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The sometimes surprising behavior of magnetic spins on a complex surface

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We have studied the unusual charge and spin properties of magnetic atoms (Mn, Co, Fe, Ti, Gd) on a complex surface as constructed by STM. This surface, a lattice of N atoms on Cu(100), was designed to be insulating in order to inhibit the Kondo effect (in which the Cu electrons would completely screen the spin). However, the magnetic adatom may be drawn down into the surface, or stay high above and attract surface atoms to it, with very different resulting properties. We show illustrations from our electronic structure calculations of these systems. The various magnetic atoms exhibit behavior ranging from spin chains to large-anisotropy atomic-scale molecular magnets to a Kondo effect for Co and Ti. Finally, when two magnetic atoms are close to one another, their magnetic spins can interact, with complex and interesting results. We show the unexpected results of a close-spaced 2D lattice of magnetic atoms as well. I will conclude with some comments about the role of large-scale calculations for nanostructures. Some references:

[1] C-Y Lin, J-L Li, Y-H Hsieh, K-L Ou, and B. A. Jones, "Magnetic Interaction between Surface-Engineered Rare-Earth Atomic Spins," Phys. Rev. X 2, 021012 (2012).
[2] R. Pushpa, J. Cruz, and B. Jones, "Spin and exchange coupling for Ti embedded in a surface dipolar network," Phys. Rev. B 84, 075422 (2011).
[3] C-Y Lin and B. A. Jones, "First-principles calculations of engineered surface spin structures," Phys. Rev. B 83, 014413 (2011).