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Enhancement of electronic, photophysical and optical properties of 5,5'-Dibromo-2,2'-bithiophene molecule: new aspect to molecular design

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ABSTRACT

The aims of this study were to enhance electronic, photophysical and optical properties of molecular semiconductors. For this purpose, the isomers of the B-doped molecule (5,5'-Dibromo-2,2'-bithiophene) have been investigated by density functional theory (DFT) based on B3LYP/6-311++G** level of theory. The isomers were first calculated using kick algorithm. The most stable isomers of the B-doped molecule are presented depending on the binding energy, fragmentation energy, ionization potential, electron affinity, chemical hardness, refractive index, radial distribution function and HOMO-LUMO energy gap based on DFT. Ultraviolet-visible (UV-vis) spectra have been also researched by time-dependent (TD) DFT calculations. The value of a band gap for isomer with the lowest total energy decreases from 4.20 to 3.47 eV while the maximum peaks of the absorbance and emission increase from 292 to 324 nm and 392 to 440 nm with boron doped into 5,5'-Dibromo-2,2'-bithiophene. Obtained results reveal that the B-doped molecule has more desirable optoelectronic properties than the pure molecule.

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1. Introduction

Recently, the molecular design has increasingly received attention for the development of optoelectronic devices to find out the best performing molecular semiconductors. In general, this process is performed by combining an electron rich donor and electron-deficient acceptor materials to get desirable optoelectronic properties. In that content, we have designed the B-doped 5,5'-Dibromo-2,2'-bithiophene isomers. It is well known the 5,5'-Dibromo-2,2'-bithiophene organic molecule is one of the derivatives of Dibromo bithiophene (DBT) which was widely used in a variety of electronic, optoelectronic [1–4], and photonic applications [5–8]. The 5,5'-Dibromo-2,2'-bithiophene has usually been used to improve materials' properties [9–12]. Recently, optoelectronic properties of the 5,5'-Dibromo-2,2'-bithiophene in different solvent environments have been investigated [13]. In the study, the band gap energy was reported to decrease as based on an increase in the concentration of the molecule [13]. It has also been used for the reduction of band gap energy of anthracene and benzotriazole units to make easier electron transfer for organic solar cells [14]. Moreover, the synthesized 5-(carbazol-9-yl)-5'-

mercapto-2,2'-bithiophene based on the organic molecule leads to enlarged emission when it is doped to the surface of CdSe quantum dot [15].

In the literature, there are no experimental and theoretical results on the electronic structures, photophysical and optical properties of the B-doped 5,5'-Dibromo-2,2'-bithiophene reported, so far. Hence, the major aim of this study is to enhance the mentioned properties for the studied molecule. Firstly, we found out the B-doped 5,5'-Dibromo-2,2'-bithiophene isomers based on the kick algorithm which is first used in molecular systems in this study. Later, among the isomers, the structure with the lowest total energy was compared with pure 5,5'-Dibromo-2,2'-bithiophene organic molecule.

2. The method of calculations

In this study, we researched the global minimum of the B-doped 5,5'-dibromo-2,2'-bithiophene on the potential energy surface using the kick algorithm. Kick method was developed by Saunders [16] to generate a large number of possible starting geometries and to search the low-lying isomeric structures. In this study, we use a kick algorithm partially based on the Saunders's stochastic kick method. The 5,5'-dibromo-2,2'-bithiophene molecule is optimized with method and basis set which is to be used in the kick algorithm. Then, the cartesian coordinates of 5,5'-dibromo-2,2'-

