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Spin-orbit coupling of 3d transition metal atoms on MgO/Ag SHRUBA GANGOPADHYAY, University of California, Davis, BARBARA JONES, IBM Research Almaden — Spin-orbit coupling is normally predominant for high Z metal atoms, but we observe Fe and Co showing significant orbital moments on a MgO/Ag surface. DFT results show that on MgO/Ag both Co and Fe prefer O top binding sites. Calculation of orbital moments using DFT is always challenging, and we compare two DFT based protocols to calculate orbital moments. Our calculations show the magnitude of orbital moments strongly dependent on a number of factors including the number of Ag layers in our unit cell and the approximation we are using. Our results exhibit significant agreement with scanning tunneling microscopy (STM) and XMCD experiments. We show that Co retains its full atomic orbital moment on the O top site of MgO whereas the orbital moment for Fe is somewhat less than its atomic orbital moment.

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