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Enhanced photoconversion efficiency in organic polymer solar cells: Synthesis, structural analysis and computational modelling of 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid-based composite

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ABSTRACT

Improving the photoconversion efficiency (PCE) of organic polymer-based solar cells (SCs) is crucial to their competitiveness with conventional SCs. This study presents a novel approach to improve PCE of an organic composite solar cell incorporating 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid. The molecular composite was designed based on the photoactive donor- π -acceptor (D- π -A) architecture and computationally modeled to optimize its efficiency. The synthesized material was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and spectral analysis, confirming the formation of a perovskite lattice. Photovoltaic performance was evaluated using simulated device measurements, which produced a fill factor (FF) of 0.708, a short-circuit current density (JSC) of 12.8 mA/cm², an open-circuit voltage (VOC) of 1.22 V, and an overall PCE of 12.78%. The active exciton diffusion path length was measured at $< 9 \text{ \AA}$, with a direct band gap of 2.05 eV. The stabilized Urbach energy of the material ranged from 110 to 220 meV. Furthermore, the active single-layer film was interfaced with both a small work function electrode (SWFE) and a long work function electrode (LWFE). The material exhibited high polarizability ($\alpha_{\text{tot}} = 483.34 \times 10^{-33} \text{ esu}$, $\Delta\alpha = 332.68 \times 10^{-33} \text{ esu}$), indicating a strong potential for efficient photoconversion. This study demonstrates the feasibility of using 4,8-dichlorobenzo [1,2-b] difuran-2,6-dicarboxylic acid-based composite for high-performance organic solar cells, offering a promising alternative to conventional SCs.

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1. Introduction

Hybrid organic cyclic compounds with π -conjugated molecular structures are associated with perovskite solar cells that effectively absorb light and generate electricity, achieving photoconversion efficiencies of up to 22%. Typically, these materials are made of 2D layered organics and are direct band gap semiconductors, which have various optoelectronic applications, including enhanced energy manipulation for light absorption and use in perovskite solar cells [1-4]. For the past two decades, conventional solar cells have played a critical role in the conversion of renewable energy sources into electricity. However, photovoltaic devices made from organic compounds have created new opportunities to reach high power conversion efficiencies (PCE), with the potential to exceed a 47% threshold [5]. Due to their low cost, lightweight nature, and ease of coating on different materials, organic solar cells are becoming promising components in green energy technology [6,7]. Since the development of second-generation solar cells,

researchers have shifted their focus to third-generation perovskite-structured organic solar cells (OSCs). These OSCs are relatively inexpensive to produce and typically exhibit excellent flexibility and stretch ability. The preparation process is manageable and straightforward, significantly improving the commercial viability of these materials. The authors suggest that there are numerous opportunities to increase PCE by modifying the chemical structure of organic materials while simultaneously altering their physical and chemical properties. All OSC materials are crafted using organic chains and ring compounds, such as polymers as the active layer, combined with various substrates to produce successful and efficient flexible OSCs. At the outset of the development of third-generation solar cells, rigid substrates were primarily used to achieve high efficiency through the design of active layer material. This approach made device optimization straightforward and mechanistic investigations easier to understand.

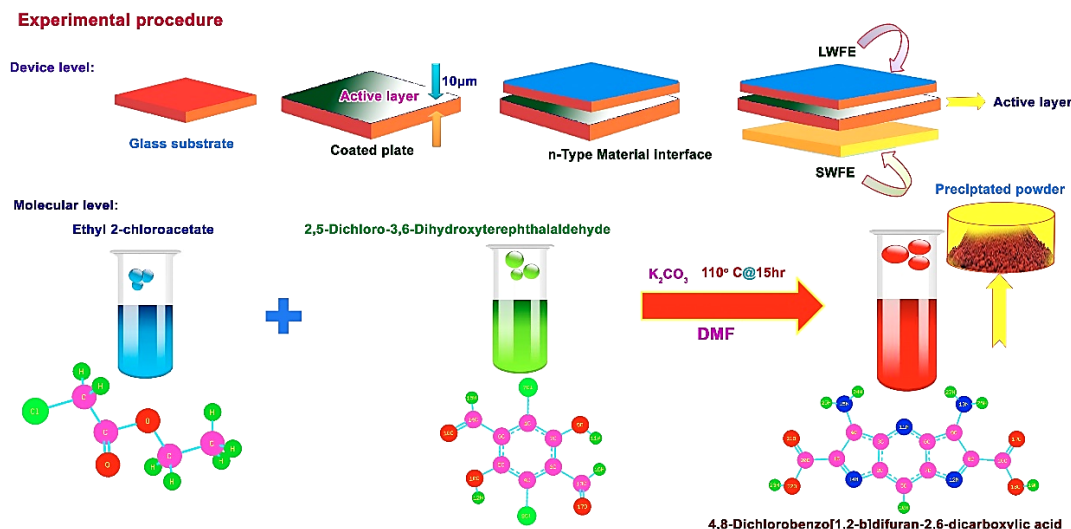


Figure 1. Experimental procedure for material preparation.

Recently, flexible solar cells have shown efficiencies comparable to rigid solar cells by adjusting the physical and chemical properties of aromatic ring and chain compounds through suitable electron-donating substitutional groups [8-10]. The active layer is prepared using a solvation model constructed with theoretical tools such as Gaussian. All organic chain and ring compounds with intrinsic π -conjugated properties contain heavily electron-populated donors and semifilled acceptors, providing significant prospects for the fabrication of OSCs with remarkable exciton production capabilities [11-15]. The ability of exciton separation and the charge transport properties of 2D perovskites can be significantly enhanced by the presence of delocalized electron clouds in organic frameworks. In particular, the π and σ conjugated intermolecular interactions between cyclic carbon arrangements lead to the formation of organic cations. This results in improved transport properties and device performance. The current literature indicates that these types of interaction provide a stronger molecular-electrostatic heterogeneous matrix stronger than standard hydrogen bonds, highlighting the cationic nature of the organic framework. A particularly interesting class of π -conjugated matrices is multifunctional dendritic and acentric ligands, which can be used to enhance the degree of intermolecular interactions. These interactions exhibit a robust electrostatic component, leading to superior bond interactions that enable charge production modifications to the optoelectronic mechanisms and enhance photovoltaic performance.

Bulk heterojunction organic solar cells (BHJ) are created by arranging carbon core conjugated systems, typically composed of hexagonal or pentagonal rings, into chains that serve as substrates. These systems generally exhibit well-defined HOMO-LUMO energy confinement. Intrinsic electron donor molecules are added or substituted at specific locations within the core ring to facilitate energy-level assignment in the desired state. As a result, the HOMO-LUMO energy gap can effectively absorb photonic energy for conversion. Typically, the morphology of a material is determined by the assignment of symmetric nucleation processes that involve heteronuclear bond units in molecular structures. Notably, the perovskite lattice structure is observed in this context. The symmetrical attachment of furan compounds to a pyridine base significantly increases the number of electron-accumulation centers within the structure. Additionally, two amino substitutions are symmetrically reinforced on the furan rings, which helps control random electron accumulation and maintain the

electron cloud over the compound's framework. An extra chlorine atom is incorporated into the center of the ring to support sufficient electron clouds. Furthermore, the introduction of COOH groups creates a diffusion pathway with a high degree of electronegativity, which helps maintain the weak attraction of excitons and prevents recombination.

In the symmetric nucleation process, the productivity of heteronuclear bonding units exceeds that of homonuclear units. It is estimated that approximately 78.256×10^6 interactive bonding units were re-established per mole of substance. However, the homonuclear bonds are enriched with proton content and dissociate from the molecule in an asymmetric manner. Both of the opposite regions interact weakly with the critical barrier potential, which can be measured by the molecular dipole moment. Each photon possesses momentum equivalent to the dissociation energy of the electron-hole pair in the active layer. This energy is then converted into the kinetic energy of the electron as it diffuses to reach the electrode [16,17].

In this study, a solvation model has been developed that utilizes base and substitutional compounds. When solved, this model causes a minor distortion in the band gap arrangement while maintaining the overall band gap. The theoretical and experimental band gap, or HOMO-LUMO energy gap, is 2.05 eV, measured in various molecular unit combinations. The measured values are consistent across all molecular units. After the model was solved, the organic material composite was prepared at an appropriate temperature, and the final product was collected in powder form and coated onto a substrate along with a supporting electrode module. All measurements were conducted, and the corresponding parameters were tabulated. From the results obtained, the power conversion efficiency (PCE) was calculated and the fill factor (FF) was also estimated.

2. Experimental

2.1. Synthesis and film preparation

To achieve accurate purity, the chemical compound, 2,5-dichloro-3,6-dihydroxyterephthalaldehyde (5 mg) was taken as seed material and dissolved in 5 mL of ethyl 2-chloroacetate, which is a liquid water-white solvent and is usually mixed as a processing aid to prepare gel or dye compounds. The well-dissolved mixture was further mixed with dimethylformamide, which acts as a solvent and potassium carbonate, which acts as catalyst and water adsorbent medium. In this chemical

reaction, ethyl alcohol and HCl are removed by heating at 80 °C and crystallization occurs. The dissolved mixture was heated to 110 °C for 15 h to obtain 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid. The final product was initially in the form of a gel and was suitable for preparing film. The complete preparation procedure is shown in Figure 1.

A high-density organic dye gel was placed on a spin coating plate and spun at 2000 rpm for 20 which was adequate for making a film. The prepared thin film was placed in a Petri dish without cover for 3 h and was then heated at 120 °C for 1 h. The film was checked to verify the uniform thickness over the plane using a screw gauge device at various places on its surface. Therefore, 6,6-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) and PCDTBT polymers are used as N and P type electrodes for making OSC composites and both are coated on the active layer film.

2.2. Measurement techniques

A well-defined and accurate XRD pattern of the prepared material was obtained with a Bruker smart CCD Apex DUO diffractometer according to the procedures in the literature [18,19]. Well-scanned IR and anti-stroke lines of Raman spectra were recorded as described in previous reports [20,21]. Regarding chemical shift concern, for present study, ¹H and ¹³C NMR spectra were recorded as described in the literature [22]. UV-vis absorption and transmission spectra for the exploration of the charge transfer (CT) complex and the electronic transition, respectively, were recorded on a PerkinElmer Lambda 365 spectrophotometer [23]. The cross section and surface of the film were clearly obtained from SEM images via a Raman scanning electron microscope (Lab RAM Soleil). In addition to UV-visible absorption, photoluminescence (PL) spectral signals were identified by a Horiba Fluorolog-3 spectrofluorometer.

2.3. Solar cell characterization

Current density versus voltage (J-V) measurements for the current photovoltaic device were performed via a using Keithley 2635 source measurement unit. A 300 W xenon lamp was used as the solar simulator and a Newport reference cell (model 71582) was used for calibration. To calibrate the light intensity of the solar simulator (100 mW/cm²), the lamp was adjusted to match the short circuit current (J_{sc}) of the reference cell under simulated light. A suitable light aperture was used for the respective active area to shadow the devices. The quantum efficiency measurements were performed by using the same lamp with a double grating monochromator. A silicon photo diode with model no. 71580 was used as the reference cell. The step size for the EQE measurement is 1 nm. The J-V measurements of the current photovoltaic device were performed on raw open cells in an open environment without preconditions.

3. Computational details

To validate the experimental results, computational calculations of the molecular structure of the title material were carried out. The parameters of the molecular mechanism such as frequency, bond interaction energy, Zero point vibrational energy, optimized parameters, and binding energy were calculated at B3LYP/6-311++G(2d,2p) level. Fundamental vibrations related to active and inactive bonds of the molecule and their analytical IR and Raman frequency calculations were performed at the B3LYP and B3PW91 theory with the same level of basis set. The entire bond parameters of optimized structures were validated with the data associated with the crystal structure and the molecular slab solvation model was predicted from the 3D translation vectors of the unit cell

arrangement. To approximate all the parameters, the Tamm-Dancoff approximation was used to implement surface field theory in the work field of time-dependent density functional theory (TD-DFT). The molecular and electronic energy of molecular geometries was calculated at the B3LYP level, and the Fermi level energy adjacent to the LUMO and below the HOMO was traced across different sets of energy levels [24]. The chemical shift of the core and the allied carbons of the present sample were calculated at the B3LYP/6-311++G(2d,2p) level from which the energy voids were identified on the core π -links.

4. Results and discussion

4.1. Molecular slab analysis of the crystal pedestal

Chains of organic cyclic components jointly generate polymers resembling structures that effectively act as binary bulk heterojunction (BHJ) solar cell materials, and these organic solar cells usually can have enhanced photovoltaic performance [25,26]. Electronic and vibrational transitions are normally considered together in organic materials where the molecular structure is formed by hybridized σ and π bonded carbons. The weakest bonded cyclic system of organic molecules abundantly results in regular crystalline arrays with considerable thermal stability. With the help of heteronuclear bonded substitutions, the cyclic weak-bond system can be easily converted to a strong molecular system with a well-defined density of states. In addition, intensive halogenations of organic cyclic compounds enhance the photoconversion efficiency [27]. Accordingly, the difuran compound was selected as the central core in which the di carboxylic acid was substituted as a non-Centro symmetry additive and the dichoro compound was injected as the photoenergy converter. The entire custom compound was investigated for the fabrication of OSCs.

