On the stability and oxidation of Pdn (n=1-7) clusters on rutile TiO2(110)\textsuperscript{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\textsubscript{n} (n=1-7) clusters supported on a TiO\textsubscript{2}(110) surface, and O\textsubscript{2} activation by such clusters, have been carried out within a gradient corrected density functional approach. It is shown that the supported Pd\textsubscript{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\textsubscript{2}(110) surface channel. When exposed to O\textsubscript{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\textsubscript{2} and its spin excitation energy. For Pd\textsubscript{n}O\textsubscript{2} (n=2-7), it is shown that while the first O is adsorbed on the Pd\textsubscript{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\textsubscript{2}.

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