

Study of the Effect of Electric Field on the Electronic Structure of C₆₀

دراسة لتأثير المجال الكهربائي على التركيب الإلكتروني للفوليرين C₆₀

¹ غيداء عبدالحافظ جابر، ² هند احمد محمد، ² وسن مناتي محمد،
¹ افراح محمد عبدالامير، ¹ علياء حفزي عباس و ¹ حامد ابراهيم عيود
¹ جامعة بابل / كلية العلوم / قسم الفيزياء
² جامعة بابل / كلية التربية للعلوم الصرفة / قسم الفيزياء
فيزياء نظرية

Abstract:

Tow strength of electric field were used to study their effects on the electronic structure for C₆₀ cage fullerene, weak and strong The results of B3LYP/6-31G** density functional calculations used in this work show that the strong electric field applied to C₆₀ cage changes the conduction and valence band energies.

In addition, electronic transition spectra of stable C₆₀ were calculated under electric field intensities.

الخلاصة :

تم دراسة تأثير شدتين للمجال الكهربائي، إحداهما قوية والأخرى ضعيفة، على التركيب الإلكتروني للفوليرين C₆₀. بينت نتائج الحسابات التي أجريت بطريقة دالة الكثافة بالمستوي B3LYP وبدوال أساس 6-31G** والمستخدم في هذا العمل أن هناك تأثير واضح للمجال الكهربائي القوي المسلط على الفوليرين C₆₀ على طاقات كل من حزمة التكافؤ وحزمة التوصيل. كما تم حساب أطيف الانتقال الإلكتروني للفوليرين C₆₀ بتأثير المجال الكهربائي وتحديد شدة الاهتزاز المقابلة لمديات المجال الكهربائي المسلط.

Introduction

Simply fullerene, a new allotropic form of carbon was first discovered in 1985 by sir Harold W. Kroto, Richard E. Smalley, Robert F. Carl and co-workers during the course of their mass spectroscopic studies on the pulsed laser vaporization of graphite [1-3].

The unique three-dimensional geometry of fullerenes with carbon spheres containing thirty or more highly reactive double bonds constitutes a rather rich scenario where a variety of different chemical reactions can be tested. The convex surface of fullerenes offers new possibilities for the study of new reactions and mechanisms under severe geometrical constraints on carbon atoms showing unusual SP^{2,3} hybridization [4].

The fullerene C₆₀ structure can work in wide fields of applications because it has special thermal, mechanical and electrical properties [5]. Many of these applications are in biology and for potential medicinal use, binding specific antibiotics to the structure to the target resistant bacteria and even target certain cancer cells such as melanoma [6]. The fullerene molecules have special photo-physical properties and due to their high electron affinity considered as the best electron acceptor in donor-acceptor systems [7-12]. And because of fullerene molecule ability to accept up six electrons, synthesized as candidates for photovoltaic devices [13-15].

Theory

The calculations in this study are carried out by Becke's three parameters Lee-Yang-Parr exchange correlation density functional theory B3LYP [16,17] with 6-31G(d,p) basis sets. Gaussian 09 package of program [18] was used to calculate the electronic properties of the studied structure.

The hybrid functional B3LYP has shown to be highly successful level for calculating the electronic properties [19]. The density functional theory partitions the electronic energy as $E = E_T + E_V + E_J + E_{XC}$, where E_T , E_V and E_J are the electronic kinetic energy, electron-nuclear attraction and the electronic-electronic respectively.

The exchange correlation energy E_{XC} is given according to B3LYP functional in the form [20]:

$$E_{XC}^{B3LYP} = E_{XC}^{LDA} + a_0(E_X^{HF} - E_X^{LDA}) + a_x(E_X^{GGA} - E_X^{LDA}) + a_c(E_C^{GGA} - E_C^{LDA})$$

The three parameters $a_0=0.02$, $a_x=0.72$ and $a_c=0.81$ and HF, LDA and GGA are the Hartree - Fock, local density and generalized gradient approximation, respectively.

The vertical ionization potential VIP and vertical electron affinity VEA can be calculated from the adiabatic method [21]:

$$VIP = E_{\text{cation}} - E_{\text{neutral}}$$

$$VEA = E_{\text{neutral}} - E_{\text{anion}}$$

Where E_{cation} and E_{anion} are the energy of the molecule derived from electron transfer (radical cation) and anion molecule, respectively.

Results and discussion

Figure 1 shows the optimized structure of C_{60} cage fullerene, and table 1 represents the results of the optimized parameters obtained at B3LYP density functional theory. These parameters include the bond length and bond angle.

