

Interfacial Properties for Phase Equilibria of Different Types and their Connection to the Phase Diagram

Jens Staubach^S, Simon Stephan^C and Hans Hasse
TU Kaiserslautern, Kaiserslautern, Germany
simon.stephan@mv.uni-kl.de

Interfacial properties of fluid mixtures in phase equilibria of different types were studied in this work: vapor-liquid (VL), liquid-liquid (LL), vapor-liquid-liquid (VLL), and gas-gas (GG) interfaces. In the phase diagram of a given mixture, different types of equilibria may occur and the phase diagram describes their relation. These relations must also play a role for the interfacial properties in the different types of equilibria, but that role is not properly understood so far, as even the basic data for their analysis is lacking. We have therefore carried out a systematic study on phase equilibria and interfacial properties of different Lennard-Jones model mixtures to elucidate these relations. All systems were studied both with molecular dynamics simulations as well as with equations of state combined with density gradient theory. The following interfacial properties were considered: surface tension, adsorption, enrichment, and interfacial thickness, and the density profiles.

Intriguing findings were obtained especially for the enrichment, which describes the height of the maximum in the interfacial density profiles of low-boiling components and is found in many systems: upon approaching a VLLE, the enrichment at a VL interface increases rapidly; the interfacial region can be considered as a precursor of the second liquid phase [1,2]. Under the influence of the gradients at the interface, the second liquid phase nucleates earlier than in the gradient-free bulk phases. The composition and density at the peak of the enrichment at the VL interface match the corresponding values of the second bulk liquid phase in the VLLE. Close to the VLLE, the thickness of VL interfaces diverges and the second liquid phase grows rapidly. It is furthermore shown, that these phenomena are closely related to the wetting behavior of the phases in the VLLE.

References

- [1] S. Stephan and H. Hasse, *Phys. Chem. Chem. Phys.* 22 (2020) 12544-12564.
- [2] S. Stephan and H. Hasse, *Mol. Phys.* 187 (2020) 1-14.