CPP 31: Modeling and Simulation of Soft Matter I (joint session CPP/DY)

Time: Tuesday 14:00–16:00 Location: PC 203

Invited Talk CPP 31.1 Tue 14:00 PC 203
The role of correlations in the collective behaviour of microswimmer suspensions — •Alexander Morozov — University of Edinburgh, Edinburgh, UK

Recent years witnessed a significant interest in physical, biological and engineering properties of self-propelled particles, such as bacteria or synthetic microswimmers. The main distinction of this 'active matter' from its passive counterpart is the ability to extract energy from the environment (consume food) and convert it into directed motion. One of the most striking consequences of this distinction is the appearance of collective motion in self-propelled particles suspended in a fluid observed in recent experiments and simulations: at low densities particles move around in an uncorrelated fashion, while at higher densities they organise into jets and vortices comprising many individual swimmers. Although this problem recieved significant attention in recent years, the precise origin of the transition is poorly understood.

In this talk I will present a numerical method based on a Lattice-Boltzmann algorithm to simulate hydrodynamic interactions between a large number of model swimmers (order 10^5), represented by extended force dipoles. Using this method we simulate dilute suspensions of self-propelled particles and show that, even below the transition, swimmers move in a correlated fashion that cannot be described by a mean-field approach. We develop a novel kinetic theory that captures these correlations and is non-perturbative in the swimmer density, and reveals the asymmetry between pusher and puller swimmers below the transition to turbulence.

CPP 31.2 Tue 14:30 PC 203
Polymer Topology by Chain Walking Polymerization Catalysis — •Ron Dockhorn[1,2], Albena Lederer[1], Jan Merna[3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]University of Chemistry and Technology Prague, CZ-16628 Praha, Czech Republic

Monte Carlo simulations of the chain walking polymerization catalysis (CW) are performed using the bond fluctuation model to investigate the influence of the walking mechanism on the polymer topology at a given molecular weight. In agreement to previous findings, for high reaction probability/slow walking the structure growths with linear chain extensions. On the other hand, for low reaction probability/fast walking the structures show dendritic growth of the polymer. The transition region is characterized by large amount of branched side chains reflecting a cross-over regime with linear global features and dendritic local sub-structures. This is in contrast to the Zimm-Stockmayer hyperbranched (ZS-HB) scaling. Static properties are investigated by means of radius of gyration and scattering function of perfect dendrimers, ZS-HB, and CW-structures. A generalized mean-field model is applied, and is found in fair agreement with the simulation data under good solvent conditions. These findings are aimed to understand the physical properties related with the topology of the CW-structures to improve the synthesis of a new class of hyperbranched molecules.

CPP 31.3 Tue 14:45 PC 203
Understanding the Dynamical Behavior of Twin Polymerization — Constantin Huster, Halit Taskin, and •Janett Prehl — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

Twin polymerization enables the formation of two different macromolecular structures of organic-inorganic hybrid materials in one single process step. To investigate the dynamical behavior and the morphology of the reaction process and the final compounds we recently developed a Monte-Carlo based reactive bond fluctuation model (rBFM) [1] that is capable to cope with the complexity of the underlying reaction mechanism. Special feature of this rBFM is the possibility to define multiple reaction centers per monomer and multiple bond vectors between two monomers that exhibit different properties.

In this presentation we introduce the rBFM and analyze first results of the diffusive behavior of the reacting twin monomers over time. By doing so we gain insights into the structure formation process of twin polymerization.

[1] K.H.Hoffmann, J.Prehl, *Reac Kinet Mech Cat* DOI: 10.1007/s11144-017-1303-y

CPP 31.4 Tue 15:00 PC 203
Bridging Time Scales with Variationally Enhanced Sampling — •Omar Valsson — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany

The usefulness of atomistic simulations is generally hampered by the presence of several metastable states separated by high barriers leading to kinetic bottlenecks. Transitions between metastable states thus occur on much longer time scales than one can simulate. Numerous enhanced sampling methods have been introduced to alleviate this time scale problem, including methods based on identifying a few crucial order parameters and enhancing their sampling through the introduction of an external biasing potential.

Here will we discuss Variationally Enhanced Sampling (Valsson and Parrinello, PRL 113 090601, 2014), a generally applicable enhanced sampling method where an external bias potential is constructed by minimizing a convex functional. We present numerous examples from physics and chemistry which show the flexibility and practicality of the method. We will furthermore show how the variational property of the method can be used to extend the method in various innovative ways, e.g.: to obtain kinetic information from atomistic simulation; to accelerate nucleation events by employing models from classial nucleation theory; and to incorporate experimental information into molecular simulations.

