

Abstract Submitted
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Electronic relaxation at a photoexcited nanostructured Si(111) surface¹ 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 Ag₃ cluster on a Si(111) surface, initially photoexcited by a short pulse, and show how surface-localized states added by the Ag cluster 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. Results from a reduced density matrix propagation over time, with Hamiltonian and rates parametrized from *ab initio* electronic structure calculations, give new insight on electronic dynamics at nanostructured surfaces.

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