Abstract for the 2014 Sanibel Symposium

Calculation of electronic photomobilities at a Si(111) nanostructured surface with adsorbed Ag clusters

Robert Hembree II , Tijo Vazhappilly*, and David A. Micha

Departments of Chemistry and of Physics
Quantum Theory Project, University of Florida
Gainesville, Florida 32611, USA

Building on previous work we extend a semiclassical treatment of mobility in semiconductors [1] to include photoexcited materials, to extract electron and hole photomobilities at Si(111) surfaces with and without adsorbed Ag clusters. This approach uses *ab initio* energy bands and orbitals generated from DFT with the PBE and HSE functionals in a plane wave basis for models of Si slabs involving large atomic supercells [2]. In our previous work we found that the addition of Ag nanoclusters creates long lived localized electronic excitations that increase the overall conductivity of the system by preventing charge carrier recombination [3]. Those results used calculated photoexcited electronic populations and available mobilities for unexcited bulk silicon. The present results contain the photoinduced mobilities along with the photoexcited electronic populations in a full semiclassical calculation of the photoconductivity. The semiclassical treatment will be described and results will be presented on changes to the photoconductivity from adding Ag clusters to the Si surface.

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

[1] N.W. Ashcroft and N.D. Mermin, *Solid State Physics*, 1st ed. (Holt, Reinhart and Winston, Philadelphia, 1976).

[2] Quantum Espresso software package. P. Giannozzi, et al J.Phys.:Condens.Matter, 21, 395502 (2009)

[3] R. Hembree II , T. Vazhappilly*, and D. A. Micha, Sanibel Symposium Poster presentation (2013)

* Present address: Chemistry Department, University of Pittsburg, USA.