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bithiophene molecule are stored as a separate file to be read by the kick algorithm every time. After this file containing cartesian coordinates is read by algorithm, a single atom is placed in the center of those coordinates. Later, a single atom (B) is 'kicked' randomly within a size-controlled sphere with a radius R (kick size), which is determined by considering the structural size of the 5,5'-dibromo-2,2'-bithiophene, due to avoid biased search. It is noted that the cartesian coordinates of 5,5'-dibromo-2,2'-bithiophene structure are fixed at its equilibrium position, i.e., no atom of it is kicked. However, in Saunders's stochastic kick method, all atoms of structure are initially placed at the same point and all atoms are kicked. Thus, a different procedure is applied in our studies here. The most important advantage of this algorithm predicts where a single atom can be connected to the pure molecule. Another advantage is also that geometry of the newly formed molecule (doped-molecule) does not change much because no atom of pure molecule is kicked. This also may be useful in situations where the structure of the molecule is undesired to change when an atom is doped to the molecule. Since the distance between two atoms (Br-Br) at the farthest distance from the planar 5,5'-dibromo-2,2'-bithiophene is 9.58 Å, the radius R of sphere should be chosen at least to be 5 Å. Otherwise, setting the radius too high will make optimization more difficult and, thus, it will cause fragmentation. The minimum and maximum radiuses (kick distance, R) are chosen to be of 0.5 Å and 6 Å in this work, respectively. To prevent the fragmentation, a single atom (B) is again placed at the same point (at the center of 5,5'-dibromo-2,2'-bithiophene) after each optimization step. Thus, there is no need to calculate atomic neighborhoods. Generated new coordinates are used as an input file in the Gaussian 09 program [17]. Initially, the kick algorithm runs at the popular B3LYP hybrid functional and 3-21 G basis set [18] up to 1000 times until no new minima appeared. After that, the same isomers were determined by comparing their geometries and energies and then eliminated for further calculations. The selected isomers were optimized again and evaluated with a relatively higher 6-311++G** basis set using the quadratically convergent self consistent field (SCF) procedure without symmetry constraints.

3. Results and discussions

3.1. The structural analysis

The optimized structures of the studied molecule and the B-doped molecule were shown in Fig. 1.

The relaxed geometries of 15 isomers with the lowest total energy of B-doped molecules are indicated in Fig. 2. In this study, we focused on the isomer with the lowest total energy (with higher stability) and compared the 5,5'-dibromo-2,2'-bithiophene organic molecule with the B-doped molecule. It is noted that the bond distances near the doped B atom are relatively distorted; however, these small geometrical distortion results give rise to significant variations in the electronic structure, photophysical and optical properties of the pure molecule. For example, B doped molecule leads to an increase in the bond distance between C and S atoms from 1.757 to 1.763 Å.

The vibrational stability of a B-doped molecule was examined based on the vibrational modes. The optimized geometry was found with the positive vibrational spectra located at the stationary point on the potential energy surface. The lowest vibrational harmonic frequency for a B-doped molecule ($35.05 \omega^{-1}$) was found smaller than the pure molecule ($38.68 \omega^{-1}$). One can conclude that the B-doped molecule is more stable than the pure molecule. This is compatible with the corresponding total energies of the pure molecule and a B-doped molecule.

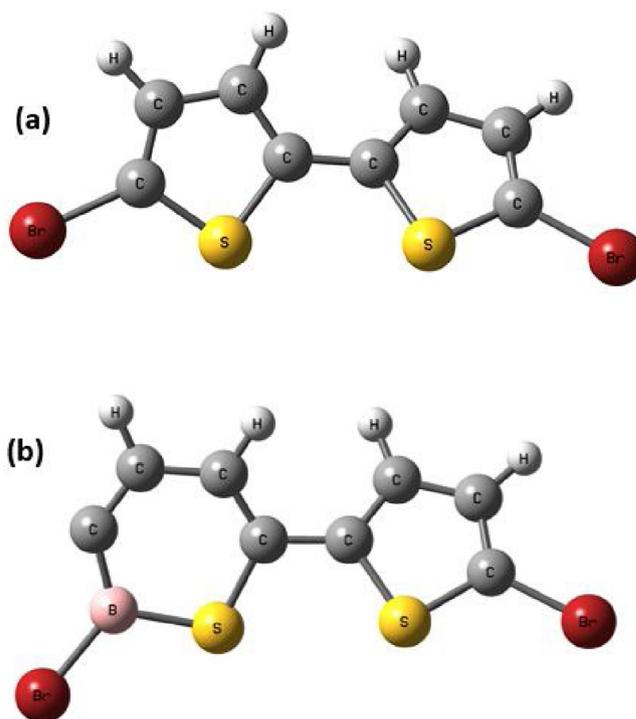


Fig. 1. Optimized geometries of (a) 5,5'-Dibromo-2,2'-bithiophene and (b) B-doped 5,5'-Dibromo-2,2'-bithiophene molecules.

