Multireference Study of Charge and Energy Transfer in Organic Semiconductors

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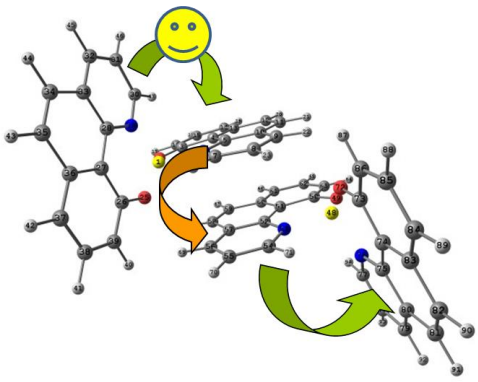
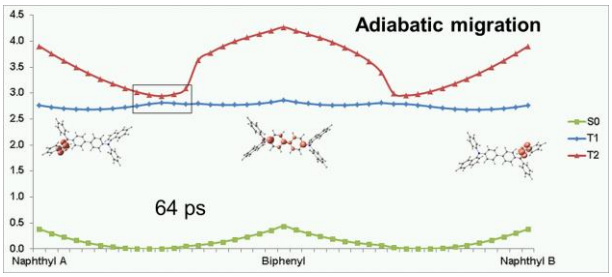
Transfer of charges and energy in organic semiconductor layers implies that the hopping quasiparticles (electrons, holes, or excitons) are localized within relatively small regions, such as small molecules or molecular fragments. However, band-like charge transport can be a key to high mobility in organic semiconductors. Charge and exciton migration is assisted by nuclear motion, and intra- and intermolecular vibronic interactions play an important role in the hopping process. Therefore, understanding how molecular structure and molecular packing affect charge and exciton localization and migration in organic semiconductors may help one in the design of efficient emissive and high-mobility transport layers. Multireference ab initio methods give a reliable tool for distinguishing between different localizations of charges or excitons, because they make it possible to treat equally important states on equal grounds. We propose a computational procedure based on CASSCF/XMCQDPT calculation to track the charge or exciton transfer path and to elucidate the role of vibrational modes in the hopping process. The examples of some typical emissive, electron- and hole-transporting materials are considered.





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