies of such hydrophobes are thus incorrect, especially in case of macroscopic solutes.

First, we develop a free energy functional for the special case of water[1–3] and its most popular models that wear 1 Lennard-Jones site and various partial point charges. In these cases, we show that the HNC (or equivalently HRF) free energy functional of the six-dimensional position and orientation solvent density can be rewritten as a simpler functional of the solvent density and a multipolar polarization density. This last quantity accounts for the full charge distribution of the water molecule. This functional for water requires as input simpler physical quantities than the full position and orientation-dependent direct correlation function: the structure factor and transverse and longitudinal multipolar dielectric susceptibilities of bulk water, extracted from experimental data or simulations.

Nevertheless, this functional still shows the thermodynamic inconsistency of HNC functionals. We overcome this by introducing a metastable gas phase for the homogeneous solvent[4] through a third order expansion of the functional around the bulk density that imposes the correct pressure of the bulk fluid. Although this theory is not limited to water, we apply it to study hydrophobic solvation in water at room temperature and pressure and compare the results to all-atom simulations. With this correction, molecular density functional theory gives, at a modest computational cost, quantitative hydration free energies and structures of small molecular solutes like n-alkanes to ones of few nanometers. The macroscopic liquid-gas surface tension predicted by the theory is comparable to experiments. This theory gives an alternative to the empirical hard sphere bridge correction used so far by several authors[5,6].

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Influence of Surface Polarity on Structure and Mobility of Binary Solvents Studied by Molecular Dynamics Simulations

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The structure, dynamics, and mobility of binary solvents at adsorbent surfaces play an important role in many processes, including adsorption and separations[1]. The information gained from experimental data is limited, because it cannot provide a microscopic view of the system. Therefore, molecular dynamics simulations offer the possibility to arrive at a better understanding of the structure and mobility of solvent mixtures at the molecular level.

In previous work, we investigated the influence of a bare silica surface on distribution and mobility of binary water-acetonitrile mixtures for a model system that mimics the conditions in hydrophilic interaction liquid chromatography (HILIC)[2]. The main focus was on the local density distribution, diffusion, residence time and hydrogen bonding system of the solvent molecules at the polar silica surface. It was shown that water forms a rigid solvent layer on the surface of the polar stationary phase. Due to hydrogen bonding, the molecules in the surface water layer show a restricted diffusion.

Here, we extend this work to study the hydrogen bonding structure and diffusive mobility of water-acetonitrile mixtures at polar and nonpolar surfaces. Additionally to the polar silica surface, a non-polar C_{18} modified silica support is investigated. This system mimics the conditions in reversed-phase liquid chromatography (RPLC). Furthermore, the behavior of solutes is shown in regard to their distribution and dynamic properties in the interface region between surface and bulk fluid region. We demonstrate that the characteristics of the solvents and solutes in the interface region differ significantly from those in the bulk region.The influence of the stationary phase on structure and mobility of solvent and analyte molecules should lead to a better understanding of the retention process in chromatography.

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Towards a Composite Benchmark Method for the Aqueous Solvation Free Energies of Organic Compounds

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Water is ubiquitous in the biosphere, and the difficulty of rigorously treating the effects of aqueous solvation currently limits the widespread use of computational methods in many areas of environmental chemistry. We propose an approach to benchmark calculations of aqueous free energies of solvation based on molecular dynamics simulation which is statistical mechanically complete and systematically improvable. The approach partitions the solvation free energy into the free energies of solvent density change, solvent cavity organization, and solvent-solute interaction, each of which is computed from first principles. A composite approach is considered for the calculation of the contributions of quantum nuclear effects to solvation free energies and the contributions of electron correlation and relativistic effects to solvent-solute interactions. Testing of the method is underway for a small set of organic compounds with Henry's law constants that are well established by experiment. However, as the proposed method contains no empirical parameters, it should perform equally well for systems where no experimental data is available.

Dielectric Response of the Water Hydration Layer and its Application on the Solvation Energy

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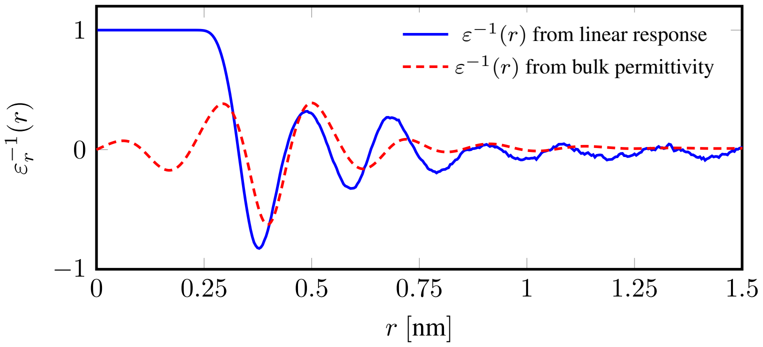
The electric field caused by a charged solute molecule introduced into a dipolar liquid solvent leads to a reorientation of the solvent molecules which is quantified by the solvent's local dielectric constant.

We calculate this dielectric response function using two different methods; linear response for a system with the explicit solute and theoretical calculations using the wave-vector dependent, non-local bulk permittivity[1,2]. The good agreement leads to our central result: while the water dielectric constant for a radial field in the hydration layer of spherical solutes *is* strongly different from bulk water, this difference is *not* due to significant restructuring of the hydrogen bond network, but can be traced back almost entirely to bulk properties of pure water.

Finally, integrating our dielectric profiles, we calculate the solvation energies for Na^+, Cl^-, I^-, and Cs^+ and find quantitative agreement with experimental data.



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Ab initio Molecular Dynamics Simulations on Wet Alumina/Isopropanol Solid/Liquid Interfaces

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The solid/liquid interface of wet and hydroxylated α-alumina/isopropanol is studied using ab-initio Car-Parrinello molecular dynamics (CPMD) simulations.

The proper description of liquid isopropanol by our PBE+D2 setup was benchmarked by comparing molecular interaction energies with basis set extrapolated coupled-cluster CCSD(T) results. Furthermore, pair correlation functions and diffusion coefficients from CPMD simulations at different temperatures were compared to experiment. The liquid isopropanol was pre-equilibrated by MD runs with a classical force field.

For the alumina slab three different surface models were taken into account: a termination with a full hydroxyl layer (**hyd**), an aluminum termination with dissociated water molecules to saturate undercoordinated surface sites (**w1**) and a third model with adsorbed water molecules between the OH groups of the **w1** structure (**w2**). In the CPMD simulations of the combined system of solid and liquid phase the recombination of dissociated water molecules is observed, especially in the case of **w2**. The mechanism and rate of these proton transfer processes is analyzed and we will discuss the influence of the surface model on the structure of the isopropanol liquid.

