

Quantum Mechanics and Molecular Mechanics for Hydrogen Bonds

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Hydrogen bonds, weak intermolecular interactions of the type AH-B pervade biology and are important in many areas of materials science. The lecture will center on the structure, energetics and dynamics of systems containing hydrogen bonds. In order to take account of complex environments, whether one is studying reactions on ice, in water, or in biology one needs to consider models that go beyond the practical limits of quantum chemistry, on the one hand, and molecular dynamics, on the other. Hybrid, so-called QM/MM (Quantum mechanics/Molecular Mechanics), methods are being developed. I will present an overview of Density Functional Theory to demonstrate the performance of different functionals in the context of a variety of hydrogen-bonded systems. At the present time the “meta-GGA” functionals which involve the Laplacian of the density and the kinetic energy density represent the state of the art. The importance of polarization effects will be brought out and I will discuss some molecular mechanical methods that take these into account. Time permitting, the question of efficient sampling during simulations will be discussed using the example of formamide-water to illustrate a hybrid approach in which two Markov chains are used, one using quantum mechanics (DFT) to calculate accurate energies and a second one based on a rapid evaluation using polarized molecular mechanics to guide the sampling.