Density Functional Theory Calculation of the Electronic Structure for C_{20} Cage Fullerene

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حسابات نظرية دالة الكثافة للتركيب الالكتروني للفوليرين C_{20}

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Abstract:

In this work, the electronic structure of C_{20} cage fullerene is studied theoretically under the effect of electric field using B3LYP density functional theory with 6-31G** basis sets. Varying strength of electric field (week and strong) was applied to the structure. Valence band, conduction band and energy gap were calculated and analyzed. The electronic transition spectra of C_{20} are calculated under strong electric field.

Key words: Fullerene, C_{20}, electric field, DFT and energy gap.

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الخلاصة :

في هذا البحث دراسة نظرية للتركيب الالكتروني للفوليرين C_{20} بتأثير المجال الكهربائي المسلط وباستعمال طريقة دالة الكثافة بالمستوى B3LYP وبتطبيق دوال أساس 6-31G**. تم تسليط مجال كهربائي ضعيف وقوي على التركيب قيد الدراسة. تم حساب حزمة التوصيل, وحزمة التكافؤ وفجوة الطاقة للتركيب بتأثير المجال الكهربائي المسلط، كما تم حساب أطياف الانتقال الالكتروني للفوليرين C_{20} تحت تأثير المجال الكهربائي.

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Introduction

Fullerenes are Cage structured carbon clusters composed of pentagonal and hexagonal faces. C_{20} fullerene is the smallest fullerene has twelve pentagons without hexagonal rings.

The table isomers of C_{20} clusters consist of bowl, ring and fullerene structures. These structures can be synthesized experimentally under suitable reaction conditions[1,2]. The C_{20} fullerene is meta stable at very high temperatures, it is predicted to be sufficiently stable at low temperatures, C_{20} fullerene is stable not only thermodynamically but also kinetically [2]. The smallest C_{20} fullerene has been recently synthesized in a gas phase by Horst Prinzbach et al.[4] and then confirmed theoretically. Each carbon atom in C_{20} cage fullerene is bonded to three other carbons with a bond angle of 180°, which is close to the tetrahedral bond angle[3-5].

Many theoretical studies, such as ab initio and density functional theory calculations have been studied the structure and the stability of C_{20} cage isomers[4].

Present work aims to study of the effect of weak and strong electric field on the electronic proportion of C_{20} cage fullerene, and investigate the electronic transition spectra of C_{20} fullerene under strong electric field by employing B3LYP density functional theory.

Method and Calculations

The Becke's three parameter Lee-Yang-Parr exchange correlation density functional theory B3LYP was used with 6-31G** basis sets. The calculations have been carried out using Gaussian 09 package of program [6].

According to B3LYP functional, the exchange correlation energy E_{XC}^{B3LYP} is given by [7]:

$$E_{XC}^{B3LYP} = E_{XC}^{LDA} + a_o \left(E_X^{HF} - E_X^{LDA} \right) + a_x \left(E_X^{GGA} - E_X^{LDA} \right) + a_c \left(E_C^{GGA} - E_C^{LDA} \right)$$

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

The vertical ionization potential IP and vertical electron affinity EA in DFT can be calculated according to the following relations[7-10].

IP= E_+ - E_n EA= E_n- E_-

Where E_+ , E_- and En are the internal energies of cation, anion and neutral molecular system, respectively.

Results and discussion

Table 1 shows the results of valence band, conduction band and energy gap corresponding to weak electric field applied to C_{20} Cage fullerene, as we see, the high occupied molecular orbital energy is (EHOMO= -2.658 eV) and the lowest unoccupied molecular orbital energy is (ELUMO= -2.406 eV), the energy band gap for C_{20} fullerene is (HOMO-LUMO=0.252eV) and this value in a good agreement with experimental data [9], that means the C_{20} Cage fullerene exhibits only a small John-Teller induced HOMO-LOMO gap. The valence band (VB) and the conduction band (CB) are very small changes under weak electric field applied to C_{20} fullerene, that due to the structure of fullerene is made by covalent bands which have only small response to the weak electric field strength, as shown in figure 1.

