CPP 32: P4: Computational Physics of Soft Matter

Time: Tuesday 14:00–16:00   Location: Poster B

CPP 32.1 Tue 14:00 Poster B

New insights into the structure of poly(p-phenylene terephthalamide: a first principles study — ●Pegah Zolfaghari[1], Ole Braukamann[1], Arno P M Kentgens[1], Robert A de Groot[1,2], and Gilles A de Wijs[1] — [1]Radboud university Nijmegen, Electronic Structure of Materials,Institute for Molecules and Materials, Netherlands — [2]Rijksuniversiteit Groningen, Solid State Materials for Electronics,Zernike Institute for Advanced Materials, Netherlands

The aromatic polyamids are a major class of polymers in recet years.This class of polyamids are of practical interest due to their high tensile strength, high elastic modulus, low elongation at breakage, and higher thermomechanical stability among other kinds of polyamids.

One of the interesting member of this class of fibres called poly, p-phenylene terepthalamide (hereafter PPTA). PPTA is a polymer which crystalizes in the form of 2D hydrogen-bonded sheets. It has enormous commerical applications, as already mentioned, and is sold under the commercial names of Kevlar and Twaron. The packing of the hydrogen-bonded sheets and phenyl group give rise to three different PPTA structures, including Northolt, Liu and Pb.

The calculations reveal that different PPTA structures which all exhibit herringbone packing of the phenyl groups between neighboring sheets, have similar stabilities. Also, The use of solid-state NMR experiments combined with Density Functional Theory (DFT) based calculations allows unambiguous assignment of all proton and carbon resonances of PPTA structures.

CPP 32.2 Tue 14:00 Poster B

Water Dynamics in Aqueous TMAO Solutions: a DFT-MD Study — ●Kota Usui[1], Marialore Sulpizi[2], Johannes Hunger[1], Mischa Bonn[1], and Yuki Nagata[1] — [1]Max-Planck Institute for Polymer Research, Mainz, Germany — [2]Johannes Gutenberg University Mainz, Mainz, Germany

Trimethylamine N-oxide (TMAO) is one of the most effective agents to stabilize proteins. It has been found that TMAO is excluded from the protein's surface, which indicates that stabilization occurs via interaction of TMAO with the solvent, i.e. water. We investigate the mechanism behind the interaction of TMAO with water using DFT and force field molecular dynamics (MD) simulations. Our DFT-MD simulation reproduces the experimentally observed ~200 cm-1 red-shift of the O-D stretch vibrational peak, in contrast to force field MD. The water reorientational motion, reflected by the anisotropy decay, is significantly retarded in the vicinity of the hydrophilic O atom of TMAO (OTMAO) for our DFT-MD simulations, which is not observed in force field MD simulations. This slow-down of the anisotropy decay is found not only for the O-D group bound to OTMAO but also for the other O-D group of the same D2O molecule. Sequentially, we elucidated why force field MD predicts significantly different dynamics from the DFT-MD. To this end, we selectively calculated the anisotropy decay of those O-D groups which remain hydrogen bonded to OTMAO, which reveals the same time scale of the anisotropy decay of TMAO, indicating that the TMAO-bound D2O loses its reorientational information by following the TMAO rotational motion.

CPP 32.3 Tue 14:00 Poster B

Electrode models for ionic liquid based capacitors — ●Kai Szuttor, Konrad Breitsprecher, and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

We compare different simulation models for ionic liquid based capacitors concerning the electrode model. Therefore molecular dynamics simulations of an explicit graphite model are compared to a plain wall electrode with adapted interaction parameters. Further we compare two simulation approaches with constant potential boundary conditions to constant charged electrodes and the influence of these different methods with regard to the differential capacitance and the layering behavior of the ionic liquid at the electrode.

CPP 32.4 Tue 14:00 Poster B

Structure and Dynamics of a Mixture of Ethylene Glycol and Water in Confinement — ●Rebecca Schmitz and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Germany

In numerous biological processes and technical applications the motion of molecules in aqueous solutions is restricted by boundary surfaces.

