Study of absorption Ag ion in C_{24} with external electrical field by DFT computational chemistry method in gas phase

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Abstract

In this work study external electrical field effect in stability between Ag ion and C_{24} in deferent places by computational chemistry method. Nowadays by theoretical calculations can be discovered many properties of materials in Nano level set so that the results with experimental results. Increasing the processing power of computers allows heavy calculations on molecules have been possible. C_{24} There is a form of carbon such as a ball is round and has unique properties that are interesting to study. In this research by simulation Ag ion in center of C_{24} and study of deferent places stability by (HOMO-LUMO-GAP) HLG energy and by replace Ag ion we found the best point in 2 A^0 center of C_{24}. When apply external electrical field With intensities 10, 20, 30 and 40 au (1 au = 27.2107 ev) Z coordinates we understand that change HLG energy with increased field was more . Study again Ag ion position with external electric field to center of C_{24}. In this paper we got conclusion that by increasing external electrical field changes are increase too and can be found the best absorption site by changing electrical field. All calculated in gas phase with Gaussian 03w package of program by B3LYP method at 6-31G* level of standard basis set.

Key words: C_{24} , Computational Chemistry , External electrical field , Absorption

1. Introduction

In recent decades, by increasing processing power of computers, new methods in computational chemistry to explore of materials at the nanoscale properties has emerged that in some cases, to accurately experimental methods answers can be expected quantum chemistry by using the Schrödinger equation and various approximations can predict various properties of nano-materials is one of the useful methods Density Function Theory (DFT) method by using the approximate real could satisfaction in quantum chemistry calculations .In This article absorption of Ag ion on Fullerenes in the presence of electric field by using Density Functional Theory (DFT) has been studied . Fullerenes are shaped carbon clusters large closed cages and have several important features are that these features previously have not been observed in other compounds. Totally Fullerenes in are interesting class of compounds that certainly will be used applied future technology. Such as many other materials in important scientific discoveries Fullerenes have been found randomly too. In 1985, Smalley interesting results in the mass spectra of carbon evaporates leading that discovered Fullerenes and stability was found the gas phase and the search for other Fullerenes started[1].
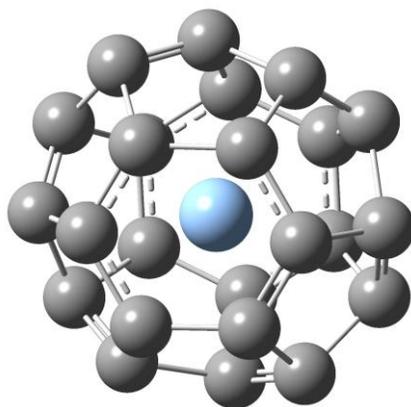

Fig 1: Shows Ag ion in center of C_{24}

2. Computational Methods

N-electron energy of a system can be expressed based on probability density it means as the electron energy is written as ρ_ε. While the density is written in methods $\rho\varepsilon$ as function of space coordinates .It is called DFT method. DFT electron energy in a system, based on the equation of Kohn-Sham is written as follows.

$$E=E_T+E_V+E_J+E_{XC}$$

E_T term is associated to kinetic energy which be come large by moving electrons. E_V is potential energy words that include interactions nuclear - electron and electron-electron. E_J term is the repulsion energy electrons - electrons and finally E_{XC} term is solidarity energy and exchange electrons. All of these terms except for repulsion nuclear-nuclear are the density function of electron and equation of N-electron system can be written as follows.

$$\varepsilon[\rho] = \frac{\hbar^2}{2m_e} \sum_{i=1}^{n} \int \Psi_i^*(r_1) \nabla_1^2 \Psi_i(r_1) dr_1 - \sum_{I=1}^{N} \int \frac{z_i}{4\Pi \varepsilon_0 r_{I1}} e^2 \rho(r_1) dr_1$$

While density base charge of $\rho_{(r)}$ at position a like this.