For the purpose of simulating the solvation model for the material structure, computations were performed along with KS DFT dispersion (DFT-D) calculations in which the program output generated a molecular strip as well as a molecular slab of the interplanar frame of the crystal. According to the calculation model, the interplanes of the material slab of t-furan were simulated in 3-different directions such as the *a*, *b*, and *c* orientations in the crystal lattice unit boundary. As in Figure 2, the molecular strip orientation on *a'* and *c'* at the 001-plane *c'* at the top (A), where all groups of atoms in such a lattice are observed to form as perovskite forms. This is the suitable place where cation liberation takes place. Another orientation appeared on the *b* and *c* sides of the lattice in which subplans with uniform slab distances were found. It is generally named as the top B(A) side of the tetragonal plane of 001 and the cation active zones appear. The third segment of the same Figure 1 shows *a* and *c* orientations such as oblique angles, and here all ligand groups were determined to be placed perpendicular to the plane of the surface. In this platform, anion liberation takes place, and because of the normal orientation on the surface, the process is very strong and equivalent anion generation is possible.

Figure 3 shows the simulated schematic diagram of the organic unit cell translation operation in crystal planes. Here, we can clearly view the repetition of the unit cell content of the molecular cluster of the title molecule. The 3D confinement of the molecular frames of unit cells has been arranged in a periodic manner in the crystal lattice. On observing the pictorial diagram, it is well-known that all the molecular slabs are associated with cation and anion chains, which are referred to as exciton couplers. The exciton generation takes place where two molecular slabs meet, which is also called the exciton regime.

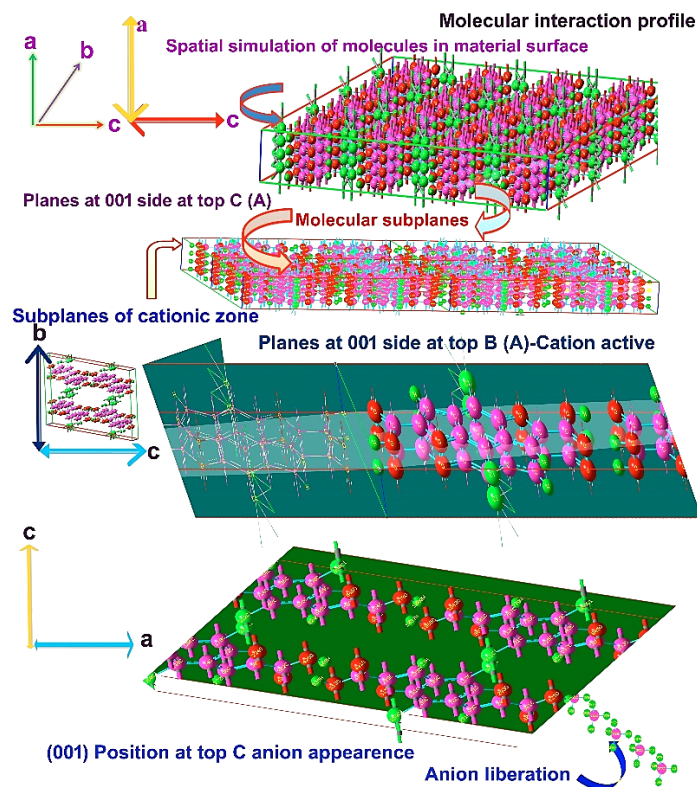


Figure 2. Molecular interaction at different planes of the lattice.

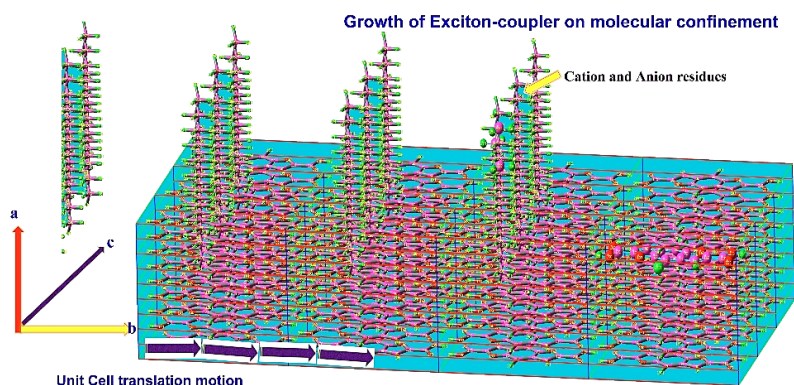


Figure 3. Simulated schematic diagram of the organic unit cell translation operation in crystal planes.

4.2. Molecular solvation model analysis

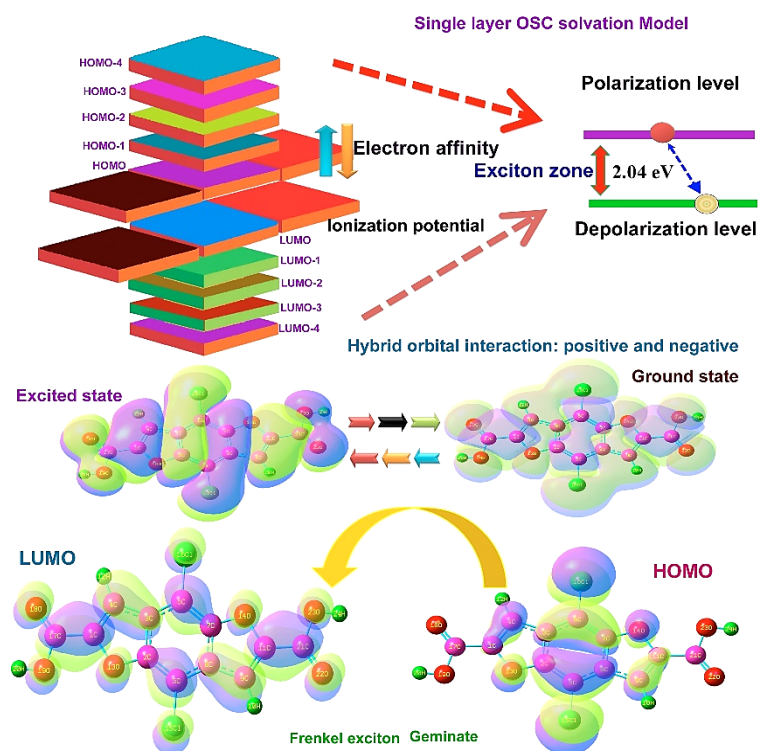
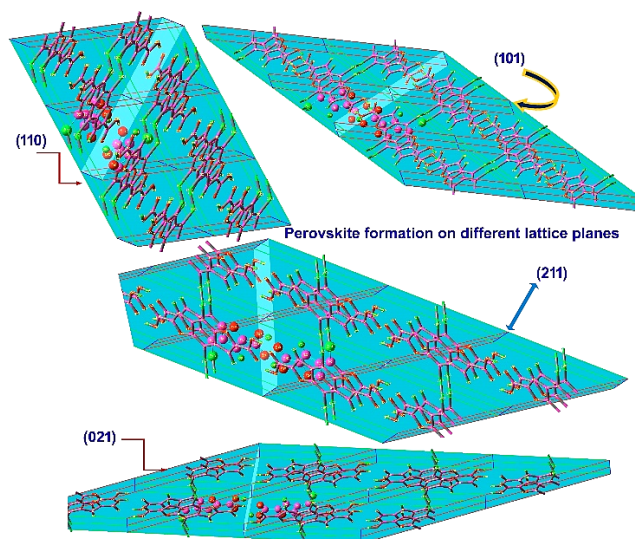
To validate the operational functions of organic solar cells (OSCs), a thorough understanding of their molecular and crystal topologies is essential. The molecular configurational topology is directly responsible for the photoconversion process in the involved material. For that purpose, the molecular solvation model is shown in Figure 4. The HOMO and LUMO sets of the present case are clearly presented in the figure where the direct energy gap between the electron affinity and ionization potential was measured as 2.04 eV which is fairly good for the reception of photon energy. The polarization level and the depolarization level of the split energy domains of the molecular material are shown in Figure 3.

During vibrations, the electronic energy states become polarized in the molecular frame, which is denoted as the excited and ground states, and between these two states the molecular configuration takes place, which generates the

exciton. The resulting configurational changes lead to the generation of excitons with moderate Coulomb attraction, which is much lower than the disintegration energy. The frenkel exciton disassociation between the HOMO and LUMO is shown in Figure 4. Different types of crystal planes are shown in Figure 5 where, depending on the phase of the planes, the plane of the molecular structure is determined to be oriented differently. Here, the molecular plane configuration at the (110) plane is entirely dissimilar to that at the (101) plane, and it deviates from the (211) plane. Because of these different orientations on different sides of the crystal, the refractive indices are different from each other. The molecular packing process is detailed in Figure 6 where the perovskite structure was formed by unit cell arrangement. The exciton length was measured as 1.75 Å between consecutive planes. When one side of the crystal plane was crossed, the same exciton length was sustained. Because of this architecture, the frequency of the light wave might be doubled.

Table 1. Crystal and optical parameters of 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid.

Parameters	Values
Space group	$P4mm$; tetragonal perovskite
Melting point	236 °C
Film dimension	65 mm×75 mm
Urbach energy	114-218 meV
Unit cell	$\alpha = \beta = \gamma = 90^\circ$
a	5.781 (Å)
b	5.023 (Å)
c	9.124 (Å)
Volume	264.94 Å ³
Refractive index	
n_1	1.592
n_2	1.637
n_3	1.523
Dielectric constant	3.6-5.9
Resistance of active thin layer	$5.6 \times 10^{-2} \Omega/\text{cm}$

**Figure 4.** Solvation model of a single-layer organic solar cell.**Figure 5.** Formation of perovskite at different planes.

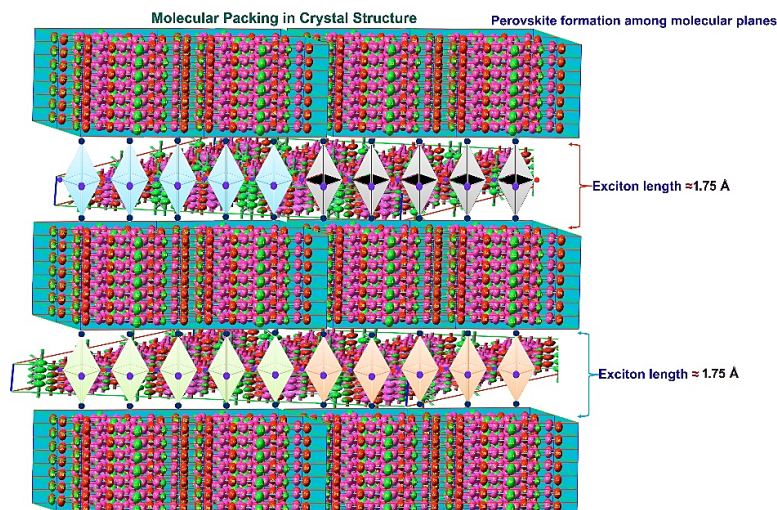


Figure 6. Molecular packing on the crystal structure.

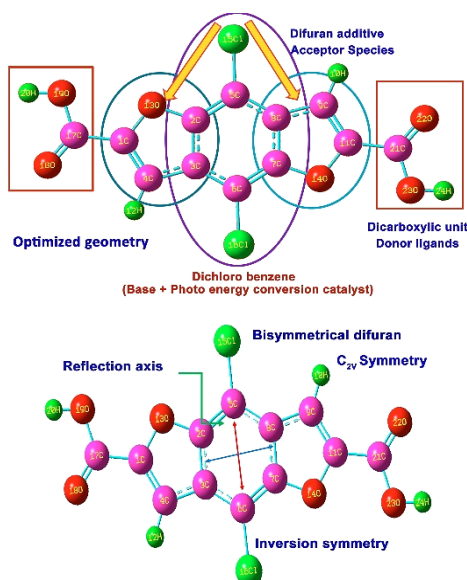


Figure 7. Optimized geometry of the molecular structure.

All crystal measurements and optical parameters of 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid are shown in Table 1. According to the computational calculations, the point group was C_{2v} , the space group was $P4mm$ (crystal class $4mm$), and the respective crystal lattice was perovskite tetragonal. The melting point of the prepared compound was 236°C whereas $\pm 18^{\circ}\text{C}$ temperature difference was observed in the stabilized state. The film dimension was measured as 65×75 mm which was designed to fit the n and p electrodes. The basic unit cell was represented by the angle separation of $\alpha = \beta = \gamma = 90^{\circ}$ and the unit cell sides were measured as $a = 5.781$ (Å), $b = 5.023$ (Å) and $c = 9.124$ (Å). Therefore, the unit was found to be translated along the c side. The total volume of the unit cell was 264.94 Å³ which is almost equivalent to 26 nm size. The estimated refractive indices of three sides of the planes were $n_1 = 1.592$, $n_2 = 1.637$ and $n_3 = 1.523$. The dielectric constant of the active material was measured as 3.92 which is adequate for generating exciton polarization, and a considerable PCE can be obtained. The resistance of the thin film was calculated using a conductivity meter and was 5.6×10^{-2} Ω/cm which was very acute to optimize the attenuation of the layer.

