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Ab initio Free Energies of Enzymatic Reactions Using Model Potentials EDINA ROSTA, ARIEH WARSHEL, University of Southern California, Department of Chemistry, Los Angeles, CA — In order to reliably model biological reactions in solutions and in proteins one has to use both high accuracy ab initio models and proper averaging over the configurations that determine the free energy. In our group, previously the Empirical Valence Bond (EVB) method was often applied successfully to determine reaction free energy profiles in proteins and in water solution. In the current work we would like to combine the advantages of the fast extensive sampling with EVB method and the accuracy of the ab initio Density Functional Theory (DFT) for Quantum Mechanics / Molecular Mechanics (QM/MM) modeling. The free energy profiles of the catalytic reaction of the dehalogenase enzyme in the protein environment and the corresponding water reaction are studied by both the reference EVB approach and the ab initio QM/MM method. Ab initio QM/MM reaction free energies and activation energies are presented in both environment utilizing the model potential.

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