Therefore it is crucial to understand the impact of nanoscale confinement on structure and dynamics of liquids. We study the behavior of a mixture of ethylene glycol and water in cylindrical silica nanopores using molecular dynamics simulations. The usage of both amorphous and crystalline nanopores provides us with further insights into the role played by the structure of the confinement. For all systems we find a considerable slowdown of the structural relaxation approaching the wall while the dynamics of the inner layer is comparable to bulk behavior. But while the dynamics of the liquid is similar in all pores, its structure depends strongly on the exact configuration of the confinement. The investigation of the liquid's density profile indicates a local microphase separation induced by the confinement as one molecular species preferentially attaches to the wall. Though reported by various groups, the physics behind this effect is not very clear yet and there is no agreement on whether water or alcohol constitutes the outer layer [1,2]. As we find a very different structure of the liquid in the amorphous and the crystalline pore, our simulation study reveals further information on the influence of various parameters of the confinement.

[1] Guo et al.; J. Phys. Chem. B 118, 34 (2014)
[2] Elamin et al.; PCCP 15, 42 (2013)

CPP 32.5 Tue 14:00 Poster B

Molecular dynamics simulation of sulfonated dimers in DMSO-Water mixtures — ●anand narayanan krishnamoorthy[1], jens smiatek[2], and christian holm[3] — [1]Institute for Computational Physics,University of Stuttgart — [2]Institute for Computational Physics,University of Stuttgart — [3]Institute for Computational Physics,University of Stuttgart

Using molecular dynamics simulations, we studied the counter ion condensation behavior of dimers with lithium ions under various mole fraction of DMSO-Water mixtures. The ionic condensation behavior show non ideal behavior for specific mole fractions of DMSO-Water mixtures. Previous study show that the non ideality of the binary mixture solution is due to the cluster formation of DMSO and Water molecules through hydorgen bonds between donor DMSO oxygen atom and hydrogen atom of Water. The non-ideal behavior, we observe can be related to solvent-solvent interactions and a preferential solvation mechanism for the dimer and the counter ions. The diffusion behavior of the binary mixture was also studied and is in good agreement with the experimental observations.

CPP 32.6 Tue 14:00 Poster B

Unravelling the conformations of di-(perylene bisimide acrylate) by molecular modelling and free energy calculations — Florian Spreitler[1], Michael Sommer[2,4], ●Manuel Hollfelder[3], Mukundan Thelakkat[2], Stephan Gekle[3], and Jürgen Köhler[1] — [1]Experimental Physics IV and BIMF, University of Bayreuth, D-95440 Bayreuth, Germany — [2]Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, D-95440 Bayreuth, Germany — [3]Biofluid Simulation and Modeling, Physics Department, University of Bayreuth, D-95440 Bayreuth, Germany — [4]Current address: Michael Sommer, Institute for Macromolecular Chemistry, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

We compare the results of Molecular Dynamics modelling and Umbrella Sampling on perylene bisimide acrylate dimers to the results from time-resolved fluorescence anisotropy experiments [F. Spreitler et al., Phys. Chem. Chem. Phys., 2014,16, 25959-25968]. It allows us to connect the experimentally found spectral signatures of three different fluorescence states with one non-stacked and two stacked (parallel and anti-parallel) molecular conformations. The experimental data can be reproduced for the parallel stacked conformation using a model of structural relaxation in the electronically excited state of the stacked aggregate. For the non stacked conformation agreement between experiment and modelling is only found if fast hopping of the electronic excitation (Förster energy transfer) between the perylene bisimide subunits is taken into account.

CPP 32.7 Tue 14:00 Poster B

Ewald summation on GPU — ●Sascha Ehrhardt and Axel Arnold — Institute for Computational Physics, Stuttgart, Germany

We implemented the Ewald summation algorithm for the computation of electrostatic energies in molecular dynamics simulations for graphic cards (GPUs) using CUDA. Our implementation is part of the open source molecular dynamics package ESPResSo (http://espressomd.org).

