Describing the Excited States in Organic Optoelectronics

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Understanding the dynamics of excited state (exciton) in organic condensed phase is very challenging because a large number of relevant processes (exciton diffusion/relaxation/dissociation, singlet fission) take place in less than 1 ps and, therefore, one cannot study them as incoherent energy transfer events between localized states (using Förster or Dexter theory). As many processes involve fairly delocalized states it is also essential to model large portions of the system of interest. Alongside the quantum coherence one should also consider the weak intermolecular interaction between molecules and the strong exciton-phonon coupling that make the dynamics of the exciton strongly coupled with that of the nuclei. One needs at the same time an accurate description of the electronic structure of a relatively large system and a theory for the exciton quantum dynamics for the same system.

In this presentation, I will introduce our recent works on methodological developments for both large scale electronic structure calculations and quantum dynamics simulation based on the renormalization group theory as well as their application for studying exciton generation/migration/dissociation /emission in organic optoelectronics.

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