Molecular simulations of enzyme catalysis

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An important goal of computational and theoretical biochemistry is helping elucidate how enzymes achieve their catalytic efficiency. The differing length and time scales of processes that contribute to catalysis, however, makes this a challenging task for molecular simulation techniques. An approach that has proved particularly powerful for the investigation of the chemical steps in enzymatic and other condensed phase reaction processes is the use of hybrid quantum chemical (QC) and molecular mechanical (MM) potentials. This talk will introduce the concept of a hybrid potential and will discuss their application to the simulation of a number of enzyme systems.