state theory is treated with standard rigid rotor harmonic oscillator assumptions. The rovibrational properties for both transition states are obtained from CASPT2 ab initio simulations. Comparisons with experiment are made over a wide temperature range (e.g., 10 to 1000 K) for $O(^3P)$ + alkene reactions and for OH + alkene reactions.

COMP 218

Parallel tempering techniques for simulation of proteins

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Rational drug design or the pathology of amyloid diseases are only two problems whose solution requires a detailed knowledge of the relation between chemical composition and structure (and function) of proteins. Despite decades of research, both experimental and in silico, this relationship is still only partially understood. Computer experiments offer one way to evaluate the sequence-structure relationship and the folding process but are extremely difficult for detailed protein models. This is because the energy landscape of all-atom protein models is characterized by a multitude of local minima separated by high energy barriers. Only over the last few years have been algorithms developed that allow one to overcome this multiple-minima problem in protein simulations. Prominent examples of these new techniques are parallel tempering and other generalized-ensemble sampling techniques. In the present talk I will focus on parallel tempering (also known as replica exchange sampling). I will discuss the underlying ideas behind this approach, its implementation to Monte Carlo and Molecular Dynamics, and strategies for further advancement of this popular approach. Recent results from folding simulations of small proteins (of order 50 residues) will illustrate the power of improved parallel tempering simulations.

COMP 219

Extracting averages and distributions from replica exchange simulations of large systems: A new version of WHAM

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