Abstract for the 2013 Sanibel Symposium

Computational Modeling of Electronic Energy Transfer between Silicon Quantum Dots Using the Foerster Theory

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Recent work has shown that Foerster resonance energy transfer (FRET) theory provides a useful tool for studying excitation energy transfer between spherical quantum dots (QDs) [1]. We calculate FRET rates for pairs of interacting crystalline $Si_{29}H_{36}$ and $Si_{35}H_{36}$ QDs and investigate how the addition of Al and P dopants or Ag adsorbates [2,3] affects electronic energy transfer. The ensemble spectral overlap between donor emission and acceptor absorption spectra are obtained from time-dependent DFT with the HSE functional and compared with available theoretical results [1,4]. Using the dipole-dipole approximation and an average over orientations, energy transfer rates of pure silicon QDs were found to be on the order of 10^{-5} ns^{-1}. Doping with either Al or P increased the excitation transfer rates by multiples of 10 to 100, partly as a result of stronger electronic coupling due to larger transition dipole moments. In addition, QDs doped in their center were found to have larger excitation transfer rates than QDs doped on their surface. The effect of QD relative orientations on transfer rates is also studied. The excitation energy transfer rates are computed as functions of inter-dot distance and compared with treatments coupling electronic density fluctuations [5] to evaluate the accuracy of the dipole-dipole approximations used in this work. We conclude that the addition of n-type and p-type dopants, or of Ag adsorbates, has the potential to enhance energy transfer between pairs of Si QDs.

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Work partly supported by the National Science Foundation, Chemistry Division, by the Dreyfus Foundation, and by the University of Florida High Performance Computing facility.