3.2. The energetic analysis

The variations of total energies of the B-doped 5,5'-Dibromo-2,2'-bithiophene isomers are indicated in Fig. 3. Point A shows the structure with the lowest total energy (-6276.88 a.u.) which is lower than that of the pure molecule (-6252.02 a.u.) and other B-doped isomers, this indicates that the B-doped on molecules are more stable than the pure molecule. Binding energy (E_b), fragmentation energy for boron atom (E_f), vertical ionization potential (VIP), vertical electron affinity (VEA), chemical hardness (η) and HOMO-LUMO energy gap (E_g) for the low-lying isomers of the B-doped molecule are tabulated in Table 1. From Table 1, E_b of the B-doped molecule increases while its VIP, VEA and η decrease comparing with the pure molecule. These results show that the energy of the molecule derived from electron-transfer for the B-doped molecule is lower than the pure molecule.

The density of states which indicates the HOMO and LUMO levels of the pure and B-doped molecules are shown in Fig. 4. The HOMO and LUMO levels are often associated with the electron donating and accepting ability of the molecules, respectively. Therefore, the high value of HOMO indicates high tendency to donate electrons to an appropriate acceptor molecule with low empty molecular orbital energy. Similarly, the low value of LUMO indicates high tendency to accept electrons from the metal surface [19,20].

The HOMO and LUMO energies of the pure molecule lie at -6.09 and -1.88 eV, respectively. Comparing with the B-doped molecule, the HOMO energy (-6.42 eV) level increased by about 1.06 eV while the LUMO energy (-2.94 eV) level increased by about 0.32 eV. The results show that the B doped molecule has higher HOMO and LUMO levels than the pure molecule.

From HOMO and LUMO energies, the gap energies of the pure and B-doped molecules are found to be 4.20 and 3.47 eV (see Table 1), respectively. This indicates that the B doped organic molecule has better HOMO, LUMO and gap energy values because

