Abstract Submitted
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Submonolayers of Au/Pd on the hematite (0001) and magnetite (111) surfaces[1] ADAM KIEJNA, TOMASZ PABISIAK, TOMASZ OSSOWSKI, Institute of Experimental Physics, University of Wrocław, Poland — Ultra-thin films and nanostructures formed by noble metals on oxide surfaces exhibit enhanced catalytic activity for CO oxidation. We used the spin-polarized density functional theory (DFT) and the DFT+U method, accounting for the strong on-site Coulomb correlations, to study the submonolayer adsorption of Au/Pd atoms on two stable iron-oxide surfaces: hematite (0001) and a magnetite (111). For each surface, adsorption on two terminations has been studied: one terminated with iron and the other with oxygen. Both Au and Pd bind strongly to hematite and magnetite surfaces and induce large changes in their geometry. DFT and DFT+U provide qualitatively similar surface geometries but they differ much in the prediction of the surface energetics and the electronic and magnetic properties of the oxides. Pd binds stronger than Au both to hematite and magnetite surfaces and the Au/Pd bonding to the O-terminated surface is distinctly stronger than that to the Fe-terminated one. For hematite, the DFT+U bonding is by 0.3-0.6 eV weaker than DFT on the Fe-terminated surface and about 2 eV stronger on the O-terminated one. For magnetite, in each case, DFT+U gives stronger bonding than DFT. The differences between DFT and DFT+U results are discussed based on the calculated electronic structure.

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