Himalayan Physics

Study of electronic structure of organic solar cell molecules

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Nirmal Diyali[1]*, Bishwas Adhikari[1], Kapil Adhikari[2]

1 Department of Physics, Prithvi Narayan Campus, Pokhara, Nepal

2 Gandaki University, Pokhara, Nepal

Abstract: This study employs the 6-311G(2d,2p) basis set and the B3LYP functional within the density functional theory (DFT) framework,using Gaussian09 suite, to examine the electronic properties of experimental molecules, including Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene, crucial components of organic solar cells. The geometrical structures of these molecules are depicted, highlighting their individual components. Frontier Molecular Orbitals (FMOs) analysis reveals the significance of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) in the electrical structure of molecules, impacting various quantum chemical parameters and predicting reactivity, stability, and solar cell efficiency. Molecular absorption coefficients, UV-visible spectroscopy data, and molecular electrostatic potential (MESP) maps further elucidate the light absorption, stability, and reactivity of these molecules. The results suggest that 2-2'bithiophene exhibits superior electron-donating capacity and nucleophilicity, while 3,4 ethylenedioxythiophene displays heightened electrophilicity. Benzo[1,2-b:5,5 b']dithiophene shows greater light absorption capability and light-harvesting potential. Understanding these electronic properties aids in optimizing the efficiency of organic photovoltaic cells.

Keywords: Organic solar cell • Density functional theory • Frontier molecular orbitals • UV-Visible spectroscopy • Molecular electrostatic potential

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I. Introduction

A solar cell, widely known as a photovoltaic cell, can convert light energy directly into electrical energy according to the photovoltaic energy conservation principle [1]. Solar cells, which are typically made of two materials; silicon and organic base material, are classified into three generation they are; first generation, second generation and third generation [2]. The organic solar cell belongs to third generation of solar cell and is divided into four categories: tandem solar cells, bulk heterojunction solar cells, single layer solar cells, and bilayer solar cells [3]. Organic solar cells face several challenges in their stability due to numerous internal and external factors, including unstable morphology, moisture, oxygen, light,

* *Corresponding Author: nirmaldiyali99@gmail.com*

heat, unstable buffer layer, electrode diffusion, mechanical stress etc. As a result, stability in organic solar cell has received a significant interest over the past few years [4]. The fundamental structure of organic solar cell is a planar-layered structure, it has an active layer made of an organic semiconductor which is sandwiched between two electrodes, namely the anode and the cathode. The performance and reliability of organic solar cells are determined by a variety of parameters, including short circuit current, open circuit voltage, short circuit current density, fill factor, internal and external quantum efficiency, and power conversion efficiency [3, 5].

Organic solar cells harness organic semiconductors to convert sunlight into electrical power directly. They have earned themselves the moniker "polymer solar cells" due to their predominant use of polymers in their construction [6]. These cells are predominantly manufactured through solution-processable and vacuum evaporation methods, which offer cost-effective and sustainable alternatives to traditional silicon solar cells [7]. Notably, their superior sunlight absorption capabilities make them ideal for a wide array of commercial applications, from wearable electronics to spacecraft and transparent solar cells [8, 9]. Moreover, the advent of ternary organic solar cells boasting a theoretical power conservation efficiency of 20.87% has prompted considerable interest, driven by the promise of reduced energy loss across various solar device applications [10, 11].

While organic solar cells have garnered significant attention in solar cell and renewable energy sectors over the past two decades, they still grapple with notable drawbacks and technical challenges [12–14]. The main challenge is the imperative to enhance overall power conversion efficiency. To address this, researchers employ a range of strategies, including morphological control of the active layer, exploration of low-band-gap organic materials to enhance light absorption, and the adoption of tandem device structures to minimize energy losses [15]. Another critical hurdle is the stability of organic solar cells, which researchers are tackling through various means such as refining fabrication processes, implementing encapsulation strategies, and engineering the molecular structure of donor materials and device components [16]. These efforts underscore ongoing advancements in organic solar cell technology as it strives towards greater efficiency and reliability.

