

Active role of oxide support during NO reduction and CO oxidation at Pd/MgO and Au/MgO.

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Abstract

The potential energy diagrams for the NO+CO reaction on 1, 2, and 3 monolayer Pd films supported by MgO(100) and for the CO oxidation on Au aggregates also supported by MgO(100) are calculated using density functional theory. Thin Pd films are generally found to be more reactive than thick films, with a notable exception for nitrogen adsorption on 2 ML Pd/MgO(100). For this system an attractive through-the-metal adsorbate-oxide interaction of 0.5 eV is identified.[1] Low coordinated gold metal atoms in various cluster-like configurations are found to bind CO and to provide a pathway for CO oxidation over the Au/MgO systems. An attractive CO-O₂ interaction is shown to play an important role in the CO oxidation, where also stabilization of peroxy species by the oxide support becomes important.[2]

[1] B. Hammer, Phys. Rev. Lett. **89**, 016102 (2002).

[2] L.M. Molina and B. Hammer, in preparation.
See <http://www.phys.au.dk/~hammer>