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Treatment of electronic photomobilities at a Si(111) nanostructured surface with adsorbed Ag clusters using electronic band structure[1]
ROBERT HEMBREE, Quantum Theory Project, Department of Physics, University of Florida, TIJO VAZHAPPILLY, Chemistry Department, University of Pittsburg, DAVID MICHA, Quantum Theory Project, Department of Chemistry and Physics, University of Florida — We report on a new treatment for computing the mobilities of photoexcited particles at Si(111) surfaces both with and without adsorbed Ag clusters. Building on previous work we develop a treatment for the mobility of photoexcited electrons and holes based on *ab initio* electronic band structure generated from generalized gradient functionals (PBE and PW91) in a plane wave basis involving large atomic supercells. Populations of photoexcited states are found using steady state solutions to the reduced density matrix in a rotating wave frame approximation. Our previous work found that the addition of Ag nanocluster creates long lived localized electronic excitations that increase the overall absorbance of the system by preventing charge carrier recombination. We explore the effects of the adsorption of the Ag cluster on the photomobility of the system due to increasing hole mobility.

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Robert Hembree
Quantum Theory Project, Department of Physics, University of Florida

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