4.3. Molecular topography analysis

The present case is an organic composite that is composed of 24 atoms in different planes and almost all of the atoms in the same plane. According to computations in higher-order theory, the molecular structure belongs to the C_{2v} point group of symmetry. Therefore, the molecule has reflection as well as inversion symmetry and has specific optoelectronic characteristics. There were 24 bonding elements present, of which 14 polar bonds and 12 nonpolar bonds are active according to the IR and Raman spectra, respectively. The molecular weight of the compound was 315 amu. The Zero-point vibrational energy was 1831.73 amu. Although the molecules in the crystal lattice were evaluated as non-Centro-symmetry systems, the molecule has bisymmetric elements as shown in Figure 7, difuran was substituted in dichlorobenzene and dicarboxylic acid groups were substituted on both sides of the compound. of the compound. Therefore, it produces high symmetry, and the molecule possesses reflection as well as inversion symmetry. The bond length, bond angle, and dihedral angle arrangements can be clearly viewed.

Table 2. Optimized geometrical parameters for 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid.

Parameters	HF	DFT		Dipole strength
	6-31+G(d,p)	6-31+G(d,p)	6-311++G(d,p)	$\times 10^{-44} \text{ esu}^2/\text{cm}^2$
Bond length (Å)				
C1-C4	1.360	1.336	1.360	45
C1-O13	1.375	1.352	1.375	969
C1-C17	1.471	1.479	1.471	673
C2-C3	1.422	1.402	1.422	36
C2-C5	1.385	1.375	1.385	33
C2-O13	1.358	1.339	1.358	3396
C3-C4	1.432	1.443	1.432	618
C3-C6	1.400	1.386	1.399	41
C4-H12	1.078	1.069	1.078	89
C5-C8	1.399	1.386	1.400	26
C5-Cl15	1.735	1.724	1.735	746
C6-C7	1.385	1.375	1.385	26
C6-Cl16	1.735	1.724	1.735	518
C7-C8	1.422	1.402	1.422	56
C7-O14	1.358	1.339	1.358	2403
C8-C9	1.432	1.443	1.431	112
C9-H10	1.078	1.069	1.078	78
C9-C11	1.360	1.336	1.360	39
C11-O14	1.375	1.352	1.375	98
C11-C21	1.471	1.479	1.470	32
C17-O18	1.208	1.182	1.208	817
C17-O19	1.347	1.317	1.348	817
O19-H20	0.969	0.947	0.969	437
C21-O22	1.208	1.182	1.208	969
C21-O23	1.347	1.317	1.347	988
O23-H24	0.969	0.947	0.969	413
Bond angle (°)				
C4-C1-O13	112.10	112.84	112.10	-
C4-C1-C17	128.56	127.95	128.56	-
O13-C1-C17	119.33	119.21	119.34	-
C3-C2-C5	123.84	123.41	123.83	-
C3-C2-O13	110.18	110.31	110.18	-
C5-C2-O13	125.98	126.28	125.99	-
C2-C3-C4	105.23	104.74	105.22	-
C2-C3-C6	120.39	120.84	120.40	-
C4-C3-C6	134.38	134.42	134.38	-
C1-C4-C3	106.24	105.48	106.24	-
C1-C4-H12	125.73	126.21	125.73	-
C3-C4-H12	128.03	128.30	128.03	-
C2-C5-C8	115.77	115.75	115.77	-
C2-C5-Cl15	122.07	122.07	122.07	-
C8-C5-Cl15	122.16	122.17	122.16	-
C3-C6-C7	115.77	115.75	115.77	-
C3-C6-Cl16	122.16	122.17	122.16	-
C7-C6-Cl16	122.07	122.07	122.07	-
C6-C7-C8	123.84	123.41	123.83	-
C6-C7-O14	125.98	126.28	125.99	-
C8-C7-O14	110.18	110.31	110.18	-
C5-C8-C7	120.39	120.84	120.39	-
C5C-8-C9	134.38	134.42	134.38	-
C7-C8-C9	105.23	104.74	105.23	-
C8-C9-H10	128.03	128.30	128.03	-
C8-C9-C11	106.24	105.48	106.25	-
H10-C9-C11	125.73	126.21	125.73	-
C9-C11-O14	112.10	112.84	112.10	-
C9-C11-C21	128.56	127.95	128.57	-
O14-C11-C21	119.33	119.20	119.34	-
C1-O13-C2	106.25	106.63	106.25	-
C7-O14-C11	106.25	106.63	106.25	-
C1-C17-O18	123.03	122.51	123.03	-
C1-C17-O19	112.87	113.14	112.87	-
O18-C17-O19	124.10	124.35	124.10	-
C17-O19-H20	107.07	108.88	107.06	-
C11-C21-O22	123.03	122.50	123.03	-
C11-C21-O23	112.87	113.13	112.86	-
O22-C21-O23	124.10	124.35	124.10	-
C21-O23-H24	107.07	108.88	107.08	-

As shown in Table 2, in terms of base geometry, C2-C5 = C6-C7 = 1.385 Å; C3-C6 = C5-C8 = 1.40 Å and C2-C3 = C7-C8 = 1.422 Å; C3-C4 = C8-C9 = 1.431 Å and all the partial segments of the bond units have similar bond distances. Similarly, in the case of the bond angle, C2-O13-C1 = C7-O14-C11 = 106.25°; C2-C3-C4 = C1-C4-C3 = 106.24° and all the angle units in the base and ligand units were found to be the same and consistent. At the boundary, C17-O18 = C21-O22 = 1.208 Å and O19-H20 = O23-H24 = 0.969 Å and all of which are the same. At the boundary,

the angle of O22-C21-O23 = O18-C17-O19 = 124.10°; C1-O13-C2 = C7-O14-C11 = 106.25° is the same.

For the carboxylic unit, C1-C17-O18 = C11-C21-O22 = 123.03° and C1-C17-O19 = C11-C21-O23 = 112.87°, although it has inversion symmetry, the reflection angles are the same. According to the optimized geometry, all the bond lengths are found to be symmetric, and bond units are equally distributed. Dual ligand units were adopted on the base unit, in which one compound acted as the core and the other two ligands acted as

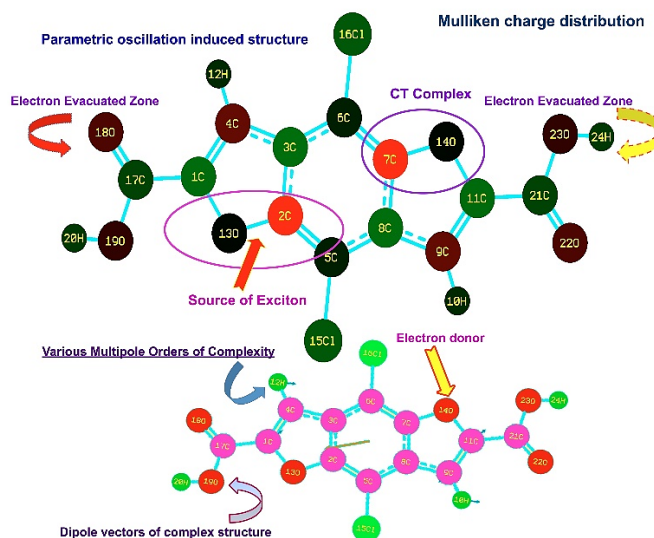


Figure 8. Mulliken charge distribution diagram.

the donor and acceptor. DMF is usually the best solvent for the manufacture of OSCs, and here it was used as both a solvent and a PCE catalyst. Because of their high symmetry, the Coulomb force of attraction and repulsion within the limit enforced electrophilic and nucleophilic depletion zones in each and every unit cell, generated excitons and was supported by incident photonic energy.

4.4. Mulliken charge profile analysis

As the present case involves organic species, the organic ring has alternating σ and π interactively hybridized delocalized orbitals. In terms of the charge pressure enforcement among the molecular site to compensate for the equilibrium forces of attraction and repulsion, an asymmetric charge distribution appears in the ring. Hence, possibly some interactive bonds are created in the atomic platform. By the application of substitutions, the charge distribution atmosphere is altered and the asymmetric charge gradient is reproduced accordingly. As a result, the substituents modify the charge distribution and enforce the production of interactive polarized and nonpolarized bonds. The modified charge allocation within the molecular is shown in Figure 8.

Typically, in organic molecular systems, some electrons (bonding electrons) are involved in the bonding process, and other electrons (non-bonding electrons) are realigned at the molecular site through the enforcement of chemical equilibrium forces of attraction and repulsion. Hence, all the energy is restored in the core of the molecular system, which is usually a bond system called the charge-transfer complex (CTC) and such a bond is a resource of all the activities of the molecular system. Here the main application of the present molecular system is photovoltaic activity, and in the CT complex, exciton production takes place while the photon energy impinges on the molecular surface of the material. Consequently, here, several CT complexes were identified as C2-O13 and C7-O14; although the molecule contains many intensified dipole bonds such as C6-Cl16, C5-Cl15, C21-O22, C21-O23, C17-O18 and C17-O19, the electronic content accumulates in these two CT complexes. The measured dipole strengths of C2-O13 and C7-O14 were 3396×10^{-44} and 2403×10^{-44} esu²/cm² respectively. In comparison to all bonds, these bonds appear to have very high dipole strengths and contain very large energy domains. In addition to such bonds, the electron content of COOH on both sides of the molecular system decreased. From this observation, it was clear that the

electronic energy was directed towards the center of the ring. Figure 8 shows the multipole complexity structure in which the individual dipole vectors appeared to be in random directions within the molecular boundary.

4.5. XRD analysis

To acquire the proper molecular pattern to form the crystal arrangement of the composite material, the sample was heated at 120 °C and made into a thin film via the spin coating method; therefore, XRD analysis was carried out. The recorded XRD pattern along with the molar absorption graph of the present sample is depicted in Figure 8. According to computations of first-principles density functional theory, the compressibility of atoms in organic composites is probed with hydrostatic pressure, revealing the negative linear compressibility of atoms and enabling anisotropic mechanical properties [28]. Therefore, the XRD pattern of organic samples usually contains many numbers of peaks with minimum to maximum intensities.

Here, the sample was heated at 120 °C to coat a film that was 10 °C greater than the melting point of the present substance; therefore, it was the annealing temperature for the compound. Therefore, the composite is further molecularly reregulated, and the order of the crystal arrangement is increased. According to the XRD pattern, the observed peaks; at 12°, 14°, 21°, 24°, 26°, 30°, 37° and 43° are attributed to the planes; (001), (110), (211), (101), (111), (220), (310) and (200) planes, respectively. The peaks of the obtained planes surely represented the perovskite lattice of the material. Some of the peaks, other than those characteristics of the tetragonal Perovskite represented a hidden and less effective lattice structure. Despite the constructive peak assignment observed in the material composite, the actual positions of all the peaks deviated. This was mainly due to the high compressibility of the organic molecular planes. The distortion of the lattice planes mentioned above also produced 2D defects in the material, which did not affect the actual semiconducting properties or optical transparency of the surface. Given the anisotropic molecular configuration atmosphere in materials, rather uncontrolled crystallization usually takes place in organic materials, resulting in a defective crystalline arrangement, which also results in incomparable transportation properties in the material domain. Therefore, the micronucleation is occurring in the molecular setup and homogeneous nucleation process were maintained in micro thin film morphology, which helped regenerate exciton reproduction.

