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**First-principles calculation of Mn Atoms on the CuN/Cu(100) Surface**[1] CHIUNG-YUAN LIN, IBM Almaden Research Center, San Jose, CA 95120-6099 and Stanford University Department of Applied Physics, Stanford, CA 94305-4090, BARBARA JONES, ANDREAS HEINRICH, IBM Almaden Research Center, San Jose, CA 95120-6099 — The electronic structure is calculated using GGA+U for one and two Mn atoms on a single CuN layer coated on the Cu(100) surface. This unique insulator-metal junction surface prevents the Mn spins from being screened by the conduction electrons and at the same time allows experimentalists to pass tunneling electrons through the Mn atoms to flip their spins. Our spin-density analysis shows that Mn atoms in such a surface preserve their atomic spins S=5/2. This result agrees with a recent STM measurement on such systems. Electron-density change and surface relaxation due to the Mn atoms are also analyzed.

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