chemisch physikalische gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag von

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Investigating multi-component polymer solutions with hybrid mesoscopic models

am Dienstag, 8. Oktober 2019, um 17:30 Uhr

Ort: Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Barrierefreier Zugang: Boltzmanngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals

Abstract

Investigating films of multi-component polymer solutions is important for basic polymer physics and technological applications, such as adhesives, coatings, lubricants, and printing optoelectronic devices. Computer simulations can significantly contribute to our understanding of complex interrelationships between structure, dynamics, and processing protocols of these materials. This understanding is crucial, e.g.for knowledge-based optimization of multi-component polymer solutions for specific applications. However, to be computationally feasible such studies frequently require mesoscopic models based on drastic simplification of original molecular structures. Here we discuss a “hybrid” strategy [1-3] where such mesoscopic particle-based models are constructed [4,5] by combining standard worm-like chain descriptions of polymers with non-bonded interactions based on functionals of local densities (order parameters). The link to a free-energy-like functional allows one to build into the model complex thermodynamic behavior in a systematic and modular way. First we validate the approach by modeling films of homopolymer melts coated on a solid substrate. The film structure in the functional-based mesoscopic model is compared with predictions of simulations performed with a “traditional” microscopic (bead-spring) model. Next we model ternary mixtures of polymer with two good solvents (solvent and cosolvent) in the dilute regime [5]. Our results demonstrate that the mesoscopic model can capture even such complex phenomena as co-non-solvency [6]. Finally, we apply the method to study films of adsorbed ternary mixtures at equilibrium with solvent vapor; a situation which is typical for solvent sorption experiments [7]. Detailed structural analysis of the adsorbed polymer layer will be presented. Interestingly, in our simulations, mesoscopic conformational properties of adsorbed polymer chains, e.g. distribution of “loops” and “tails”, match early analytical predictions [8] obtained for concentrated binary solutions. We conclude with a short outlook on further applications and methodological developments.

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Kaffee und Getränke werden bereitgestellt

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