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**Electronic relaxation of a photoexcitation of AgSi(111):H surface**[1]

DIMITRI KILIN, DAVID A. MICHA, University of Florida — A combination of time dependent density matrix and *ab initio* electronic structure methods provide details of the relaxation pathways of photo-induced charge redistribution at nanostructured semiconductor surfaces, giving their changes in energy and space over time. They are applied to a Ag cluster on a Si(111) surface, initially photoexcited by a short pulse, and show that the Ag cluster adds surface-localized states that enhance electron transfer. Population density distributions in energy and in space, for valence and conduction bands, explore the energy band landscape of a Si slab, with various relaxation pathways ending up in a charge-separated state, with a hole in the Si slab and an electron in the adsorbed Ag cluster. Calculated electronic relaxation times for Si(111):H are of the same order as experimental values for similar semiconductor systems. We have also noticed that average non-adiabatic coupling and transition dipoles have similar dependence on numbers of orbitals involved in transition. Results from a reduced density matrix propagation with Hamiltonian and rates parametrized from *ab initio* electronic structure calculations give new insight on electronic dynamics at nanostructured surfaces.

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