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A new bonding insight of Ti adatom on MgO/Ag system BARBARA JONES, IBM Research - Almaden, SHRUBA GANGOPADHYAY, University of California, Davis — Atomic scale magnetism attracts attention due to both possible applications in nanoscale spintronic devices and interest in the basic quantum mechanical interactions. First principle simulations of these type of systems are challenging, especially where transition metal oxygen bonding plays key role. In our talk we will show a comparison of two sets of calculations i) DFT+Hubbard U and ii) DFT+U+spin orbit coupling (SOC), for a system of a Ti adatom (which is magnetic in this environment) on a monolayer of MgO, on bulk Ag. In our work we calculated U using linear response theory, for the specific adatom site. Scanning tunneling microscopy data shows more resemblance to DFT+U+SOC results. Though our system has a 3d Ti, where relativistic effects are not expected to play a significant role, we nonetheless found inclusion of SOC drastically changes the electronic and magnetic structure of Ti-O bonding compared to DFT+U results. Our findings reinforce the fact that magnetic transition metal -oxygen bonding in a complex surface system demands extra care and can show surprises compared to similar bulk systems.

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