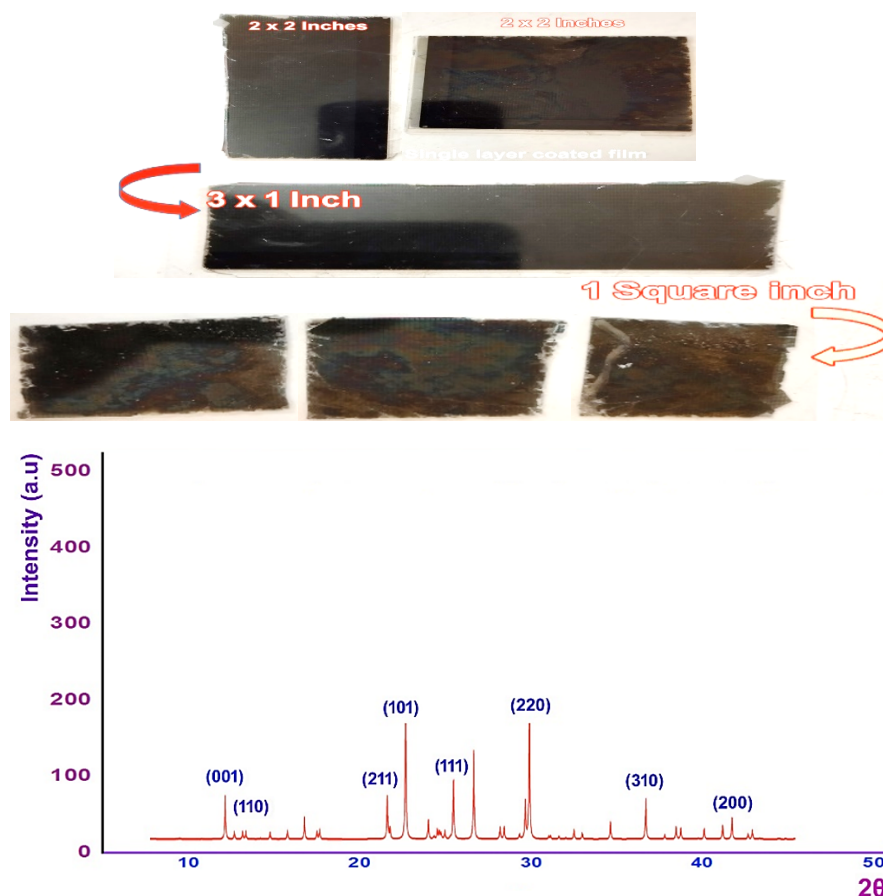


Figure 9. XRD graph of the prepared sample.

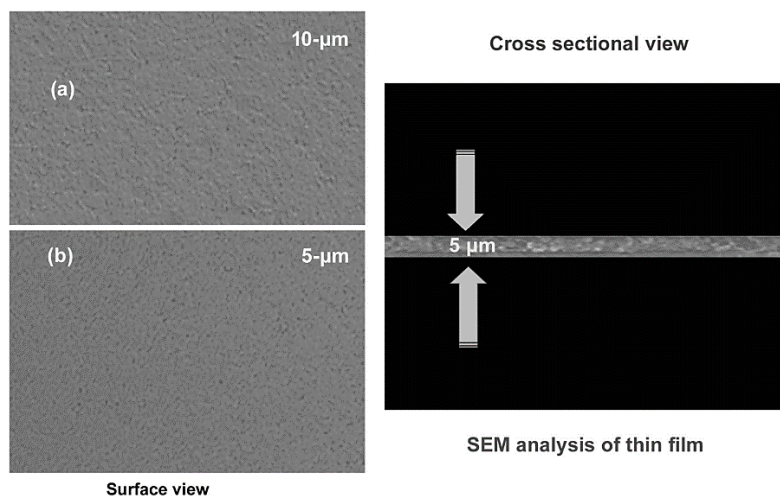


Figure 10. SEM images of thin film.

Figure 9 shows the plot between the absorption of the photon energy and the wavelength of light radiation for the present material. Typically, an efficient absorber has 95% absorption in the spectral range of 400-800 nm; accordingly, the present case has efficient absorption in the region of 350-720 nm. This proves the absorption efficiency and good transport properties.

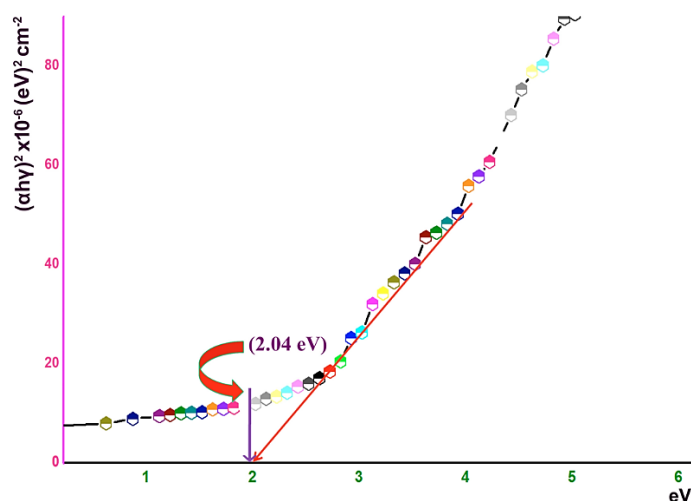
4.6. SEM examination

The active layer of the present compound was coated on a p-substrate followed by a glass substrate via the spin coating method. The thickness of the active layer of the thin film was

measured as 5 μm which is the optimized penetration depth of the photon energy. An SEM image of the coated film is shown in Figure 10. Figure 10a shows 5 μm and 10 μm SEM images and both photographs show the micro-porous molecular composites and smooth surface with a uniform distribution, which means that the film has an elevated harvesting rate of incident light. When the film is very deep, the annulled material is scrubbed and has a loosely packed net-like structure. To measure the thickness of the film and cross-sectional uniformity, we obtained the cross-sectional view by masking both sides of the film. Initially, the sample was taken as a gel, heated at 120 $^{\circ}\text{C}$ and coated on a substrate, so that the film was forcefully uniform.

Table 3. Photovoltaic values (PV) of 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid and comparison with polymer cell.

No	Parameters	Values	ITO with polyethylene naphthalate (PEN)	Poly-pyrrole polymer
1	Direct band gap calculated from slope	2.05 eV	-	-
2	Birefringence(Δn) $K\lambda/t$	1.960	-	-
3	$1/d_{\text{hkl}}^2 = (h^2 + k^2)/a^2 + l^2/c^2$	$264.94 \text{ \AA}^3$	-	-
4	Open circuit voltage (V_{oc})	0.60 V	0.660	0.727
5	Short circuit current (J_{sc})	14 (mA/cm^2)	8.97	10.20
6	Power conversion efficiency	4 %	2.65%	3.12%
7	Attenuation of n-type	0.69 V	-	-
8	Attenuation of p-type	0.89 V	-	-
9	Photon energy loss	0.19 V	-	-
10	Fill factor (FF)	0.476	0.45	-0.42

**Figure 11.** Band gap from $\alpha\chi$ versus energy diagram.

A clear picture of the frottage of perovskite crystals with well-reduced molecular boundary conditions was also obtained. As the present case was organic, the process of coating with homogeneity is not very difficult and the existence of molecular amalgamation in the material for obtaining the perovskite lattice is quite standard. During testing, it was clear that the surface of the film was in good contact with the hole-transport layer (PEDOT: PSS) and the electron transport layer (PC61BM) for the construction of a good shunt path with very much reduced attenuation for the photocurrent.

4.7. Photovoltaic (PV) measurements

To measure the band gap of the material, the absorption ability of the compound per photon energy was determined and the corresponding graph is shown in Figure 11. The observed values were plotted as $\alpha\chi$ versus energy in eV, and the slope was drawn from which the band gap was estimated as 2.04 eV, which is close to the HOMO-LUMO energy gap. As shown in the graph, the curve started at 9 eV/cm^2 at 0 eV and reached 89 eV/cm^2 at 5.2 eV. The birefringence (Δn) $K\lambda/t$ was estimated for the material to be 1.960 which clearly reflects the atomically anisotropic atmosphere of the compound that has a non-uniform atomic distribution of optical properties in different subplane directions. As shown in Table 3, the volume ($1/d_{\text{hkl}}^2 = (h^2 + k^2)/a^2 + l^2/c^2$) of the unit crystal was $264.94 \text{ \AA}^3$ which was due to the very dense packing of the crystal.

Photovoltaic recitation of the present OSC was observed via a J-V plot, as shown in Figure 12. According to the electrical scanning protocol, the test was performed from reverse to forward bias conditions at a scanning rate of 0.05 V/s. All photoconversion processes were studied in the Keithley-2400 apparatus in which the open circuit voltage (V_{OC}) was estimated to be 0.60 V at a short circuit current (J_{SC}) of 14 (mA/cm^2). Therefore, the calculated power conversion efficiency (PCE) was 4%. This observed J-V characteristic was considerably greater than that of PV performance of

polyethylene naphtholate and polypyrrole polymer solar cells (SC). According to the $J_{\text{SC}}-V_{\text{OC}}$ curve, the reverse bias current starts to flow at $-15 \text{ mA}/\text{cm}^2$ at a potential of 0 V. The current was slowly increased and passed through 0 mA/cm^2 at 0.7 V, and the forward current was further increased to 2.5 mA/cm^2 at 1.1 V. The forward current suddenly increased at random and reached 14.8 mA/cm^2 at 1.2 V. All power conversion parameters were calculated under the n- and p-type partner layers with attenuation of 0.69 and 0.89 V, respectively. Therefore, the maximum photon energy loss was estimated to be 0.19 V, and the fill factor was 0.526, which is the ultimate parameter for exploring the PCE of the solar cell. Usually, charge carriers avoid recombination under reverse bias conditions, but in this case, fewer recombination processes take place because of an application of strong electric field. In addition, the recombination of charge carriers has taken a weaker effect, and the bias current is independent of the influence between the electron and the hole.

4.8. Vibrational study

4.8.1. Vibrational assignments

The organic species present in the OSC was composed of 24 atoms in which 14 polar bonds and 12 nonpolar bonds were present. Because polar bonds have a high force constant, they consume more IR radiation than polar bonds. Moreover, the nonpolar bonds have high polarization constants; therefore, they are more Raman active than the polar bonds. Due to its molecular bisymmetry, its point group belongs to the C_{2v} type. So, according to group theory, the stretching, in-plane, and out-of-plane bending vibrations can be classified via Equation 1,

$$\Gamma_{66}\text{-Vib} = 24A_1 + 9A_2 + 21B_1 + 12B_2 \quad (1)$$

Usually, the stretching and in-plane bending modes are under the irreducible representations of A_1 and B_2 , respectively.

Table 4. Observed and calculated vibrational frequencies of 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid.

Symmetry species	Observed frequency (cm ⁻¹)		Methods			Vibrational Assignments	Interaction energy (kJ/mol)
	FT-IR	FT-Raman	HF	B3LYP	B3PW91		
C _{2v}			6-311++G(d,p)	6-311++G(d,p)	6-31++G(d,p)	Polar (P) / non-polar (NP)	
A ₁	3300w	3300w	3318	3306	3302	(O-H) υ/P	16.4
A ₁	3290w	3290w	3300	3295	3294	(O-H) υ/P	16.3
A ₁	3080m	3080s	3056	3110	3111	(C-H) υ/P	13.9
A ₁	3070m	3070s	3065	3095	3092	(C-H) υ/P	13.6
A ₁	1700s	1700w	1719	1706	1703	(C=O) υ/NP	14.6
A ₁	1680s	1680w	1698	1688	1688	(C=O) υ/NP	14.6
A ₁	1650w	-	1659	1654	1658	(C=C) υ/NP	14.7
A ₁	1620m	1620w	1630	1637	1621	(C=C) υ/NP	12.1
A ₁	1610m	-	1620	1616	1613	(C=C) υ/NP	12.1
A ₁	-	1600m	1608	1606	1609	(C=C) υ/NP	12.1
A ₁	1520s	-	1536	1526	1512	(C=C) υ/NP	11.8
B ₂	1500s	1500m	1518	1509	1502	(O-H) δ/P	11.9
B ₂	1490s	-	1500	1500	1493	(O-H) δ/P	11.5
A ₁	-	1450w	1466	1459	1457	(C-C) υ/NP	10.5
A ₁	1420m	-	1438	1430	1418	(C-C) υ/NP	10.5
A ₁	1400m	-	1409	1402	1398	(C-C) υ/NP	10.8
A ₁	1340w	1340w	1392	1387	1381	(C-C) υ/NP	9.4
A ₁	1300m	1300m	1315	1298	1296	(C-C) υ/NP	9.2
A ₁	1275w	-	1289	1281	1269	(C-O) υ/P	9.8
A ₁	1230w	-	1265	1259	1248	(C-O) υ/P	8.9
A ₁	1190w	-	1256	1248	1236	(C-O) υ/P	8.9
A ₁	1180m	1180w	1165	1175	1174	(C-O) υ/P	8.9
A ₂	1175s	1175w	1165	1161	1201	(O-H) γ/P	7.9
A ₂	1125s	1125m	1129	1129	1119	(O-H) γ/P	7.0
A ₁	1100m	1100w	1123	1108	1103	(C-O) υ/P	7.0
A ₁	1060s	-	1075	1071	1061	(C-O) υ/P	7.0
B ₂	1010s	-	1025	1020	1009	(C-H) δ/P	7.0
B ₂	950w	950s	971	958	951	(C-H) δ/P	7.0
B ₂	940w	-	956	941	943	(C-C) υ/P	7.0
B ₂	920w	-	932	925	924	(C-C) υ/P	14.6
B ₁	900s	-	912	901	908	(C-H) γ/P	14.2
B ₁	875w	875s	888	876	876	(C-H) γ/P	7.8
B ₂	860w	-	875	865	863	(CCC) δ/NP	-
B ₂	850m	850w	866	847	851	(CCC) δ/NP	-
B ₂	780w	-	791	790	782	(CCC) δ/NP	-
B ₂	770s	-	781	778	776	(CCC) δ/NP	-
B ₂	750s	750w	766	761	751	(CCC) δ/NP	-
B ₂	720s	-	738	729	718	(COC) δ/P	10.8
B ₂	710w	710w	721	706	697	(COC) δ/P	10.8
B ₂	690w	-	710	694	688	(C-O) δ/P	-
B ₂	-	680w	694	687	679	(C-O) δ/P	-
A ₁	650s	650w	667	659	643	(C-Cl) υ/NP	-
A ₁	640m	640w	653	648	637	(C-Cl) υ/NP	-
A ₂	620s	620w	630	618	621	(CCC) γ/NP	-
A ₂	610s	610w	622	606	608	(CCC) γ/NP	-
A ₂	605s	-	610	600	600	(CCC) γ/NP	-
A ₂	590s	590w	595	591	588	(CCC) γ/NP	-
A ₂	550w	550w	568	561	548	(CCC) γ/NP	-
A ₂	540w	-	554	548	529	(COC) γ/NP	-
A ₂	520s	520m	532	519	519	(COC) γ/P	-
B ₂	510w	-	510	508	506	(C-Cl) δ /NP	-
B ₂	480m	-	498	483	488	(C-Cl) δ /NP	-
B ₁	460m	-	578	465	462	(C-O) γ /P	-
B ₁	390w	-	398	397	392	(C-O) γ /P	-
B ₁	350m	-	365	361	356	(C-Cl) γ /NP	-
B ₁	320w	-	332	331	322	(C-Cl) γ /NP	-
B ₂	300m	-	309	305	302	(C-COOH) δ /NP	-
B ₂	260w	260w	268	264	261	(C-COOH) δ /NP	-
B ₂	250m	250w	259	248	256	Ring δ	-
B ₂	220w	220w	235	230	218	Ring δ	-
B ₁	190m	190w	200	197	192	(C-Cl) τ/P	-
B ₁	160m	160w	185	168	168	(C-COOH) γ /NP	-
B ₁	-	120w	137	118	121	(C-COOH) γ /NP	-
B ₁	110w	-	121	110	115	(O-H) τ/P	-
B ₁	90w	-	112	94	100	(O-H) τ/P	-
B ₁	80w	-	98	84	96	Ring γ	-

