Structural and electronic properties of Pt_n (n = 3, 7, 13) clusters on metallic single wall carbon nanotube

Cuong N.T., Chi D.H., Kim Y.-T., Mitani T.

Materials Science School, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Tatsunokuchi, Ishikawa, Japan; Center for Strategic Development of Science and Technology, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Tatsunokuchi, Ishikawa, Japan; Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Viet Nam

Abstract: A systematic study of Pt_n (n = 3, 5, 7) clusters adsorbed on the metallic (5, 5) single wall carbon nanotube was carried out using theoretical calculations within Density Functional Theory. The geometrical and electronic structure and interaction between the Pt clusters and the single wall carbon nanotube were investigated. The bridge adsorption sites on the outer wall of the carbon nanotube are found favorable for Pt atom. We found that the average C-Pt and Pt-Pt bond length, binding energy, and the amount of charge transfers from the Pt cluster toward the nanotube increase with the size of cluster. The calculated density-of-states suggest a mixing of ionic and covalent character for the binding nature of this system. ?? 2006 WILEY-VCH Verlag GmbH & Co. KGaA.

Year: 2006
Source title: Physica Status Solidi (B) Basic Research
Volume: 243
Issue: 13
Page : 3472-3475
Cited by: 4
Link: Scorpus Link
Correspondence Address: Chi, D.H.; Center for Strategic Development of Science and Technology, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Tatsunokuchi, Ishikawa, Japan; email: dam@jaist.ac.jp
ISSN: 3701972
DOI: 10.1002/pssb.200669166
Language of Original Document: English
Abbreviated Source Title: Physica Status Solidi (B) Basic Research
Document Type: Conference Paper
Source: Scopus
Authors with affiliations:

1. Cuong, N.T., Materials Science School, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Tatsunokuchi, Ishikawa, Japan
2. Chi, D.H., Center for Strategic Development of Science and Technology, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Tatsunokuchi, Ishikawa, Japan, Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Viet Nam

3. Kim, Y.-T., Materials Science School, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Tatsunokuchi, Ishikawa, Japan
4. Mitani, T., Materials Science School, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Tatsunokuchi, Ishikawa, Japan

References:

1. Antolini, E., (2005) Appl. Catal. B, Environ., 63, pp. 137-149
2. Frackowiak, E., (2005) Electrochem. Commun., 8, pp. 129-132
3. He, Z., (2004) Mater. Chem. Phys., 85, pp. 396-401
4. Matsumoto, T., (2004) Catal. Today, 90, pp. 277-281
5. Kim, Y.-T., Ohshima, K., Higashimine, K., Uruga, T., Takata, M., Suematsu, H., Mitani, T., (2005) Angew. Chem. Int. Ed., 45, pp. 407-411
6. Hohenberg, P., Kohn, W., (1964) Phys. Rev., 136, pp. B864
7. Kohn, W., Sham, L.J., (1965) Phys. Rev., 140, pp. A1133
8. Ozaki, T., (2003) Phys. Rev. B, 67, p. 155108
9. Perdew, J.P., Burke, K., Ernzerhof, M., (1996) Phys. Rev. Lett., 77, p. 3865
10. Ozaki, T., Kino, H., (2004) Phys. Rev. B, 69, pp. 195113-195113
11. Troullier, N., Martine, J.L., (1991) Phys. Rev. B, 43, p. 1993
12. http://staff.aist.go.jp/t-ozaki/openmx/, DFT OpenMX code is available on the web site