We will also introduce the VES code (http://www.ves-code.org), an open-source library for the PLUMED 2 plugin that implements methods based on Variationally Enhanced Sampling.

CPP 31.5 Tue 15:15 PC 203
Kinetics of defects in self-assembled block-copolymers using continuum models — •Juan Carlos Orozco Rey and Marcus Mueller — University of Goettingen, Institute of Theoretical Physics, Goettingen, Germany

The computational study of directed self-assembled (DSA) of copolymeric materials is a challenging task due to the disparity of length scales involved in the structure formation process. Fast simulation techniques, which enable us to conciliate the periodicity of the self-assembled structures with the large scale of devices targeted in the manufacturing of these materials, are of significant interest. Continuum models provide the highest level of coarse-graining where the polymer system is no longer described by the molecular degrees of freedom but only in terms of a local collective variable - the difference in composition. We study the ability of two continuum models - Ohta-Kawasaki and Swift-Hohenberg - to describe key aspects of defects and their dynamics: the limits of stability, the shape of the internal AB interfaces and the kinetics of motion.

We use particle-based simulations and self-consistent field theory to compare and identify the most promising model for the study of DSA. We show that in spite of the caveats of a highly coarse-grained description, a continuum model provides valuable insights into the kinetics of self-assembly as well as into the surface-directed structure formation of device-oriented structures like T-junctions. The combination with more detailed models enables us to gain better understanding of the process while reducing the computational cost.

CPP 31.6 Tue 15:30 PC 203
Higher coordination of cross-links improve toughness of fiber bundles — •Huzaifa Shabbir and Markus Hartmann — Sensengasse 8 , 1090 Vienna Austria

(Physical) cross-linking is an effective strategy to tailor the mechanical properties of polymeric systems. Often, these cross-links are weaker than the covalent backbone that holds the structure together. If reversible, cross-links provide the material with some self-healing behavior.

We use Monte Carlo simulations to investigate the mechanical behavior of (reversibly) cross-linked polymeric systems. The framework of a multi-body potential is utilized to control the coordination of cross-links (coordination is defined as the number of monomers participating in one cross-link). Displacement controlled computational loading experiments are conducted to evaluate the mechanical properties of fibrous systems.

Previous work shows that the coordination of cross-links significantly influences the mechanical performance of a linear chain [1]. In this talk, the influence of the coordination of cross-links on the mechanics of aligned fiber bundles will be discussed. In particular, it will be shown that the coordination of cross-links has a large impact on the toughness of fiber bundles as higher coordination inhibits the premature rupture of the covalent backbone observed for classical cross-links of two fold coordination [2]. Special emphasis will be put on the influence of the topology of cross-links that show a much richer variety for a higher coordination compared to the classical coordination of two.

CPP 31.7 Tue 15:45 PC 203

Permeability maximization in polymer gels: Modeling and simulation — •Won Kyu Kim[1], Matej Kanduč[1], Rafael Roa[1], and Joachim Dzubiella[1,2] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

Permeability measures the ability of soft matter, such as polymer-based networks (hydrogels), to transport solvents and solutes, defining important control parameters in soft functional material applications, e.g., for filtration, drug release, and transport of reactants in responsive nano-reactors [1-4]. We study permeability by means of coarse-grained simulations and theory of a model polymer network. We find that the permeability can be maximized by optimal polymer volume fractions and inter-particle interactions between the polymer and the penetrating solutes. This nontrivial phenomenon is triggered by a competition between solute partitioning [1-3] and diffusion [2]. Throughout a wide range of parameter space of the solvent quality, solute coupling, and gel volume fraction, a rich topology of the partitioning is found. The solutes' diffusivity is highly correlated to gel structures, resulting in a drastically nonmonotonous permeability. Possible applications to hydrogel based devices such as responsive nanoreactors for catalysis [2,4] are discussed.

[1] W. K. Kim et al, Macromolecules 50, 6227 (2017). [2] R. Roa et al, ACS Catalysis 7, 5604 (2017). [3] M. Kanduč et al, Phys. Chem. Chem. Phys. 19, 5906 (2017). [4] S. Wu et al, Angewandte Chemie 51, 2229 (2012).