The Ewald summation splits up the Coulomb energy sum in two sums, where one is calculated in real space and the other in reciprocal space. Because the two sums can be computed independently of each other, the real space part will be computed on the CPU using the efficient short range routines of ESPResSo, whereas the reciprocal space part will be computed on the GPU. The results are compared to the existing particle-particle particle-mesh (P3M) algorithm without GPU support. For moderate densities, the GPU-accelerated Ewald summation is comparable in efficiency with the better scaling P3M algorithm up to about 3000 particles, but allows for much higher accuracies without drastic penalties if desired.

CPP 32.8   Tue 14:00   Poster B
Monte Carlo Studies on dendrimers with special terminal-groups at different solvent conditions — •Martin Wengenmayr, Jens-Uwe Sommer, and Ron Dockhorn — Leibniz Institute of Polymer Research Dresden, Germany

Monte Carlo Simulations of high generation dendritic polymers at different solvent conditions are performed using the Bond Fluctuation Model on CPU and GPU. Different solvent conditions are applied using explicit solvent. In order to comply with the wide range of dendrimer modifications different terminal groups, for instance flexible linear chains, were attached. Static and dynamic properties like the radius of gyration, the gyration tensor and the conformation of subunits are investigated in detail. We expect that our results help to understand the swelling and collapse of a dendrimer as a carrier molecule for drug delivery processes.

CPP 32.9   Tue 14:00   Poster B
Comparison of passive and active microrheology for an unentangled polymer melt — •Anja Kuhnhold and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg, Halle, Deutschland

We use molecular dynamics simulations to study the microrheology (MR) of an unentangled polymer melt. Microrheology aims at the estimation of the complex shear modulus of a probe from the motion of suspended micro- or nanoscopic particles in the probe.
This motion can either be purely thermal, similar to the Brownian motion, or forced to a specific form, like an oscillation. The former is called passive MR and the latter active MR.
In passive MR the complex modulus is calculated by using a generalized Stokes-Einstein relation. In active MR a corresponding relation depends on the specific form of the motion.
Our system is a melt of short bead-spring polymer chains including one nanoparticle. For the active MR we use an oscillating harmonical potential, similar to the experimental optical tweezer, to force the particle to oscillate with a certain frequency. Passive and active MR give similar results in the linear response regime independent of temperature, and at high temperatures these are equal to the true (reference) bulk modulus. The lower frequency range is better accessible by passive MR while with active MR one can generally reach higher frequencies.

CPP 32.10   Tue 14:00   Poster B
Effects of Stiffness on a Generic Polymer Model and where Knots come into Play — •Martin Marenz and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We give an overview of the influence of bending stiffness on the conformational phases of a generic homopolymer model and study especially the occurrence of knots as stable pseudo phases. Thus we present the pseudo-phase diagram for the complete range of semi-flexible polymers, ranging from flexible to stiff ones. Although it is a simplistic model, we have observed a rich variety of conformational phases which are comparable to conformations observed for real polymers and proteins. Just by changing the internal bending stiffness, the polymer model features different pseudo-phases like bended, knot-like, hairpin or toroidal phases. To identify these phases we have calculated, besides standard observables, the complete gyration tensor and the knot type of the polymer via the Alexander polynomial. Due to the relative complex phase space with numerous pseudo-phase transitions and the large parameter space, we used a recently developed parallel variant of the multicanonical algorithm to cope with all problems arising from the transitions and the slow dynamics at very low energies.

CPP 32.11   Tue 14:00   Poster B
Parallelized Event Chain Algorithm for Dense Hard Sphere and Polymer Systems — •Tobias Alexander Kampmann, Horst-Holger Boltz, and Jan Kierfeld — TU Dortmund University

We present a parallelized event chain algorithm for hard sphere systems. Analyzing the performance gains for the parallelized event chain in two dimensions we find a criterion for an optimal degree of parallelization. Furthermore we discuss the extension of the algorithm to other systems with hard sphere interactions with a special focus on dense polymeric systems (polymer melts).

