

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**A DFT Study of Palladium Clusters and their Reactions with H<sub>2</sub> and O<sub>2</sub>: Application to catalyzed H<sub>2</sub>O<sub>2</sub> synthesis<sup>1</sup>** ADAM PELZER, Central Michigan University/Argonne National Lab, KOBLAR JACKSON, Central Michigan University, JULIUS JELLINEK, Argonne National Lab — Adsorption of oxygen and hydrogen in both atomic and molecular forms on small Pd<sub>n</sub> clusters (n=2-13 and 19) is investigated using density functional theory. An extensive search for the energetically preferred structural forms and spin states of the clusters is performed. The geometries and energetics of the cluster-adsorbate systems and their transition states are mapped out as well. Cases of both single and multiple adsorptions are considered, and trends in the saturation coverage of the clusters versus cluster size are examined. Edge sites are found to be energetically preferred for O<sub>2</sub> adsorption, whereas the atop sites favor binding of H<sub>2</sub>. Atomic adsorption of hydrogen is examined as well and limits to the number of H atoms that can be dissociated on each size cluster are found. In order to understand how trends in the results extend to larger cluster sizes, limited calculations have also been performed for Pd<sub>55</sub>. The role of Pd<sub>n</sub> clusters as catalysts for production of H<sub>2</sub>O<sub>2</sub> from H<sub>2</sub> and O<sub>2</sub> is discussed as well.

<sup>1</sup>AWP and KAJ were supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, U.S. Department of Energy under Award Number: DE-SC0001330. JJ was supported by the Office of Basic Energy Sciences, Division

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Date submitted: 10 Nov 2011

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