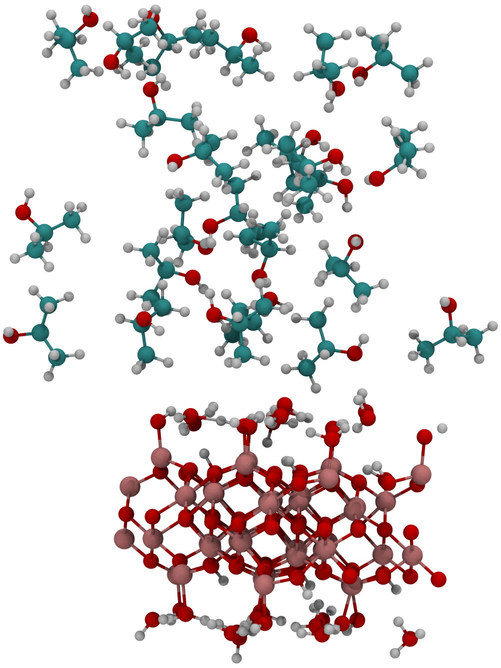

Figure 1. Slab w2 with 24 isopropanol molecules after short equillibration

Pressure Correction of Solvation Free Energy - Calculations with Classical DFT

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Solvation Free energy is a very important quantity which allows ones to compute many useful properties of substances in solution.
Unfortunately, the solvation free energy calculations are computationally expensive.
That's why there exist alternative, faster but sometimes less accurate methods, like Poisson Boltzmann calculations or Matubayasy technique.
From these methods the Classical Density Functional Theory (DFT) and connected with it integral equation theory of liquids are one of the most promising techniques for energy calculations.
However, the accurate solvation free energy calculation in the Classical DFT approach appeared to be a challenging task.
Although the methods based on the simplest Hyper Netted Chain (HNC) approximation can give a qualitatively correct estimation of the solvent structure around the solute the calculated values of the solvation free energies are unrealistic and far from experimental ones.
It was noticed, that the error in the solvation free energy calculations is proportional to the partial molar volume of the solute.[1]
There were proposed the empirical correction models for the RISM and 3DRISM, which used this observation and were able to predict the solvation free energies of simple solute with accuracy of 1 kcal/mol.[2]
In our recent paper we were able to show that these empirical corrections can be explained by the difference in pressure in HNC approximation and in experiments.[3]
Although the explanation given in the paper is not perfect, we will show below that the final formula for the solvation free energy calculation is still correct. This is explained by the fact that pressure in the HNC model is extremely (>10 KBar), which make it possible to neglect the atmospheric pressure contribution.
In this way we derived the expression which was free of empirical fitting coefficients and was able to predict the solvation free energies with accuracy of 1.5-2 kcal/mol.
Another approach to the solvation free energy calculations is to improve the HNC model itself. The aim of improvements is to include the three and many body interactions to the model. Some of the models include the empirical three-body terms for improvement the water structure, another use the three and many-body interactions from the simplified models.
The models which use the experimental c-functions, and include the many-body interactions from the Fundamental Messure Theory (FMT) are called FMSA or the models with the Hard Sphere bridge.

It was shown, that using these models it is possible to predict accurately the solvation energies of alknes [Maximillien], and also more complex solutes [Wu]. The accuracy in some cases was better than the accuracy of the HNC calculations with the Partial Molar Volume correction.
One of the disadvantages of these models is the fact that they still contain the empirical parameter: diameter of the hard sphere.
The result of the calculations are very sensitive to it, and the optimal choice of the proper diameter is a challenging task.
And of course, the predictability of the model with fitting parameters is always a question, because one cannot fully trust the model which one does not fully understand.
In our work we demonstrate that the sensitivity of the model to the hard sphere radius is due to the difference in pressure in the model and in experiments.
We give the unambiguous algorithm for the choosing the hard sphere diameter which results in the correct pressure in the model, and thus get rid of the empirical parameter.
We show the results of calculations with the optimal hard sphere radius and compare them to the HNC and experimental results.

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Predicting Aqueous Speciation of Environmentally Relevant Halogen Oxidants: Chloramines, Bromamines, and Bromochloramines

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Chloramines, bromamines, and bromochloramines are halogen-containing oxidants that arise from the reaction between ammonia and hypohalous acids during the disinfection of drinking and wastewaters. Although involved in the formation of toxic disinfection byproducts, these molecules are difficult to study by experimental means, and their speciation remains poorly defined. To bridge this gap, we successfully designed a benchmark level computational method, called TA14,[1] adapted from the Weizmann theory and the Feller-Peterson-Dixon procedures, to establish the thermodynamics of these species in gas phase. Our composite method combines a systematic sequence of wavefunction theory calculations (up to CCSDTQ), relativistic effects, diagonal Born-Oppenheimer corrections, and anharmonic vibrational modes.

To evaluate the effects of aqueous solvation on halamine formation and decomposition, free energies of solvation were modeled with the SMD[2] implicit solvation model together with the cluster-continuum approach developed by Bryantsev in 2008.[3] These gas phase and solution phase thermodynamic data are used to predict aqueous equilibrium constants describing the formation reactions of chloramines, bromamines, and bromochloramines. Based on the comparisons with available experimental data, we propose uncertainties ranging from 1 to 2 logarithm units for computed aqueous equilibrium constants. These newly reported estimates of reaction thermodynamics will enable us to place constraints on the formation rate constants of these reactive halogenated species, leading to more accurate predictions of speciation of halamines during water treatment.

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Characterization of Structural and Electronic Properties of 2'-Palmitoyluridine (2UP) and 3'- Palmitoyluridine (3UP) in Vacuum and in Solvents

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A new class of molecules was developed, the lipophilic nucleosides[1]. They are capable of anchor/form membranes and also capture nucleic acids/pieces of DNA. These characteristics allow them to be used to design new drug-delivery mechanisms or biological sensors. It was observed that they can anchor in lipid membranes and not cause any significant alteration in the system and are still capable of attracting DNA or RNA fragments from the solution. 2'-palmitoyluridine (2UP) and 3'-palmitoyluridine (3UP)[2] belong to this new category of molecules. So far, only experimental studies were done with 2UP and 3UP. Here, Quantum Mechanics was used to analyze electronic and structural properties of 2UP and 3UP in comparison with Uracil and Uridine in vaccum, showing that they are very similar. 2UP and 3UP were also analyzed considering two solvents, water and chloroform, as PCM using Quantum Mechanics, and the same solvents as explicit molecules, using Molecular Dynamics. Also using Molecular Dynamics, it was observed that 2UP and 3UP present different geometries in vacuum and in chloroform, the bending of the two molecules is very similar in vacuum and in water, but in chloroform, 2UP is more stretched than 3UP during the dynamics. With chloroform as explicit solvent, the UV-Vis spectrum was calculated and is in excellent agreement with experimental results, validating the geometry parametrization for 2UP and 3UP in the Gromos53a6 force field[3].

