Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Band transport of PbS quantum dot superlattices YUN LIU, NOLAN PEARD, JEFFREY GROSSMAN, Massachusetts Institute of Technology — The efficiency of PbS based quantum dot (QD) photovoltaics (PV) has risen to the current record of 11.3%. However, continued increase in QDPV efficiency requires substantial improvements in the electronic transport within QD films. Recent reports of bandlike transport in QD superlattices have been shown to enhance carrier mobility due to increased coupling and reduced energetic disorder. In this work, we systematically investigated the effects of ligands and packing geometry on the transport properties of PbS QD superlattices. Treating each QD as a pseudo-atom, conductivities were calculated using density functional theory and Boltzmann transport theory as a function of their various lattice arrangements. Our results show that shorter atomic ligands enhance transport properties compared to longer organic ligands. We also find that higher packing density does not always increase the conductivity; rather the specific coupling facet is also important. Coupling through {100} facet in the simple cubic lattice enhances the conductivity by around 50% compared to coupling through {111} facet in body centered cubic configuration. The improved understanding allows us to design superlattice based devices that further enhance the carrier mobilities and improve the PV efficiency

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Date submitted: 11 Nov 2016 Electronic form version 1.4