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Two- and three-state conical intersections in complex systems
SPIRIDOULA MATSIKA, Temple University, KURT KISTLER, ZONGRONG XU, AKIHIKO YOSHIKAWA — Nonadiabatic processes play an important role on the excited state dynamics of chemical systems. Conical intersections (actual potential energy surface crossings) of two states have been established to facilitate nonadiabatic processes of molecules and radicals in the gas phase. More recently three-state conical intersections have made their appearance and may also play a key role in nonadiabatic processes. Here we present studies where the importance of conical intersections is being investigated in photoinitiated processes of biologically relevant systems, and particularly the nucleobases and their analogs. Large scale ab initio multireference configuration interaction methods (MRCI) are being used. Our results show the presence of many seams of two- or three-state conical intersections that can complicate the potential energy surfaces and dynamics of these systems. Solvent effects on conical intersections are first being investigated using clusters of water with the system. A mixed quantum mechanical/ classical mechanical (QM/MM) approach where the solute is described with the MRCI method will also be presented as a means to study the effect of the solvent on excited states.

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