The behavior of valence and conduction band as a function of a strong electric field applied to C_{20} fullerene was illustrated in table 2. There is a large change in both valence and conduction bands will produced by arising the strength of applied electric field, the valence band maximum and conduction band minimum are made from bonding states only, as shown in figure 2. The applied electric field weakness the antibonding states of valence band and conduction band and enhances the bonding states of valence and conduction bands. There is large change for both valence and conduction band under the strong electric field because of the skeleton of fullerene is made by bonds which have large response to the strong electric field.

Table 1: The results of valence band, conduction band and energy gap for C_{20} fullerene corresponding to weak electric field

Electric field intensity(a.u)	Valence band(eV)	Conduction band(eV)	Energy gap(eV)
0.000	-2.645	-2.410	0.235
0.0001	-2.648	-2.412	0.236
0.0003	-2.649	-2.413	0.236
0.0005	-2.650	-2.412	0.238
0.0007	-2.650	-2.412	0.238
0.001	-2.650	-2.412	0.238

Table 2: The results of valence band, conduction band and energy gap for C_{20} fullerene corresponding to strong electric field

Electric field intensity(a.u)	Valence band(eV)	Conduction band(eV)	Energy gap(eV)
0.000	-2.645	-2.410	0.235
0.01	-2.615	-2.105	0.510
0.02	-3.965	-3.863	0.102
0.03	-4.322	-4.257	0.065
0.04	-4.445	-4.025	0.420
0.05	-4.465	-3.990	0.475
0.06	-4.478	-4.098	0.560
0.07	-4.480	-3.920	0.560

Figure 3 show change energy gap with increasing the applied strong electric field, This change oscillates due to the strength of electric field lowest value of energy gap in (Eg = 0.065 eV) at electric field of (0.03 a.u) , and the largest (Eg = 0.560 eV) at electric field (0.06 a.u).

Figures 4 and 5 illustrate the behavior of electronic transition oscillation of C_{20} fullerene as a function of weak and strong electric field respectively. At weak electric field applied to C_{20} fullerene, there is no change in the 1st excited state and the transition remain approximately in the range of wave length (2050 - 2100) nm, that means the state of absorption spectrum stable and applied electric field do not effects on this state.

