Abstract Submitted
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Density functional theory and DFT+U study of transition metal porphines adsorbed on Au(111) surfaces[1] KEVIN LEUNG, SUSAN REMPE, PETER SCHULTZ, Sandia National Laboratories, EDUARDO SPROVIERO, VICTOR BATISTA, Yale University, MICHAEL CHANDROSS, CRAIG MEDFORTH, Sandia National Laboratories — We apply Density Functional Theory (DFT) and the DFT+U technique to study Pd(II) and Mn(II) phosphines adsorbed on atomistically flat Au(111) surfaces. PdP is found to adsorb preferentially on gold in a flat geometry, not in an edgewise geometry, in qualitative agreement with experiments on substituted porphyrins. The DFT+U technique is found to be crucial for reproducing the correct magnetic moment and geometry of the isolated manganese porphine (MnP) molecule. Adsorption of Mn(II)P on Au(111) substantially alters the Mn ion spin state and electronic structure. Its strong binding to the gold surface can be partially reversed by applying an electric potential, which leads to significant changes in the electronic, magnetic, and structural properties of the adsorbed MnP.

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