**419b Calculation of Solvation Properties Using a Combined Expanded Ensemble – Transition Matrix Monte Carlo Approach**

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Solvation properties play an important role in the design of many chemical and biological processes. Such properties help to describe the association of solute particles, phase equilibrium, nucleation properties, and are used to calculate Henry's Law coefficients. In this presentation we describe a novel approach for calculating equilibrium solvation properties (free energies, entropies, etc.) using molecular simulation. Two methods for calculating solvation properties at a given density or pressure are presented: one that provides these properties at a specific temperature and a second that enables one to obtain solvation properties over a range of temperatures. In both cases an expanded ensemble is used to gradually increase the strength of interaction between a solute particle and the solvent through a series of subensembles. Transition matrix Monte Carlo techniques are used to evaluate the relative free energy of each subensemble. Solvation free energies at a specific temperature are calculated using transition probabilities from Monte Carlo moves that attempt to transfer the system to a neighboring subensemble. Transition probabilities in two dimensions, energy (or enthalpy in the constant pressure case) and subensemble, are necessary when calculating solvation free energies over a range of temperatures Once transition probabilities are collected at a specified temperature, standard reweighting techniques are used to evaluate probabilities at different temperatures. These techniques are applied to the water-methane system as a means to examine the performance of the method.