Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Calculating exciton downconversion rates in Coulombically coupled chromophores CRAIG CHAPMAN, GEORGE SCHATZ, Northwestern University — Exciton downconversion is a second order energy transfer process that splits a high energy exciton in a donor chromophore into multiple lower energy excitons in acceptor chromophores. Downconversion has been seen in a variety of materials including rare-earth doped glassy matrices, organic crystals, and semiconductor nanocrystals, and has the potential to efficiently convert a single high energy photon into a broad distribution of lower energy excitons. A comprehensive mechanistic understanding of the energy conversion process will allow for the rational engineering of materials that can control the flow of energy in a guided fashion. To this end we formulate and implement a method for calculating multi-chromophore Förster-like exciton transfer rates using transition charges obtained from time-dependent density functional theory.

Craig Chapman
Northwestern University

Date submitted: 14 Nov 2014 Electronic form version 1.4