The out-of-plane bending and torsional modes are grouped under the notations of A₂ and B₁, respectively. As per the vibrational assignments of an cyclic system of organic molecule, a total of 66 vibrations are classified into 24 stretching modes, 12 in-plane bending and 21 out-of-plane bending, and 9 torsional bending modes. The active FT-IR and FT-Raman bands are presented in Table 4, and their respective spectra (experimental and theoretical) for the present compound are obtained in Figures 13 and 14, respectively.

When the sharing of electrons is unequal, the covalent polar bond becomes stronger than nonpolar bonds. Moreover, intramolecular covalent bonds are the hardest and most indestructible to facilitate strong intramolecular interactions. A greater number of polar bonds than nonpolar bonds in a molecule normally results in good chemical stability and reacts with the atmosphere without breaking bonds. Such ambience arrangements at the molecular site led to interactions of the bonds, which provide the interaction energy.

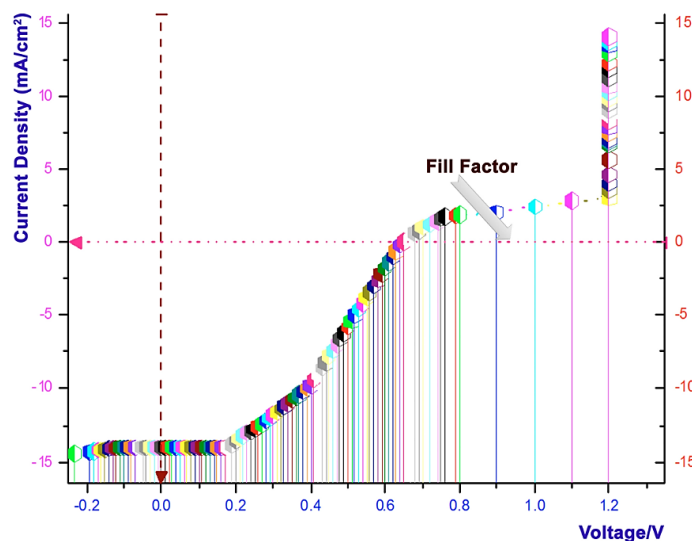


Figure 12. J-V plot for the prepared compound.

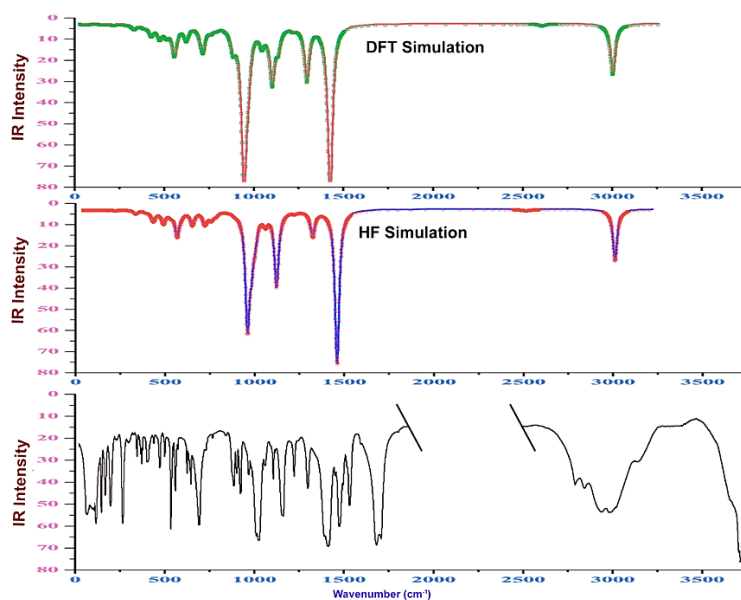


Figure 13. Observed and simulated FT-IR spectra.

Each and every bond has its own interaction energy and is usually affected by influence of non-bonding electrons in the molecular site. Therefore, the energy of interaction restored at the molecular site affects the vibrational energy of the bonds, which generates energy to develop the nonradiative lifetime. This condition of bonds in the molecule creates a steep optical absorption edge in the molecular arrangements of the molecular slabs of the crystal. Second, the polar bonds are active in the IR region and non-polar bonds are active in visible region, and both are possible when the bonds are elastic. Thus, when photoenergy is absorbed by a material, vibration of the molecular bonds occurs, which will induce the photoconversion process. This perspective of the vibrational energy linked with polar and non-polar bonds was investigated along with the bond interaction energy and is discussed below.

4.8.2. Furan vibrational modes

Although the main base was the benzene ring, the attached species was a furan derivative, in which C-H bonds were present. According to the complementary spectroscopic rules

[28,29], furan C-H bond vibrations, such as C-H stretching vibrations, belong to the region 3180-3000 cm^{-1} , in plane bending with medium to strong intensity at 1310-1080 cm^{-1} and out-of-plane bending vibrations with medium intensity at 935-900 and 835-750 cm^{-1} , respectively [30,31]. Consequently, in the present study, the stretching was observed at 3080 and 3070 cm^{-1} , in-plane bending was observed at 1010 and 950 cm^{-1} and out-of-plane bending modes were observed at 900 and 875 cm^{-1} . Most of the bands observed to be strong and the assigned vibrational bands were highly coherent with the defined region. This observation revealed that furan has been actively involved in the production of chemical properties.

Similarly, the C=C and C-O stretching bands for furan derivatives appeared in the regions of 1610-1560, 1520-1470 and 1100-1075 cm^{-1} , respectively [32,33]. The C=C stretching modes were observed at 1610 cm^{-1} and the C-O stretching modes were observed at 1190, 1180, 1100 and 1060 cm^{-1} . On the basis of the support of carboxylic acid group, the C=C stretching belongs to the first observed region. Two bands of C-O stretching were observed well beyond the characteristic region, whereas two bands were found within the region.

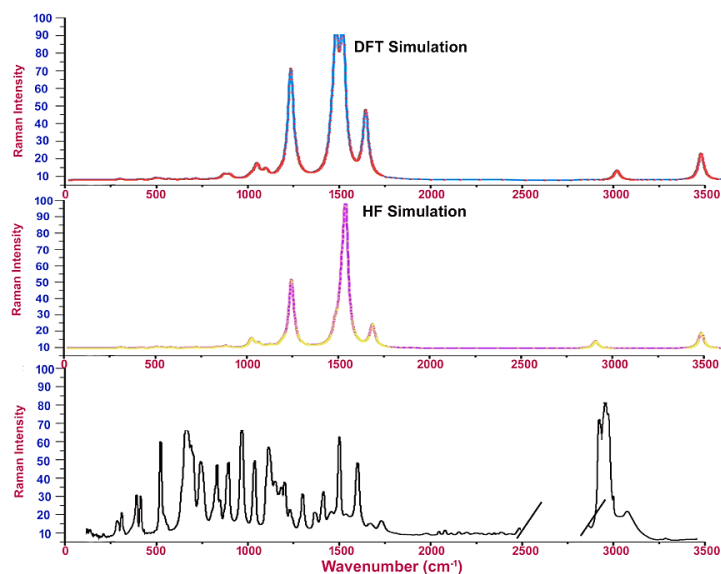


Figure 14. Observed and simulated FT-Raman spectra.

The elevated internal vibrational energy was due mainly to the association of the heavy electronegative group, and the maximum interaction energy played an important role.

4.8.3. Carboxylic group vibrations

To support the scattering polarization to induce a penetration path for exciton movement, a dicarboxylic group was attached to the furan compound, which enhanced the interaction energy of the individual dipole moment and forces drift motion at the molecular site. It is very important to check the activity of such groups in molecular composites. Activeness is directly reflected by the vibrational bond energy and elastic interaction characteristics. In fact, the vibrations of the O-H, C=O, and C-O groups are elevated in the supervibration region if they are active in terms of molecular composition. This can be ensured by analyzing the observed vibrational regions of the bond species. For that purpose, the vibrational energy along with the interaction energy of the bond was verified.

The carboxylic (CB) groups are attached to both sides of the compound and are involved in the property conversion and are placed symmetrically on the furan ring. Because of the dominant position, the related vibrational bands for several carboxylic groups are broadened. Hence, the interaction energy of the O-H bond was 16.4 kJ/mol. and the corresponding stretching peaks are usually observed at higher wavenumbers with weak to very weak intensities. Consequently, it is usually observed in the region of 3500-3350 cm^{-1} , but here, the stretching band was observed at 3300 and 3290 cm^{-1} . As mentioned above, its control temperament was strained in the IR region similar to that of Raman. The associated in-plane and out-of-plane bending bands were located at 1500 and 1490 cm^{-1} and at 1175 and 1125 cm^{-1} , respectively. However, according to the literature [34], the O-H in plane and out of plane bending modes are generally for carboxylic groups and appear in the zones of 1610-1240 cm^{-1} and 980-780 cm^{-1} , respectively. In terms of the characteristic wavenumber, in-plane bending bands were found well within the limit, whereas out-of-plane bending above the allowed region exhibited a reigned character.

The core bond in the carboxylic acid group is the C=O bond, which is typically stretched in the region of 1790-1670 cm^{-1} [35], Specific modes appear binarily at 1700 and 1680 cm^{-1} . The related C-O stretching bands are detected at 1275 and 1230

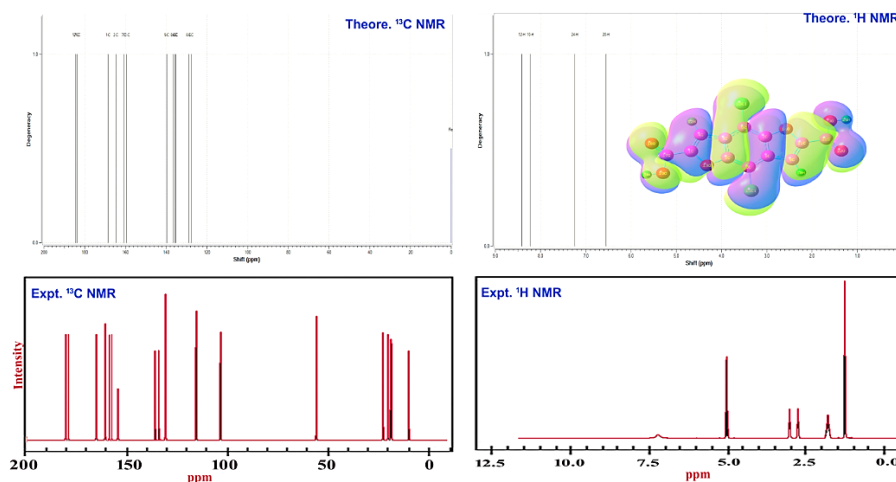
cm^{-1} and, additionally, in-plane and out-of-plane bending peaks are observed at 720, 710, 690 and 680 cm^{-1} as well as 540, 520, 460 and 390 cm^{-1} respectively. Furthermore, C-O-C stretching vibrations, COC in-plane bending, and COC out-of-plane bending vibrations are generally observed in the regions of 1320-1200, 760-660, and 570-490 cm^{-1} , respectively [36]. To achieve a high interaction energy of 14.6 kJ/mol, the C=O bond is significantly outstretched and these vibrational eclipses actively contribute to the creation of a photoactive property. The unexpected interaction energy at the carboxylic boundary leads to an increase in the number of vibrational bands. Additionally, the C-C interligand link between the furan and CB groups is a crucial connection that energizes the base hub system. There are two C-C bonds that provide stretching, with in-plane and out-of-plane bending peaks observed at 940 and 920 cm^{-1} , 300 & 260 cm^{-1} and 160 & 120 cm^{-1} , respectively. These vibrations demonstrate that the interaction energy contributes to the final bond of the COOH boundary, which also induces the photoactive chemical property.

