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Adsorption of CO and O2 molecules on supported small Au clusters MARTIN AMFT, NATALIA SKORODUMOVA, Uppsala University, DIVISION FOR MATERIALS THEORY TEAM — We investigate the catalytic activity of metal-oxide/metal supported tiny gold clusters towards the carbon monoxide oxidation by means of density functional theory calculations. Our focus lies on cluster-size effects, the influence of different support materials and co-adsorption of other molecules, e.g. water. In agreement with experimental data we could explain, why Au ad-atoms and dimers on MgO do not show any catalytic activity towards CO oxidation and why a Langmuir-Hinshelwood reaction mechanism via co-adsorption is possible for the trimer and tetramer. Furthermore we thoroughly studied the influence of spin-orbit coupling, a hitherto widely neglected effect in these systems, on the adsorption of gold clusters on the surface and of small molecules on the cluster/surface system. Last but not least clusters consisting of an odd number of gold atoms carry a spin moment from one unpaired 6s electron. We studied its coupling to the moments of a magnetic metal beneath a thin supporting metal-oxide layer.

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