

Abstract Submitted
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Electron hopping between Wurtzite CdSe Quantum Dots Linked by Molecules¹ IEK-HENG CHU, Dept of Physics and QTP, Univ of Florida, MARINA RADULASKI, Dept of Physics, Univ of Belgrade, Serbia, NENAD VUKMIROVIC, Lawrence Berkeley National Lab, HAI-PING CHENG, Dept of Physics and QTP, Univ of Florida, LIN-WANG WANG, Lawrence Berkeley National Lab — Recent experimental results show that the transport properties of quantum dot (QD) arrays will be tremendously improved after attached by cross-linking molecules. Here, we present an *ab initio* study on the electron hopping rates between wurtzite CdSe QDs connected by Sn₂S₆ molecules. The conduction band minima (CBM) transports among connected QDs are calculated. The charge patching method (CPM) is used to construct the charge density of the QDs and the connected systems. The folded spectrum method (FSM) was applied to find the band edge states and the electronic coupling between the neighboring QDs. Electron-phonon couplings are calculated to yield the reorganization energy. The electron hopping rate is then calculated by Marcus theory and its corresponding quantum treatments. Hopping rates for three different sizes of QDs, and two different types of molecular attachments are also presented here for comparison.

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