ISSN 2587-1943

MOLECULAR ORBITAL CALCULATION FOR ANTHRADITHIOPHENE (ADT) COMPLEX BY USING HARTREE-FOCK THEORY

Hunar Hama Khalid 1 , Hazhar Rasul 2

Original scientific paper

In this study, we investigate the Hartree-Fock (HF) of Anthradithiophene (ADT) complex in detail. Hence, before quantum mechanical calculations were optimized using various basis sets. For appropriate calculation level. The highest occupied molecular orbital (HOMO) and the lowest occupied molecular orbital (LUMO) were plotted. Also, based on the obtained results, the band gap energy was calculated. Finally, we have a demonstration of the average band gap for ADT molecule.

Anahtar Kelimeler: *Hartree-Fock, Molecular Orbital, Anthradithiophene, Energy Band Gap.*

1 Giriş

Organic thin-film transistors depending on oligothiophenes or pentacene have reached device efficiency with mobility ranging from of 0.1-1 cm^{-2}/Vs and on/off current ratios greater than 10^6. In fact, monolithic incorporation of plastic transistors and organic lighting systems offers prospective applications not only in low-end information storage, such as intelligent cards or identifying tags but also as switching equipment in active matrix displays. ADT is a successful organic thin-film transistor material: it can be viewed as an intermediate among pentacene and oligothiophenes from its molecular structure. Particularly interesting is the significance of its sulfur orbit on electronic transport characteristics [1].

Hartree-Fock's theory is crucial for most electronic structure theory. It is the basis of the description of molecular orbital (MO) that indicates that each electron's motion can be described by a single particle (orbital) characteristic that does not depend explicitly on the instantaneous movements of the other electrons. Hartree-Fock's theory often provides a good beginning point for more elaborate theoretical methods easier evaluated for Schrodinger's electronic equation [2].

The Hartree – Fock method is widely used in quantum chemistry for calculated electronic structure computations. Hartree–Fock 's theory is the variability of this minimizing issue [3]. The HF estimate is not only the foundation of nearly all conventional methods, such as wave function depend on quantum chemical methods, but is also of good theoretical significance [4]. The HF treats exchange exactly but neglects correlation completely. While the HF complete energy is an upper limit to the real ground-state complete energy [5].

In this study, we have focused on the molecular orbital of ADT molecule, by investigating the HF theory by using some basis sets. The molecular orbital theory has to turn into a strong technique for exploring molecules ' electronic structure, enlightening some chemistry regions. The theory of MO originates from early studies in band spectroscopy of diatomic molecules and has been broadly used to explain most aspects of molecular structure and various molecular characteristics such as electronic dipole moments, optical absorption spectra, electron and nuclear magnetic resonance [6].

2 Computational Detail

In literature, there have been some experimental results about the ADT molecule. It was synthesized as a thin film with a (10um) mm^2- sized platelets of ADT single crystals were grown from the vapor phase in a stream of gas [1]. The material crystallizes in a layered structure similar to rigid rod-like oligomers of thiophene. Consequently, the electrical and optical properties are expected to be highly anisotropic. For electrical measurements, ohmic contacts were prepared by thermal evaporation of gold through a shadow mask. An annealing step in a flow of hydrogen at 150 ^oC was applied after contact preparation to reduce trapping states within the samples and to improve the quality of the ohmic contacts. Current-voltage characteristic was measured in a helium atmosphere in the temperature range from 30 to 350 K using a highly sensitive electrometer [1].

In this work, the input files of the relevant complex were prepared with GaussView 5.8. All other calculations were performed with Gaussian 09 using Hartree-Fock calculation. The HF calculations were carried out using 3-21G, 6-31G, 6-31G (d, p), 6-311G, LanL2DZ, and SDD basis sets. The geometry was fully optimized in its ground states.

3 Result and Discussion

After running Gaussian program, the optimized geometry obtained as shown in Figure 1.

