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First principles study of adsorption and dissociation of H_2, O_2, and CO on α-Al_2O_3 (0001) supported Pt-Co alloy[1] T.J. DHILIP KUMAR, C. ZHOU, B. NADUVALATH, Department of Chemistry, University of Nevada Las Vegas — Recently, there has been several investigations carried out to improve the electro-catalytic activity of Pt and Pt based alloys for the oxygen reduction reaction in fuel cell electrodes. In particular, Pt-Co alloy systems have been often employed. To gain physical insight into the catalytic properties of these systems we have performed a systematic study of the electronic structures, bonding and growth patterns of nanoclusters of Pt-Co alloy using first principles density functional calculations. The 3:1 ratio of Pt-Co alloy has been constructed as nanoclusters and thin film supported on α-Al_2O_3. The geometry optimized tetrahedron, and the square planar structures of Pt_3Co are placed over the slabs of six layers α-Al_2O_3(0001) surface. Activity of H_2, O_2 and CO on these structures from various approaches has been explored. In all our calculations the non-locality in the exchange correlation functional is taken into account by considering spin polarized generalized gradient approximation as proposed by Perdue and Wang. Brillouin zone integrations have been performed using Monkhorst-Pack grids with (2 X 2 X 1) k-point meshes. The electronic structures of these systems have been analyzed by computing the electronic density of states.

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