When solar light strikes the organic solar molecules, excitons (bound electron-hole pairs) are generated on active layers. Commonly, aluminum and indium tin oxide are used as the cathode and anode in organic solar cells, respectively [17]. Lijun Huo and Jianhui Hou introduced a new polymer material, Benzo[1,2:4,5-b']dithiophene (BDT), as an electron donor to boost power conservation efficiency in organic solar cells, and it serves as an essential for solar materials [18]. The symmetric and planar structure of BDT is frequently deployed by researchers due to its expected high mobility in BDT-based polymers. However, one of the most important challenges is controlling morphology through the synthesis of molecular structures [18]. Rasool et al. identified five novel architectural molecules of benzodithiophene derivatives, focusing on enhancing the photovoltaic and opto-electronic properties of small molecules

based on benzodithiophene [19]. It was found that these new molecules have a band gap of 1.90 eV to 2.09 eV [19]. The benzotrithiophene-based small molecule benzo [1,2-b:3,4-b':6,5-b"]trithiophene (BTT) has promising photovoltaic properties when used as an electron donor active material in small-molecule organic solar cells (SM-OSCs). Cristian Castillo et al. found that this organic molecule shows broad light absorption and a 2.04% power conversion efficiency (PCE) from 420 nm to 670 nm. This efficiency is attributed to improved electron transfer dynamics, reduced charge carrier recombination, and favorable energy band alignment. Further optimization of cell architectures could potentially enhance the efficiency of the molecules [20].

The purpose of the study is to discuss the several electronic properties of some materials and performance of organic solar cell. Additionally, the paper discusses the challenges and strategies for improving the stability and efficiency of OSCs. It could provide a better understanding of solar cell technology and its capacity to generate power.

II. Methodology

Experimental geometry of the molecules (Benzo[1,2-b:5,5 b']dithiophene, 3,4-Ethylen-edioxythiophene Molecule and 2,2'- Bithiophene) were obtained from ChemSpider, which is an accessible database of molecules owned and managed by the Royal Society of Chemistry [21]. Density functional theory (DFT) using the B3LYP functional and 6-311G(2d, 2p) basis set in the Gaussian09 software suites [22] is carried out. The physical and electronic properties of molecules can be accurately replicated by DFT. The obtained geometrical structure of organic solar cell molecules (Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene and 3,4 ethylenedioxythiophene) including their separate components and distances between adjacent atoms are demonstrated in Fig. 1. The variations in bond lengths reflect the differences in atomic connectivity and electron distribution within each molecule.

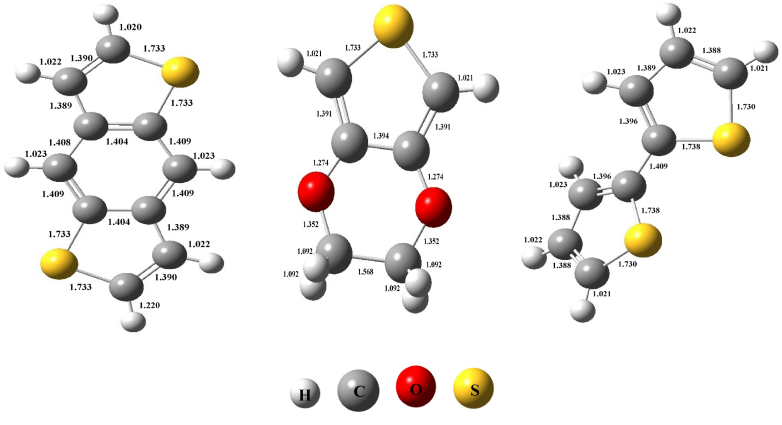

Figure 1. The optimized structures and bond lengths of the investigated molecules Benzo[1,2-b:5,5 b']dithiophene, 3,4 ethylenedioxythiophene and 2-2'bithiophene respectively

A UV-VIS spectrophotometer measures electromagnetic radiation in the UV-Visible spectrum, passing through matter between 200 nm and 700 nm. Light is reflected, scattered, and absorbed by the substance by exciting electrons. The transmittance of light is determined by dividing the intensity of light reaches the detector by the intensity of light emitted. The energy differences between states are due to electrons changing energy levels due to incident light. According to Lambert-Beer's law, the absorbance of incoming radiation (I_0) and transmitted radiation (I) determines the amount of light absorbed or reflected from a sample, expressed as absorbance or transmittance [24]. Mathematically,

$$T = \frac{I}{I_0}$$

$$or, \quad \%T = \frac{I}{I_o} \times 100 \tag{1}$$

The amount of absorbance can be written as;

$$A = -\log(\frac{I}{I_o}) = abc \tag{2}$$

where a is the extinction coefficient or absorptivity, which quantifies how strongly the material absorbs light at a specific wavelength, b is the path length of the light through the material, often the thickness of the sample or the length of the light path and c is the concentration of the absorbing species in the material.

