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**First-principles Calculations of Engineered Surface Kondo Atom**

CHIUNG-YUAN LIN, Department of Electronics Engineering, National Chiao Tung University, Taiwan, BARBARA JONES, IBM Almaden Research Center — In recent STM experiments, a surface Kondo atom (Co) is studied under the influence of a second magnetic atom or magnetic anisotropy on a specially designed CuN/Cu(100) surface. The Kondo properties of Co on such a surface were not studied before. We have done density functional calculation of this system, and obtain several properties that is important for the surface Kondo effect. We calculated the Co's surrounding local density of states and the on-site Coulomb  $U$ , and compare and contrast the behavior of Co and Mn. Our calculations also confirm that the Co spin of this structure is  $3/2$ , as also measured indirectly by STM. [Ref. of experiments: Nature Physics, 4, 847 (2008); Phys. Rev. Lett. 103, 107203 (2009).]

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