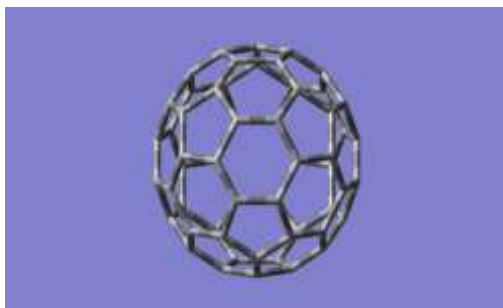


Figure1: optimized structure of C_{60} cage fullerene

Table1: The optimized parameters of fullerene C_{60}

| Description | Length(Angstrom) | Angle(Degree) |
|-------------|------------------|---------------|
| C-C | 1.4638 | |
| C=C | 1.3846 | |
| C-C=C | | 120.001 |
| C=C-C | | 119.997 |
| C-C-C | | 97.6331 |

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Figure 2 declare the results of effect of the weak electric field on the valence band, conduction band and energy gap of C₆₀ fullerene, the applied electric field is in the range (0.0001-0.0009) a.u. Without electric field, the C₆₀ fullerene has high occupied molecular orbital lie at (E= -8.33 eV) and the lowest unoccupied molecular orbital lie at (E= -0.63eV). Therefore, the energy gap for C₆₀ fullerene is (E_g=1.832 eV). The vertical ionization potential $VIP=E_{\text{cation}}-E_{\text{neutral}}$ and the vertical electron affinity $VEA=E_{\text{neutral}}-E_{\text{anion}}$ values determined by DFT energy calculations are defined by adiabatic method. The VIP and VEA of C₆₀ have been calculated(7.78 and 2.57)eV, respectively.

The electronic configuration of C₆₀ consists namely a five – fold degenerate highest occupied molecular orbital and a triply degenerate lowest unoccupied molecular orbital. The result of energy gap means that C₆₀ has high reactivity toward both electrophilic and nucleophilic, the LUMO is predicted to be triply degenerate and energetically low lying, making a good electron acceptor capable of having six reduction states. Means, C₆₀ fullerene is an electron from the nucleophilic.

Figure 2 declare that there is no clearly effect of electric field appear on valence and conduction band. This means the weak electric field cannot be used to change the states of C₆₀ fullerene. Figure 3 shows the effect of strong electric field on valence band, conduction band and energy gap of C₆₀ fullerene. CB and VB both change with increasing the applied electric field, the valence band maximum and the conduction band minimum are made from bonding states only. The applied electric field enhanced the bonding states of valence and conduction bands, and weakness the antibonding states of valence and conduction bands.

The change in the band gap energy of C₆₀ was illustrated in figure 4, increasing the strong applied electric field changes the energy gap. The lowest value of energy gap (E_g=0.092 eV) at electric field (0.03 a.u) and the largest (E_g=2.134 eV) at electric field (0.01 a.u).

The electronic transition oscillations of C₆₀ fullerene as a function of weak and strong electric field was illustrated in figures 5 and 6, respectively. As we see in figure 5, the transition approximately remain the same and there is no change in the first excited state, the transition is in the range (697 -703) nm. The result means the absorption spectrum has stable states, they are unaffected by the applied weak electric field. While these states are varying by increasing the electric field, the wave length of the first excited state was oscillating in the range (665 -1178)nm. At (0.04 a.u) electric field and it reaches (1178 nm) wave length as we see in figure 6.