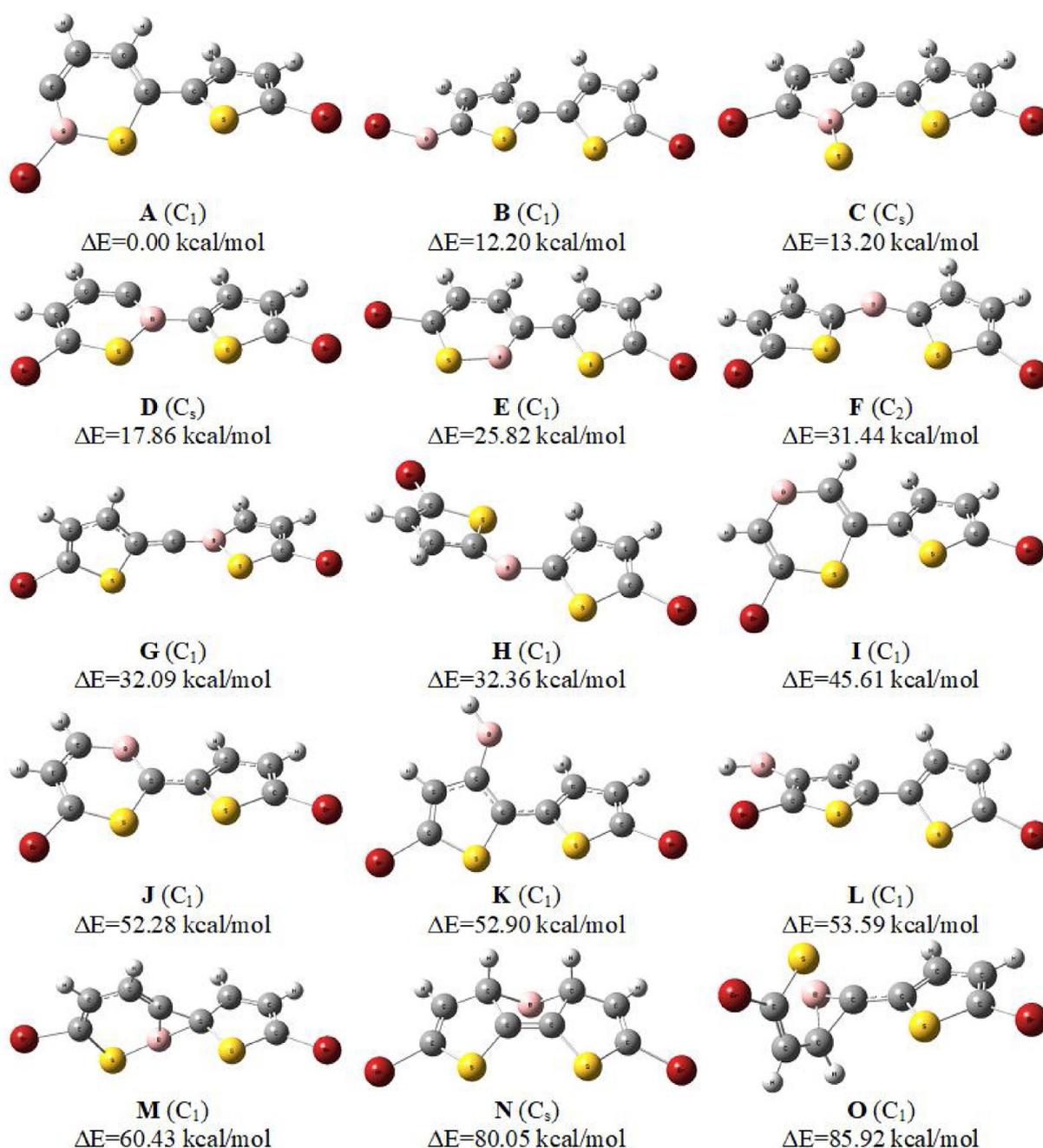


Fig. 2. Optimized geometries of B-doped 5,5'-Dibromo-2,2'-bithiophene isomers.

the electronic transfer is easier, that is the B-doped molecule allows easy excitation of electrons from HOMO to LUMO.

Therefore, the presence of B atom improves the conductivity and enhances reactivity of the pure molecule. The results in Table 1 show that B-doped isomers cause a decrease in the energy gap. There are also among isomers structures with lower gap energies than these of the structure with lowest total energy, compared with the pure molecule, however, we are related to the structure with the lowest total energy. From results, one can conclude that the B-doped molecule is the more suitable candidate for organic electronics because the small band gap makes promotion of electrons from the ground state to the excited-state very easy upon photo-excitation of organic compound involved in photovoltaics. Higher

electron mobilities in a B-doped molecule are desirable as electron transport material to improve and control charge injection and transport in OLEDs. The B-doped molecule have also sufficiently deep HOMO energy (-6.42 eV) to block holes in OLEDs. The HOMO and LUMO levels of B-doped molecule (HOMO= -6.42 eV and LUMO -2.94 eV) is similar to TAZ (HOMO= -6.4 eV and LUMO -2.8 eV) and TPBI (HOMO= -6.3 eV and LUMO -2.8 eV) molecules used in blue phosphorescent OLEDs [21]. In addition, one of the molecular design criteria, particularly for OLEDs, is large electron affinities and ionization potentials (>6.0 eV) to achieve high electron mobility [22]. The electron affinity (1.47 eV) and ionization potential (8.42 eV) of the B-doped molecule is larger than the pure molecule about 1.0 eV.

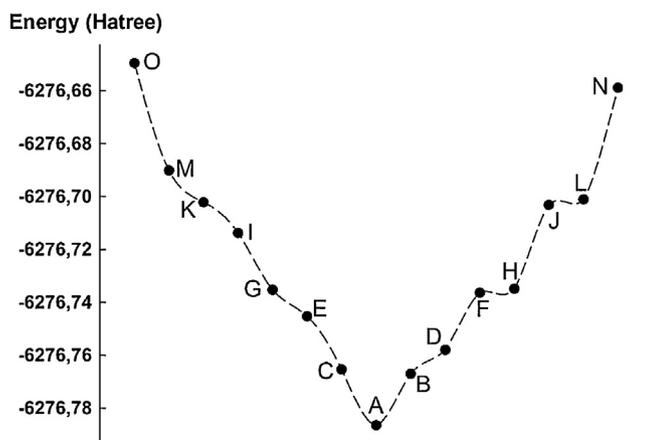


Fig. 3. The variations of total energies of B-doped 5,5'-Dibromo-2,2'-bithiophene isomers.

