Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Defect states and charge transport in quantum dot solids[1]
NICHOLAS BRAWAND, MATTHEW GOLDEY, Institute for Molecular Engineering, University of Chicago, MARTON VOROS, Materials Science Division, Argonne National Laboratory, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago and Materials Science Division, Argonne National Laboratory —
Defects at the surface of semiconducting quantum dots (QD) give rise to electronic states within the gap, which are detrimental to charge transport properties of QD devices. We investigated charge transport in silicon quantum dots with deep and shallow defect levels, using ab initio calculations and constrained density functional theory.[1] We found that shallow defects may be more detrimental to charge transport than deep ones, with associated transfer rates differing by up to 5 orders of magnitude for the small dots (1-2 nm) considered here. Hence our results indicate that the common assumption that the ability of defects to trap charges is determined by their position in the energy gap of the QD, is too simplistic, and our findings call for a reassessment of the role played by shallow defects in QD devices. Overall, our results highlight the key importance of taking into account the atomistic structural properties of QD surfaces when investigating transport properties. [1] N. P. Brawand, Matthew B. Goldey, Marton Voros, and Giulia Galli, submitted

[1]Center for Hierarchical Materials Design, funded by National Institute of Standards and Technology 70NANB14H012; Center for Advanced Solar Photophysics, funded by the U.S. Department of Energy (DOE); and U.S. DOE, Contract No. DE-AC02-06CH11357

Nicholas Brawand
Institute for Molecular Engineering, University of Chicago

Date submitted: 10 Nov 2016 Electronic form version 1.4