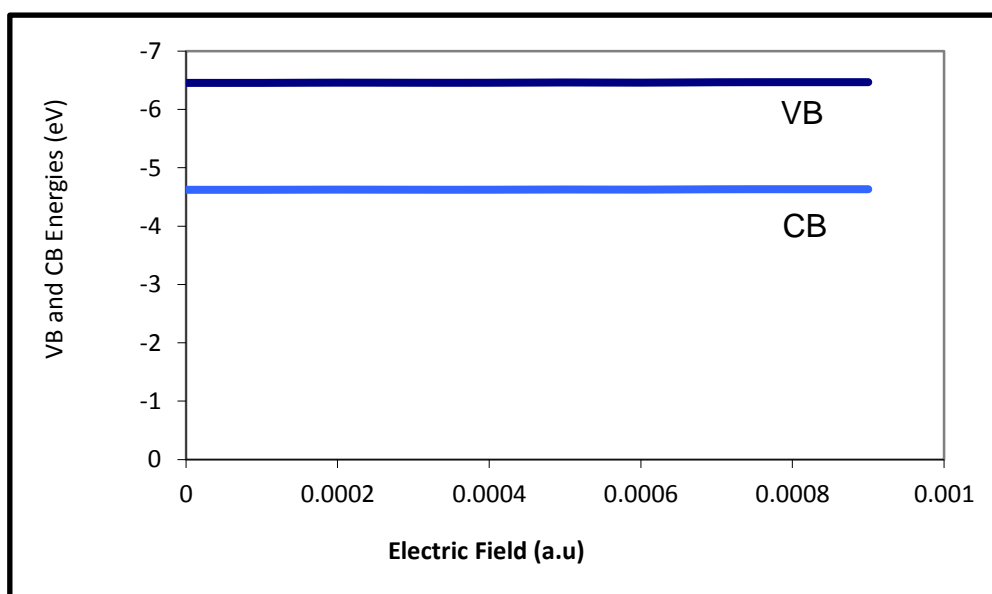


Figure 2: VB and CD behavior as a function of weak electric field

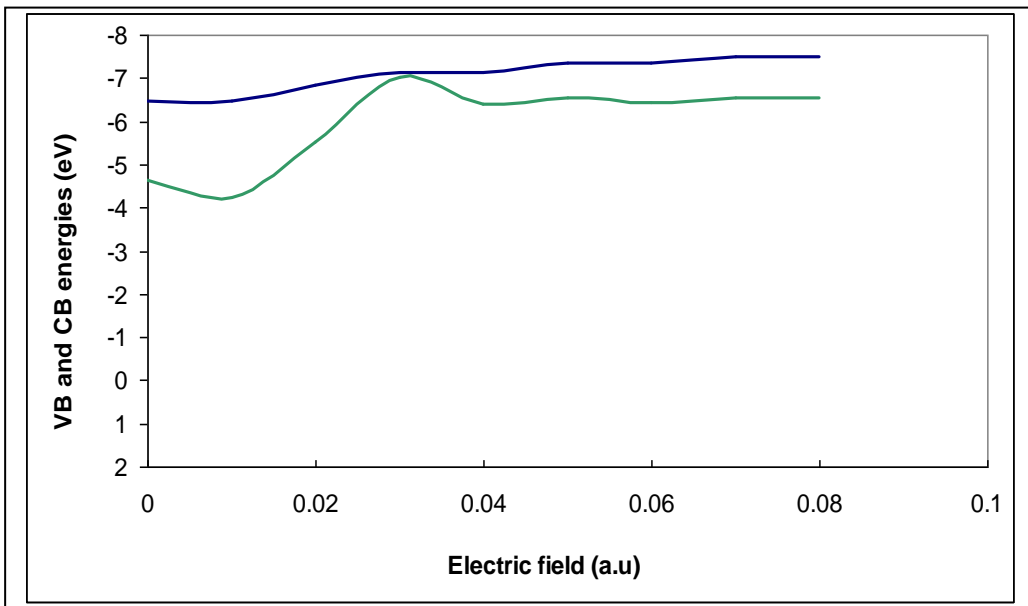


Figure 3: VB and CB behavior as a function of strong electric field

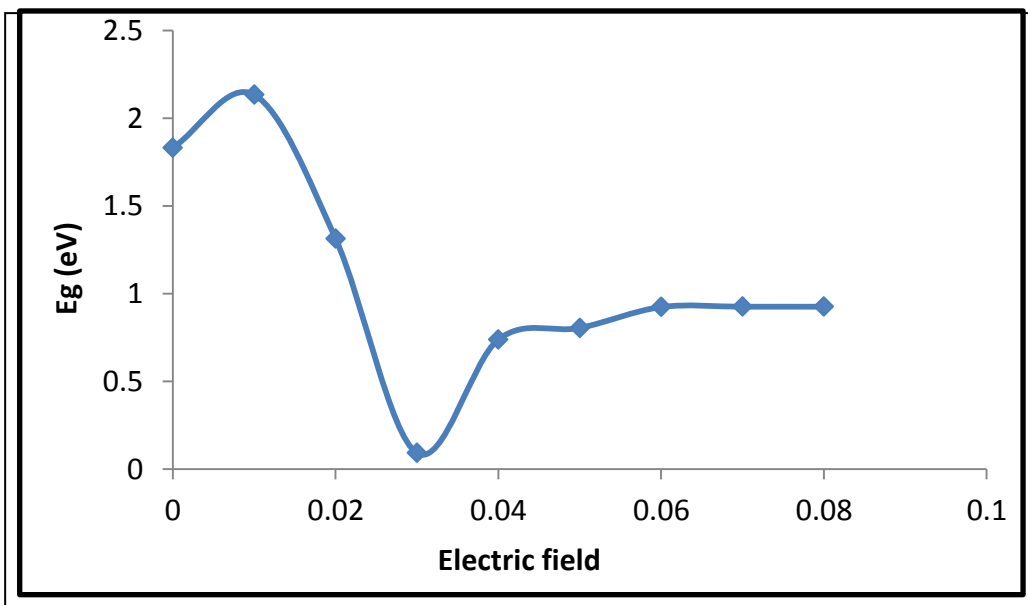


Figure 4: The band gap energy of C_{60} as a function of strong electric field

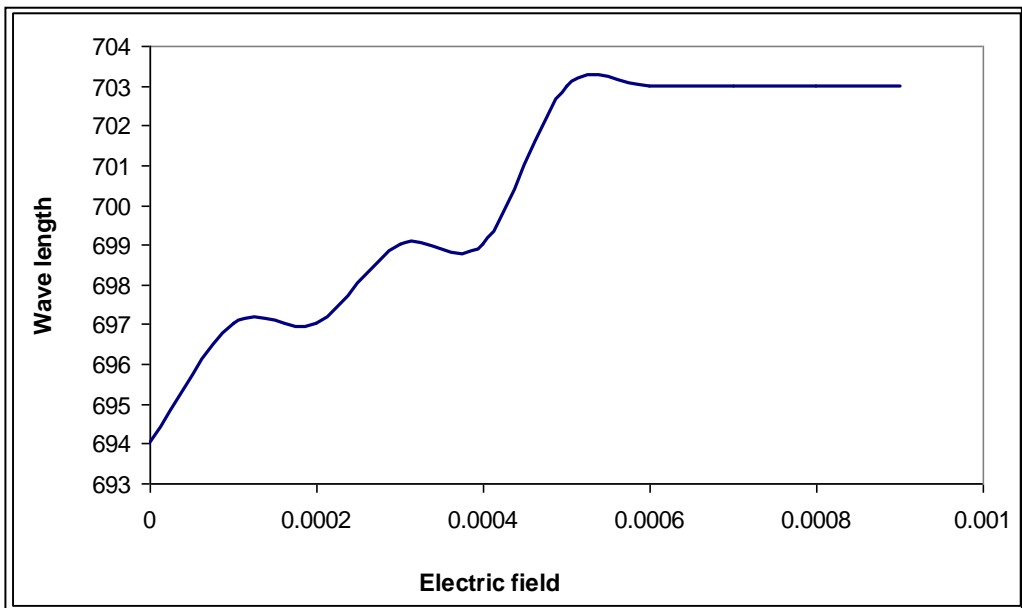


Figure 5: The first excited state of C_{60} fullerene as a function of weak field

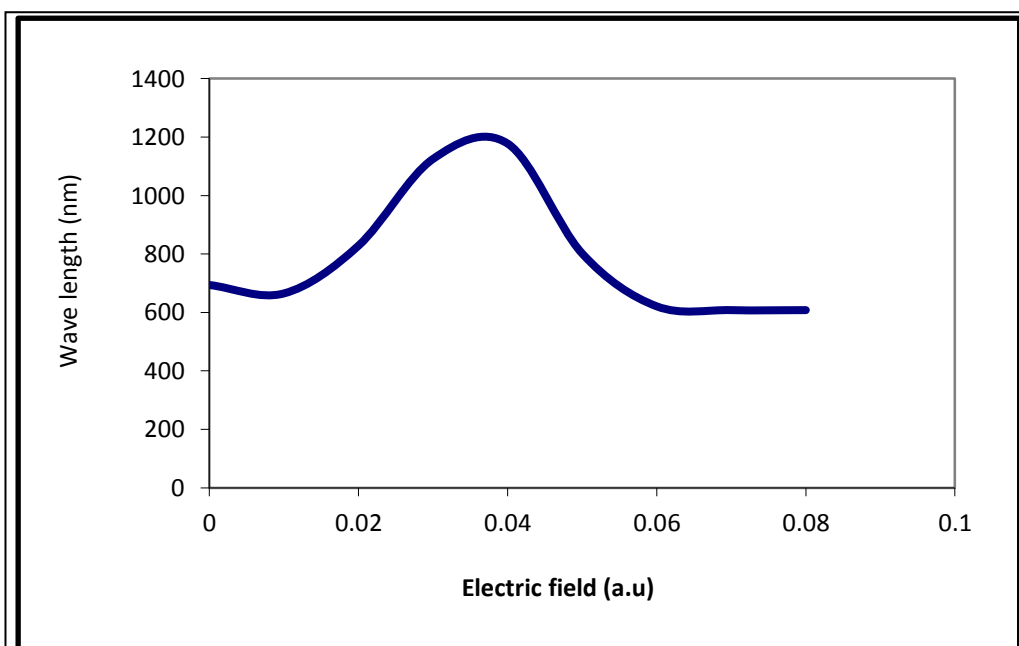


Figure 6: The first excited state of C_{60} fullerene as a function of strong electric field

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conclusion:

1. The energies of the studied structure are not change with weak electric field applied to the structure, while the strong electric field changes the valence and conduction bands of the fullerene.
2. The energy gap varying due to increasing the strength of the strong electric field applied.
3. The absorption spectrum has stable states, they unaffected by the applied weak electric field. While these states are varying by increasing the electric field.
4. The wave length of the first excited state was oscillating in the range (665 -1178)nm.

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