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Effect of physisorbed molecules and an external external fields on the metallic Shockley surface state of Cu(111): A density functional theory study[1]

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— To manipulate the Cu(111) partially-filled Shockley surface state, we study its response to an external field[2] E and physisorbed PAHs and quinone molecules. We use density-functional theory calculations with periodic-boundary conditions. The van der Waals density functional version vdW-DF2 accounts for the molecular adsorption. The issue that the Kohn-Sham wave functions couple to both sides of the Cu slab is handled with a decoupling scheme based on a rotation in Hilbert space. A convergence study reveals that to obtain a proper Shockley surface state, 6 Cu layers is sufficient, while 15 is optimal. We use 6 layers for the response to the molecules and 15 to external field. We find that the surface state displays isotropic dispersion (up to order k^6), free-electron like until the Fermi wave vector but with a significant quartic component beyond. The shift in band minimum and effective mass depend linearly on E, with a smaller fractional change in the latter. Charge transfer occurs beyond the outermost copper atoms, and most of the screening is due to bulk electrons. We find that the molecular physisorption increases the band minimum, with the effect the of a quinone being much stronger than the corresponding PAH.

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[2] KB, TLE, PH; arXiv 1109:6706

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