Conformal Solution Theory of Vapor-Liquid Interfaces

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In the present work, the well-known Conformal Solution Theory (CST) was extended to interfacial properties and tested using results from two independent methods: molecular dynamics (MD) simulation and density gradient theory (DGT). We focus on vapor-liquid (VL) interfaces, which are important in many applications. Different interfacial properties are studied: surface tension, adsorption, enrichment, and interfacial thickness, and the density profiles. It is shown that, for a wide range of systems including pure components and mixtures of different types, the VL interfacial properties are directly linked to the mean interactions in the liquid phase: a mono-variate dependency of the different interfacial properties on the configurational internal energy is revealed [1] - similar to the entropy-scaling principle.

This facilitates establishing a link between macroscopic phase equilibrium properties and nanoscopic interfacial properties [2,3]: a model for predicting the enrichment of components at the interface from readily available bulk VLE data was developed; it was trained only on data for simple dispersive systems. The model was then tested using the entire set of data on the enrichment available in the literature (appr. 2000 data point from 100 publications), form many different classes of mixtures. The enrichment was predicted with an average error of about only 10 %. This strongly supports the established conformal solution theory.

References

[1] S. Stephan and H. Hasse, Phys. Rev. E 101 (2020) 012802.

[2] S. Stephan and H. Hasse, Int. Rev. Phys. Chem. 39 (2020) 319-349.

[3] S. Stephan and H. Hasse, Mol. Phys. 187 (2020) 1-14.