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

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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.

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