Table 1

Binding energy per atom (E_b), fragmentation energy for boron atom (E_f), vertical ionization potential (VIP), vertical electron affinity (VEA), chemical hardness (η) and HOMO-LUMO energy gap (E_g) for the low-lying isomers of B doped 5,5'-Dibromo-2,2'-bithiophene molecule. All values are eV.

Isomers	E_b	E_f	VIP	VEA	η	E_g
pure	5.49	–	7.63	0.41	3.61	4.20
A	5.48	5.29	8.42	1.47	3.48	3.47
B	5.45	4.76	7.37	0.73	3.32	2.68
C	5.45	4.72	7.65	3.09	2.28	1.89
D	5.44	4.51	7.46	1.29	3.08	3.57
E	5.42	4.17	7.82	1.22	3.30	3.55
F	5.40	3.93	6.86	0.77	3.04	2.40
G	5.40	3.90	7.75	1.54	3.10	2.99
H	5.40	3.89	6.83	0.78	3.03	2.39
I	5.37	3.31	7.07	0.57	3.25	2.56
J	5.35	3.02	6.85	1.28	2.79	1.96
K	5.35	3.00	7.24	0.82	3.21	2.54
L	5.35	2.97	7.49	0.44	3.53	2.74
M	5.33	2.67	6.12	0.96	2.58	1.71
N	5.28	1.82	7.76	0.94	3.41	3.67
O	5.26	1.56	7.12	0.94	3.09	3.18

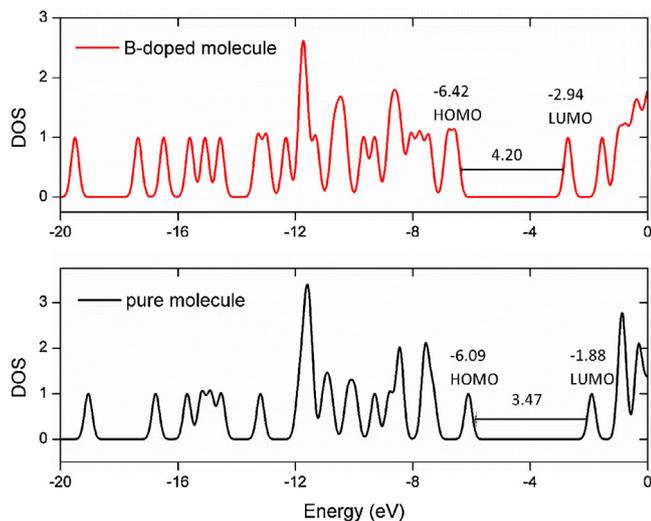


Fig. 4. DOS for 5,5'-Dibromo-2,2'-bithiophene and B-doped 5,5'-Dibromo-2,2'-bithiophene molecules.

3.3. The refractive index (n)

The refractive index (n) values of the pure molecule and B-doped molecule were calculated from Ravindra relation [23], which represents a linear relation including the E_g , which is defined as:

$$n = 4.084 - 0.62E_g \quad (2)$$

The relation is more compatible with experimental results [24,25]. n values are found to be in orders: the pure molecule (1.596) < the B doped molecule (1.932). The n value of the pure molecule obtained from experiment was found between 1.6 and 1.7 in solvent environment [13]. The solute-solvent interactions give rise to the significant changes in the chemical and physical characteristics of the solute from gas phase to solvent phase [26]. Thus, when we ignore the solvent effect on molecule, our theoretical n value in gas phase is compatible with experiment for pure molecule (1.596). When it comes to B-doped molecule, based on a decrease on the band gap, n value of it inherently increases from refractive index relation. The n value also changes depend on the type of organic molecule. For example, we found the n value higher 2.8 of the PTCDI-C8 organic nanostructure [26], which is usually used in organic field effect transistors and solar cells.

