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Stochastic QM/MM Models for Proton Transport in Condensed Phase: An Empirical Valence Bond (EVB) Approach ANTON BURYKIN, University of Southern California, Department of Chemistry, SONJA BRAUNSAND, University of Southern California, Department of Chemistry, ARIEH WARSHEL, University of Southern California, Department of Chemistry — Proton transport (PT) plays a major role in biophysics in general and bioenergetics in particular. In view of the crucial role of biological PT processes it is important to gain a quantitative molecular understanding of the factors that control such processes. While modeling actual time-dependent PT in biological systems one has to deal with up to microsecond time scales which are not accessible to QM/MM methods. In order to overcome this problem we have developed a new type of hybrid quantum/classical approach which combines explicit QM (EVB) representation of the chain of donor and acceptors and implicit representation (via the effective coordinates) of the environment (the rest of the protein/water system). The dynamics of the whole QM/MM system is described by stochastic (langevin) equations. This model takes into account the correct physics of proton charge delocalization and the reorganization of solvent polar groups during the PT process. The description of QM/MM langevin dynamics method is given and several applications to biological systems (PT in Gramicidin A channel and Carbonic Anhydrase) are presented.

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