Computational Modeling of Electronic Energy Transfer between Oriented Silicon Quantum Dots with Adsorbates and Dopants

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Electronic energy transfer rates K_{EET} between selected pairs of crystalline silicon quantum dots (SiQDs) systems, either bare, doped with Al or P, or with adsorbed Ag, have been calculated and analyzed to extend previous work [1] on light absorption of QDs . The effect of their relative orientation on energy transfer rates for each system has also been considered. Using Time-Dependent Density Functional Theory and the hybrid functional HSE06 [2], the Foerster resonance energy transfer (FRET) treatment [2,3] was adopted in a model for calculating electronic energy transfer rates under the dipole-dipole interaction approximation. Calculations with adsorbed Ag show that: (a) addition of Ag increases rates up to ten times; (b) collinear alignment of permanent dipoles increases transfer rates by an order of magnitude compared to parallel orientation; (c) there is a red-shift in the absorption spectra; and (d) smaller QD-size increases transfer due to a greater electronic orbital overlap. Calculations with dopants show that: (a) p-type and n-type dopants enhance energy transfer up to two orders of magnitude; (b) surface-doping with P and center-doping with Al show the greatest rates; and (c) K_{EET} is largest for collinear permanent dipoles when dopant is on the outer surface and for parallel permanent dipoles when dopant is inside the QD.

1. D. M. Stewart, M. G. Mavros, and D. A. Micha, J. Phys. Chem. C, 2012, *116*, 2310.
2. H. Freitag, M. G. Mavros, and D. A. Micha, J. Chem. Phys. 137, 144301 (2012).
3. R. Baer and E. Rabani, J. Chem. Phys. 128, 184710 (2008).