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Diffusion in Crowded Cytoplasm-Like Environments

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We report results from an ongoing study using Brownian dynamics to simualte diffusion of macromolecules in crowded cytoplasm-like environments. The study is focused on the dependence of the diffusion and the crossover to the anomalous subdiffusion on the composition of the environment in terms of volume fraction and relative concentration of the different macromolecule types. In accordance with previous theoretical and experimental studies, diffusion slows down with increasing volume fraction. Contrary to expectations, there is also a strong dependence of diffusion on molecular composition. The crossover time to the anomalous subdiffusion regime decreases and the diffusion slows down when the smaller macromolecules start to dominate. Interestingly, the diffusion is faster in a cytoplasm-like (more polydisperse) system, than in a two component system, at comparable packing fractions or even when the cytoplasm packing fraction is larger.

The Behaviour of the Von Willebrand Factor in Blood Flow

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The von Willebrand factor (vWF), a large multimeric protein, is essential in haemostasis. Under normal conditions, vWF is present in blood as a globular polymer. However, in case of an injury, vWF is able to unwrap and bind to the vessel wall and to flowing platelets. Thus, platelets are significantly slowed down and can adhere to the wall and close the lesion[1]. Nevertheless, it is still not clear how the unwrapping of the vWF is triggered. To better understand these complex processes, we employ a particle-based hydrodynamic simulation method to study the behaviour of vWF in blood flow. The vWF is modelled as a chain of beads (monomers) connected by springs. In addition, the monomers are subject to attractive interactions in order to represent characteristic properties of the vWF[2]. The behaviour of vWF is investigated under different conditions including a freely-suspended polymer in shear flow and a polymer attached to a wall. We also examine the migration of vWF to a wall (margination) depending on shear rate and volume fraction of red blood cells (RBCs) and compare it to recent results of platelet margination[3]. Furthermore, the stretching of the vWF in flow direction depending on its radial position in a capillary is monitored. Our results show that attractive interactions between monomer beads increase margination efficiency and significantly affect the extension of vWF at different radial positions in blood vessels.

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Tumbling Dynamics of Sheets in Shear Flow

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The behavior of soft matter systems in shear flow is distinctively different from their equilibrium behavior. For example, a broad class of soft matter systems such as polymers, membranes, cells, vesicles etc. are deformed and show a preferred alignment in the flow, resulting in a shear rate dependent viscosity. They also undergo a tumbling motion in the flow, with a power-law dependence of the tumbling frequency and relaxation times on the shear rate.

Motivated by experimental studies on graphene sheets in shear flow, we study, using mesoscopic hydrodynamic simulations, the behavior of a two-dimensional sheet in shear flow. We find, in agreement with experiments, a preferred alignment of the sheet in the flow. The alignment angle decays as a power-law for small shear rates, and in contrast to, e.g., rods, it saturates for high shear rates. We also find that the tumbling frequency, relaxation times, viscosity etc. show a power-law dependence on the shear rate, with exponents being different from those of theoretically solvable systems such as rod-like or flexible polymers in shear flow.

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Fast Approximation of the Multipolar Real Space Ewald Sum

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There is currently ongoing efforts to achieve higher accuracy in molecular simulations by implementing advanced potential energy surfaces through the addition of higher order multipoles to fixed point charge electrostatics. Naturally, a lot of the work has focused on development for the Particle Mesh Ewald (PME) method[1–3].
The Ewald sum[6] has two main components, a real space and a reciprocal space. For charge-charge electrostatics, PME[4] is very efficient because the bulk of the computational work is moved to the reciprocal space and efficiently evaluated using FFT and the real space scales as $O(N)$. However, for higher order multipolar interactions the real space sum is still a significant bottleneck. As an example, on a single core, for 96000 atoms with multipolar interactions up to quadrupoles, the cost of the real space is about four times that of the reciprocal space.
Our present work is aimed at addressing this bottleneck. We are investigating a Barnes-Hut treecode algorithm[5] approach to reduce the cost of the real space. The goal is to be able to tune the algorithm to achieve an acceptable accuracy at lower cost. The poster will present results on our progress.

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Simulation of Diffusional Association 7 (SDA 7): Brownian Dynamics Simulations of Biomacromolecular Association

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Accurate modelling of the ways in which biomacromolecules associate in solution is important for the understanding of cellular processes. Simulating the dynamics of these large molecules in solution with an explicit solvent representation is a highly complex problem. One route to reduce the dimensionality of this problem is through the use of a continuum solvent (CS) description, in which the solvent is represented as a polarisable dielectric medium. Brownian dynamics (BD) simulations provide a way in which the diffusive motion of molecules can be represented within such a scheme. The simulated trajectories are propagated by a combination of systematic forces due to specific interactions between solute pairs, and random forces that mimic the molecular buffeting caused by solvent molecules.

The Simulation of Diffusional Association (SDA) BD software package was initially developed to allow bimolecular association rate constants of macromolecules to be calculated.[1] It has also been applied to the study of electron transfer rates[2] and protein–protein docking.[3] More recently, it has been modified to permit simulations of many solutes in a periodic volume.[4]

In this work we discuss the most recent version of SDA, SDA 7, and its associated webserver, webSDA.[5] SDA 7 has been developed using a new parallelisation scheme to exploit modern computer architectures. We describe the processor scaling obtained with this scheme during simulations of a number of test cases. We also outline future developments of the software.

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Parallel Algorithm for the Lowe Andersen Thermostat

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Molecular dynamics (MD) simulations in the canonical ensemble require a reliable method to control temperature under the condition to conserve mechanical properties and statistical distributions[1] The control usually mimics an energy exchange with a given thermostat in order to mimic the canonical ensemble. A variety of methods were developed for the MD based on different princples, i.e. deterministic methods (velocity scaling[2], Berendsen[3], Nosé-Hoover[4], Nosé-Hoover chains[5]) or stochastic methods (Andersen[6], Langevin[7], Bussi velocity rescaling[8], Dissipative Particle Dynamics – DPD[9] and Lowe Andersen – LA[10]). Only two of these thermostats conserve linear and angular momentum, i.e. DPD and LA since by construction forces and velocities are modified in a symmetric manner for pairs of particles along the inter-particle connecting line. Both thermostats operate on the local environment and can be considered efficient. The two methods are equivalent for very short time steps, but for large time steps the LA thermostat provides a more reliable description of the system dynamics compared with the DPD thermostat[11].

