CPP 4 SYMPOSIUM: Dynamics of multi-component fluids IV

Zeit: Freitag 15:45–17:00 Raum: TU C243

Hauptvortrag

CPP 4.1 Fr 15:45 TU C243

Hybrid models for Mixed Soft Systems: Lessons from Computer Games — •Johannes Fraaije — Leiden Institute of Chemistry

We all know computer games, and we dot not think it at all strange that in one gaming environment one encounters many different visual and physical entities: smoke, bullets, and cars, ... Yet, in our professional practice of simulating soft matter systems, it suddenly seems if we have forgotten the joy of a good game, and we limit ourselves, to either field models (smoke), or particle models (bullets), or finite element models (cars). Why the restriction? There are many soft matter systems simulations, which would profit enormously from having, in one simulation environment, a field model for fast degrees of freedom, a coarse-grained model for molecuar dynamics and on top of that, a finite-elemenet description of (bio)colloidal surfaces. Although the logic and necessity of such hybrid modelling is clear, no such general purpose method exist, other than the new Culgi scripting language we have developed. I present results which combine mesoscopic field simulations (Mesodyn) and DPD polymer particle simulations, for the purpose of understanding mixed formulations. These are systems consisting of a few tens percent of surfactant, and a few percent of block copolymer. With either pure method, it would be impossible to simulate such formulation, even with very big computers, but with the hybdrid model it is a task for a PC - a lesson learned from computer games.

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Dynamics of structural transitions in amphiphilic systems followed by small-angle scattering experiments — •Gradzielski Michael — Lehrstuhl Physikalische Chemie I, Universität Bayreuth, D-95440 Bayreuth

Morphological transitions in amphiphilic systems can be induced by mixing with other surfactants or additives. In our experiments fast mixing phenomena were investigated by means of coupling the stopped-flow technique with the observation by means of SANS/SAXS, whereby detailed structural information can be obtained with a time resolution of 5-50 ms. Different types of structural investigations were studied, e. g. formation of unilamellar or multilamellar vesicles by mixing with oppositely charged surfactant or a cosurfactant. For instance the slow formation of monodisperse unilamellar vesicles was observed, that is driven purely by diffusive processes, and proceeds via a well-defined disk state. In general kinetics, intermediately formed structures and final state depend subtlely on the electrostatic conditions of the amphiphilic system and the molecular composition. In other experiments the disintegration of micelles initiated by mixing with a bad solvent was studied. Interestingly this this process does not proceed via a simple dissolution step by through a minimum aggregation state, which is followed by the reformation of small micellar structures. In general, it can be stated that the dynamics of amphiphilic systems can be complex but its detailed knowledge is pivotal for using self-aggregation as a tool for forming complex nanostructured materials.

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Computer simulations of ethanol/water mixtures - from the atomistic to the mesoscale — •Jörg R. Silbermann, Sabine H. L. Klapp, and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin, Germany

We consider fluid mixtures of ethanol (E) dissolved in water. Atomistic simulations[(1)] permit us to extract the center of mass (cm) pair distribution function $g_{EE}(R)$ of the ethanol molecules. Based on $g_{EE}(R)$ we seek for an effective pair potential $U_{EE}(R)$ capable of describing the system on a mesoscopic scale, where the solvent is no longer treated explicitly and the ethanol molecules are represented by isotropic beads. Using mesoscale computer simulations, we study this issues for several compositions of the mixture. At small ethanol densities the potential of mean force $U_{mf}(R) = -kT \ln g_{EE}(R)$ turns out to reproduce the atomistic $g_{EE}(R)$ in a satisfactory way, indicating that three- and more-body interactions are negligible. For systems with larger ethanol densities, however, corrections for higher order interactions are nessecary. In this context we investigate the capabilities of integral equation techniques to extract $U_{EE}(R)$. Moreover, we investigate prospects to recover the dynamics of the prestine system on a mesoscopic scale by means of dissipative particle dynamics concepts.

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Slow dynamics of block copolymer melts in different ordered morphologies — •C.M. Papadakis[1], F. Rittig[2], P. Stepanek[3], K. Mortensen[4], and K. Almdal[4] — [1]Physikdepartment E13, TU München — [2]BASF AG, Ludwigshafen — [3]Institute of Macromolecular Chemistry, Prague — [4]Risø National Laboratory, Denmark

Diblock copolymers in the melt state form a variety of mesoscopically ordered morphologies, depending on their composition and on temperature. They can thus serve as a model system for studying the dynamics in different ordered morphologies with the disordered state as a reference state.

We have studied the slow dynamics in the disordered, the lamellar, the gyroid, the hexagonal and the body-centered cubic phase combining small-angle neutron scattering, dynamic light scattering and pulsed field gradient NMR. The dimensionality of the morphology has a great influence on the dynamics: The copolymer diffusion along the interfaces is anisotropic, in contrast to the isotropic disordered phase, and collective motions like undulations of lamellar interfaces or the fluctuation of the micellar distance in the body-centered cubic state become possible.