Increasing the strength of the applied electric field leads to varying in the wave length of the 1st excited state with increasing the electric field intensity. The wave length oscillates in the range (700 - 1200) nm, it reaches approximately(800) nm wave length at 0.02 a.u electric field. Figures 4 and 5 are drawn from the CIS calculation for the studied structure under the applied electric field.
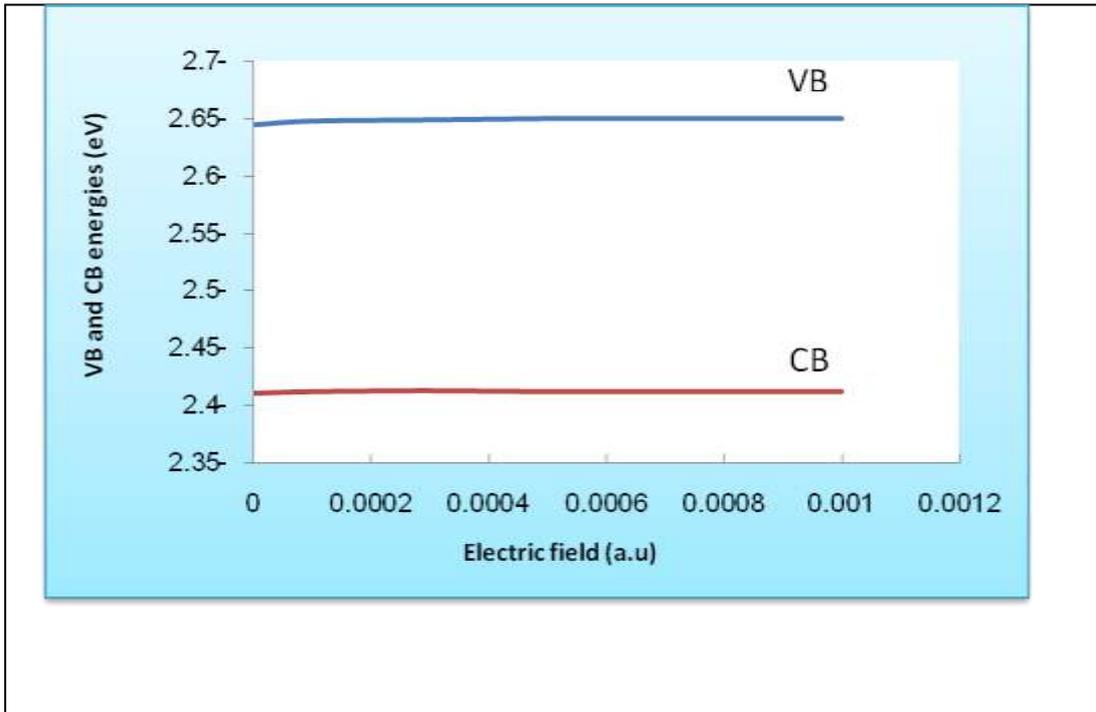
Figure 1: The relation of valence band and conduction band with weak
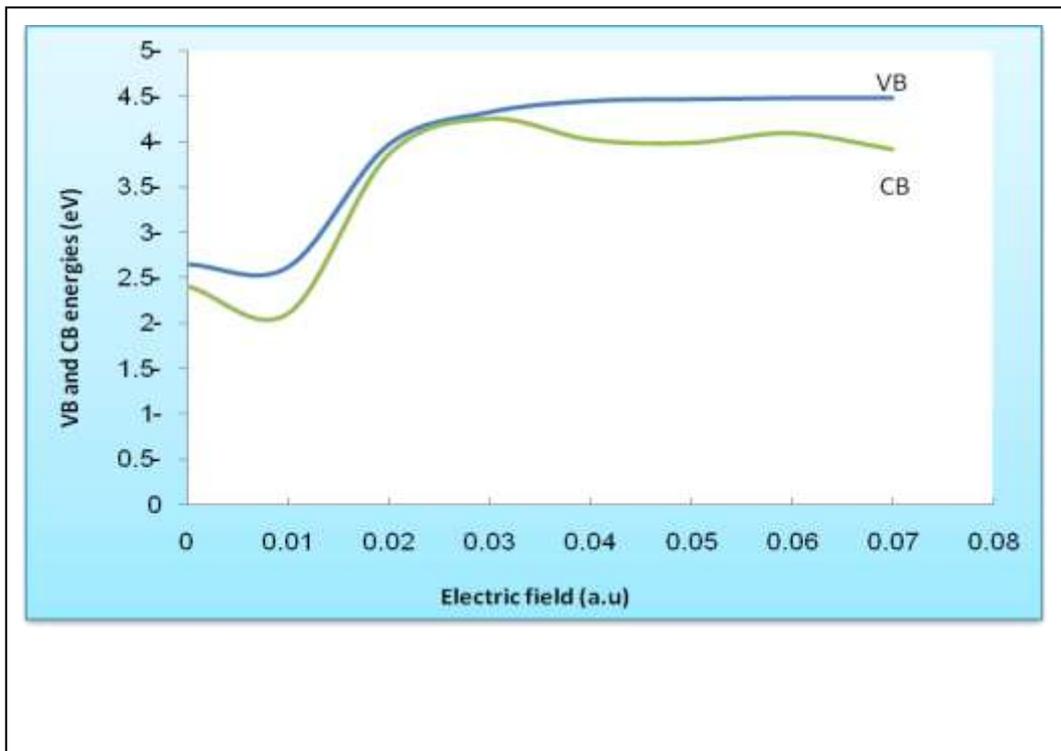electric field

