Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-Principles Studies of the Excited States and Optical Properties of Xanthene Derivative Chromophores[1] SAMIA HAMED, UC Berkeley Department of Chemistry, SAHAR SHARIFZADEH, Molecular Foundry at LBNL, JEFFREY NEATON[2], UC Berkeley Department of Physics — Elucidation of the energy transfer mechanism in natural photosynthetic systems remains an exciting challenge. In particular, biomimetic protein-pigment complexes provide a unique study space in which individual parameters are adjusted and the impact of those changes captured. Here, we compute the excited state properties of a group of xanthene-derivative chromophores to be employed in the construction of new biomimetic light harvesting frameworks. Excitation energies, transition dipoles, and natural transition orbitals for the low-lying singlet and triplet states of these experimentally-relevant chromophores are obtained from first-principles density functional theory. The performance of several exchange-correlation functionals, including an optimally-tuned range-separated hybrid, are evaluated and compared with many body perturbation theory and experiment. Finally, we will discuss the implication of our results for the bottom-up design of new chromophores.

[1]This work is supported by the DOE and computational resources are provided by NERSC.
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Date submitted: 14 Nov 2013 Electronic form version 1.4