MAR14-2013-007584

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Modeling Charge Mobility in Nanoparticle Solar Cells[1]

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Nanoparticle (NP) solar cells show the promise to enhance the efficiency of solar cells over the Shockley-Queisser limit due to quantum confinement enhanced charge multiplication processes [1]. A fundamental challenge of NP solar cells, however, is that the very reason that leads to enhanced charge generation also tends to hinder charge transport. To address this challenge, we outline a multi-scale transport modeling scheme based on our previous calculations [2] that involves determining NP parameters from ab-initio and semi-empirical calculations, such as energy level structures, charging energies. This is then embedded in a Kinetic Monte Carlo hopping transport framework to calculate electron and hole mobilities in NP devices as a function composition, disorder, temperature. As a first demonstration, we apply our method to PbSe NP Schottky devices.

Work done in collaboration with Ian Carbone, Physics Department, University of California, Santa Cruz and Marton Voros, Physics Department, University of California, Davis.

[1] Matthew C. Beard et al., Acc. Chem. Res. 46, 1252 (2013).
[2] Ian Carbone, S.A. Carter, G.T. Zimanyi, accepted in J. of Appl. Phys.

[1]Work supported by NSF-Solar DMR-1035468.