Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Towards the Ultimate Limit of Connectivity in Quantum Dots with High Mobility and Clean Gaps HUASHAN LI, DAVID ZHITOMIRSKY, SHREYA DAVE, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Colloidal quantum dots (CQDs) are especially promising for commercial electronic and optoelectronic applications, yet there is a considerable lack of fundamental understanding of their electronic structure as they couple within thin films. In this work, we applied a combination of computational and experimental techniques to gain insight into the impact of connectivity in CQD assemblies. High Resolution Transmission Electron Microscopy demonstrates that a range of connectivity between dots in the film is attainable by tuning the CQD size and ligand treatment. These results were complemented by ab-initio simulations within the phonon-assisted charge hopping scenario. We find that both the orbital hybridization and interfacial dipole moment can change the electronic structure substantially; thus, control over the interface structure beyond stoichiometry is necessary to eliminate trap states. In addition, carrier mobility has a strong dependence on the type of connectivity (i.e., bridge vs. necking), the connectivity orientation, carrier energy, and defect states. Based on our calculations, we propose a scheme for improved carrier mobility, by necking the dots for the advantage of large electron coupling, followed by excess I ligand passivation to recover the wavefunction delocalization.

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Date submitted: 02 Nov 2015 Electronic form version 1.4