Prediction of Interfacial Properties of Binary Mixtures with a Density Functional Theory Based on the SAFT-VR Equation of State

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A detailed knowledge of the interfacial behaviour is required to deal with many industrial technological processes, especially those ones related to separation and extraction. However, the modelling of interfacial properties remains a challenge due to the inhomogeneous nature of the system. We develop a theoretical framework to predict the interfacial properties of mixtures of different nature and industrial interest. We use the well-known SAFT-VR [1] equation of state coupled with a density functional theory (DFT) to describe the interface. SAFT has been successfully used to describe the phase behaviour of complex fluids. Based on a rigorous statistical mechanics basis, the SAFT description is expressed as a sum of contributions to the total free energy of the system and provides a framework in which the effects of molecular shape and interactions on the thermodynamic properties can be separated and quantified. The DFT free energy functional is constructed by partitioning the free energy density into a local term (which accounts for the short-range ideal, repulsive and association interaction contributions), and a non local term (which considers the long-range dispersion interactions). Two different approaches are compared for the short-range interactions: the local density approximation (LDA) and the fundamental measure theory (FMT) [2]. The non-local term is also described following two different methodologies: a mean-field approach and a specific treatment inspired by the ideas of Toxvaerd [3]. The new methodology is used then to describe the vapour-liquid and liquid-liquid interface of a variety of non-associating and associating molecules ranging in size from small molecules to long chains, with particular attention to n-alkanes, perfluoroalkanes, carbon dioxide and water. Predictions for the interfacial tension predictions are compared with experimental data in order to check the accuracy of the method and test the different approaches made in the theory. An examination of the interfacial density and composition profiles and surface adsorption is also presented.

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