The energy gap, defined as the disparity between the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), serves as a crucial metric for assessing the physical characteristics of molecules. Equation (3) is used to determine the energy gap [25].

$$E_g = E_{LUMO} - E_{HOMO} \tag{3}$$

where, E_{LUMO} and E_{HOMO} are energy of highest occupied molecular orbital and energy of lowest unoccupied molecular orbital respectively.

To calculate the ionization potentials (IP) and electronic affinities (EA), equations (5) and (6) were employed [26].

$$IP = -E_{HOMO} \tag{4}$$

$$EA = -E_{LUMO} \tag{5}$$

Global Reactivity Parameters (GRPs) such as, electronegativity (χ), chemical hardness (η), chemical softness (S), chemical potential (μ), and electrophilicity index (Ω) are obtained as [27]

$$\mu = \frac{(E_{HOMO} + E_{LUMO})}{2} \tag{6}$$

$$\eta = -\frac{(E_{HOMO} - E_{LUMO})}{2} \tag{7}$$

$$\chi = \frac{-E_{HOMO} - E_{LUMO}}{2} \tag{8}$$

$$S = \frac{1}{2\eta} \tag{9}$$

$$W = \frac{\mu^2}{2\eta} \tag{10}$$

III. Results and Discussion

Frontier molecular orbitals (FMOs) analysis

The locations of HOMO and LUMO have been provided to have a substantial impact on the electrical structure of molecules in organic solar cells. The bond theory classifies HOMO and LUMO as valence and conduction bands, respectively. Many quantum chemical parameters, including chemical reactivity, electronic characteristics, chemical stability, charge transfer, UV-visible spectrum, and solar cell PCE, are predicted by the FMOs energy gap [28]. The energy gap is the amount of energy required to get from a higher energy level to a lower energy level. A higher energy band gap corresponds to lower solar absorption and greater open circuit voltage. Due to poor solar absorption, there is also a small amount of electrical production [29]. The energy gap is used to measure the kinetic stability and chemical reactivity of molecules. The large frontier energy band gap implies high kinetic stability and low chemical reactivity, and vice versa. Similarly, LUMO energy was used to identify the compound's electrophilicity, while HOMO energy was used to determine their nucleophilicity. Higher HOMO energy indicates that during chemical reactions, they have a greater tendency to donate electrons, whereas higher LUMO energy indicates a greater tendency to accept electrons [30]. To check the strength, energy

required to separate molecules, stability of molecules, binding energy per atom, and HOMO-LUMO gap were calculated, and they are listed in Table 1 and Fig. 2.

Table 1. The HOMO–LUMO values and energy band gap of the solar cell molecules Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene and 3,4 ethylenedioxythiophene.

Molecules	**HOMO (eV)**	**LUMO (eV)**	E_g **(eV)**
Benzo[1,2-b:5,5 b']dithiophene	-5.41	-1.33	4.07
2-2'bithiophene	-5.53	-1.37	4.16
3,4 ethylenedioxythiophene	-5.52	-0.032	5.48

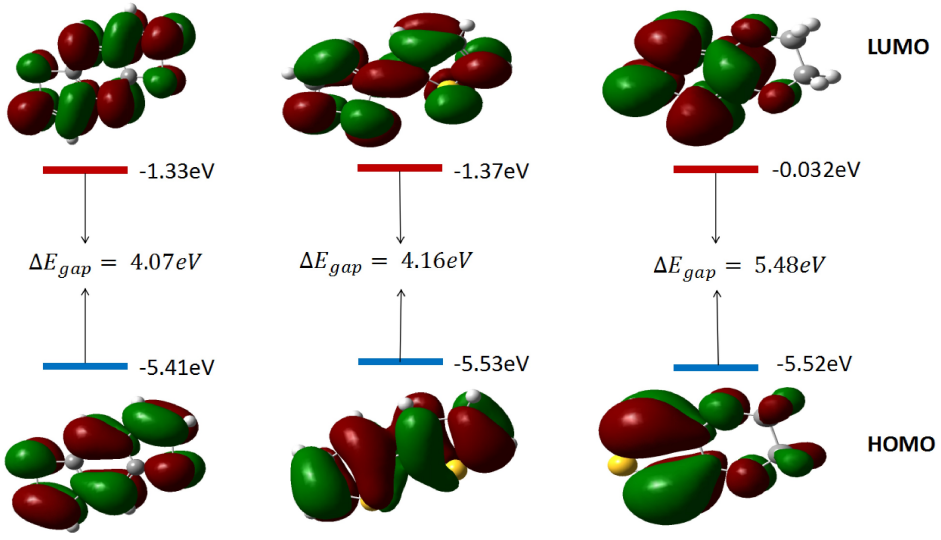

Figure 2. The optimized structures of the investigated molecules Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene and 3,4 ethylenedioxythiophenet

