Abstract for the 2015 Sanibel Symposium

Density Matrix Theory and Modeling of Photomobilities at Nanostructured Semiconductor Surfaces: Thickness Dependence for Si Slabs from Electronic Band States

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A reduced density matrix formulation of photoconductivity allows for the interaction of electron and hole currents with medium phonons and excitons. We report on a new implementation of the theory using electronic band states obtained from an energy-gap corrected DFT, and voltage induced electronic displacements. This allows calculation of the mobilities of photoexcited particles in Si(111) slabs for varying thickness, generated by supercells of octahedral symmetry, with and without adsorbed Ag clusters [1]. Populations of photoexcited states are found using steady state solutions to the reduced density matrix in a rotating wave approximation [2]. The adsorption of Ag nanocluster creates long lived localized electronic excitations that increase the overall absorbance of the system by preventing charge carrier recombination, and increases hole conductivity [3]. We explore the effects of changing slab thickness on the photomobility of electrons and holes.

Work partly supported by the NSF (USA) and by the HPC computing facility of the University of Florida.

[1] Tijo Vazhappilly and D. A. Micha, J. Phys. Chem. C **118,** 4429, (2014)

[2] D .S. Kilin and D.A. Micha, J. Phys. Chem. C **113**, 3530 (2009)

[3] Robert Hembree and D.A. Micha, J. Chem. Phys. **138**, 184708 (2013)

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