Pipat Khongpracha 2006: Structure and Reactivity of Nanostructured Materials and Their Metal Complexes with CO Molecules. Doctor of Philosophy (Chemistry), Major Field: Physical Chemistry, Department of Chemistry. Thesis Advisor: Professor Jumras Limtrakul, Ph.D. 110 pages.
ISBN 974-16-1922-7

The adsorptions of CO and NO on Ag-ZSM-5 have been studied by using the Surface Charge Representation of External Embedded Potential (SCREEP) embedded cluster model at the density functional theory. It was found that CO adsorbs on the Ag+ ion in the linear configuration with the bond distance of 1.130 Å and binding energy of 18.63 kcal/mol. Adsorbed NO, on the other hand has a bend configuration with the AgNO angle of 127.5 ° and the Ag-N bond distance of 1.150 Å. The binding energy for NO is 9.24 kcal/mol. By using natural bond orbital analysis (NBO), it could be seen that the former has stronger a σ donation and also a greater π-back donation. The Madelung potential has only a small perturbation on the structure and binding energy of the adsorption complexes. This environmental effect, however, improves the agreement between the calculated frequency shifts and those of experimental observations.

The interaction of a gold atom with single-wall carbon nanohorn (SWNH) and single-wall carbon nanotube (SWNT) tips and their complexes with a CO molecule were studied using the density functional theory (DFT). The analysis of the pyramidalization angle (θ_p) as well as the π-orbital misalignment angles (ϕ) lead to an elucidation that there would be many reactive carbon sites on the tips of both SWNH and SWNT, the former provides reactive sites that can more selectively interact with the target atom. The CO probe molecule binds tightest with the Au/SWNH tip and the Au/SWNT tip with the interaction energies of -22.34 and -18.29 kcal/mol, respectively. The main contribution of the metal interacted with both carbon nanostructures stemmed from the interactions of σ-donation and π-back bonding. The results suggest the potential of the use of an SWNH for the development of a high-specific nanosensor.

ภิพัฒน์ คงประชา 24 / 05 / 2006

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