Abstract Submitted
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Short time evolution of electronic charge transfer and separation, and quantum coherences, at photoexcited crystalline and amorphous Si surfaces: Adsorbate and dopant effects[1] DAVID MICHA, ANDREW LEATHERS, University of Florida, DMITRI KILIN, University of South Dakota — The short time evolution of populations of electronic states and their quantum coherence at nanostructured surfaces of semiconductors provide insight on mechanisms of electronic charge transfer and separation. Starting from atomic structure, density matrix (DM)equations of motion (EOM) have been generated from a general formulation of dissipative quantum dynamics and have been parametrized in a basis set of Kohn-Sham orbitals, for both crystalline and amorphous Si slabs [1] with metal cluster adsorbates and with group III and V dopants. Integrodifferential EOMs have been solved for an initial ground state excited by femtosecond light pulses [2] to provide the time evolution of direct and indirect electron transfer at the surfaces. Results show that one of the transfer mechanisms can lead to long term separation of electronic charge, and what material properties contribute to large charge transfer and separation.

[1] T. W. LaJoie et al., Intern. J. Quantum Chem. 110, 3005 (2010).
[2] A. S. Leathers et al. J. Chem. Phys. 132, 114702-1(2010)]

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