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Mixing and Demixing Dynamics in Binary Liquid Mixtures

Anna Luisa Upterworth*, Till Hanke and Daniel Sebastiani****

*Institute of Chemistry, Martin-Luther-University Halle-Wittenberg
anna-luisa.upterworth@chemie.uni-halle.de
** Institute of Chemistry, Martin-Luther-University Halle-Wittenberg

Phase transition such as solution processes occur in a wide variety of chemical systems and therefore also cover a broad range of time scales. An easily accessible method to study and understand them are Molecular Dynamics (MD) simulations, which allow for analysis at both microscopic and macroscopic scale. However, the simple question of how far the mixing or phase separation of the components has progressed at any given moment in a MD simulation cannot be answered by most common analysis methods, as they are limited to equilibrium states.
By computing the configurational entropy of mixing ΔS based solely on the set of atomic coordinates, we are able to gain quantitative information also from non-equilibrium states[1]. This enables a more detailed and on the fly analysis of mixing and demixing processes and their dynamics. We demonstrate the potential of our approach for the semi-automatic prediction of mixing and demixing temperatures of binary liquid mixtures. In this context, we investigate the influence of system size, temperature and chemical structure of the components with a special focus on the mixing behavior of different alkanes with (per)fluorinated compounds.

[1] Hanke, T., Upterworth, A. L. , Sebastiani, D., Explicit Configurational Entropy of Mixing in Molecular Dynamics Simulations, *J. Phys. Chem. Lett.* **2024**, 15(45), 11320-11327, DOI: 10.1021/acs.jpclett.4c02819