ELECTRONIC STRUCTURE OF CARBON NANOCAGE WITH BIPARTITE STRUCTURE: A *DFT* study

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Introduction

The carbon is one of the chemical elements most found in nature. A of its main characteristics is the formation of polymorphs under various conditions of temperature and pressure. The figure. 1 shows some of the main forms allotropic of the carbon.

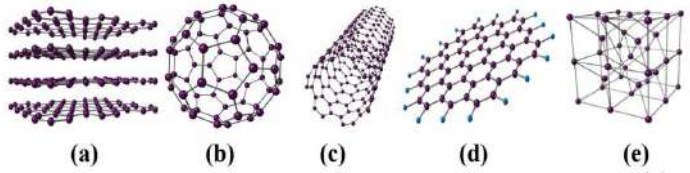

Figure 2 *– Schematic representation of different allotropes of carbon: (a) graphite, (b) fullerene, (c) nanotube, (d) graphene e (e) diamond.*

Although nanotubes and graphene are the most studied elements of the carbon nanostructures family, cage-like structure, like fullerenes[1], are subject de constant interest in the area. Such structure have potencial applications drug delivery(fig. 2a)[2] or as elements in nanojunctions(fig. 2b). For exemple[3].

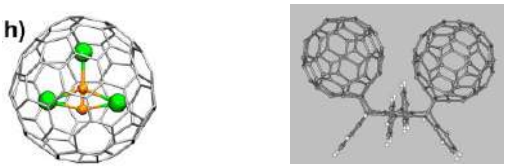

Figure 2 *– Schematic illustration of fullerene in applications (a) in drug transport and (b)in heterijunctions.*

Metodologia

The figure illustrate the geometric structure(semiocta) constructed from the FORTRAN computational language.

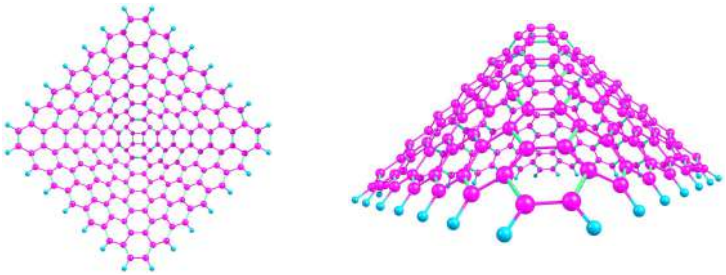

Figure 2 *– Schematics illustrations of the geometric structure of the semi-octahedron of size 6 viewed through chamcraft software.*

As usual in many-body electronic structure calculations, the nuclei of the treated molecules or clusters are seen as fixed (the Born–Oppenheimer approximation), generating a static external potential V in which the electrons are moving. A stationary electronic state is then described by a wavefunction Ψ(r1→,...,rN→) satisfying the many-electron time-independent Schrödinger equation

$$\hat{H}\Psi = \left[\hat{T}+\hat{V}+\hat{U}\right]\Psi = \left[\sum_i^N\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right)+\sum_i^N V(\vec{r}_i)+\sum_{i<j}^N U(\vec{r}_i,\vec{r}_j)\right]\Psi = E\Psi$$

This complicated many-particle equation is not separable into simpler single-particle equations because of the interaction term Û. DFT provides an appealing alternative, being much more versatile as it provides a way to systematically map the many-body problem, with Û, onto a single-body problem without Û. In DFT the key variable is the electron density n(r→), which for a normalized Ψ is given by

$$n(\vec{r}) = N\int \mathrm{d}^3r_2\cdots\int \mathrm{d}^3r_N\,\Psi^*(\vec{r},\vec{r}_2,\ldots,\vec{r}_N)\,\Psi(\vec{r},\vec{r}_2,\ldots,\vec{r}_N).$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V_s(\vec{r})\right]\varphi_i(\vec{r}) = \varepsilon_i\varphi_i(\vec{r})$$

Resultados e discussão

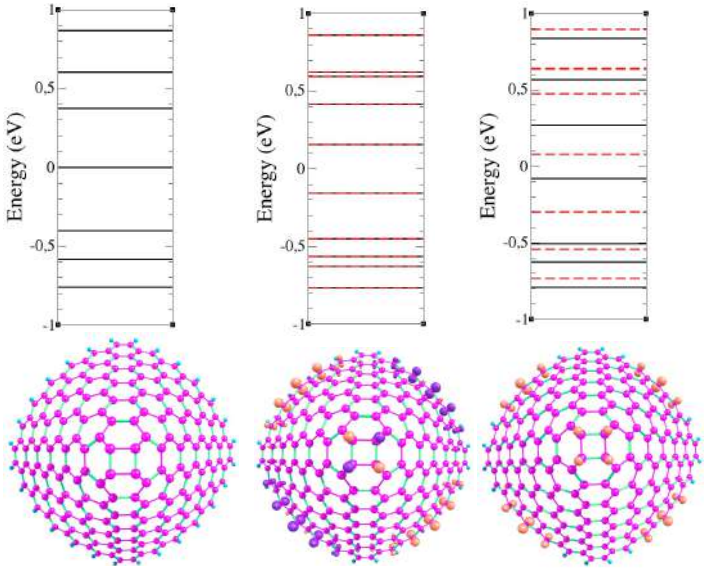

Figure 3 *– Electronic structure of the carbon half-octahedron of size 6 (C 196). The black and continuous color lines represent the "up" spin state and the red and dashed lines represent the spin state "dw".*

It is worth mentioning that the electronic levels for *spins up* and *down* are similar for AFM and PM configurations. This is due to the simple fact that the amount of polarized edges with spin up alignment is of the same amount of *spin down*, that is, we have two edges with *spin up* polarization and two edges with spin polarization *down*, with both configurations have a property of *spin up* symmetry and *dw*. In the PM configuration, since no edge has spin polarization, it also obeys the property of symmetry between the charge distribution *spin up* and *down*. In the TFM configuration, the electronic levels for spin up and dw do not coincide. This is due to the fact that the amount of polarized edges with spin up alignment is different from the amount of polarized edges with spin dw alignment. In the TFM configuration, all edges are biased with *spin up*..

Conclusão

We verified the existence of spin polarizations for the carbon half-octahedra, so that all possible magnetic configurations (PN, AFM, TFM) were observed from the size 6 (C 196) structure. As can be seen in the energy levels, we can modulate the HOMO-LUMO gap by choosing the magnetic state. Therefore, these structures, if inserted in nanodevices, may be potential systems for applications in spintronics.

Agradecimento

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Referências

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