Figure 2: The relation of valence band and conduction band with strong
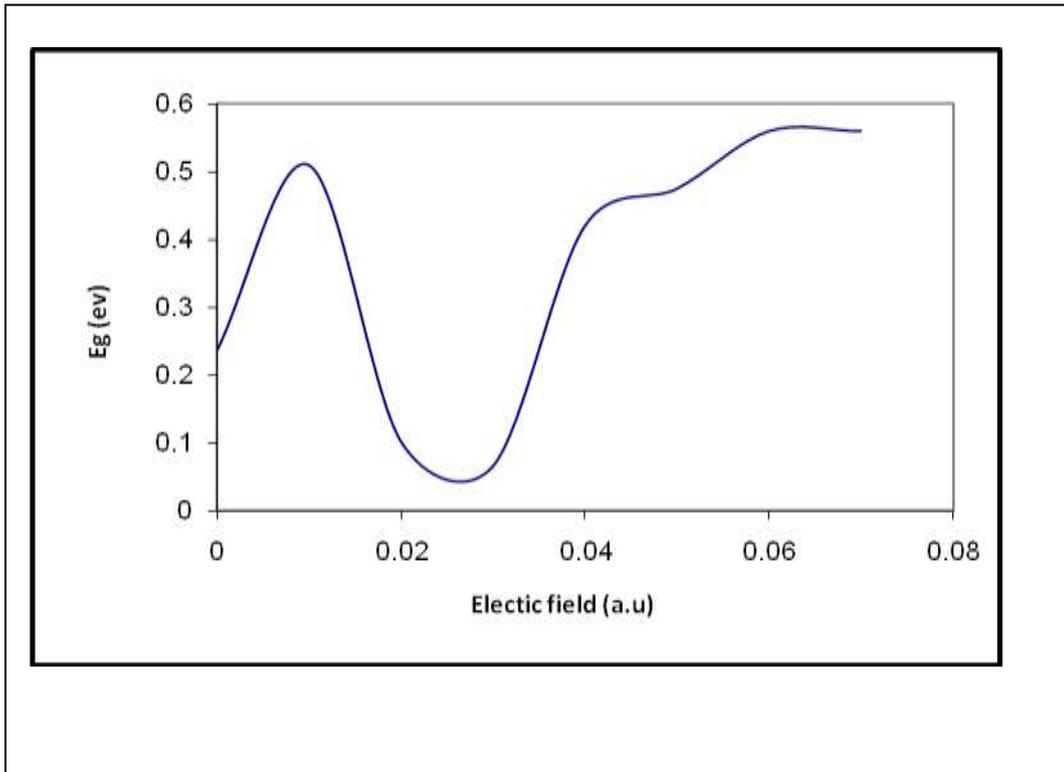electric field