The HOMO energies of Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene were measured at -5.41eV, -5.53eV, and -5.53eV, respectively, while their LUMO energies were -1.33eV, -1.37eV, and -0.032eV, respectively. Notably, 3,4 ethylenedioxythiophene exhibited the highest LUMO energy (-0.032eV), whereas 2-2'bithiophene displayed the lowest HOMO energy (-5.53eV). Consequently, 2-2'bithiophene molecules possess a greater electron-donating capacity compared to the other two molecules, rendering them more likely to donate electrons during chemical reactions and thus exhibiting enhanced nucleophilic behavior. Conversely, due to its higher LUMO energy, 3,4 ethylenedioxythiophene demonstrates a greater propensity to accept electrons during chemical reactions, indicating its more electrophilic nature.

The energy gap (E_g) highlights an essential aspect of organic solar cells and other photovoltaic devices. It is very important tool to analyze the energy required for electronic excitation, absorption of sunlight, open-circuit voltages, and conductivity. The relation between energy band gap and conductivity (σ) is seen in equation (11).

$$\sigma \propto e^{\left(\frac{-E_g}{KT}\right)} \tag{11}$$

A small energy gap indicates greater charge transfer, resulting in low open-circuit voltages and the ability to capture more sunlight and this enhances the number of charge carriers (electrons and holes) and current production in the device [29, 31]. The studied molecules Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene have energy gaps of 4.07 eV, 4.16 eV, and 5.48 eV, respectively. In terms of the energy gap, Benzo[1,2-b:5,5 b']dithiophene exhibits the lowest band gap compared to the other two compounds under study, making it the ideal molecule for solar cells among the three.

Electronic properties analysis

The Gaussian09 suite program was used to calculate the values of Global Reactivity Parameters (GRPs) such as ionization potential (I), electron affinity (A), electronegativity (χ), chemical hardness (η), chemical softness (S), chemical potential (μ), and electrophilicity index (Ω) using the basis set 6-311G(2d,2p) and functional B3LYP. The computed GRPs values are presented in Table 2.

Table 2. Estimated global reactivity parameters of molecules Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene and 3,4 ethylenedioxythiophene using DFT/B3LYP/6-311G(2d,2p).

Molecules	**IP(eV)**	**EA(eV)**	μ**(eV)**	η**(eV)**	**S(eV)**	**Ω(eV)**	χ**(eV)**
Benzo[1,2-b:5,5 b']dithiophene	5.41	1.33	-3.37	2.04	0.25	2.78	1.37
2-2'bithiophene	5.53	1.37	-3.45	2.08	0.24	2.86	3.45
3,4 ethylenedioxythiophene	5.52	0.032	-2.78	2.74	0.18	1.41	2.78

The IP and EA reflect the electron donating and accepting tendencies of molecules, respectively, and both are influenced by the HOMO and LUMO energies. Additionally, the values of chemical potential indicate the chemical stability of compounds. Similarly, the energy gap, chemical potential, stability, and hardness of molecules are strongly correlated with reactivity [32]. A higher EA is observed in the molecules of 2-2'bithiophene (1.37 eV), suggesting that it could serve as a superior material for electron transport. The softness of molecules, measuring their polarizability, is higher in the Benzo[1,2-b:5,5 b']dithiophene molecule compared to the other two, rendering it softer and more polarizable. While hardness and softness are opposing properties of molecules, with higher hardness values corresponding to greater stability and lower reactivity under normal circumstances, there is minimal variation in the calculated hardness values of Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene, which are 2.04 eV, 2.08 eV, and 2.74 eV, respectively. Based on its hardness value, 3,4 ethylenedioxythiophene exhibits slightly greater hardness than the other examined molecules, indicating lower reactivity

and higher stability. The electrophilicity scale, a tool used to measure electrophilic power, reveals that Benzo[1,2-b:5,5 b']dithiophene is more electrophilic (2.78 eV) than the other molecules, owing to its higher electrophilicity.

