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First-principles Calculation of the Single Impurity Surface Kondo Resonance CHIUNG-YUAN LIN, IBM Almaden Research Center, San Jose, CA 95120-6099, ANTONIO CASTRO NETO, Department of Physics, Boston University, Boston, MA 02215, BARBARA JONES, IBM Almaden Research Center, San Jose, CA 95120-6099 — We have performed first-principles calculation of the surface and bulk wavefunctions of the Cu(111) surface and their hybridization energies to a Co adatom, including the potential scattering from the Co [1]. By analyzing the calculated hybridization energies, we have calculated the Kondo temperature to remarkable accuracy. We find the bulk states dominate the contribution to the Kondo temperature, in agreement with a recent experiment [2]. Furthermore, we also calculate the tunneling conductance of a scanning tunneling microscope on this system and compare our results with recent experiments of Co impurities in the Cu(111) surface. Good quantitative agreement is found at short parallel impurity-tip distances (< 6 angstroms). Our results indicate the need for a new formulation of the problem at larger distances. [1] C.-Y. Lin, A. H. Castro Neto, and B. A. Jones, Phys. Rev. Lett. 97, 156102 (2006). [2] N. Knorr, M. A. Schneider, L. Diekhoner, P. Wahl, and K. Kern, Phys. Rev. Lett. 88, 096804 (2002).

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