Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Asymmetric tunneling rates for electrons and holes at CdSe quantum dot/carbon nanotube interfaces[1] SOHRAB ISMAIL-BEIGI, JIE JIANG, Yale University — Decorating carbon nanotubes with CdSe quantum dots (QDs) is one potential approach for creating high efficiency photovoltaics. Our collaborators at Yale recently produced a ligand-free covalent attachment of CdSe QDs to carbon nanotubes through an organic ligand exchange mechanism. Our prior first principles work described the energetics of the various binding processes and rationalized the experimental growth methodology. After a brief review of the system, we will describe our intriguing finding that excited electrons and holes tunnel with different rates out of the QD and into the carbon nanotubes. The asymmetric tunneling rate itself can, in principle, boost the separation of photo-excited charge at the interface even if there are insufficient band energy differences across the interface. We describe our results for the tunneling rates computed using (i) a brute force approach with increasing simulation cell size to remove periodic effects, and (ii) a Green's function method that directly connects the QD to a thermodynamically large electron reservoir (e.g., a very long pristine nanotube).

[1]Supported by NSF SOLAR DMR 0934520

Sohrab Ismail-Beigi
Yale University

Date submitted: 14 Nov 2013 Electronic form version 1.4