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Response of the Shockley surface state on Cu(111) to an external electrical field: A density-functional theory study[1] KRISTIAN BERLAND, PER HYLDGAARD, Chalmers U. of Tech., T.L. EINSTEIN, U. of Maryland — We study the response of the Cu(111) Shockley surface state to an external electrical field E by combining a density-functional theory calculation for a finite slab geometry with an analysis of the Kohn-Sham wavefunctions to obtain a well-converged characterization. We find that the surface state displays isotropic dispersion, quadratic until the Fermi wave vector but with a significant quartic contribution beyond. We find that the shift in band minimum and effective mass depend linearly on E. Most change in electrostatic potential profile, and charge transfer occurs outside the outermost copper atoms, and most of the screening is due to bulk electrons. Our analysis is facilitated by a method used to decouple the Kohn-Sham states due to the finite slab geometry, using a rotation in Hilbert space. We discuss applications to tuning the Fermi wavelength and so the many patterns attributed to metallic surface states.

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