Biothermodynamics
Prof. Dr.-Ing. habil. Mirjana Minceva

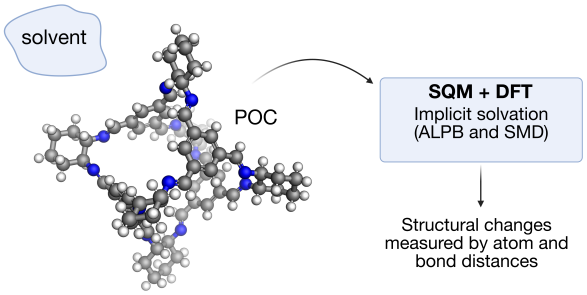
Master's Thesis

Solvent effects on the structure of porous organic cages: a computational study

Background Porous organic cages (POCs) are solid molecules that can be dissolved in a solvent in order to form *porous liquids*—combining liquid processability with permanent porosity. These materials show great promise for gas separation, storage, and catalysis applications. Some studies have suggested that solvents can dramatically alter cage structure due to pore-size changes. Understanding this effect at a molecular-level becomes crucial for the rational design of porous liquids.

Project Description This thesis will investigate how different solvents influence POC structure and CO_2 adsorption capacity at the molecular level by means of computational methods. The student will:

- Optimize cage geometries using semi-empirical quantum mechanics (SQM) and density functional theory (DFT)
- Evaluate the effect of implicit and explicit solvation on POC structure, comparing DFT calculations with nuclear magnetic resonance (NMR) measurements
- Calculate CO_2-POC binding free energies



Requirements:

- Background in physical chemistry, chemical physics, or related field
- Interest in computational chemistry and molecular modeling
- Programming experience beneficial but not required

Start date: Immediately

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