

Predicting the Influence of Complex Solvent Environments on Thermophysical Properties

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Part I:

Functional organic materials composed of dye-based molecules that stack into various structures by non-covalent intermolecular forces have fascinating optical and mechanical properties. These novel materials are of increasing importance for many high-technology applications. There is a need for a rational design of such materials based on the engineering of dye-dye interactions and the prediction of how these interactions impact the properties of nano- or bulk state materials. Perylene di-imide derivatives (PDIs) emerged as a prototype class of molecules for the elucidation of the transition from monomeric to bulk materials via the supramolecular state. We discuss the influence of the molecular architecture and the solvent composition on the thermodynamic fingerprint of the aggregation and investigate the ability of classical molecular dynamics simulations to be used in rational materials design.

Part II:

Deep eutectic solvents (DES) are used for biocatalysis reactions more and more. Low saturation vapor pressure, low flammability as well as little toxicity are only a few advantages compared to previously used substances. Choosing the right solvent composition can lead to low viscosities with simultaneously low water activity which are required conditions for reactions and process design. In this project static and dynamic mixture properties for a DES based on choline chloride and glycerol mixed with water are investigated due to their concentration and temperature dependence using means of molecular dynamics simulations.