

Abstract Submitted  
for the OSF19 Meeting of  
The American Physical Society

**Configurational contribution to the Soret effect of a protein ligand system**<sup>1</sup> JUTTA LUETTNER-STRAETHMANN, University of Akron — 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.

<sup>1</sup>Support: Research Center Juelich and the University of Halle (DFG - SFB TRR 102)

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Date submitted: 24 Sep 2019

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