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First-Principles Studies of the Excited States of Chromophore Monomers and Dimers SAMIA HAMED, University of California at Berkeley, SAHAR SHARIFZADEH, Boston University, JEFFREY NEATON, University of California at Berkeley — Elucidation of the energy transfer mechanism in natural photosynthetic systems remains an exciting challenge. Through the careful analysis of excited states on individual chromophores and dimers – and the predictive first-principles methods used to compute them – we are building towards an understanding of the nature of excitation transfer among arrays of chromophores embedded in protein environments. Excitation energies, transition dipoles, and natural transition orbitals for the important low-lying singlet and triplet states of experimentally-relevant chromophores are obtained from first-principles time-dependent density functional theory (TDDFT) and many body perturbation theory. The effect of the Tamm-Dancoff approximation and the performance of several exchange-correlation functionals, including an optimally-tuned range-separated hybrid, are evaluated with TDDFT, and compared to MBPT calculations and experiments. This work has been supported by the DOE; computational resources have been provided by NERSC.

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