42f Interfacial Properties and Structure of Polymer Blends and Solutions from Interfacial-Saft (Isaft) Density Functional Theory

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A multitude of industrial applications such as polymer coating and thin films, paints, separations, catalysis, wettability or emulsions have motivated studies of complex macromolecular systems (hydrocarbons, proteins, polymers) in confined geometries, and at solid-fluid and fluid-fluid interfaces. Experimental studies of such systems are difficult because of their small scale. Consequently, experimental results for interfacial properties are sparse. Molecular simulations become computationally expensive for long chain molecules and polymers, hence the need for a computationally simple, thermodynamically consistent theory for structure and thermodynamics of inhomogeneous polymeric solutions and blends.

We have recently developed a density functional theory (DFT) to describe phase behavior and microstructure of mixtures of polymeric fluids in inhomogeneous environments. We demonstrate the success of the theory in capturing the effects of size and shape of the fluid molecules and system parameters such as fluid-fluid and surface-fluid interaction strengths on fluid structure and interfacial properties. Our DFT shares a common basis with the Statistical Associating Fluid Theory (SAFT), one of the most accurate and widely used theories for bulk polymer solutions. This self-consistency of the bulk and interfacial models is crucial; it enables us to predict the interfacial properties of the considered systems with a set of molecular parameters obtained from the readily available bulk properties. Results from iSAFT are presented for interfacial tension, surface forces and molecular structure of polymer blends and solutions. They are compared with Monte Carlo simulation results, as well as with experimental data for these systems.