



SCHOOL OF NATURAL SCIENCES CHEMISTRY SEMINAR 291

Obtaining Accurate QM/MM Free Energies Using Novel Sampling and Reweighting Approaches

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ABSTRACT

To accurately compute free energies of complex condensed phase systems there are two key prerequisites: the accurate description of inter- and intramolecular interactions, and adequate sampling of all relevant conformational degrees of freedom. The hybrid quantum mechanical / molecular mechanical (QM/MM) framework is the current tool of choice when accurate computations of macromolecular systems are essential. However, robust and efficient approaches that employ the high levels of computational theory needed to accurately describe highly polarizable systems (i.e., ab initio, DFT), while also including explicit solvation effects and accounting for extensive conformational sampling are essentially non-existent. Herein, we describe new methods that greatly improve both the accuracy and efficiency of carrying out QM or QM/MM free energy simulations. Initially, these have been applied to calculate solvation free energies and free energy profiles along reaction paths.

BIO:

H. Lee Woodcock received degrees in Chemistry and Biology from Appalachian State University. Subsequently, a PhD in computational quantum chemistry was awarded under the direction of Prof. H.F. Schaefer from the University of Georgia. An extended post-doctoral fellowship followed at that the National Institutes of Health under the direction of Dr. Bernard Brooks. During this time, work primarily focused on the development and application of QM/MM approaches (specifically working on CHARMM and Q-Chem software packages); this continues to be a major focus of research in the Woodcock Group. However, work has also expanded in the area of drug discovery and development of web-based interfaces for biomolecular computation. Additionally, Prof. Woodcock also serves as Program Chair for the ACS Division of Computers in Chemistry.