

Physical Properties of Anthra [2,3-b;6,7-b'] Dithiophene Organic Material

^{a,b,*} Hazhar Hamad Rasul, ^b NiyaziBulut, ^c Bayram Gündüz

^a Department of Physics, College of Science, Salahaddin University, Erbil-Iraq

^b Department of Physics, Faculty of Science, Firat University, 23169 Elazig Turkey

^c Department of Science Education, Faculty of Education, Mus Alparslan University, 49250 Mus, Turkey

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ABSTRACT

Anthradithiophene (ADT) is a front-runner in the world of small molecule semiconductors for photo electronics and organic electronics (OE), especially in OPV is abbreviated organic photovoltaics and OFET is abbreviated organic field effect transistors. In this study, ADT was optimized using the Hartree-Fock (HF) and the density functional theory (DFT). The highest occupied molecular orbital (HOMO), "conduction band" and lowest occupied molecular orbital (LUMO), "valance band" were computed and from here band gap energy was obtained. In addition, electrostatic potential map for the ADT molecular levels were indicated and explained in detail. Results of using two methods such as DFT and HF theory, confirmation of DFT is much better than the HF theory.

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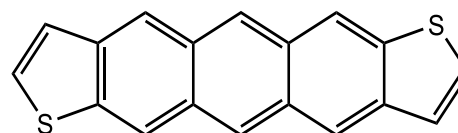
1. Introduction

At the moment, computers have become an essential part of the world of science, particularly when it comes to calculator problems. For problems which cannot be solved numerical methods and analytically, computers are of essential importance.

In a world where we are dependent on matter properties that help us improve our lifestyle, it is necessary to study their properties so that we can use them in our service. Matters are due to electronic properties. These matters consist of various types of particles, each with mass and size. These materials are constituted by clouds of electrons that oscillate around a set of nuclei, where every particle interacts with each other within some order, and the key features of the material are as a result of the electronic properties [1].

Since the improvement of quantum mechanics in the 1920s and with the introduction of the Schrödinger equation (SE) in 1926, different approaches to solve the SE have conventional substantial attention by chemists and physicists around the world.

The first steps to deal with the analytically and complex not accessible many body SE were achieved by Hartree and Fock (HF), who derived a set of self-consistent (SC), wave function (WF) based equations which allowed an iterative computation of energies and other wanted parameters.[2, 3]. The HF method has been used intensively up to now, in atomic and nuclei physics as well as theoretical chemistry.



Chemical Formula: $C_{18}H_{10}S_2$

Molecular Weight: 290.40

Elemental Analysis: C, 74.45; H, 3.47; S, 22.08

Figure 1. Molecular structure of Anthradithiophene (ADT).

* Corresponding author:

E-mail (hazharhrm@gmail.com)

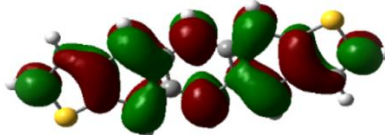
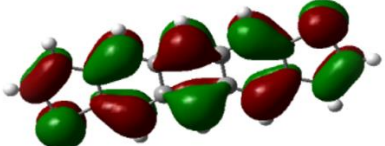
Experimental	DFT-Method	HF-Method	
-2.02 eV	-2.47107eV	-1.01362eV	
2.79eV	2.593791eV	5.80909eV	
-4.48eV	-5.06486eV	-6.82271eV	

Figure 2. Boundary molecular orbitals and energy levels for HOMO and LUMO orbitals of $C_{18}H_{10}S_2$.



Figure 3. These figures represent the Potential Energy Surfaces for molecules of ADT. For Basis (6-311G) and different methods DFT and HFT

This also obvious the birth of the density functional theory (DFT) that is developed to the main parts. In chemistry, in 1998 Kohn was awarded the Nobel Prize for his development of the DFT [4, 5]. Kohn and Sham derived a set of SC in 1965, iteratively solvable equations which lastly allowed to use the up to that point only theoretical concept of Hohenberg and Kohn (HK) also in actual calculate simulations[6]. Annotation the fact the WF is a much complex quantity than the electron density, the computation times of DFT calculations are essentially lower. The electron density, a variable only depending on three spatial variables, in principle includes all information about the ground state properties of a system.

We report here the show physical properties of ADT molecule, such as band gap (BG) and the potential energy surface (PES). To indicate the influence using the wavefunction and electron density to describe the energy of molecule.

2. Theory

In this paper, all atomic calculations and simulations were made using Gaussian software. The theoretical distance

between atoms was optimized by using the density functional theory (ADT), along with (B3LYP) and Hartree Fock (HF) theory. Both methods by using basis 6-311G. Usually, the HF method accounts for about 99.5% percent of the electronic energy, and several chemical properties, such as force constants, polarizabilities, dipole moments, magnetizabilities and excitation energies are typically off by less than 10 percent [7]. The problem with HF is that it does not include all effect of electron correlation. The broadest definition of electron correlation is to say that the position of the single electron depends on all other the position of electrons.

In quantum chemistry, the DFT approach is the most broadly used method. The basis for DFT is the proof by HK that the ground state electronic energy is determined wholly by the density of electron, In other words, there exists a one-to-one correspondence between a system and the electron density of the energy. The idea behind DFT is that the energy of a molecule can be determined by the density electron density that is depended on it instead of a wave function.

Electron density is expressed in this formulation as a linear combination (LC) of basis functions similar in mathematical form. A determinant is then formed from these functions, known as orbitals of Kohn Sham (KS). It is the

electron density that is used to compute the energy from this determinant of orbitals.

To compute the energy gap some researchers use molecule computations to estimate the band gap (BG) from the HOMO-LUMO energy separation. The energy difference between the top of the highest filled band and the bottom of the lowest empty band is called the BG and is corresponding to the HOMO and the LUMO gap in molecular systems [8]. The unoccupied molecular orbitals are called virtual orbitals. A gap means nothing else than the difference between two states. Electrons are able to jump from one band to another. In order for an electron to jump from a HOMO band to a LUMO band, it requires a specific minimum amount of energy for the transition is called the BG energy [9].

3. Results and Discussion

We presented a shorted study of Anthradithiophene (ADT) as shown molecular structure in Figure 1. And to obtain a band gap by different methods for knowing which way is better than others for ADT by comparing the experimental data [10], as shown in Figure 2. In the result, DFT is much better than the HF theory, because the DFT is not used the wave function to describe the energy of a molecule, instead the electron density is used, the basic variable is the density rather than the WF and it is description of interacting electrons in the ground state, including exchange and correlation. The problem with HF is that it does not include all effect of electron correlation. Also HF approach field, each electron interacts only through an average potential with the other electrons and fails to account for the instantaneous repulsion effects of electron-electron. Also, determine the potential energy surface by two different methods, that it is suitable with properties of ADT, as shown in Figure 3.

The red region of this diagram corresponds to the region of greatest electronegativity. Also, the blue color represents a small electronegativity. About yellow and green color, they have more electronegativity than blue but less than red color. As shown that it is nonpolar due to their high ratio of carbon to hydrogen.

4. Conclusion

In conclusion, we computed the band gap energy (BG) and determined the potential energy surface (PES) by two different methods such as density functional theory (DFT) and Hartree-Fock (HF) theory, also we indicated which methods is better than others. These results, showed density functional theory is much better than the Hartree-Fock theory.

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