Abstract for the 2013 Sanibel Symposium

Time Dependent Photoconductivity at Nanostructured Silicon Surfaces From a Dissipative Kinetics Model With Ab Initio Electronic Parameters

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We report on a treatment of photoconductivity based on density matrix calculations of photoexcited electronic populations with *ab initio* electronic parameters which are then applied to a kinetics treatment of conductivity involving photoexcited electrons in delocalized and localized states [1-3]. This leads to an extension of the Drude treatment of conductivity for delocalized electrons, and of the Drude-Lorentz treatment for localized electrons [4]. An atomic structure model of Si(111):H with an adsorbed Ag_3 planar nanostructure on the surface is created and modeled using DFT to get input parameters for the kinetics treatment [1]. Under photoexcitation by visible light some electrons will excite and localize to the nanostructure while other electrons will excite within the Si slab forming particles and holes. Calculated photoexcited population densities are derived from reduced density matrix diagonal elements, solutions from equations of motion including dissipative dynamics. Preliminary results are presented for the conductivity vs light wavelength and vs applied voltage.

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Work partly supported by the National Science Foundation, Chemistry Division, and by the University of Florida High Performance Computing facility.