Employing ONIOM calculations to investigate the abilities of simple and N, B, S-doped carbon nanotubes in sensing of carbon monoxide

Hossein Tavakol[1], Fahimeh Hassani[1], and Dana Shahabi[1]

[1]Isfahan university of technology

May 5, 2020

Abstract

In this work, geometries, stabilities and electronic properties of carbon monoxide (CO) molecule as an adsorbent on simple carbon nanotube (CNT) and N, B, S-doped carbon nanotubes (NCNT, BCNT and SCNT) with parallel and perpendicular configurations are fully considered using ONIOM, natural bond orbital (NBO), and quantum theory of atom in molecule (QTAIM) calculations. The adsorption energies (Ead) demonstrate that CO molecule could be adsorbed on the surface of the simple carbon nanotube with parallel configuration (CNT-p) and N-doped carbon nanotube with perpendicular configuration (NCNT-d) in exothermic process. QTAIM calculations are showed the close-shell (non-covalent) interactions between CO molecule and CNT or N, B, S-doped CNTs. Also, the energy gap (Eg) values between the highest occupied molecular orbital and the lowest unoccupied molecular orbital are calculated. In accordance to the results of energy gap, simple and N-doped carbon nanotubes could be used as CO-sensors.

Hosted file

`final manuscript.docx` available at https://authorea.com/users/288390/articles/413698-employing-oniom-calculations-to-investigate-the-abilities-of-simple-and-n-b-s-doped-carbon-nanotubes-in-sensing-of-carbon-monoxide