UV-Visible spectroscopy analysis

The UV-visible spectroscopy was used to study the absorption profile of the respective molecules. Results of the UV-Visible Spectroscopy Analysis is demonstrated in Fig. 3 and Table 3.

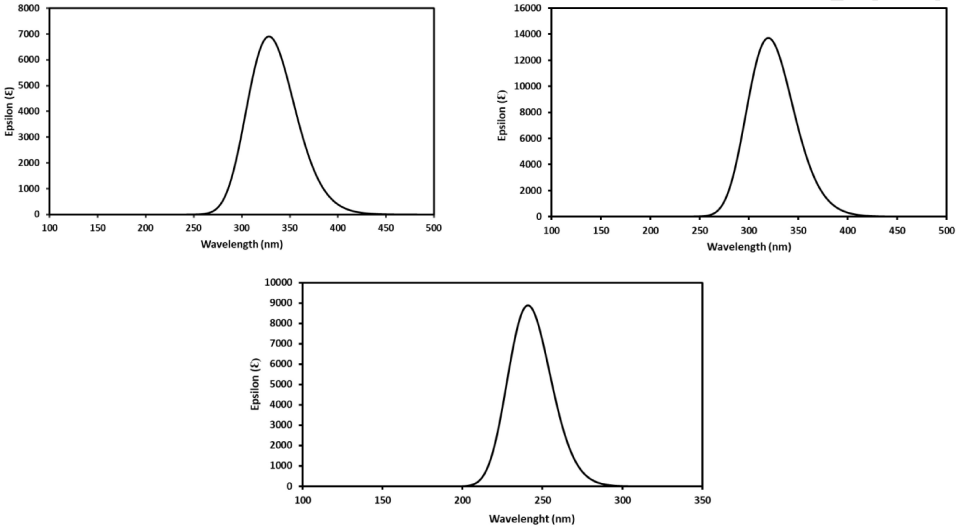

Figure 3. Absorption profile of Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene and 3,4 ethylenedioxythiophenet molecules respectively, calculated by using functional B3LYP and 6-311G(2d,2p) basis set.

Table 3. Calculated maximum wavelength (λ_{max}), wavelength range and molecular absorption coefficient (ϵ) of examined molecules Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene and 3,4 ethylenedioxythiophene.

Molecules	λ_{max} (nm)	**Wavelength Range** (nm)	ϵ $(Lmol^{-1}cm^{-1})$
Benzo[1,2-b:5,5 b']dithiophene	328.28	250-350	700
2-2'bithiophene	319.68	260-410	14000
3,4 ethylenedioxythiophene	249.29	205-280	9000

A broader visible spectrum indicates increased light absorption, thereby enhancing the efficiency of converting solar energy into electricity [33]. All examined molecules displayed absorption peaks between 245 nm and 330 nm. Particularly, the wavelength range of 2-2'bithiophene molecules spans from 260 nm to 410 nm, with a higher peak centered at 319.68 nm. Similarly, 3,4-ethylenedioxythiophene molecules exhibited the smallest wavelength ranges and maximum wavelengths of 205 nm to 280 nm and 249.29 nm, respectively, while the wavelength range of benzo[1,2-b:5,5 b']dithiophene molecules is 250 nm to 350 nm, with its maximum wavelength at 328.28 nm. The broader range of wavelengths observed in

2-2'bithiophene molecules enables them to absorb more sunlight and convert it into electricity, thereby maximizing the overall energy conversion efficiency of the solar cell. Higher molecular absorption coefficients typically correlate with better light absorption and greater solar efficiency in photovoltaic devices [34]. The molecular absorption coefficients of the investigated molecules—Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene are calculated as 700 $Lmol^{-1}cm^{-1}$, 14000 $Lmol^{-1}cm^{-1}$, and 9000 $Lmol^{-1}cm^{-1}$, respectively. Compared to the other two molecules, 2-2'bithiophene molecules exhibit superior light absorption quality and excellent solar efficiency due to their higher molecular absorption coefficient of 14000 $Lmol^{-1}cm^{-1}$. Similarly, the maximum absorption wavelength values of Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene molecules are 328.28 nm, 319.68 nm, and 249 nm, respectively. The higher wavelength observed in Benzo molecules makes them a favorable choice for producing photovoltaic materials.