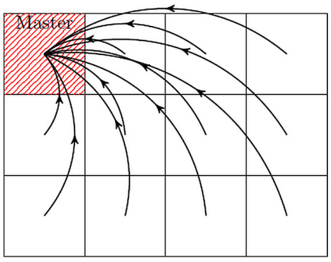

Figure 1. The naive slave - master communication scheme for the Lowe Anderson thermostat.

Due to the need for simulations of large particle systems and long time trajectories, efficient and scalable parallel algorithms are highly needed. In contrast to an LA thermostat, a DPD version of a thermostat is straight forward to be parallelized by domain decomposition as the forces that act on the particles are additive and can be calculated separately on the different processors based on the particle velocities of the local particles and those located on the neighbour boundaries of the domains of the neighbour processors. Up to now, a reliable parallel implementation for LA is unavailable, due to a missing proper schedule of thermostat particle updates, which have to be carefully designed. The LA thermostat is difficult to be parallelized as the velocity of a given particle is updated based on the relative velocity of the particle and the neighbour particles within an LA cut-off distance. Therefore, the particle velocities must be treated in a prescribed sequence, in order to avoid a simultaneous update of he velocity of a given particle neighboured processors. The simplest, but not the most efficient method is to send the velocities of the particles from the entire system to a master processor that can correct the velocities of all the particles and sends the updated velocities to the home processors. In the present contribution we present a new version of a parallel implementation which completely avoids the master-slave concept and fully relies on a domain decomposition approach, i.e. avoiding excessive memory allocation on the nodes. An implementation is suggested which minimizes data communication by respecting the correctness of the LA thermostat, therefore conserving linear and angular momentum and correctly reproducing distribution functions of particle velocites.

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Modeling of Cells, Blood Flow and Nanocarriers

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This abstract is an overview of two major projects I was involved with, during the last year. The first project combines work from various people within our lab, where the second project is part of the research I did to complete my Master's thesis.

SEM ++ is a particle method to model biological systems. Here, we model a cell by assuming that it is composed of a collection of smaller particles, the sub-cellular elements (SCEs). To model the mechanical properties of a cell, the particles interact with each other through a parameterized force field. This field includes potential forces for the interactions between two particles, which can be repulsive or attractive depending on the distance between them. In addition, the particles are subject to forces due random kicks from thermal fluctuations and viscous forces. SEM++ has been extended to include hydrodynamic interactions between the particles. In order to find a model that best fits the experimental data, an approximate Bayesian computation will be employed to calculate the SEM++ parameters. The two models, with and without hydrodynamic interactions, will then be compared to find the most plausible viscoelastic physical model for cell stretching.

The second project deals with the modeling of blood flow and nanoparticle transport in solid tumors. This work was done in the Cancer Biophysics Lab at the University of Cyprus. Conventional drug delivery systems for solid tumors are composed of a nanocarrier that releases its therapeutic load. These two-stage nanoparticles utilize the enhanced permeability and retention (EPR) effect to enable preferential delivery to tumor tissue. We employed a mathematical model to study the effect of particle size, drug release rate and binding affinity on the distribution and efficacy of nanoparticles to derive optimal design rules. Furthermore, we introduced a new multi-stage delivery system. The system consists of a 20-nm primary nanoparticle, which releases 5-nm secondary particles, which in turn release the chemotherapeutic drug. We found that tuning the drug release kinetics and binding affinities leads to improved delivery of the drug. Our results also indicate that multi-stage nanoparticles are superior over two-stage nano-carriers provided they have a faster drug release rate and for high binding affinity drugs. Furthermore, our results suggest that smaller nanoparticles achieve better treatment outcome.

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Block Preconditioners in Fluid Flow Simulation

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Fluid flow simulation is the basic tool to gain insight to the possible behavior of many natural processes which directly impact on human life. Among the mathematical equations in fluid modeling, possibly the most studied ones are the Navier-Stokes equations since they describe the motion for a fluid with constant density, which is the case for a large class of situations.

We want to solve the steady incompressible Navier Stokes system posed in the two dimensional unit square $\Omega = [0,1]^2$. In dimensionless form they read as follows:

$$-\frac{1}{Re}\Delta\vec{u} + \vec{u}\cdot\nabla\vec{u} + \nabla p = \vec{f} \quad \text{in } \Omega \tag{1a}$$

$$\nabla\cdot\vec{u} = 0 \quad \text{in } \Omega, \tag{1b}$$

where $\vec{u}$ and p denote the velocity and the pressure of the fluid, and Re is the Reynolds number. To gain insight on the necessary techniques to achieve this goal we start with the limiting case $Re \ll 1$ and consider the Stokes system:

$$\Delta\vec{u} + \nabla p = \vec{f} \quad \text{in } \Omega \tag{2a}$$

$$\nabla\cdot\vec{u} = 0 \quad \text{in } \Omega. \tag{2b}$$

Discretization of (2) via stable Mixed Finite Elements (MFE) lead to solve a saddle point problem with the following block matrix structure:

$$\begin{bmatrix} \mathbf{F} & \mathbf{B}^\top \\ \mathbf{B} & \mathbf{0} \end{bmatrix}. \tag{3}$$

In the case of (1) a MFE discretization produces a non linear system of equations, which we solve using a so called Newton-Krylov method. The linearized problem at each step has the same structure as (3). For preconditioning we rely on the factorization:

$$\begin{bmatrix} \mathbf{F} & \mathbf{B}^\top \\ \mathbf{B} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{B}\mathbf{F}^{-1} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{F} & \mathbf{0} \\ \mathbf{0} & -\mathbf{B}\mathbf{F}^{-1}\mathbf{B}^\top \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{F}^{-1}\mathbf{B}^\top \\ \mathbf{0} & \mathbf{I} \end{bmatrix}. \tag{4}$$

In either case, the operator on the block (1,1) is treated with the Algebraic Multigrid Method (AMG)[2]. The Schur complement in the (2,2) block is replaced by the pressure mass matrix in the Stokes case and for the Navier-Stokes system it is treated with the least squares commutator preconditioner (BFBt)[1]. In order to test our solver we work out (1) and (2) with proper boundary conditions and forcing term based on analytical solutions.

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Prediction of Optimal Drug/Polymer Matches in Block-Copolymer Nanoparticle Formulations for Drug-Delivery Applications: Parameterization of Coarse-Grained Models

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Micelles formed by block copolymers are widely investigated as drug carriers. Drug encapsulation into copolymer micelles increases drug circulation in the blood stream and thus enhances drug accumulation in the tumor or inflammation areas due to the so-called enhanced permeability and retention (EPR) effect[1]. Until now all the available nanoparticle-drug formulations were developed by an experimental trial and error approach because so far no methodology exists which is able to predict optimal co-polymer compositions for a given drug in nanoparticle formulations.

