Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

DFT+U studies of atomic scale magnetism: A curious case study for future spintronic devices[1] SHRUBA GANGOPADHYAY, IBM Almaden Research Center, HOSSEIN HASHEMI, University of Michigan, BARBARA JONES[2], IBM Almaden Research Center — Atomic scale magnetism attracts interest due to both its possible application to nanoscale spintroic devices, and due to its inherent interest as a source of basic quantum mechanical interactions. We work together with the local Scanning Tunneling Microscopy (STM) team to match our calculations to experiment, and in the process learn much which can't be measured with the STM. In particular we use DFT+U to calculate the properties of magnetic atoms on nanolayers of insulator on top of a metal such as silver. In this talk we report the results of detailed calculations of singles and dimers of Mn on MgO/Ag. As time permits we may include our calculations of other magnetic adatoms for comparison. We find that the local interactions are very different for the three stable binding sites on this surface, both for charge and spin densities. Using on onsite Hubbard U parameter which we determine from first principles, we are able to study the variability of the magnetic moment between the binding sites, as well as determine the lowest energy binding site. The magnetic adatoms affect the surrounding interface layer in unexpected ways. We are able to obtain interesting insights which help us understand how magnetism propagates along surfaces as well as between interfaces.

[1]Research for this project is partially funded by KAUST.
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Date submitted: 31 Oct 2012 Electronic form version 1.4