

Ab initio investigation on the magnetization of Pd thin films

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Strain induces magnetization on the Pd which is non-magnetic in its bulk form. Depending on the substrate, the pseudo-morphically grown Pd surfaces can exhibit an induced magnetic moment even with the scarce interfacial hybridization, solely due to the strain effect. In this study, we report our first-principles investigation on the Pd magnetization in various environments. The effects of strain, substrate, and the external electric field on the electronic and magnetic properties are examined from the electronic structure calculations in the framework of DFT (Density Functional Theory) within both the local density approximation and the generalized gradient approximation. Different behavior of the surface and interfacial Pd atoms especially in their magnetic properties will be discussed.