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Ni adsorption on MgO(001)**: A Comparison of DFT and DFT+U**
OLIVER ALBERTINI, AMY LIU, Georgetown University, BARBARA JONES, IBM Almaden Research Center — The study of magnetic atoms on surfaces has drawn recent attention due to possible applications in the realm of magnetic storage and quantum computing. Researchers are looking across the 3d transition metal series for candidates with high magnetic anisotropy. Here we examine the MgO/Ag surface with a Ni adatom using DFT and DFT+U computational approaches. We investigate the preferential binding site and the interesting physics involved in the resulting magnetic moment, drawing comparisons with a recent study of Co on MgO/Ag.

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