3.4. Mulliken atomic charge and dipole moment

The charge distribution is an important electronic parameter for optoelectronic applications. The Mulliken charge distributions of the atoms in the pure molecule in the same position are found to be different than these of the B-doped molecule. For example, the charge of Br atom connecting to B atom is negative (-0.008), however, the charge of the same atom in the pure molecule is positive (0.271). The other C and S atoms connecting B atoms in the B-doped molecule have lower charge value than that of the pure molecule. The charges of C and S atoms in the pure molecule are of -0.766 and 0.747, respectively, however the charges of C and S atoms in the B-doped molecule are of -0.178 and 0.455, respectively.

We also performed the dipole moments (μ) of the pure and B-doped molecule. The μ of the B-doped molecule is found to be greater than that of the pure molecule. The highest value of component of μ along the y-axis ($\mu_y = 3.6917$ Debye) predicts large charge separation in the B-doped molecule. The corresponding total dipole moment (μ_T) was found to be 4.1204 Debye. For the pure molecule, it has a value of 2.3049 Debye along the y axis. These results indicate that the B-doped molecule has the stronger intermolecular interaction than the pure molecule.

3.5. UV-vis absorption spectroscopy

The optical absorption of the pure and B-doped molecules was performed by TD-DFT calculations based on the CAM-B3LYP level [see Fig. 5(a)] [27] because the basis set gives better results than B3LYP basis set for TD-DFT calculations [26]. The absorbance maxima of pure molecule in solvent environment is experimentally measured of about 324 nm [13]. When we ignore the solvent effect on molecule (because the solute-solvent interactions give rise to the significant efficiency to molecule), our theoretical absorbance maxima (about 292 nm) in gas phase is compatible with experiment for pure molecule. In the present study, the maximum value of optical absorption (324 nm) of the B-doped molecule is found to be greater than that of pure molecule (292 nm). From the calculated absorption values, the B-doped molecule gives rise to the enhancement of visible light absorption. Thus, the B-doped molecule which is more stable (in terms of the total energy and the lowest vibrational frequency) is very promising optoelectronic applications.

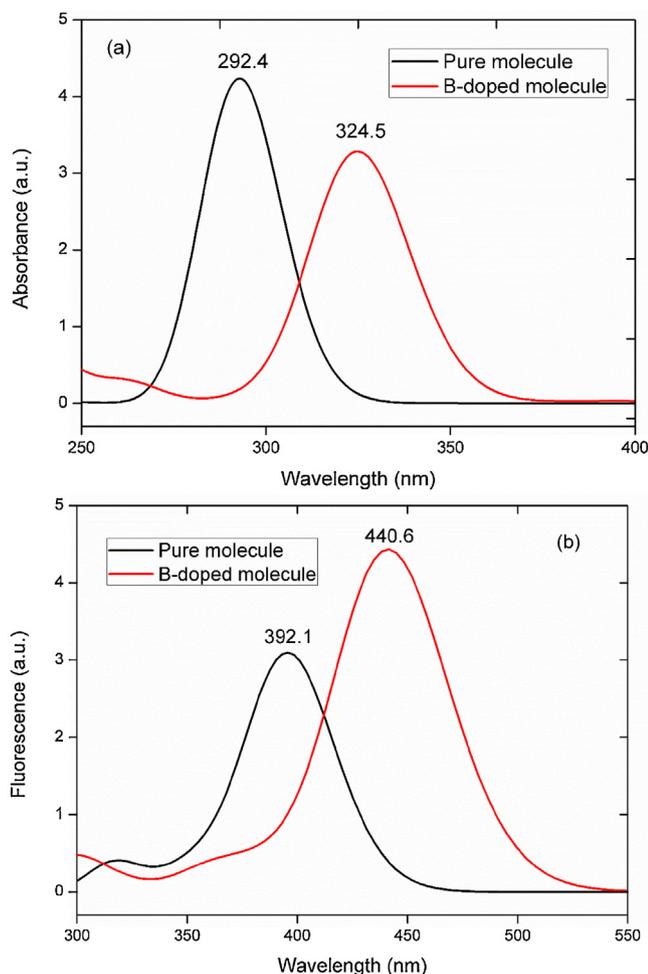


Fig. 5. (a) Absorption (b) emission spectra of 5,5'-Dibromo-2,2'-bithiophene and B-doped 5,5'-Dibromo-2,2'-bithiophene molecules.

