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Exciton fission, dissociation and transport in organic conjugated materials: Modeling insights

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Electronic excited states in conjugated organic materials involve an admixture of localized (Frenkel-like) and charge-transfer (CT) excitations. We will first review some recent modeling work showing that this mixed Frenkel-CT character steers the Davydov splitting, mediates singlet fission and prompts triplet energy migration in oligoacenes crystals. Ultrafast and efficient charge separation occurs at interfaces between properly designed molecular donors and acceptors, despite the large electron-hole Coulomb binding energy. In a second part of the talk, we will describe the various mechanisms for such a dissociation process and assess them from atomistic simulations based on a combination of force-field, quantum-chemical and model Hamiltonian calculations.