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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.

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