Our goal is to develop such a methodology based on molecular simulations. Due to the size of the systems under consideration the fully-atomistic description of the molecules is computationally not feasible. Therefore we decided to use so-called coarse-grained (CG) models, where several atoms are represented by one interaction site – "bead"[2]. Coarse-graining not only reduces the number of interaction sites but also allows using larger molecular dynamics simulation time steps compared to a fully atomistic description. As a result coarse-grain modeling leads to a reduction of computational consumptions by 2 - 5 orders of magnitude, however it requires careful parameterization to be able to reproduce target properties of the system.

In this poster presentation we review our approach for coarse-grain model parameterization. We aim at predicting the drug loading into co-polymer nanoparticles. Thus, in this project it is crucial to design a coarse-grain model which can accurately reproduce free energy changes associated with the drug partitioning between hydrophilic and hydrophobic compartments. Therefore, we parameterize the non-bonded interaction potentials by fitting against experimental thermodynamics data. We focus on reproducing solvation free energies and densities of small molecule representatives of the polymer material in their pure liquids. In this oral presentation we demonstrate the results of building the CG model for a selected polymeric material and discuss advantages/limitations of the proposed methodology.

The work is supported by a European Commission grant: Marie Curie Initial Training Network "NANODRUG" (grant agreement number: 289454).

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A Revised Basin-Hopping Monte Carlo Algorithm for Global Optimization of Nanoparticles

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Theoretical investigations and experiments suggest that nanoparticles (NPs) are able to provide significant contributions in the field of designing new materials with specific and tailored properties. Such materials could be exploited in a myriad of possibilities, such as catalysis, biological sensors and markers, optoelectronics, to name a few. However, in contrast with what happens in bulk materials, the correct assessment in a laboratory of the atomic structure of NPs is still a challenge due to the intrinsic difficulties in accessing it directly, e.g., surface reconstruction, no long range order, reduced symmetry and quantum-sized effects.

Given this scenario, from a theoretical perspective the most suitable approach to obtain a better understanding of the atomic structure of NPs are global search algorithms. The principal hindrance in finding the ground state structure of a NP by the means of a configuration space search lies in the fact that the potential energy surface (PES) describing the allowed configurations is endowed with a large number of local minima, usually scaling exponentially with the number of atoms. In face of that and other hurdles, an efficient algorithm is a requirement. One algorithm that has been very successful for global optimization of NPs is the Basin-Hopping Monte Carlo (BHMC) algorithm, in which the PES is explored by Metropolis sampling its local minima. Despite its success in the case of unbiased randomly initialized NPs, BHMC as a standalone technique has been restricted to well known empirical systems and a small sets of first-principles NPs.

In this poster we present suggestions for improving the BHMC algorithm for unbiased global optimization of NPs[1]. The standard BHMC algorithm is enhanced by bringing together novel strategies along with techniques employed in different global optimization methods. However, care has been taken to keep the underlying scheme of BHMC unchanged, in the spirit of allowing existing codes to be modified without any major complications. The improvements include a large set of local and nonlocal trial operators tailored for NPs, allowing an efficient and thorough exploration of PES. In addition to the trial operators, different strategies (static and dynamic) of operator selection are proposed, and also a filter operator designed to handle unphysical solutions in first-principles NPs.

To assess the efficiency of our strategies, our implementation was applied to several classes of systems, including Lennard-Jones and Sutton-Chen NPs with up to 148 atoms, a set of larger Lennard-Jones NPs with sizes ranging from 200 to 1500 atoms, binary Lennard-Jones clusters with up to 100 atoms, $(AgPd)_{55}$ alloy clusters described by the Sutton-Chen

potential, and aluminum clusters with up to 30 atoms described within the generalized gradient approximation of density functional theory.
Unbiased global searches carried out by our implementation were able to not only accurately reproduce published results, but also identify global minima previously missed by the standard BHMC algorithm, and in many cases with more efficiency. published results for these systems, and in many cases with more efficiency The set of ideas and strategies encompassed in the revised BHMC algorithm presented in this paper has been proven a valuable asset for theoretical investigations of the atomic structure of NPs.

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Self-Assembly of Water-Methanol Mixtures at the Surface of Graphite

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AFM experiments showed the formation of regular "stripe" patterns at the interface between a solution of methanol and water and a surface of graphite. This effect is also visible for very low relative concentrations of methanol. We have performed molecular dynamics simulations to investigate the microscopic mechanism that underlies the self-assembly of these structures.

The size and time scales that are needed to explore this phenomenon is such that a direct first principles study is prohibitively expensive. Therefore, we used conventional empirical forcefields for the water/methanol mixture from literature, and combined them with Lennard Jones terms to describe the interaction between molecules and the graphite layers. The parameters were obtained by fitting the energetics of different geometries of isolated water and methanol molecules adsorbed on graphite, computed with a dispersion-corrected density functional calculation. Short DFT simulations of water, methanol and a 50/50 solution show qualitative agreement with the forcefield calculations, validating our empirical model.

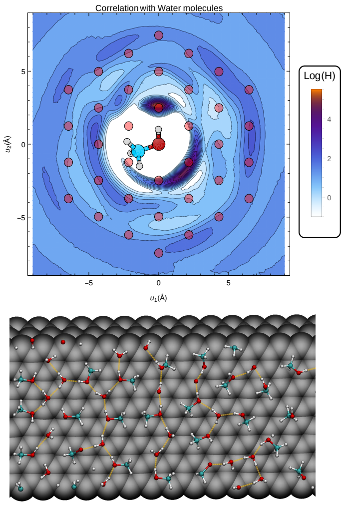

Figure 1.
above: The Hbond correlations around a MeOH molecule on graphite. The red dots correspond to the graphite lattice.
below: Simulations show a tendency to the formation of 1D chains of Hbonds.

Unfortunately, the glassy dynamics of the MeOH/H_2O system means that the direct observation of the formation of regular structures at the surface is beyond reach of even empirical FF molecular dynamics. We observe preferential segregation of methanol at the surface, a corrugated potential of mean force for methanol molecules that follows the symmetry of the graphite lattice, and a qualitative tendency of forming 1D "wires" of alternating MeOH/H_2O molecules (See Fig. 1).