4.8.4. Benzene and Cl vibrations

As a major part of the core system, the benzene ring appears at the center and has strong C=C bond interactions, increasing the intensity of the crystallinity. The characteristics region of the spectrum could be verified, and the binding energy of the bonds could be used to explore the viable molecular site for making a good platform for exciton production and penetration. As predicted, the C=C and C-C stretching modes usually originate in the regions of 1625-1550 and 1540-1430 cm^{-1} , respectively [37]. The respective semicircle CCCs in-plane and out-of-plane bending vibrations are allocated in the regions of 650-410 and 400-310 cm^{-1} , respectively [38]. The bands at 1650, 1620 and 1610 cm^{-1} were assigned to C=C stretching, and the bands at 1450, 1420 and 1400 cm^{-1} are allotted to C-C stretching with strong to medium intensity. The semicircles in plane and out of plane bending modes were allotted at 860, 850 and 780 cm^{-1} and 620, 610 and 605 cm^{-1} , respectively. By considering this observation, it was clear that the bond interaction energy strongly supported the ring and that the consistency of the core charge accumulation enables the random formation of exciton voids. It holds the exciton and reserves steeping photon energy.

Table 5. Experimental and calculated ^1H and ^{13}C NMR chemical shifts (ppm) of 4,8-dichlorobenzo [1,2-b]difuran-2,6-dicarboxylic acid.

Atom	TMS-B3LYP/6-311++G(2d,p)	Solvent phase, DMSO		Experimental
	Gas			
C1	168	168		165
C2	164	164		164
C3	135	135		135
C4	135	135		135
C5	127	127		129
C6	128	128		130
C7	160	161		161
C8	136	136		134
C9	139	139		136
C11	159	159		155
C17	184	184		180
C21	183	183		179
H10	8	8		7.2
H12	8	8		7.1
H20	6	6		5
H24	7	7		5.5
O13	273	274		-
O14	254	253		-
O18	477	478		-
O19	213	213		-
O22	464	464		-

**Figure 15.** Observed and simulated ^{13}C and ^1H NMR spectra.

In this case, the halogen ligand injected on the benzene ring supplies the inherent electron domains and provides an additional recoiling effect on electrons with less kinetic energy. It is also helpful for the production of saturated excitons (yet ultimately separated) and eliminates recombination on the molecular platform. It is very important to ensure the restored energy of the dichlorine species in terms of vibrational energy. According to the IR and Raman table for organic vibrations, the C-Cl stretching modes, in-plane and out-of-plane bending modes, are located in the regions of 760-505, 385-265 cm^{-1} and below 250 cm^{-1} , respectively [39]. Here in this compound, the stretching peak was found at 650 and 640 cm^{-1} , in-plane bending was at 510 and 480 cm^{-1} and out-of-plane bending peaks were at 350 and 320 cm^{-1} , respectively. As we expected, the Cl ligand in the base ring produced an enormous amount of interaction energy that can energetically produce electron clouds for exciton.

4.9. NMR spectral analysis

The diffusion and drift paths of electron-hole motion during exciton production are normally at the nodal points of the core called the core carbon, which can be identified from their chemical shift characteristics. The chemical shift is simply the amount of proton shield breaking of carbon, and it is also used to measure the asymmetrical and symmetrical ligand substitu-

tions in the respective proton, and to measure how the shield is fractured. If the shield is broken much, the diffusion enforcement will be higher, and if it is moderate, drift will be possible. For the measurement of the chemical shift, the NMR spectra are shown in Figure 15 along with the simulated one. The chemical shifts of the core and allied carbons are depicted in Table 5.

The symmetrical and asymmetrical disintegration of the proton shield depends on the type of ligand groups added to the respective carbon. When the asymmetry of the ligand group is increased, the chemical shift is increased simultaneously. Therefore, the nodal point is left on the carbon and this carbon is ready to transport the charge carrier to a greater extent. Thus, the nodal points are grouped, and the nodal region framework is produced within and around the molecular site. By measuring the chemical shift of each core and allied carbon, the path can be identified. The chemical shifts of C2, C3, C5, C6, C7 and C8 were δ 164, 135, 127, 128, 160, and 128 ppm, respectively. Here, the strong CT complex was C2-O13, where the exciton was identified to start the diffusion motion and reached C11 through C5, C8, and C9 through the COOH group, the electron was sent to the partner layer. Another CT complex was traced at C7-O14, where the electron transferred through C6, C3, and C4 reached C1, and in that way, drift motion was attained to reach COOH. For each process, two electron-hole pairs were created per molecule.

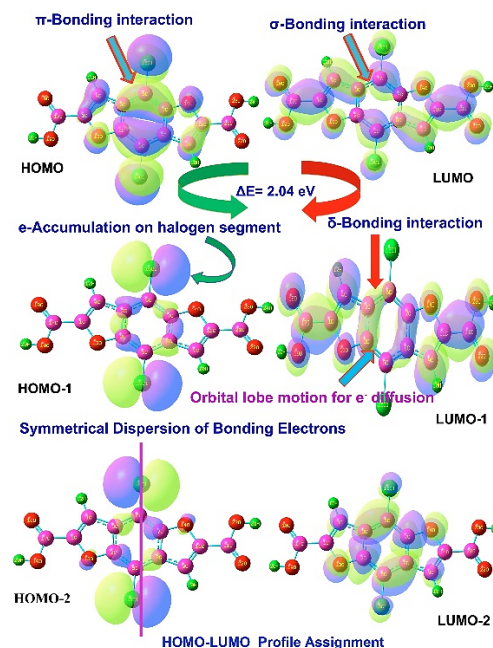


Figure 16. Frontier molecular map of the prepared compound.

In addition to that, according to the high value of the chemical shift (δ 287 ppm), two Cl atoms in the para positions of the core provide one electron of each. Due to the high degree of chemical shift, O18 and O22 acted as good nodal points in which the electron and hole pair emerged. Chemical shifts of all core and allied carbons were estimated to be above δ 125 ppm, implying that the entire core C worked as active nodal zones for the production and disintegration. So, the number of photon energy conversions is directly proportional to the presence of molecules per unit cell of a number of molecules per unit mole of substance.

4.10. HOMO-LUMO interaction analysis

As a single-layer active solar cell sheet, the crystallization architecture acts as a feasible conducting layer for exciton transport. Among these, the molecular clusters in different coordinates form a molecular strip matrix system in the thin film that forms an electronic platform for exciton production and transport. The energy absorption and transduction (photon energy converted into electronic energy) are directly proportional to the existence of the bandgap of the material. The band gap can be measured from the HOMO and LUMO domain arrangements in the molecular system, and thus the crystal material. As the active layer is a semiconductor material made of organic groups, the material should have an acute bandgap that is equal to the energy of photons for photovoltaic energy conversion. Consequently, the calculated band gap of the HOMO (donor) and LUMO (acceptor) interval was 2.04 eV. For that built band gap built from a suitable composition of organic elements, the bonding interaction profile is a very significant parameter. The frontier molecular setup for the photoconversion compound is presented in Figure 16. Here, to make good donors of electron clouds, the π -bonding setup was purposively arranged in the HOMO where the π -interaction appeared over the CCC of the center ring and highly polarized C-O bonds were linked. The electron accumulation in the ring was isolated by C-C bonding in the furan ring, which protected against electron leakage to promote electron-hole recombination. To achieve adequate acceptor (hole reservoir) σ -bonding interactions over the LUMO, no π -bonding was

occurred on the LUMO segment. The strangled π -bonding layout appeared at the C-C position of the molecular link, which further terminated the electron trapping pool in the COOH group.

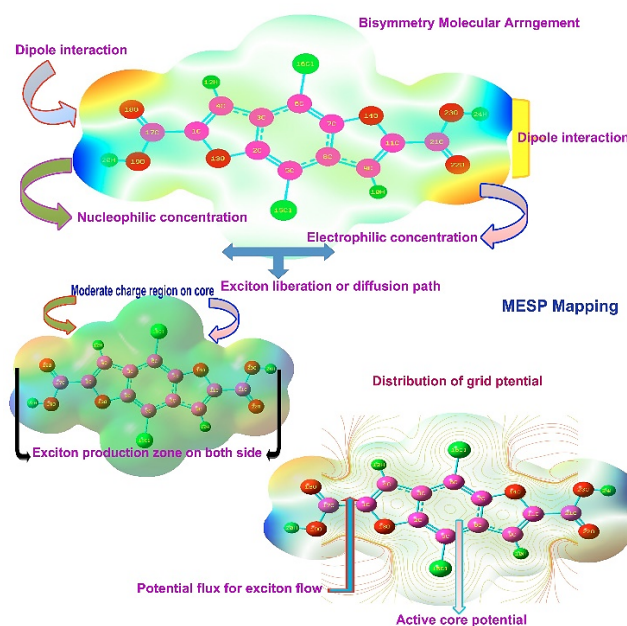
In the case of HOMO-1, with the exception of electron accumulation on Cl, all non-bonding electrons are concentrated on the internuclear places on the benzene ring. This did not occur frequently since all the forces of equilibrium centripetally acted at the center of the core. The δ -bonding arrangement was discovered at the entrance core in LUMO-1, where the orbital lobe motion was trapped, which spontaneously induced the electron diffusion. In HOMO-2, the electron cloud was covered on only one halogen ligand that sites all electron domains, and all atoms have a protonic content only. LUMO-2 appeared to be a π -bonding segment that overlapped with the pedals and tracked the acceptor domains. From the LUMO-HOMO organization in the molecular site, exploring the viable process of excited exciton production in the molecular system is most possible and the electron-hole transport is authorized by a further HOMO-LUMO cascade. Therefore, the photoconversion efficiency is very high.

4.11. Electrostatic potential map (EPM) - comprehensive studies

The chemical equilibrium forces of attraction and repulsion around intermolecular sites usually lead to the accumulation of electron domains against the protonic content, which displays the electrophilic and nucleophilic configuration of the molecular structure. The asymmetrical charge distribution is always a random allocation of available charges, which are normally portrayed by color gradients. The entire electronic and protonic contents are indicated by two identities, such as red and blue regions, which clearly show a very acute displacement of the molecular dipole moment. For this molecule, Figure 17 presents the colour gradient of the intermolecular charge assignment to notify the energy restoration. Those regions with a high charge gradient are the electron-hole production agents.

Table 6. Theoretical electronic absorption spectra of 4,8-dichlorobenzo [1,2-b]difuran-2,6-dicarboxylic acid.

λ (nm)	E(eV)	f	Transition level	CT complex identity/ Photoexcited state	Assignment/ Energy region	Photo-excited state/ Exciton binding energy	Bands
Gas							
383	3.23	0.36	H $\rightarrow$ L (80%)	Exciton production on C=O	n $\rightarrow$ π^* / visible	1.71	K-band
314	3.93	0.026	H+1D1 $\rightarrow$ L (79%)				
311	3.97	0.501	H+2D2 $\rightarrow$ L (69%)				
DMSO							
384	3.22	0.37	H $\rightarrow$ L (80%)	C=O	n $\rightarrow$ π^* / visible	1.85	K-band
314	3.93	0.03	H+1D1 $\rightarrow$ L-1 (90%)				
312	3.96	0.50	H+1D2 $\rightarrow$ L ((69%)				

**Figure 17.** Molecular electrostatic potential diagram.

The present compound has bisymmetry, because of which the electronic and protonic contents can be distinguished clearly in the intermolecular segments. In this molecule, absolute electrophilic and nucleophilic displacement occurs in two COOH groups, and harsh dipole moment interactions take place. In addition to that, no strong dipole species seem to be present in other places. Although highly electronegative atoms were present in the center core, there was no significant electrophilic or nucleophilic attack at the molecular site. This observation of the complex assignment of CT data is highly controversial. However, this method is used to ensure the dipole moment of a molecule as a whole, according to which the mechanical condition of the molecule was very strong, and stereoisomers. Such stereoisomers usually have photophysical and physical supporting properties. The grid potential is displayed in the same figure, where all the sources of the photoactive region can be clearly viewed. The present case consists of a three-ring core where the chemical potential flux source was tracked.

