Quantum Dynamics Simulations Exploring the Influence of Quantum Beats on Excitation Energy Transfer and Charge Separation Dynamics in Extended Light Harvesting Systems

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We use partial linearized density matrix (PLDM) propagation to explore excitation energy transfer and charge separation dynamics in an extended dissipative model of Photo System II (PSII). Our studies include excited state energy transfer inside the CP47 and CP43 light harvesting complexes, between the CP47/CP43 complexes and the reaction center (RC), and finally the dynamics of conversion of excitation energy to charge separation inside the RC complex. Parts of our model pathways involve strongly coupled pairs, or dimers of chromophores that often act as intersections between transmission paths composed largely of monomers. These dimers give rise to quantum beats and we explore their influence on the partitioning of amplitude flow between different intersecting pathways for realistic parameterization of the pigment-protein environment coupling as well as the influence of static site disorder in our model. Time permitting we will also present new results exploring excitation energy transfer pathways in the PC645 system where we find that dissipation to high frequency vibrational modes plays a key role in determining the dominant pathway for energy transfer through this extended complex.