

Internal Webinar

Effect of Inter-system Crossing in bimolecular collision reactions and Exciton transfer Using a Mapping Hamiltonian

Mrinmoy Mandal

University of Hawai'i Manoa, USA

Non-adiabatic dynamics simulations have rapidly become an essential tool for understanding the many key molecular processes in the field of chemistry, specially, approaches that involve intersections between neighboring electronic states of different spin multiplicity. So, I will discuss about the effect of intersystem crossing in $C(^3P) + SiH_4$ reaction, though SOC is reasonably small for molecules involving first, second and third row atoms of the periodic table.

In the recent past years organic semiconductors have become widely used materials in electronic devices and exciton transfer plays an important role. I will talk on exciton transfer between the dimer using a Mapping Hamiltonian.

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10:00 AM

