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On the stability and oxidation of Pdn (n=1-7) clusters on rutile TiO2(110)[1]

S. VINCENT ONG, SHIV KHANNA, Virginia Commonwealth University, DEPT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — First principles theoretical studies of the atomic and electronic structure of Pd_n (n=1-7) clusters supported on a $TiO_2(110)$ surface, and O_2 activation by such clusters, have been carried out within a gradient corrected density functional approach. It is shown that the supported Pd_n cluster geometries are driven by competing effects including intra-cluster interactions favoring compact geometries and cluster support interactions that favor geometries that flatten out in the $TiO_2(110)$ surface channel. When exposed to O_2, a single Pd atom only activates the O-O bond while all other clusters energetically favor a broken O-O bond. The differing behavior of the Pd atom is proposed to originate from the minimal amount of charge transferred from Pd to O_2 and its spin excitation energy. For Pd_nO_2 (n=2-7), it is shown that while the first O is adsorbed on the Pd_n cluster, the second O occupies a site above a lattice Ti site at the Pd-Ti interface and is indicative of spill over O atoms. The theoretical finding are compared with recent experiments on the structure and oxidation of CO by supported clusters in the presence of O_2.

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