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Optical excitation and electron relaxation at the Si (001) 2x1 surface: A combined approach of density functional and density matrix theory NORBERT BUECKING, Technische Universität Berlin, D-10623 Berlin, Germany, PETER KRATZER, Universität Duisburg-Essen, D-47048 Duisburg, Germany, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, D-14195 Berlin, Germany, ANDREAS KNORR, Technische Universität Berlin, D-10623 Berlin, Germany — We present a microscopic theory to describe optical excitation and the subsequent phonon-induced relaxation dynamics of non-equilibrium electrons at a Si(001)(2x1) surface. Density matrix formalism is used to derive dynamical equations for the electronic occupations and polarizations in a surface/bulk system, where the electron-optical and electron-phonon interaction up to second order are considered. The matrix elements that govern the dynamics in the equations and the band structure of the surface system are determined by density functional theory calculations within the local-density approximation. These are performed on a slab geometry in order to take the buckled dimer surface reconstruction into account in the dynamics. The interplay of the population dynamics of the D_{down} state with the bulk conduction bands after an optical excitation is discussed and the typical deexcitation timescales for non-equilibrium surface electrons are deduced and compared to two-photon photoemission experiments.

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