Adhesion of rhodium, palladium, and platinum to alumina and the reduction of nitric oxide on the resulting surfaces: a theoretical analysis

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Author(s) Ward, Thomas R.; Alemany, Pere; Hoffmann, Roald
Author(s) at UniBasel Ward, Thomas R. ;
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Approx. MO calcns. were made of adhesion and NO redn. in the 3-way catalyst (modeled by a monolayer of either Rh, Pd, or Pt on the (0001)O and (0001)Al faces of ?ś-Al2O3). The support is not electronically innocent, but affects NO redn. capability significantly. Both Pt and Pd form stable interfaces with both O and Al faces. Only the Al interface is stable with Rh. Depending on the nature of the interface, the Fermi level of the composite systems varies dramatically. This, in turn, affects the adsorption mode (mol. or dissociative) of NO. Apparently, an O-Pt interface is best suited for both dissociative adsorption of NO as well as the coupling of 2 adsorbed nitrosyls to form a reduced dinitrosyl species with significant N-N double-bond character.

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