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Quantum-classical master equation approach to energy transfer dynamics in multichromophoric systems AARON KELLY, Dalhousie Univ, WILLIAM PFALZGRAFF, ANDRES MONTOYA-CASTILLO, THOMAS MARKLAND, Stanford University — Quantum-classical and semiclassical dynamics methods offer a hierarchy of rigorous approaches to treat non-equilibirum condensed phase relaxation processes, such as electronic excitation energy transfer in multi-chromophore systems. Each tier of this hierarchy offers a different balance between accuracy and computational cost. However, for problems containing large numbers of degrees of freedom, or that involve many quantum states, or where an ab initio treatment of the electronic states is required, only the lowest tiers of this hierarchy are likely to be practical due to computational limitations. In this talk I will discuss our recent work related to combining these methods with the generalized quantum master equation (GQME) framework. In many cases these techniques can be made both more accurate and more efficient, allowing large systems to be simulated with good accuracy. I will demonstrate the abilities and benefits of this approach in describing electronic energy transfer processes in multi-chromophoric light harvesting systems, such as LHC-II, and in developing new theoretical tools for modeling nonlinear optical spectra.

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