SFB TRR 102

Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

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Tuesday,
16th April 2019

at: **5.15pm**

VDP 4 1.27,
Von-Danckelmann-Platz 4
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"Configurational contribution to the Soret effect of proteins and ligands - An investigation with density-of-states simulations "

Many of the biological functions of proteins are closely associated with their ability to bind ligands and change conformations in response to changing conditions. Since binding state and conformation of a protein affect its response to a temperature gradient, they may be probed with thermophoresis. In recent years, thermophoretic techniques to investigate biomolecular interactions, quantify ligand binding, and probe conformational changes have become established. To develop a better understanding of the mechanisms underlying the thermophoretic behavior of proteins and ligands, we employ a simple, off-lattice model for a protein and ligand in explicit solvent. To investigate the partitioning of the particles in a temperature gradient, we perform Wang-Landau type simulations in a divided simulation box and construct the density of states over a two-dimensional state space. This method gives us access to the entropy and energy of the divided system and allows us to estimate the configurational contribution to the Soret coefficient. For dilute solutions of hydrophobic proteins, we find that a hard-sphere solvent model captures important aspects of protein-ligand interactions and allows us to relate the binding energy to the change in Soret coefficient upon ligand binding. To study more hydrophilic systems and compare with experimental data, we employ more complex solvent models to investigate thermodiffusion in aqueous solutions.