TIFR Centre for Interdisciplinary Sciences
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Seminar

Localized Operator Partitioning Method for Electronic Energy Transfer

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A fundamental understanding of electronic energy transfer (EET) is crucial, as EET plays a central role in natural processes such as photosynthesis, as well as in technological applications like solar cells and light emitting diodes. A key gap in our understanding of EET results from the lack of a reliable first-principles tool that can 1) spatially partition the electronic energy of a system into its fragments, 2) partition in a fragment-additive manner at all inter-chromophoric distances, 3) account for electron indistinguishability and 4) have the ability to interpret the fragment energies in terms of one- and two-electron contributions in a straightforward manner. We present the localized operator partitioning method (LOPM) - an electronic fragment Hamiltonian that possesses all the features above - that enables us to obtain the fragment energy in EET dynamics using any time-dependent electronic wave function or electron density. However, the implementation of the local operator for realistic chromophoric systems is non-trivial because of the difficulties in real space partitioning of one- and two-electron integrals. I discuss some of these challenges and our strategies to overcome them. As a first application to revealing electron-nuclear dynamics of EET, I will then present our recent results on static and dynamic applications of LOPM on bichromophoric systems.

Thursday, Aug 18th 2016

4:00 PM (Tea/Coffee at 3:45 PM)

Seminar Hall, TCIS