Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic coherence and the kinetics of energy transfer in light-harvesting systems PENGFEI HUO, University of Rochester, DAVID COKER, Boston University, THOMAS MILLER, Caltech — Recent 2D-spectroscopy experiments have observed transient electronic coherence in natural and artificial light harvesting systems, which raises questions about the role of electronic coherence in facilitating excitation energy transfer (EET) processes. In this talk, we introduce the recently developed partial linearized path-integral (PLPI) method, which can accurately simulate exciton transfer dynamics across multiple reaction regimes, as well as reliably describe the electronic coherence among excitonic states. Further, we develop a strategy that enables the analysis of the relative impact of static and dynamic electronic coherence. With PLPI simulations, we find that energy transfer dynamics are almost entirely dominated by static coherence effects; dynamic coherence is found to cause only minor effects. These conclusions are consistent with the historical view that emphasizes the importance of energy-level alignment for efficient incoherent energy transfer,while suggesting a less important role for more exotic electronic coherence effects that have been recently emphasized.

Pengfei Huo
University of Rochester

Date submitted: 05 Nov 2015 Electronic form version 1.4