CPP 32.12   Tue 14:00   Poster B
The evaporation of nanodroplet on a heated substrate — •Jianguo Zhang, Frederic Leory, and Florian Müller-Plathe — TU Darmstadt

Two non-equilibrium methods (called bubble method and splitting method, respectively) developed to study the steady-state evaporation of a droplet surrounded by its vapor, where the evaporation continuously occurs at the vapor-liquid interface while the droplet size remains constant [1]. Then we present our activity dealing with the evaporation of nanometer sized droplets. The evaporation mechanisms of nanodroplets on surface which are chemically both homogenous and heterogeneous are studied by MD simulations under nonequilibrium conditions [2-4].
[1] Zhang, J., Müller-Plathe, F., Yahia-Ouahmed, M., & Leroy F., J. Chem. Phys. (2013), 139, 134701. [2] Zhang, J., Leroy, F. & Müller-Plathe, F., Langmuir (2013), 29, 9770-9782 [3] Zhang, J., Leroy, F. & Müller-Plathe, F., PRL (2014), 113, 046101. [4] Zhang, J., Leroy, F. & Müller-Plathe, F., in preparation.

CPP 32.13   Tue 14:00   Poster B
Implicit-solvent coarse-grain models of thermosensitive polymers — •Richard Chudoba[1,2], Jan Heyda[3], and Joachim Dzubiella[1,2] — [1]Dept. of Physics, Humboldt-University Berlin, Germany — [2]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Germany — [3]Dept. of Physical Chemistry, Institute of Chemical Technology, Prague, Czech Republic

Functionalized, thermosensitive polymers have become an integral building block for the development of "smart", environment-sensitive materials with tunable properties. In particular close to their lower critical solution temperature (LCST) copolymers show dramatic changes in their material properties in response to only tiny changes in the solvent environment, e.g. a salt concentration. Solution theory based but still empirical route towards the quantitative prediction of ion-specific effects on polymer folding has been proposed recently.

We employ implicit-solvent coarse-graining strategy to verify this concept on the models of thermosensitive polymers. Our primary targets are poly(ethylene)glycole (PEG) and poly(N-isopropylacrylamide) (PNIPAM), both widely experimentally studied and characterized due to their potential not only in biological applications.

Replica exchange molecular dynamics have been employed to gather equilibrium statistics for polymer in explicit solvent at temperatures around LCST and serve as a reference for the coarse-graining step. The iterative Boltzmann inversion is here the method of choice and the resulting implicit polymer models are then simulated within Monte Carlo and/or Brownian dynamics.

CPP 32.14   Tue 14:00   Poster B
Two dimensional nanomaterials as sensors and drug delivery agents — Hakkim Vovusha[1], •Suparna Sanyal[2], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden. — [2]Department of Cell and Molecular Biology, Uppsala University, Uppsala, Sweden

Two dimensional nanomaterials have emerged as promising agents for enabling fabrication of data storage devices, sensors for molecular detection, e.g., sensing of gas molecules involved in environmental hazards and drug delivery agents due to their ultrathin size with all surface effects, exotic electronic and mechanical properties. Understanding of electronic structures of these materials is important to design new materials for better sensitivity and selectivity of molecules. In this context, adsorption characteristics of different molecules such as DNA/RNA nucleobases, explosive molecules and polycyclic aromatic hydrocarbons with 2D graphene, graphene oxide, boron nitride and hybrid boron nitride-graphene in both nano flake and infinite 2D sheet geometries have been studied by density functional theory (DFT). Also,

time-dependent DFT has been used for calculations of optical properties for identifying features due to adsorption. Our results provide important insights in gas sensing and drug delivery issues.

CPP 32.15   Tue 14:00   Poster B

About the time dependency of the Van der Waals equation of state — ●Peter Friedel — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

The Van der Waals equation is one of the prototypes of the equation of states for realistic systems because of the first time introduction of excluded volume and particle interactions into theoretical considerations. On the other side the simulated annealing (and the similar simulated compressing) approach applies the time dependency to one of the variables of state performing simulations of realistic systems as quasi static state changes. The combination of this time dependency and the VdW-EoS enables a generalization of such considerations up to the simulations of time dependent processes like phase transitions and the obtaining of phase transition kinetics. Simple mathematical deductions starting with the time dependent Van der Waals equation allow the derivation of two so called differential simulated changes of state methods under isobar and isotherm conditions. These new methods enable simulations of crossing phase transition points of hypocritical substances without the danger that the simulations crash because of the achievement of infinite values of the corresponding susceptibility coefficients.