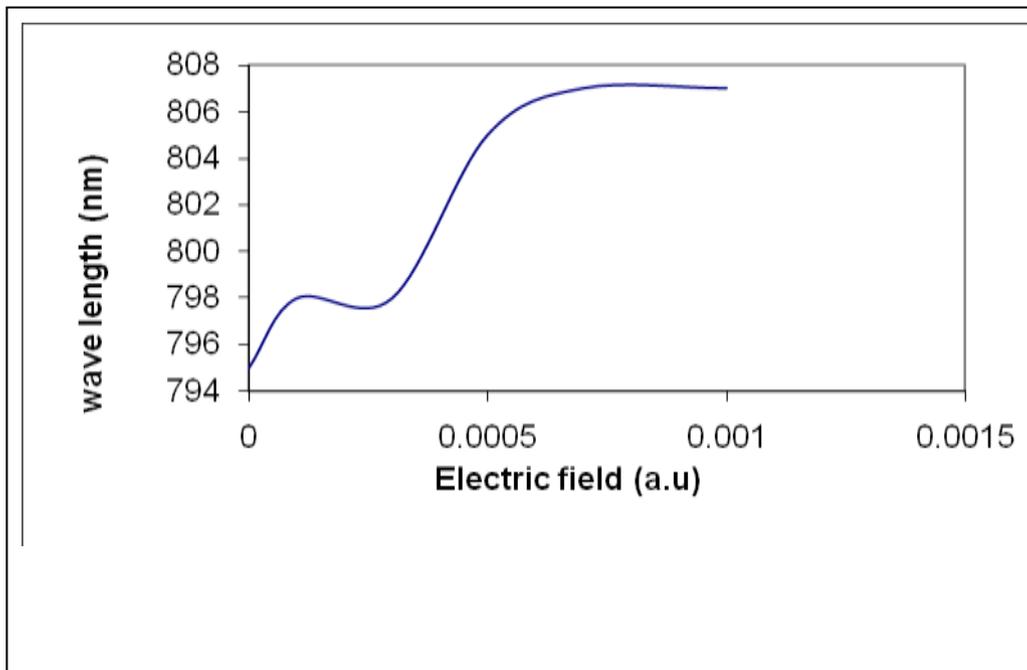Figure 3: The energy band gap of C_{20} fullerene as a function of strong electric field
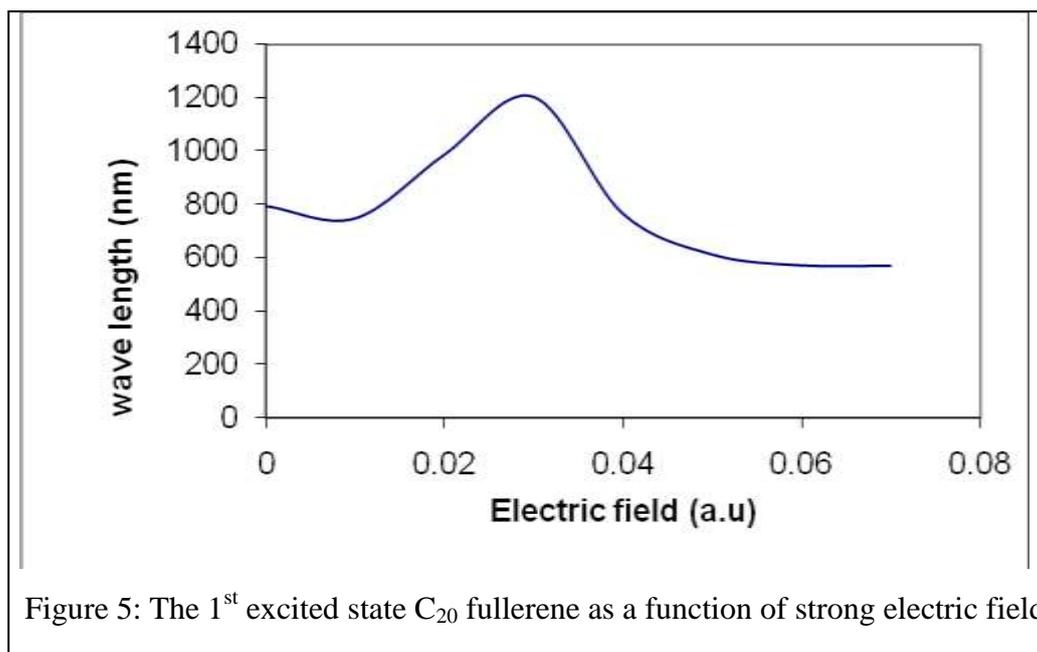

Figure 4: The 1st excited state C_{20} fullerene as a function of weak electric field

Figure 5: The 1st excited state C_{20} fullerene as a function of strong electric field

Conclusions

From the results produced in this study, we can conclude that the method used in analyzed calculations is a best method in which we cannot found previous studies in this field. 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, therefore the energy gap varying due to increasing the strength of the strong electric field applied. The applied electric field enhances the bonding states of valence and conduction bands and weakness the antibonding states of valence band and conduction band.

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