4.12. UV-Vis spectral studies

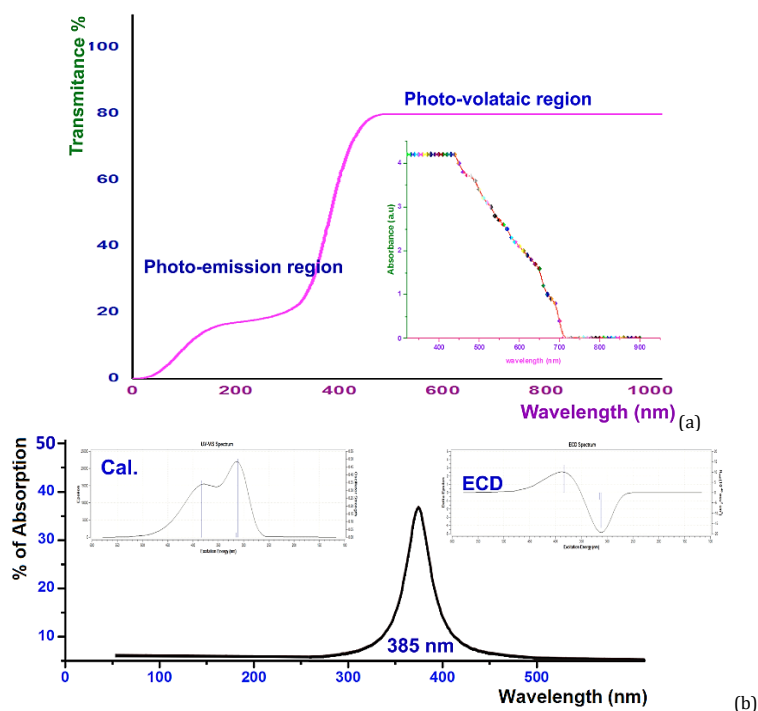
The present compound was used for the analysis of photovoltaic performance, and the analysis of UV-visible transmission and absorption spectra is very important to emphasize the photovoltaic background and response of the material [40]. Consequently, both spectra were recorded and are presented in Figure 18, and the corresponding parameters are presented in Table 6. Figure 18 (a) shows the transmittance spectrum in which the light signal passes through the material and is transmitted. The transmission started at 100 nm and

increased to 410 nm, and in this region, the photoemission process occurred instead of the photovoltaic activity. The light signal transmission characteristics were abruptly changed at 420 nm and became saturated at 800 nm. Therefore, the above condition clearly shows the behaviour of the material as photovoltaic.

Figure 18 (b) displays the UV-vis absorption spectrum, along with both the experimental and simulated absorption spectra. This figure illustrates the electronic spectra of the compound, which consists of 66 vibrational bands, organized according to the density of energy states. Due to the high dipole moment and polarizability of the heteronuclear and homonuclear bond units, the absorption spectrum exhibits a prominent electronic peak with maximum intensity. According to UV-visible spectral selection rules, the simulated electronic peaks were observed at 311 and 383 nm, while the experimental peak was recorded at 385 nm. Theoretically, in the gas state, the electronic spectra degenerate into three energy states: 283, 314, and 311 nm, corresponding to energy gaps of 3.23, 3.93, and 3.97 eV, with oscillator strengths of 0.36, 0.026, and 0.501, respectively. For the DMSO solvent, three degenerate energy states were also identified at 384, 314, and 312 nm, with energy gaps of 3.22, 3.93, and 3.96 eV, and oscillator strengths of 0.37, 0.03, and 0.50, respectively. All these energy regions correspond to n $\rightarrow$ π^* transition states in the visible region, with the central charge transfer (CT) complex being C=O, which is the main source of exciton production. The first transition was assigned as H(D) $\rightarrow$ L(A) at 80%, the second as H+1(D) $\rightarrow$ L-1(A) at 90%, and the third as H+1(D) $\rightarrow$ L(A) at 69%.

Table 7. Physicochemical parameters of 4,8-dichlorobenzo [1,2-b]difuran-2,6-dicarboxylic acid.

Parameter	IR region	UV-Visible region	Electrophilicity charge transfer (ECT) ($\Delta N_{\max}$) _A -($\Delta N_{\max}$) _B
E_{total} (Kcal/mol)	1831.7	1867.9	-12.011
E_{HOMO} (eV)	7.138	6.997	
E_{LUMO} (eV)	5.115	4.899	
$\Delta E_{\text{HOMO-LUMO gap}}$ (eV)	2.023	2.098	
$E_{\text{HOMO}+1}$ (eV)	8.408	7.489	
$E_{\text{LUMO}-1}$ (eV)	4.261	3.987	
$\Delta E_{\text{HOMO}-1-\text{LUMO}+1 \text{ gap}}$ (eV)	4.147	3.502	
Chemical hardness (η)	1.011	1.210	
Electronegativity (χ)	6.126	6.248	
Chemical potential (μ)	5.187	5.211	
Chemical softness (S)	2.023	2.098	
Electrophilicity index (ω)	18.550	17.433	
Dipole moment	3.187	3.110	

**Figure 18.** (a) UV-visible transmission spectra and (b) absorption spectra.

Concerning the energy gaps of the electronic transitions, the binding energies of the excitons were measured at 1.71 and 1.85 eV in dual states. This energy of electronic states closely matches the band-gap energy of the HOMO-LUMO state, and it is also used as the offset energy for the dissociation of electron-hole pairs. The radical of the CT complex, C=O, was identified at the K-band, indicating its molecular stability for the photovoltaic process without loss of energy from photon absorption.

4.13. Physicochemical properties

The physical and chemical parameters are crucial for discussion, as the complete physicochemical profile of a compound provides valuable information regarding its stability and the mechanism of the photoconversion process. All parameters were calculated from direct band gap measurements and are summarized in Table 7. According to the table, the total energy stored in the compound was 1831.7 kcal/mol, reflecting the sum of the potential and kinetic energy of the bonding elements within the compound. This means that the compound can absorb and manage an equivalent amount of optical energy. In particular, it was slightly higher in the UV region, recorded at 1867.9 kcal/mol. The dipole moment of the molecular polarization gradient was measured at 3.187 Debye

for the infrared (IR) region and 3.110 Debye for the UV-visible region. This indicates the ability of the chemical equilibrium forces to shift two opposite charge levels within the molecular structure. The energy values of the highest occupied molecular orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) were 7.138 and 5.115 eV, respectively. Both of these values are quite high and represent second-order energy segments of degeneracy. The associated direct band gap was 2.023 eV, which is slightly lower than the band gap observed in the UV-visible region. Due to the photo response characteristics of the compound, the Fermi level of the semiconductor band gap was found to be 6.126 eV. This is favorable for generating consistent excitons with restored kinetic energy equivalent to 3.06 eV.

The second order energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were measured at 8.408 eV (HOMO+1) and 4.261 eV (LUMO-1), respectively. The control factor for the second-order orbital setup was approximately 0.64 eV, reflecting the influence of the orbital cascading arrangement within the molecular structure of the crystal. Consequently, the overlapping band gap for the second-order orbital was found to be 4.147 eV in the infrared (IR) spectrum and 3.502 eV in the ultraviolet-visible (UV-vis) spectral region.

Table 8. The polarizability α (a.u.) and first hyperpolarizability β (esu).

Parameter	Value (a.u.)	Parameter	Value (a.u.)
α_{xx} [Phase I]	120.11	β_{xxxx}	6319
α_{yy} [Phase II]	13.41	β_{xxyy}	1742
α_{yy} [Phase III]	130.44	β_{xyyy}	1740
α_{zz}	0.006	β_{yyyy}	2140
α_{yz}	0.01	β_{xxxx} [I order Phase I]	130
α_{zz}	125.24	β_{xyzz} [I order Phase II]	1221
α_{tot}	332.68	β_{yyzz} [I order Phase III]	15
$\Delta\alpha$	483.34	β_{tot}	310
μ_x	1.221		
μ_y	1.011		
μ_z	-2.087		
$\Delta\mu$	1.477		

The Fermi level is situated at 4.357 eV, which indicates a short potential barrier for the sequential flow of charges to the subsequent order. Due to its low chemical hardness of 1.011 eV, the compound is reactive with other substances, enhancing its photomechanical properties. The electronegativity (χ) of the compound in the IR and UV-Vis regions was estimated at 6.126 eV and 6.248 eV, respectively. These values suggest that the electronic structure experiences a gradual decrease in its negative gradient. Typically, if the electronegativity exceeds 3.1 eV, the compound exhibits specific spontaneous electronic domains. In this case, the crystal displays a higher order of negative electronic symmetry compared to its protonic content, facilitating the easy formation of excitons. The chemical potential, a thermodynamic property representing the chemical energy per mole of a substance, was measured at 5.187 eV in the IR region and 5.211 eV in the UV-visible region. Generally, this chemical potential can be converted into other forms of energy depending on the material's characteristics. As a photovoltaic material, the chemical potential corresponds to an electronic energy equivalent of 5.187 eV. The chemical softness of the compound, indicating its ability to accept ligand groups to enhance physical and chemical properties, was measured at 2.03 eV, which is adequate for associating with organic molecules. The electrophilicity index of the compound was found to be 18.55 eV, indicating a very high conductivity ability, suggesting that its conductivity surpasses that of typical conductors. This implies that the crystal material exhibits remarkable carrier transport properties. The electrophilicity charge transfer (ECT) of the organic semiconductor film (OSC) was measured at -12.01 eV, demonstrating a unique flow of chemical potential directed from the ligand to the core of the compound. This distinctive flow of chemical energy primarily results from the attachment of the chlorobenzene-furan compound to dicarboxylic acid.

4.14. Polarizability and the first hyperpolarizability analysis

In addition to the dielectric medium, because of the existence of homonuclear bond units in organic compounds, the polarization is organized. Therefore, the drift and diffusional motion of charge carriers are supported in the material medium. Hence, the first-order and second-order of the polarization take place via the hyperactivity of the dipoles and polarized species therefore; photoelectron transport is adequately carried out. The polarization mechanism in the present molecular system is studied by calculating the polarizability of the connected bonds in 4D and presented in Table 8. According to the internal coordinate system of molecular structure, the first order polarizations were measured in 3D and are arranged in Phase I, II and III as α_{xx} , α_{xy} , α_{yy} and α_{zz} to be 120.11×10^{-33} , 13.41×10^{-33} , 130.44×10^{-33} and 125.24×10^{-33} esu, respectively. The observed values of polarization at different coordinates illustrate the isotropic and anisotropic polarization conditions of the material. Each coordinate has a separate polarization constant which varies

with its coordinate. Therefore, the nature of the material normally has fragmented refractive indices. The resulting total and average polarizations were calculated as $\alpha_{tot} = 483.34 \times 10^{-33}$ esu $\Delta\alpha = 332.68 \times 10^{-33}$ esu, respectively. Whenever the polarizability of the medium crossed 100×10^{-33} esu, it is said to be anisotropic. However, in the present material the medium presents elevated polarizability. Therefore, the first-order polarizations were active, and it is adequate to produce a photoconversion mechanism. The dipole moment is an important factor in determining the asymmetric charge distribution that results in increased polarization due to the availability of polar atoms [41]. Typically, material with high crystallinity has a low dipole moment due to the elimination of opposite dipole vectors at the molecular site that are able to produce superior symmetry. Accordingly, the present molecule has 1.47 Debye (calculated theoretically), owing to which the present material is able to have high degree of charge transfer.

In the material medium, hyperactive polarization was identified and distinguished from first-order polarization via measurement. Accordingly, the hyperpolarizability (HPL) was determined to be 310×10^{-33} esu. The hyperaction of molecular polarization was also calculated using the Gaussian program in 4D coordinates; β_{xxxx} , β_{xxyy} , β_{xyyy} , and β_{yyyy} as 6319.1×10^{-33} , 1742×10^{-33} , 1740×10^{-33} and 2140×10^{-33} esu, respectively. Furthermore, hyper-second-order polarizability established the dynamic response of the electron with a nucleolus-bound system to the response of the local electric field. With respect to the second-order polarizability concerns, as a crystal material, in β_{xxxx} coordinate, hyperactivity was found to be very high, and a finite matrix dielectric track down was observed for a particular molecular slab. In the 4D internal coordinate system, the molecular strips in each direction have a specific dielectric density, which creates a tunnel path for electron and hole transport.

4.15. Exciton binding energy (EBE) and charge mobility profile

The transition electron density is a significant parameter for examining excitons, electron delocalization in relation to holes, and charge transition sites. To investigate the charge dissociation properties of a compound, understanding the electronic potential of the molecules within the material is crucial. For effective charge carrier transport, the molecules in the crystal planes must achieve a minimum energy level, which is necessary to dissociate excitons into free electrons and holes [42]. This understanding is essential to determine the strength of Coulombic interactions, which result in the nominal binding forces of excitons. To study the optical ability and charge-transfer mechanisms associated with binding energy, the Bethe-Salpeter equation (BSE) has been employed. The binding energy of the core atoms, along with their partner atoms in the molecular ring, is presented in Table 9.

