Adhesion of Rh, Pd, and Pt to Alumina and NO Reactions on Resulting Surfaces

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We report here approximate molecular orbital computations of adhesion and NO reduction in the Three Way Catalyst, modeled by a monolayer of either Rh, Pd or Pt on the (0001)O and (0001)A1 faces of α-A12O3. Platinum and palladium form stable interfaces with both oxygen and aluminum faces. Only the aluminum interface is stable with rhodium. Depending on the nature of the interface, the Fermi level of the composite systems varies dramatically. This, in turn, affects the adsorption mode, molecular or dissociative, of nitric oxide. From our study, it appears that an oxygen-platinum interface is best suited for both dissociative adsorption of NO as well as the coupling of two adsorbed nitrosyls to form a reduced dinitrosyl species with significant N-N double bond character.
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