In order to give a quantitative assessment of these observations, and to infer indirectly an explanation of the experimental observations, we proceeded to analyze the interplay between the corrugated potential of mean force and the topology and geometry of the Hbond network. We first constructed the adjacency matrix of the HB-network, using a machine-learning approach (a probabilistic analysis of molecular motifs, PAMM[1]) to define structural parameters for the hydrogen bonds between the different components. This analysis shows a strong preference for alternated (methanol and water) hydrogen bonds, that becomes even more pronounced at the surface of graphite. Secondly, we analysed the potential of mean force to the surface. What is more, this topological ordering corresponds to a very strong geometric structure of the coordination environment of molecules within the first layer in contact with graphite. These geometric are closely related to the periodicity of the underlying graphite, but exhibit a small mismatch.

We believe that a possible explanation of the experimental observations can be given in terms of the formation of an array of wires, perpendicular to the direction of the stripes. The AFM data might actually be showing an ordered array of defects that are induced by the slight mismatch between the lattice parameter of graphite (and the corresponding potential of mean force) and the intrinsic geometry of the ordered Hbond network formed by MeOH/Water 1D wires.

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Structure and Thermodynamic Stability of Graphene Oxide

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A large set of possible atomic configurations of graphene oxide with different composition and coverage were investigated by density functional theory.
The adsorption of hydroxyl groups and the formation of epoxides and endoperoxides was systematically evaluated. In a first series of calculations the mutual interaction and the preferred relative position of pairs of these adsorbates was determined (compare Figure 1).

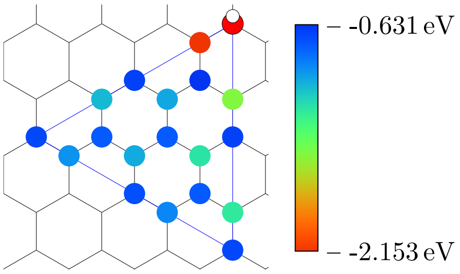

Figure 1. Energies for different adsorption positions of a second OH-group on the opposing side in a 6 × 6 supercell of graphene.

Based on these results, promising low-energy adsorption pattern at a high coverage of various compositions were derived and their relative thermodynamic stability was analyzed in terms of a surface phase diagram (Figure 2), relating the stability of a compound to the availability of surface reactants.

Finally, a detailed study concerning the possibility for formation of 1,4-endoperoxides, and similar adsorbate moieties with high ring-strain, on graphene oxide under influence of high coverage patterns was performed.

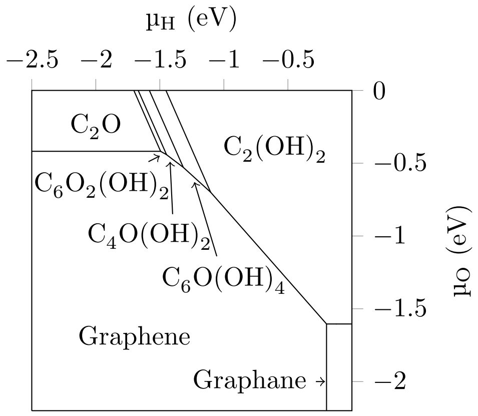

Figure 2. Surface phase diagram for graphene oxide species.

Optimal Control of a Semi-Discrete Cahn-Hilliard/Navier-Stokes System with Variable Densities

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In this poster the coupled Cahn-Hilliard/Navier-Stokes model by Abels, Garcke, Grün[1] with variable densities is considered. For a suitable time-discretization we study an optimal control problem where the control acts as a distributed force on the fluid part. Special emphasis is placed on the case of the double-obstacle potential leading to an optimization problem with nonconvex, nonsmooth constraints given by a variational inequality (MPEC). We discuss the existence of minimizers and derive first-order optimality conditions. This is done by means of a mollified Yosida-type regularization and limit passage within the regularization parameter. For the limit system optimality conditions of C-stationarity type are derived.

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Protein Stabilization and Counteraction of Denaturing Property of Urea by Glycine Betaine

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The proteins are marginally stable biomolecules, however, when present with osmolytes, small naturally occurring organic molecules, can be stable and remain functional even in extreme conditions such as those found in icy lands, abyssal water, and deserts. There have been many studies on how osmolytes stabilize proteins from these extreme conditions and counteract them. However, the exact mechanism is still a matter of debate. Exploration of the mechanism of osmolyte action on proteins can be helpful in designing new synthetic osmolytes to stabilize a range of proteins which in turn, might find use in the field of medicine, biotechnology, and agriculture. The present work explores the mechanism of protein stabilization by osmolytes and the counteraction of denaturing effect of urea by using classical molecular dynamics simulations. The results indicate that the direct interaction between glycine betaine (GB) and urea and the increase in the solvation of GB and urea are the mains reasons for the counteraction of denaturing effect of urea. The enhanced hydrogen bonding network of water also contributes to counteraction of denaturing property of urea. It was also found that in GB-urea mixture, GB acts as stronger osmolyte and urea becomes a weaker denaturing agent.

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Simulation of Contaminant Adsorption in Functionalized Membranes

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The contamination of our water resources by pharmaceuticals is highly concerning, both for the possible impact on human health and the effect on our environment[1]. Levels within aquatic environments of particular drugs have reached unprecedented levels, and have become a focus of agencies such as the world health organization[2,3]. As such, research into methods of contamination removal from water is essential.

The use of functionalized membranes to purify water is becoming increasingly popular. The functionalization of these membranes involves altering the chemical structure of the pore–wall such that certain contaminants are adsorbed and captured[4,5]. Such modification means that membranes with larger pores than traditional alternatives may be used, which reduces the required operational pressure drop and energy consumption. However, designing an efficient membrane is not a straightforward process; experimental testing and refinement of prototypes is an expensive and time consuming procedure. Due to this, mathematical modeling and numerical simulation has an important role to play in the design process, aiding membrane designers to optimize the membrane efficiency through alteration and refinement of membrane characteristics, such as the pore–size, membrane tortuosity and the type of functionalized used, as well as operational parameters such as the flow rate or pressure drop.

In this poster we present a pore–scale mathematical model to describe the transport and adsorption of a contaminant within a fluid in a functionalized membrane. Using a pore–scale model, as opposed to the associated Darcy–scale description, allows for a more accurate representation of the processes under consideration. The motion of the fluid is described by the Navier-Stokes system of equations, while the transport of the contaminant is represented by an advection–diffusion equation, with a Robin boundary condition characterizing the reversible adsorption of the contaminants at the pore–wall. Numerical simulation of the resultant system of equations is achieved by a sophisticated software package, FiltEST – Chem, which is capable of solving reactive flow directly on images using the finite volume method in conjunction with a Chorin timestepping method for the flow[6]. Here we illustrate the interplay between the flow rate, diffusion coefficient and the rates of reaction on the membrane efficiency within a virtually generated geometry which is representative of a real microfiltration membrane. The results from this research will be highly beneficial to membrane designers and manufacturers, informing them of how to alter their membranes and tune operating conditions so as to maximize contaminant capturing.

