TCI SEMINAR

Hydrogen Exchange Tunnelling: Large Curvature Reaction Path Dynamics

Monday, October 5, 2009
3:30 p.m. Room 8335

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Hydrogen exchange tunnelling processes are ideal for studying the role of intramolecular vibrational energy redistribution in chemical processes through the vibrational dependence of tunnelling splittings. The interpretation of the results requires a detailed model of the underlying quantum dynamics, for which the Reaction Path Hamiltonian (RPH) would appear particularly suitable. However, the RPH constitues an approximation with fundamental limitations in the case of strongly curved paths, which are typical for Hydrogen exchange tunnelling. I will discuss an alternative non-orthogonal representation of the Hamiltonian that has an exact variational limit for all curvatures, is stable with respect to variations of the path and can in principle treat bifurcating paths.

Theoretical Chemistry Institute Seminar Series