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First-principles Calculation of Atom-scale Magnetic Interaction
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— The advance of manipulating atoms on surfaces by STM has made it possible to study atomic magnetism. It has been shown that STM can build chains of magnetic atoms and measure magnetic excitation of such chains [1]. This new technique has potential application to explore the limits of magnetic data storage, by engineering the energy required to flip the collective orientation of a small number of magnetically coupled atoms. We have applied GGA+U to determine the atomic spin and calculate the exchange coupling J (several meV) for Mn chains on a CuN/Cu(100) surface. Our spin-density analysis shows that Mn atoms in such a surface preserve their atomic spins S=5/2. To demonstrate the potential to engineer the coupling between atomic spins, we calculate the J's for the Mn dimers atop Cu atoms and atop N in the CuN layer, and find the Cu-site dimer has its J twice as large as the N-site. The local structures of the Mn dimers on these two sites determined by relaxation account for this difference in J.The charge transfers between Mn and its neighboring atoms are also calculated. [1] C. F. Hirjibehedin, C. P. Lutz, A. J. Heinrich, Science 312, 1021 (2006).

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