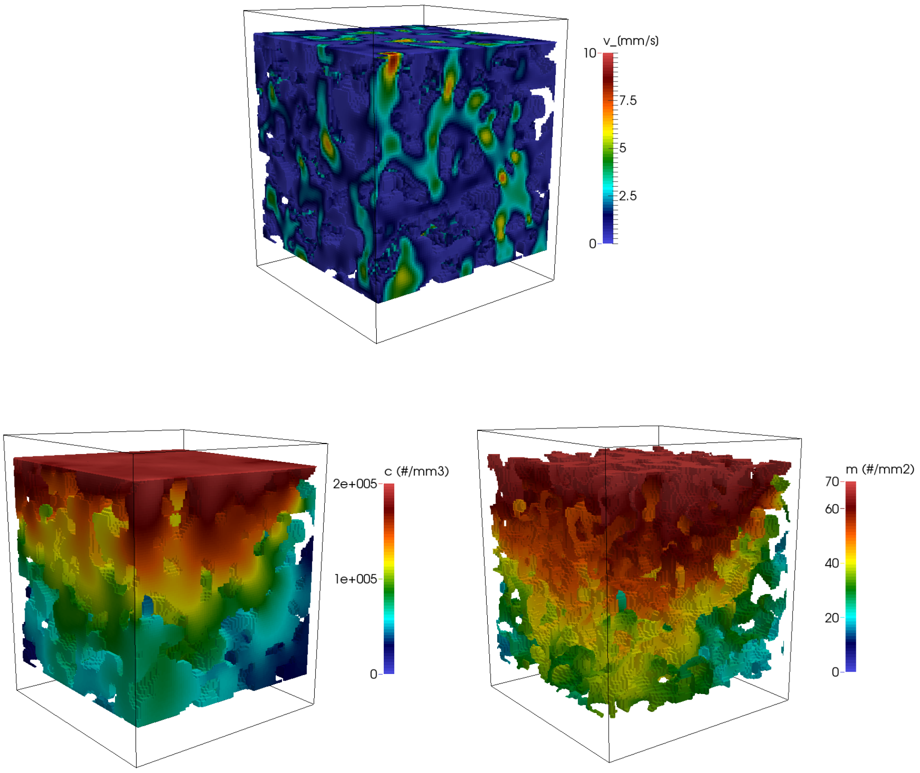

Figure 1. Pore–scale velocity magnitude (top), fluid phase concentration (bottom left) and solid phase concentration (bottom right) of a contaminant within a microfiltration membrane, at a snapshot in time.

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From Stripe to Slab Confinement in Macromolecules Linearization in Nanochannels

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Understanding of conformation and dynamics of biomacromolecules confined to a nanochannel or slit is relevant to clarification of several biological mechanisms and processes. By linearization of these biomacromolecules in the confinement of slab (rectangular nanochannel) or stripe-like channel geometry (channel of one-monomer thickness), it is possible to study the structural properties of biomacromolecules. The extension of semiflexible polymers in strong confinement in a channel is well described by the relation due to Odijk[1]. In weak confinement it is successfully described by the de Gennes blob theory[2]. Recent simulation studies analyzed also new intermediate regimes, the extended de Gennes regime[3] and Gauss de Gennes regime[4]. Interestingly in stripe geometry there is absence of these intermediate regime[5].

In the present work we have investigated recently suggested advantageous analysis in the chain linearization experiments with macromolecules confined in a stripe-like channel[5] using Monte Carlo simulations. The enhanced chain extension in a stripe geometry which is due to the higher excluded volume interactions between monomers in two dimensions geometry weakens considerably on transition to an experimentally feasible slit-like geometry. Based on the chain extension-confinement strength dependence and the structure factor behavior for a chain in a stripe we infer the excluded volume regime (de Gennes regime) typical for two-dimensional systems. On widening of the stripe in direction perpendicular to the stripe plane, i.e. on the transition to the slab geometry, the chain extension decreases significantly and the pseudo-ideal regime is observed for not very long semiflexible chains. The evidence of the pseudo-ideal regime in confined chains is based on analysis of the extension curves, variation of the extension with the persistence length P, and the structure factor analysis. The slab behavior can be observed when the two-dimensional stripe reaches the reduced thickness D larger than approximately $D/P \approx 0.2$ in the third dimension. The maximum height of a slab at which the advantage of a stripe is retained is very low and has implications for linearization experiments.

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Molecular Dynamics Simulation of Sulfone Linked Sulfonated Dimers

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This project focuses on the investigation of structural properties of sulfone linked sulfonated dimers in lithium form via all atom molecular dynamics simulations. Previous research has been primarily focused on sulfonated polyelectroytes in apolar and aprotic solvents in sodium form. But it is quite interesting to study the conformations and binding mechanisms of these typical dimers in lithium form in a broad range of solvents. The results show that the typical conformations of these dimers plays a vital role in determining the suitable ion binding mechanism to the dimer. Triple binding mechanism is favored for sulfonic acid ortho form of the dimer where as single and double binding mechanism is favored for the meso form. Also the condensation behavior of these dimers were studied under various aprotic, protic, polar and apolar solvents.

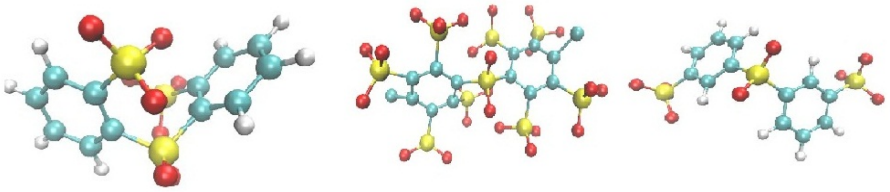

Figure 1. Corresponding dimer structures: ortho-form (left), meso-form (right) and full form (middle). The ortho and meso form have a net charge of (-2e), whereas the full form has a net charge of (-8e). These dimers are denoted as S220 dimers.

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Structure and Dynamics of Hybrid Polymer/Gold Nanoparticle Systems through Atomistic Molecular Dynamics Simulations

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Hybrid polymer/nanoparticle systems are a relatively new class of materials that has attracted growing scientific and technological interest[1–5]. In this work, the properties of polyethylene chains around of a gold nanoparticle at a temperature of 450 K are investigated using classical atomistic molecular dynamics simulations.
A classical Morse-type potential, which was parameterized based on the results of density functional calculations[2], used in order to describe the interaction between the polymer and the gold nanoparticle. Several gold nanoparticles[3] with Wulff construction were studied, with diameter ranging from around 2.5’5 nm and polyethylene chains consist of 22 monomers[4]. A typical snapshot of the model system is shown in Figure 1.

