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Structural Oscillation in Pd_{13} During Oxidation/Reduction[1] D.R. ROY, J. ULISES REVELES, S. VINCENT ONG, S.N. KHANNA, Virginia Commonwealth University, A.M. KÖSTER, P. CALAMINICI, CINVESTAV, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION, DEPARTAMENTO DE QUíMICA, CINVESTAV COLLABORATION
— First principles electronic structure calculations within a gradient corrected density functional formalism have been carried out to investigate the electronic structure and magnetic properties of bare and oxidized Pd_{13} clusters. It is shown that the ground state of neutral Pd_{13} is a bilayer structure that can be regarded as a fragment of the bulk, while a compact icosahedron is higher in energy. The addition of an electron, however, reverses the ordering of structures and Pd_{13}^- has an icosahedral ground state. Similar reordering of structure occurs as an O_2 molecule is added to the neutral cluster. The talk will focus on the oscillations between the two structures during catalysis process.

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