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

Year: 2006
Source title: Chemical Physics Letters
Volume: 432
Issue: 3-Jan
Page : 213-217
Cited by: 19
Link: Scorpus Link
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ISSN: 92614
CODEN: CHPLB
DOI: 10.1016/j.cplett.2006.10.063
Language of Original Document: English
Abbreviated Source Title: Chemical Physics Letters
Document Type: Article
Source: Scopus
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