Abstract Submitted
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First principles study of adsorption and dissociation of H_2, O_2, and CO on Pt_4 and Pt_3Co clusters[1] T. J. DHILIP KUMAR, CHENGGANG ZHOU, BALAKRISHNAN NADUVALATH, Department of Chemistry, University of Nevada Las Vegas, NV 89154, ROBERT C. FORREY, Department of Physics, Penn State University, Berks-Lehigh Valley College, Reading, PA 19610, HANSONG CHENG, Airproducts and Chemicals Inc., 7201 Hamilton Boulevard, Allentown, PA 18195 — Pt and Pt based alloy nanoparticles have received much attention recently in designing improved catalysts for the oxygen reduction reaction in fuel cell electrodes. In particular, Pt-Co alloy systems have attracted significant interest in proton exchange membrane fuel cells. To gain physical insight into the catalytic properties of Pt and Pt-Co alloys we have performed fundamental studies on Pt_4 and Pt_3Co alloy clusters using first principles density functional calculations. The structural and physicochemical properties of the pure metal and the alloy have been analyzed, and for Pt_4, the tetrahedral geometry is found to be more stable than the square planar geometry. On the optimized tetrahedral geometries the interactions of H_2, O_2, and CO with different orientations have been studied. The calculated energies of adsorption indicate H_2 and CO prefers to adsorb on Pt atop while O_2 prefers Co atop. The adsorption energy of CO is found to be the highest of all the three adsorbing species in both pure Pt_4 and Pt_3Co alloy clusters.

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