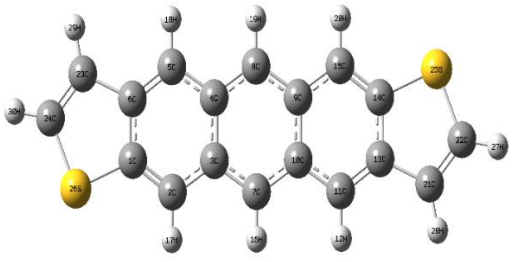

Figure 1. The symbolic optimized structure of ADT.

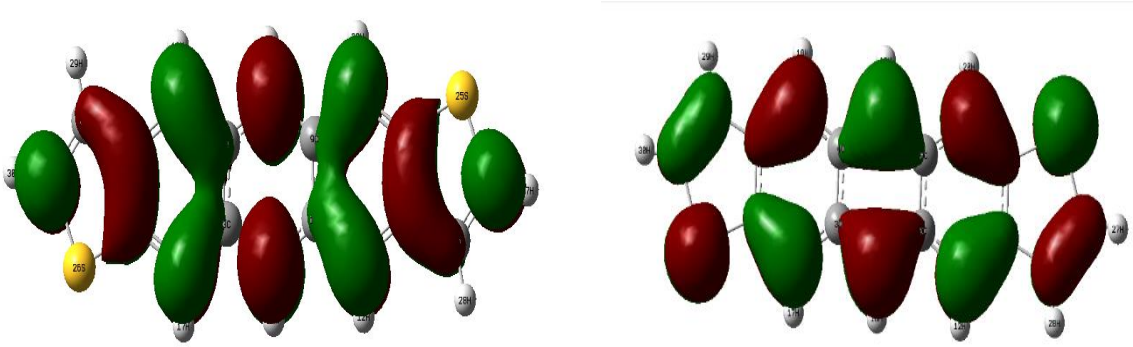

Figure 2. Demonstration the HOMO and LUMO of ADT molecule

Table 1. Determination of the bandgap energy of ADT

	HF method		
Basis Sets	HOMO	LUMO	Band-Gap (eV)
3-21G	-6.84993	1.159478	8.009
6-31G	-6.69727	1.18424	7.881
6-31G(d, p)	-6.50325	1.329821	7.833
6-311G	-6.82462	1.014985	7.839
LanL2DZ	-6.82652	0.892806	7.719
SDD	-6.817	0.914575	7.731

The energy distinction between the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) indicates the molecule's type and nature. The geometry and its energy correspondence are shown in Figure 2. The obtained energy gaps are sown in the Table which is calculated by subtracting HOMO and LUMO energy levels.

4 Conclusion

In this study, several molecular orbital of ADT molecule was investigated. The molecule was simulated by using Gaussian 09 program and then quantum mechanical based model calculations have been implemented to obtain molecular orbital for HOMO and LUMO energy level. In the end, average band gap energy is obtained as 7.835 eV, by using six basis sets.

4 Kaynaklar

[1] Schön, J., Kloc, C., Siegrist, T., Laquindanum, J., and Katz, H., 2001. Charge transport in anthradithiophene single crystals, Organic Electronics, 2(3-4), 165-169.

[2] Sherrill, C.D., 2000. An introduction to Hartree-Fock molecular orbital theory, School of Chemistry and Biochemistry Georgia Institute of Technology.

[3] Hantsch, F.C., 2012. The Hartree-Fock equations in quantum mechanics.

[4] Koch, W. and Holthausen, M.C., 2015. A chemist's guide to density functional theory, John Wiley & Sons.

[5] Fiolhais, C., Nogueira, F., and Marques, M.A., 2003. A primer in density functional theory, Springer Science & Business Media.

[6] Pople, J.A. and Beveridge, D.L., 1970. Molecular orbital theory, C0., NY.

Authors' addresses

Hunar HAMA KHALID 1
Firat University
Faculty of Science,
Department of Physics, Elazığ, Turkey

Hazhar RASUL2
Firat University
College of Science,
Salahaddin-University, Erbil-Iraq