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Correlated Wavefunction Description of Kondo States on Metal Surfaces SAHAR SHARIFZADEH, Princeton University, Dept. of Electrical Engineering, PATRICK HUANG, Physics and Life Sciences Directorate, Lawrence Livermore National Laboratory, EMILY A. CARTER, Princeton University, Dept. of Mechanical and Aerospace Engineering — At low temperatures, a variety of magnetic impurities adsorbed on metal surfaces form a Kondo state, where the conduction electrons are thought to screen out the spin on the impurity to yield a many-body singlet, based on analogy with bulk Kondo physics in which magnetic quenching is observed at low temperatures. In scanning tunneling spectroscopy (STS), this state manifests as a narrow resonance in the density of states at the Fermi level. However, qualitative differences in the Kondo resonance lineshape are seen between specific adatom-substrate systems, for reasons that are not understood. We present a many-body correlated wavefunction study of Co on transition metal surfaces. We apply an embedded configuration interaction (CI) approach, where a finite cluster containing the impurity is described by a many-body CI wavefunction, while the effects of the extended background are included via a periodic density functional theory-based embedding potential. We discuss the nature of the correlated wavefunction and impurity orbital structure on different surfaces, and discuss implications for the observed STS data.

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