Molecular electrostatic potential (MESP) analysis

The MESP is the most important tool for investigating both electrophilic and nucleophilic attacks on molecules [35]. The electrostatic potential maps of Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene are represented in Fig. 4. The MESP map appears in several colors, including green, blue, and red. The color portions that are red and blue depict the maximum negative (acceptor portion) and positive regions (donor portion) and also represent suitable for electrophilic and nucleophilic attacks due to their low and high electronic densities. On the other hand, green is a color of zero potential.

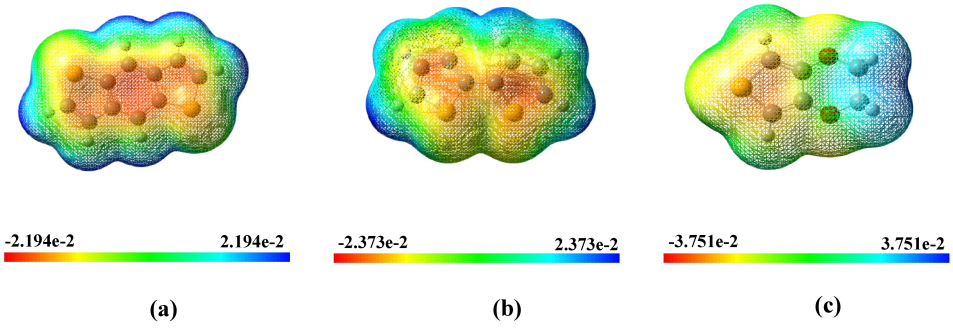

Figure 4. Molecular Electrostatic Potential maps of (a) Benzo[1,2-b:5,5 b']dithiophene, (b) 2-2'bithiophene and (c) 3,4 ethylenedioxythiophenet molecules calculated by using functional B3LYP and 6-11G(2d,2p) basic set.

Surface analysis of the MESP for Benzo[1,2-b:5,5 b']dithiophene molecules revealed distinct charac-

teristics: carbon atoms exhibited maximum negativity with low electronic densities, whereas sulfur and hydrogen atoms displayed maximum positivity and high electron density. This analysis indicates that the center of the molecule is highly susceptible to electrophilic attraction, suggesting potential reactivity at this region. Similarly, in the 2-2'bithiophene molecule, the central atoms, carbon, and sulfur, are depicted as negative regions (indicated by the red portion) in the electrostatic potential map. Conversely, hydrogen atoms are represented by the green color, suggesting a neutral charge potential. This observation implies that the central region of the molecule is readily susceptible to electrophilic attraction, given its predominantly negative charge, thus facilitating such interactions. Moreover, in 3,4 ethylenedioxythiophene molecules, oxygen atoms are depicted in blue color, while sulfur atoms are represented in red. This color variation indicates distinct electrostatic potentials within the molecule. Oxygen atoms display a negative potential with low electron density, making them preference to electrophilic attraction. Conversely, sulfur atoms exhibit maximum positive potential and high electron density, suggesting a propensity for nucleophilic attraction. This analysis highlights the contrasting reactivity of oxygen and sulfur atoms within the molecule, with oxygen being more prone to electrophilic interactions and sulfur to nucleophilic interactions.

IV. Conclusions

The electronic properties of molecules are calculated using the B3LYP function and 6-311G(2d,2p) basis set through Gaussian09 suites program. We use frontier molecular orbitals (FMOs), UV-Visible Spectroscopy, and electrical properties to investigate the stability, conductivity, and light absorption of Benzo[1,2-b:5,5 b']dithiophene, 2-2'bithiophene, and 3,4 ethylenedioxythiophene molecules. While molecules Benzo[1,2-b:5,5 b']dithiophene show more nucleophilicity, molecules 3,4 ethylenedioxythiophene exhibit stronger electrophilicity due to their higher LUMO and HOMO energies. The HOMO-LUMO gap of all investigated molecules indicates that the benzo[1,2-b:5,5 b']dithiophene molecule has a greater capacity to absorb light and light-harvesting ability. However, organic photovoltaic cells face major challenges in terms of stability and high efficiency. Compared to the other two compounds, the 3,4-ethylenedioxythiophene molecule exhibits greater stability and lower reactivity. It is clearly seen that 2-2'bithiophene molecule has wider spectrum and greater molecular absorption coefficients so boosting their efficiency in converting sunlight into electricity.

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