



REACTION DYNAMICS OF MULTIPOLE PROTON TRANSFER

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Reaction dynamics of proton transfer is one of most fundamental and important topics in chemistry. Multiple proton transfer is an essential process in the proton relay in enzyme, protropic tautomerization, proton transfer in water, etc., however detailed dynamics of these process is not very well understood yet. In order to understand dynamics of the multiple proton transfer in detail, it is necessary to obtain global potential energy surface (PES) of the reaction, but it is very difficult or requires great effort and huge amount of computing time to get the multidimensional PES of large molecular systems. Direct dynamics and recently developed MCMM methods have been applied to study the multiple proton transfer in several hydrogen bonded clusters, and the results will be presented.

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