

Study of the effect of gold on the structural properties of carbon nanotubes and its ability to absorb carbon monoxide

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The unique and unique properties of nanotubes, including the high modulus of young and good tensile strength on one side and their carbon dioxide content (Because carbon is a low-weight material, very stable and simple to process, which is cheaper than metals for production)), being had caused, in the past decade we see important research and good performance in growth of nanotubes. At first, in this project, single-wall carbon nanotubes was drawing by the software of nanotubes modeler. and then, structure of desired view by (gauss view 5) and input_file was built by it, too. By Gaussian software, by functional density theory, the DFT (B3LYP) hybrid function, and the LANL2DZ base series, the desired compound structure was optimized at K298 and atm1 pressures, and eventually performed on optimized compositions of frequency studies and NBO Became. In this study, quantities such as, ionization energy, electron, potential of chemical electron, hardness and softness, homo luno gap, enthalpy and free energy of Gibbs was calculated. The result showed that, blocked of gold in the nanotubes is possible a position of having favorable enthalpy and entropy and negative Gibbs energy. Stable has increased with increasing ionization energy in blocked nanotubes to pure nanotubes. Attractive physical has been investigated in two cases of blocked nano tubes. that in both modes, the absorption is taken. so, and this material can be used as carbon monoxide sensor.

Keywords : Nano tube carbon, Blocked nano tube, Mechanical Gold physical properties, the theory of density function

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