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Comparison between GGA+U and LSDA-GGA on CuN/Cu(100)

PUSHPA RAGHANI, CPN, Stanford University, CA, CHIUNG-YUAN LIN, National Chaio Tung University, Taiwan, BARBARA JONES, IBM Almaden Research Center, CA, USA, CPN COLLABORATION — It has become possible to study atomic magnetism by the Scanning Tunneling Microscope. The spin of a magnetic atom is often screened when it is adsorbed on a metal surface. However, a CuN layer reduces this screening and the atomic spins become detectable by STM. We have applied DFT to calculate the charge transfer, binding energies of the CuN layer on a Cu(100) surface. Within DFT, we use two different techniques for exchange correlation interaction: GGA+U and LSDA-GGA. Then we will calculate the atomic spins for Mn on CuN/Cu(100) using these two techniques. We will compare and discuss the results.

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