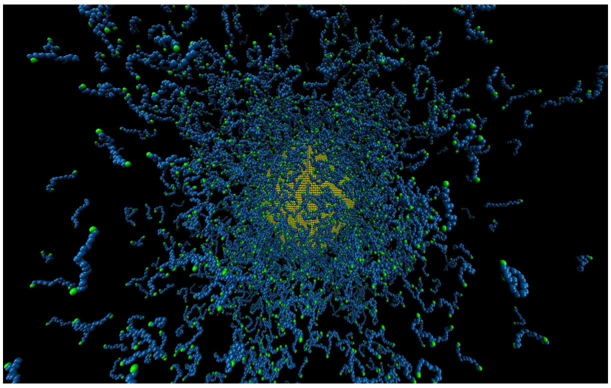

Figure 1. Snapshot from MD simulation of hybrid polyethylene/gold nanocomposite at 450K. Au nanoparticle (3101 atoms, diameter of 5.02 nm) and polyethylene (5040 chains, 22-mers per chain) are shown. With yellow is the Au and with grey are the edges of Au nanoparticle. With blue are the CH2 and with green the CH3 monomers.

The structural, conformational, and dynamical properties of the chains were analyzed and compared to the behavior of the bulk polyethylene system. In more detail, we report data concerning polymer density profiles, bond order parameter, segmental and terminal dynamics (Figure 2). All properties are examined as a function of distance from the Au NP.

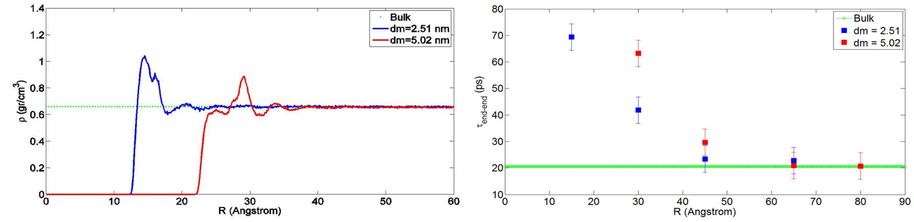

Figure 2. Monomer density profiles of polyethylene as a function of R (distance from the center of mass of the gold nanoparticle) for the two hybrid systems (left). Relaxation time of polyethylene segment v1-3 along R (distance from the center of mass of the gold nanoparticle) for the two hybrid systems (right).

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Water Dynamics in AOT Reverse Micelle

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Reverse micelles are sizable water nano-inclusions dispersed in organic solvent and surrounded by a detergent monolayer, widely used as micro-reactors in heterogeneous chemistry and templates for nano-particle synthesis, and also for enzyme catalysis and drug delivery.[1] The water core has complex dynamics due to the influence by both electrostatic interaction with the highly-charged surfactant layer surface and nano-confinement in geometry. Compared to bulk water, the confined water has limited mobility, greater viscosity, smaller polarity, less hydrogen bonds per molecule and smaller dielectric constant. By varying the size of a common reverse micelle, Aerosol OT (Dioctyl sodium sulfosuccinate), one can detect the effects of confinement and hydration on the structure and stability of biomolecules such as peptides, proteins and nucleic acids.

The current work presents our efforts towards understanding the hydration environment in reverse micelles by molecular simulation methods. Specifically, we use a recently-developed 2PT calculation method to map the absolute entropy of the water inside the reverse micelle for better understanding of the water heterogeneity in the confinement.[2] Briefly, the partition function of the system, which contains all the information necessary to extract the relevant thermodynamic properties, is extracted from the total density of states (DOS). Practically, the DOS is the Fourier transform of the atomic velocity autocorrelation function. The DOS is then self-consistently partitioned into a hard-sphere (anharmonic) and a solid (harmonic) component. Using the appropriate quantum weighting functions, the total system thermodynamics can be recovered by a linear combination of the two DOS.[3] The efficiency of the 2PT method means that the system thermodynamics are evaluated dynamically along the trajectory for typically only a 10 - 20.

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Phase Separation of Self-Propelled Rods with Length Bidispersity

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The collective behaviour of microswimmers has gained considerable attention in the recent years. Examples of microswimmers span from biological cells and bacteria to human-made nano-robots. Here, we propose a model for self-propelled rods in two dimensions that interact with a physical interaction potential. We model each rod by a number of beads to calculate the rod-rod interactions. In contrast to previous models with excluded-volume interactions[1], our capped interaction potential allows rods to cross. Our simulations thus combine the computational efficiency of two-dimensional simulations with a possibility to mimic an escape to the third dimension when two rods collide[2].

Depending on the density and the self-propulsion, we find a rich phenomenology for this system: a disordered phase at low densities and low self-propulsion, a segregated phase with a giant cluster at medium densities and medium self-propulsion, a laning phase at very high densities and a cluster break-up phase at very high self-propulsion.

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Structure of Microgels with Coulomb Interactions

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Microgels are cross-linked polyelectrolyte networks. Their ability to undergoing reversible volume phase-transitions in respond to external conditions renders them potential candidates for numerous applications. Hence, various simulation studies of the swelling of polyelectrolyte gels have been performed during the last decade. Such simulations typically focus on regular polymer lattice under periodic boundary conditions, *i.e.*, only the bulk properties of the gel are examined. However, comparably little is known about finite-size cross-linked polyelectrolytes.

To elucidate the influence of explicit ions on the structural properties of finite-size cross-linked polyelectrolytes, we perform large-scale computer simulations. Thereby, molecular dynamics simulations for the polymers are combined with the Brownian multiparticle collision dynamics approach[1]. A microgel particle itself is comprised of a regular network of self-avoiding polymers internally connected by tetra-functional cross-links and with dangling ends at its surface (df. figure). Electrostatic interactions between the charged monomers and the counterions are taken into account by the Coulomb potential. In addition, systems with Debye-Hückel interaction, *i.e.*, counterions are taken into account implicitly only, are considered[2]. The emerging structural properties will be presented, which shed light onto the swelling behavior of microgels.

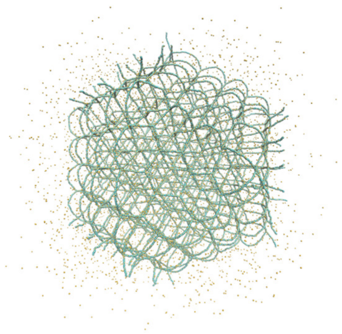

Figure 1. The snapshot of a fully swollen microgel in the presence of counterions.

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