Abstract Submitted
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Optical properties of crystalline and amorphous silicon slabs with adsorbed metal clusters and with dopants: A combined ab-initio electronic structure and density matrix treatment[1] DIMITRI KILIN, University of South Dakota, DAVID MICHA, JESSICA RAMIREZ, University of Florida — The optical absorbance and surface photovoltage of slabs of Si with varying number of layers have been calculated starting from their atomic structure. Results have been obtained for nanostructured surfaces with adsorbed metal clusters and for group III and V dopants, from ab initio DFT with periodic boundary conditions for extended systems, and from time-dependent DFT for supercells. Density matrix equations of motion (EOM) have been parametrized in a basis set of Kohn-Sham orbitals, for both crystalline and amorphous Si slabs [1]. Results for properties and from electronic charge distributions provide insight on slab confinement effects for electronically excited states and for particle-hole creation. In addition, the integrodifferential EOMs have been solved for an initial femtosecond pulse excitation [2] to analyze the nature of electron transfer at the surfaces, relevant to photovoltaics.

[1] T. W. LaJoie, J. J. Ramirez, D. S. Kilin, and D. A. Micha Intern. J. Quantum Chem. 110, 3005 (2010).
[2] A. S. Leathers, D. A. Micha, and D. S. Kilin, J. Chem. Phys. 132, 114702-1(2010)]

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