

Interaction of Transition Metal Adatoms with Ultrathin MgO/Fe(001) Films

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Recent works of ultrathin oxide films showed that the charge states of metal adatoms on the ultrathin oxide films supported by metal substrates, such as MgO/Mo(001) and MgO/Ag(001), play important roles. In this work, we investigated the electronic properties of transition metal adatoms (Au, Pd, and Pt) adsorbed on MgO/Fe(001) by carrying out first-principles electronic-structure calculations. The calculations in this study showed that the negative charging of the Au adatom occurred through the charge transfer from Fe to Au as in the other metal substrates of Mo and Ag. It was also found that the negative charging happened even for Pd and Pt with lower electron affinity than Au. Interestingly, Pd and Pt became spin-polarized with the presence of the magnetic Fe substrate contrary to Pd/MgO/Mo(001). Our calculation results clearly suggest that the magnetic Fe substrate of MgO/Fe(001) can offer a new way to modify the spin states as well as the charge states for metal adatoms on ultrathin oxide films.

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