Electronic structures of Pt clusters adsorbed on (5, 5) single wall carbon nanotube

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Abstract: We present a DFT study for the adsorption of single Pt atom and Pt clusters on graphene surface and carbon nanotube. Adsorption of a Pt atom shows a heavy dependence of binding energy on the graphene curvature. The adsorbed Pt atoms tend to form clusters, than to disperse on the graphene surface. The Pt-Pt bond length and the charge transfer from Pt clusters to the nanotube vary as a function of cluster size. A simulation of oxygen adsorption suggests higher performance for catalytic activities of Pt clusters adsorbed on the nanotube, in comparison with free Pt clusters. ?? 2006 Elsevier B.V. All rights reserved.

Index Keywords: Adsorption; Binding energy; Carbon nanotubes; Catalysis; Charge transfer; Electronic structure; Catalytic activities; Graphene; Graphene surface; Single wall carbon nanotube; Platinum

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