Figure 5(b) indicates the curves of emission spectra of the pure and B-doped molecules. As seen in Fig. 5(b), B-doped molecule displays the maximum peak (440.6 nm) in the visible region, while the pure molecule displays the emission maxima (392.1 nm) in the near ultraviolet region. The changes in emission efficiency is of about 49 nm. These results suggest that the B-doped molecule is suitable for OLED devices.

3.6. Radial distribution function

The radial distribution functions (RDFs) are related to the probability of finding a particle in the distance from another particle. We compared the RDF results of the pure with B-doped molecule (From Fig. 6). The RDF of B-doped molecule is greater than that of the pure molecule. Both the maximum peaks of the RDFs of the pure and B-doped molecules are found to be in the range of 1–1.5 Å. The radial distribution function (RDF) describes how the density of surrounding matter varies as a function of the distance from a point. It gives the information concerning the frequency with which certain distances occur. The RDF of the B-doped molecule having a value of about 3 is greater than the pure molecule having a value of about 2.5 in this range. This means that it is three times more likely that two molecules would be found at this separation for the B-doped molecule. Thus, the chances of finding two atoms with this separation are less for the pure molecule. It also has a narrower peak than that of the pure molecule.

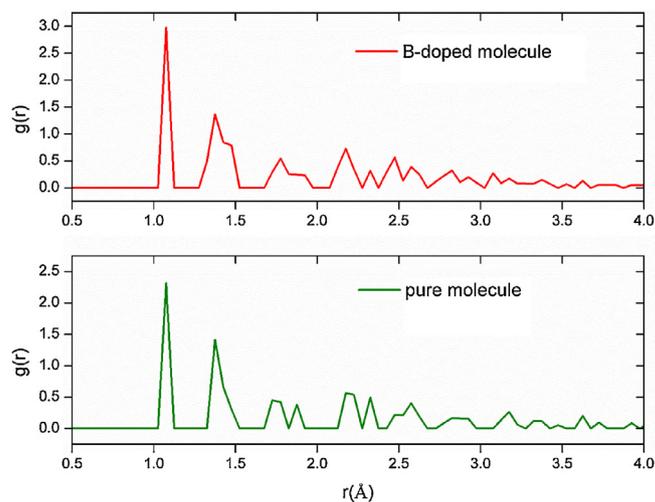


Fig. 6. Radial distribution function (RDF) of 5,5'-Dibromo-2,2'-bithiophene and B-doped 5,5'-Dibromo-2,2'-bithiophene molecules.

4. Conclusions

We performed a theoretical investigation to enhance the electronic structure, photophysical and optical properties of semiconductor molecules using kick algorithm which is first used in this study to get an insight a new aspect to molecular design. Comparing with the pure molecule, the B-doped molecule has more desirable properties. For example, the B-doped molecule is more stable than the pure molecule. The band gaps of the isomers of the B-doped molecule are found to be smaller than those of the pure molecule which means that the electronic transfer is easier. The refractive index increases when it comes to the B-doped molecule. B-doped molecule has stronger intermolecular interaction due to a larger dipole moment value. The charge distributions of the pure molecule are significantly changed based on the B atom. The B-doped molecule becomes preferable in terms of the formation energy than the pure molecule. The energy of the molecule derived from electron-transfer for the B-doped molecule is lower than the pure molecule. The B-doped molecule gives rise to an enhancement in visible light absorption and emission. The radial distribution function of the B-doped molecule is greater than that of the pure molecule. We hope that the B-doped 5,5'-Dibromo-2,2'-bithiophene molecule has many unexplored molecular designs which will influence the performance of optoelectronic devices.

CRediT authorship contribution statement

İ. Muz: Investigation, Methodology, Visualization, Writing - original draft, Writing - review & editing, Data curation, Software.
M. Kurban: Supervision, Investigation, Conceptualization, Writing - original draft, Writing - review & editing, Data curation, Validation, Software.

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