

Effect of Chain Length on Wetting Transition at Fluid Interfaces of Lennard-Jones Chains Mixtures

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The description of wetting behavior in terms of state variables (i.e temperature, pressure, composition) and conformational parameters (i.e chain lengths, interaction solvent-solute, etc) becomes relevant in various technological applications. Particularly, the variation of these properties with process conditions is one of the main factors governing the design and operation of the equipment involved in physico-chemical processes and in chemical transformations. In the present work we report predictions of sub-critical vapor-liquid-liquid equilibrium (VLLE) and interfacial properties for binary composed by tangent spherical segments of equal size. Two complementary methods, namely Molecular Dynamics simulations (MD) and Density Gradient Theory (DGT) have been used for describing the interfacial region, thus allowing predicting both the macroscopic and molecular details of mixtures exhibiting wetting behavior. DGT calculations rely on the prediction of the VLLE by means of the soft-SAFT equation of state (soft SAFT-EoS). Preliminary results show that a wetting transition along the three-phase line (from partial a total wettability) is obtained when the chain length increases, from a monomer + monomer case of type-V Lennard-Jones.