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**Atomic-scale magnetism of Fe and Co on a complex surface** BARBARA JONES, IBM Almaden Res Ctr, SHRUBA GANGOPADHYAY, University of California Davis, OLIVER ALBERTINI, Georgetown University — Miniaturization is one of present challenges for development of future spintronic devices. Our goal is to exploit the unusual properties of magnetism of transition metal atoms on complex surfaces. In collaboration with Almaden's Scanning Tunneling Microscopy team, we use DFT+U to calculate the properties of transition atoms on nanolayers of insulator on top of a metal such as silver. In this talk we report the results of detailed calculations of Fe and Co on MgO/Ag. MgO is a common spintronic insulator, but in a nanolayer on metallic Ag, its behavior is not that of the bulk. We find that Fe and Co have very different local spin and charge interactions with this surface. Using an onsite Hubbard U parameter which we determine from first principles, we are able to study the variability of the magnetic moment and nature of bonding. 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.

Barbara Jones  
IBM Almaden Res Ctr

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