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Study of the Ionization Potential, Electron Affinity and HOMO-LUMO Gaps in the Smal Fullerene Nanostructures

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ABSTRACT

In this work, the theoretical investigations on the buckyball systems including C_{20}, C_{24}, C_{26}, C_{28}, C_{30} and $C_{19}Si$ were done to study the structures and properties of different carbon nanoclusters. The geometries of all species were performed at the B3LYP and PBE1PBE levels using the 6-31+G (d) basis set. The HOMO–LUMO energy gap, ionization potential, electron affinity, chemical potential, electronegativity, global hardness and softness, electrophilicity and maximum amount of electronic charge of studied clusters were computed. The results showed that the computed electronic properties were considerable influenced by the size of different carbon nanoclusters. The Si atom doped instead of the carbon atom in C_{20} was investigated

1. Introduction

The use of nanomaterials is extensively increased in many aspects [1]. A molecule of carbon in the shape of a hollow sphere, ellipsoid, tube and many other forms, is called buckyballs [2]. In 1985, Kroto and co-workers discovered the first fullerene molecule that called buckminsterfullerene (C_{60}) [3]. The fullerene has opened the new area of appropriate designing of nanomaterials with full of novel attributes [4–7]. Important thermodynamic properties including ionization potentials, electron affinity and other parameters have been carried out on fullerene and its different derivatives [8–12]. Experimental research of the vertical ionization potentials of fullerene and its hydrogenated derivatives namely $C_{60}H_{18}$ and $C_{60}H_{36}$ have performed [8], which the results indicated that the first ionization potentials of the hydrogenated fullerenes are lower than that of the fullerene C_{60}. Recently, the theoretical study of size dependence of ionization potential and dissociation energies of neutral and charged carbon clusters (C_n; n=40–70) have investigated at the B3LYP/6-31G(d) level [9]. The fullerene C_{50}, C_{60} and C_{70} have known as magic number fullerenes, because of the largest ionization potentials and dissociation energies. The aim of this research is to investigate the effect of size on the ionization potentials, electron affinities and other electronic properties of different carbon clusters with hybrid density functional B3LYP and PBE1PBE using 6-31+G(d) basis set at gas phase and 1atm pressure. It has been shown that the size has notable influence on the electronic properties of nanostructures.

2. Computational details

The ground state geometries were optimized at the DFT level using the B3LYP and PBE1PBE functionals and the 6-31+G(d) basis set. The energy required to release an electron from the system at the ground state is defined to the vertical ionization potentials (IP). The energy difference between the neutral and the anionic species is defined as the vertical electron affinity. The quantum molecular descriptors for nanocarbons were determined as follows:

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