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Mn Adsorption on MgO/Ag(100): DFT and DFT+U Calculations HOSSEIN HASHEMI, Martin-Luther-Universität Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany, BARBARA JONES, IBM Almaden Research Center, San Jose, CA 95120-6099, USA — The adsorption properties of a Mn adatom on MgO ultrathin films deposited on a Ag(100) substrate are determined from first principles DFT calculations and compared with the corresponding adsorption characteristics from DFT+U calculations. First, we investigate the properties of a pure Ag (100) surface and a MgO/Ag(100) system. The structural relaxation, work function and surface energy for the Ag(100) surface, as a function of thickness dependence, is discussed. Next, we discuss the addition of a Mn adatom. Regular (U=0) DFT calculations show that the most stable site for Mn adsorption on MgO/Ag(100) is the bridge site, followed closely by the Oxygen site, and a very unlikely position, the Mg site. We have also investigated the role of strong electron correlations in the substrate on the chemisorption properties of a Mn adatom. DFT+U calculations predict the Oxygen site to be the most stable site, instead of the bridge site, in contrast to U=0 DFT calculations. The energies, geometry, and magnetic properties of the Mn adatom are all influenced by adding a Coulomb energy. Altogether our results show that the on-site Coulomb repulsion in the Mn d band plays an important role in the description of adsorption on MgO/Ag(100).

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