$$\rho(r) = \sum_{i=1}^{n} |\Psi_i(r)|^2$$

That The sum is over all occupied orbital by KS .Considering the above relationships, if the KS orbital be achieved ground state electron energy molecule can be calculated . KS equations for single-electron orbital is as follows [2].

$$\hat{H}_i^{KS} \Psi_i^{KS} = \varepsilon_i^{KS} \psi^{KS}$$

Where the Hamiltonian operator contains 4 single-electron kinetic operator electron-electron attraction between potential energy Repulsion energy between electrons, is the exchange potential correlation . Several DFT methods including B3LYP energy combined with various exchange obtained by functions correlation[3]. All calculations have been performed in gas phase using Density Functional Theory (DFT) method of B3LYP at 6-31G* standard basis set is used Gaussian 03w package of program[4].

3. Results and Analysis

In this paper by examining different parameters such as Total of energy system Homo Lumo Gap(HLG) energy that most stable Ag ion in different modes C_{24} we could reach the external electric field changes the stability is studied . Basic studies were found with applied electric field in the Z axis influence the most on Fullerenes that studied by applying electric field in the Z axis to investigate the gap energy gap we have discussed . Difference between Homo and Lumo is called gap energy the amount they that whatever the difference is we have more stability that this is a good descriptor for this stability is . To do this first Fullerenes in gas phase using Density Functional Theory (DFT) and level calculated 6-31G * optimized that we reach full stability, and then absorption places for Ag ions we determined that the center of Fullerenes to 3 A^0 is continued distance . With reviews conducted and plotted energy in chart 1 can most stable state with out electric field in distance 2 A^0 from the center we predict . Then, by applying electric field to the 10 , 20 , 30 and 40 au (1au = 27.2107 ev) to review sites that did so absorbed was determined in the presence of stable electric field is associated with changes in a graph is visible .Has had greatest impact in two angstrom place which from the state of most stability as low-lead stability and distance 1 Å from the center of the most stable point can be considered that with increasing electric field distance 2 Å begin to sustainability that Chart 1 .
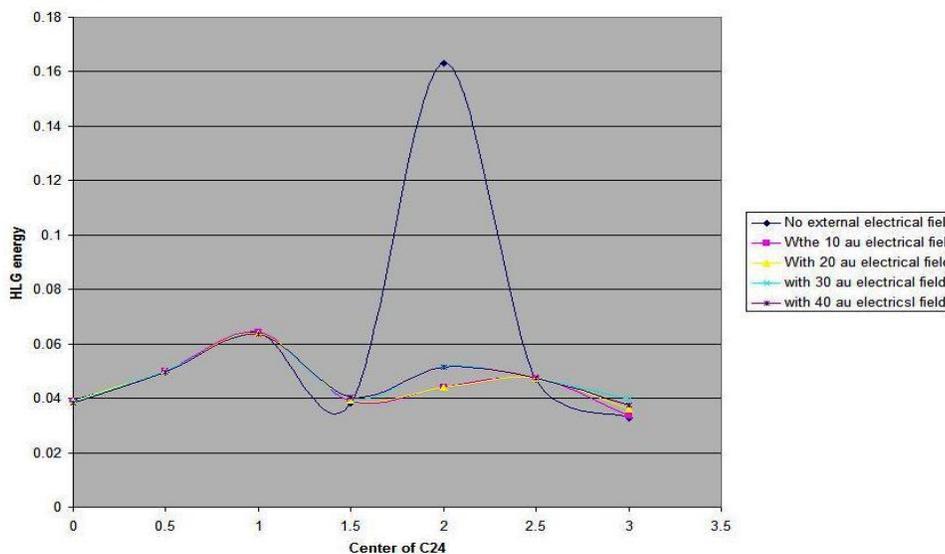
Chart 1 : HLG energy of C_{24} and Ag ion in deferent place

4. Conclusions

With reviews conducted on Fullerenes by theoretical chemistry and careful study of energy we reached this conclusion that can be applied electric field changes across the stability of Fullerenes and to a controlled element or absorb the isolated Fullerenes That it would be in medicine and electronics we useful . Theoretical chemistry and density function method and the method was very useful for this paper and nano materials .

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