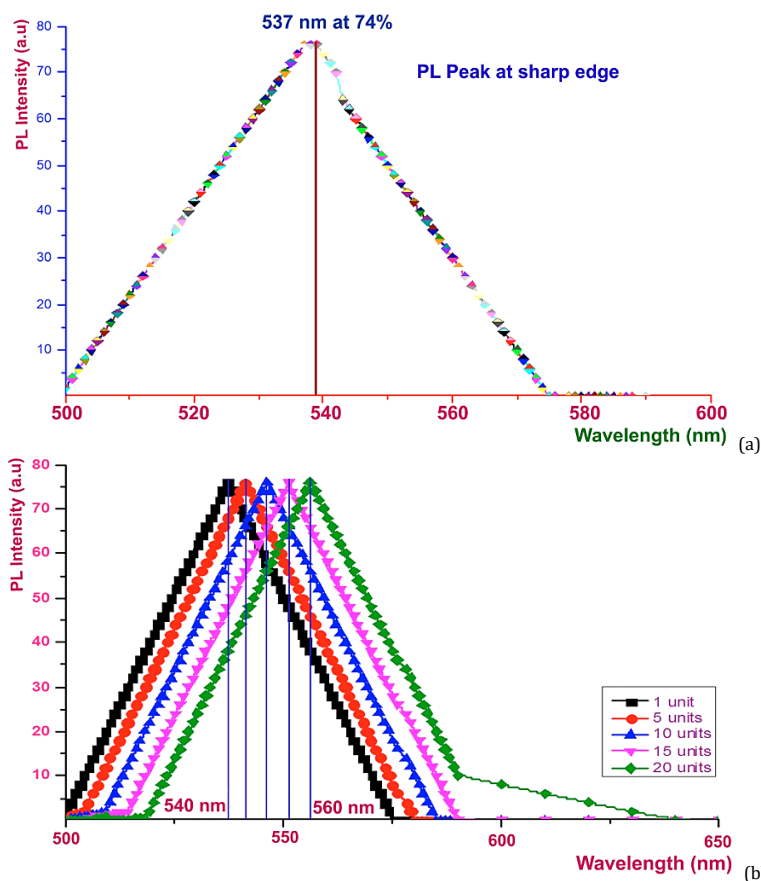
The binding energy was calculated for the core carbons C1, C2, C3, C4, C5, C6, C7, C8, C9, C11, C17, and C21 to assess the required energy for disassociation.

Table 9. Exciton binding energy and charge mobility.

Core atoms	Binding energy $E_B = E_g - \Delta E$ (eV)	Reorganization energy (λ_e)	Reorganization energy (λ_h)	Charge mobility e_{mob} ($cm^2 V^{-1}s^{-1}$)
C1	0.23	0.023	0.089	17.85
C2	0.58	0.079	0.032	18.18
C3	0.27	0.056	0.049	19.80
C4	0.29	0.062	0.042	19.23
C5	0.29	0.029	0.098	15.87
C6	0.26	0.041	0.061	19.60
C7	0.59	0.061	0.006	30.30
C8	0.27	0.075	0.039	17.54
C9	0.29	0.056	0.061	17.09
C11	0.23	0.087	0.021	18.51
C17	0.31	0.067	0.039	18.86
C21	0.31	0.089	0.021	18.18

Table 10. Optical parameters of perovskite at the (110) plane deposited films at different molecular units.

Molecular unit	Band gap (eV)	Refractive index	Extinction coefficient	Dielectric constant (real part)	Dielectric constant (imaginary part)	PL intensity
1	2.06	1.52	1.37	1.4	-	69.2
5	2.26	1.62	2.62	2.6	0.2	70.1
10	2.27	1.71	4.84	3.1	1.8	76.5
15	2.26	1.86	3.26	4.2	2.3	81.3
20	2.27	1.86	3.24	7.1	2.8	81.3
25	2.29	1.86	3.22	8.2	3.6	81.3

**Figure 19.** (a) Photoluminescence spectra for one unit and (b) Photoluminescence spectra for different units.

The calculated binding energies were 0.23, 0.58, 0.27, 0.29, 0.29, 0.26, 0.59, 0.27, 0.29, 0.23, 0.31, and 0.31 eV, respectively. In organic materials, the effective binding energy generally ranges from 0.23 to 0.53 eV. All core atoms, along with their partner atoms, exhibited low binding energies primarily because of weak interactions among the core atoms in the molecular structure. This weak interaction between electrons and holes at the molecular site promotes the spontaneous movement of charges toward opposite electrodes, thereby increasing the current density. This perspective on molecular formation within the crystal planes indicates the potential for

high levels of charge transport and considerable power conversion efficiency (PCE). Although the PCE in this case was estimated using photovoltaic parameters, evaluating the efficiency of organic composites is essential for estimating charge transport rates and charge mobility, which can be readily determined through the reorganization energy (RE) of electrons and holes [43]. The RE values for electrons and holes associated with each core carbon atom are shown in Table 9. These results indicate that all carbons possess low RE values for both electrons and holes, facilitating effective charge dissociation rather than recombination.

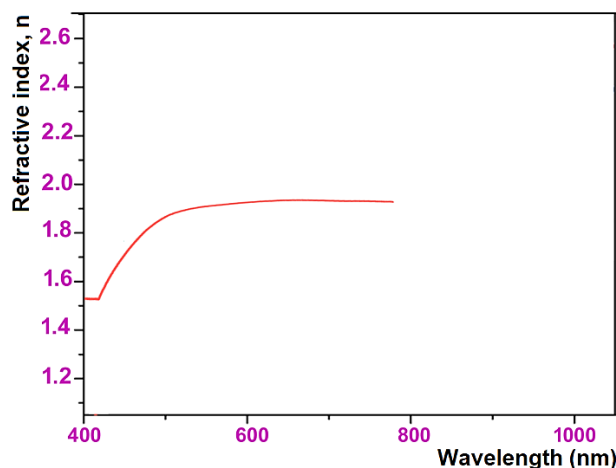


Figure 20. Refractive indices for different wavelengths.

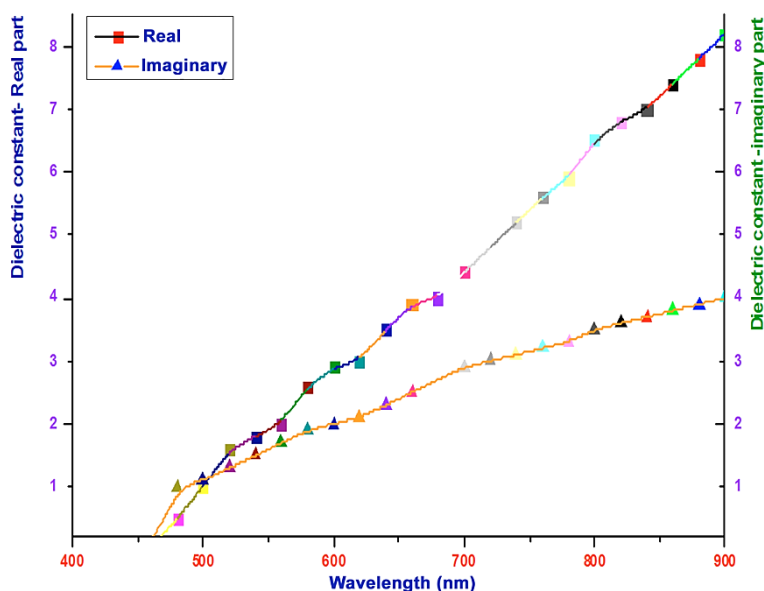


Figure 21. Dielectric constant (DC) variation at different wavelengths.

The lower RE value of electron-hole interactions signifies increased charge mobility, enhanced charge transfer, and reduced electron-hole recombination, which can be attributed strongly to the presence of electron-donating groups in the molecular structure. Typically, charge mobility is inversely proportional to RE. Consequently, the charge mobility of all core carbons was found to be high as a result of the low RE values, which suggesting that this case demonstrates a high charge mobility rate.

4.16. Photoluminescence on photoexcitation studies

A band gap of 2.06 eV was observed for a single molecule with a refractive index of 1.54, with an extinction coefficient of 1.37 (Table 10). As the number of molecular combinations increased, all related parameters also showed an elevation. Specifically, as the number of molecular units increased from 5 to 25, the band gap rose from 2.26 to 2.29 eV, the refractive index increased from 1.62 to 1.86, and the extinction coefficient increased from 2.62 to 4.84 before decreasing to 3.22. Photoluminescence (PL) increased from 69.2 to 81.3%, saturating at 25 molecular units. One mole contains approximately 2.50×10^{22} molecules, which should exhibit strong PL absorption with

minimal energy loss. The excitations of excitons from the ground state to the excited state at a particular wavelength are illustrated in Figure 19, which also shows the photoenergy absorption per molecule as well as for different molecular units within the crystal structure. In Figure 19 (a), the excitation profile of the present compound is displayed at 537 nm with 74% intensity. In Figure 19 (b), multiple PL peaks illustrate photoluminescence absorption for molecular combinations ranging from 1 to 20 units. According to the calculations used to determine the PL peak positions, a single peak was observed at 540 nm for one molecular unit, with intensity of 74%. Subsequently, for 5, 10, 15, and 20 molecular units, peaks were observed at 544, 548, 552, and 560 nm, respectively. As the number of molecular units increased from 5 to 20, the peak positions shifted slightly to higher wavelengths.

4.17. Refractive index (RI) analysis

In terms of the material composition, for light rays, the material medium generally behaves as a dispersive medium, as demonstrated by the observation of different refractive indices for different combinations of molecular units [44]. For incoming radiation, the material medium reacts as chroma-

tically dispersed, so the medium behaves differently for different colors. As shown in Figure 20, for the present organic film, the RI is plotted against the wavelength of light in the region of 400-800 nm. The RI was found to change from 1.52 to 1.86 as the wavelength of 550 nm became saturated in the 1.86 to 800 nm region. This observation shows that the electronic transition was initiated from 400 nm and it become saturated at 540 nm and extended up to 600 nm. The electronic transition at 540 nm confirmed the strong absorption of the present case.

4.18. Dielectric examination

The dielectric properties of organic compounds are key for the photoconversion operation and performance of OSCs [45]. Dielectric screening played an important role in PCE enhancement since high dielectric constant strongly reduces the exciton binding energy and Coulomb capture radius and increases the electron-hole pair dissociation energy between the photoexcited electron and hole [46]. The variation in the dielectric constant (DC) with respect to the real and imaginary parts with respect to the wavelength of the radiation is obtained in Figure 21. For this case, the dielectric constant in the real part was calculated to be 8.2 (singlet-triplet band gap) at the maximum, which increased from the minimum of 1.4. This was mainly due to the Cl substitutions in the main ring, which increased the spontaneous polarization in the molecular planes when it was irradiated in the visible region. It improves the dissociation probability, which suggests efficient transport of charge and prevents energy loss. The virtual dielectric constant represents the energy loss factor or the irradiated energy absorbed per m^3 . Here, the imaginary dielectric response started at 0 and ended at 470 nm and continuously increased up to 4.0. Low energy loss occurs when light radiation irradiated with light. The calculated instantaneous Coulomb capture radius (CPR) was 3.9 nm at a dielectric constant of 4.0, whereas when the DC was increased by 8.1, the resulting CPR was 1.67 nm. Simultaneously, the energy loss is possibly condensed as the dielectric constant decreases.

5. Conclusions

To analyse the photovoltaic performance of the organic composite, a new compound, 4,8-dichlorobenzo[1,2-b]difuran-2,6-dicarboxylic acid, was synthesized by addressing challenging root processes. A thin film of the prepared compound was created to obtain single-layer organic solar cells (OSCs), and this film underwent experiments to gather crystallographic information. The single-layer solvation model was simulated using Gaussian software to determine the molecular mechanisms associated with the power conversion efficiency (PCE). Molecular topographic and Mulliken charge analyses were conducted to identify viable active molecular nodal exciton production centers. Furthermore, dielectric screening was performed to determine the exciton binding energy, which facilitates the dissociation of electron-hole pairs. Consequently, favorable lattice architecture formation of single-layer organic material medium was observed. All experimental and theoretical results related to PCE parameters were satisfactory, leading to the following conclusions.

- The present organic thin-film material possessed an ABX₃ patterned tetragonal perovskite lattice with the space group P4 *4mm* and the point group C_{2v}.
- From the unit cell measurements, the cell sides were measured as $a = 5.781$ (Å), $b = 5.023$ (Å), and $c = 9.124$ (Å), and the symmetry operation showed that the unit translated along the c side. The total volume of the unit cell was 264.94 Å³.
- The main CT complexes were identified as C2-O13 and C7-O14 and their dipole moment was 3396×10^{-44} and 2403×10^{-44} esu²/cm², respectively. The electronic transitions of that dipole produce a functional dielectric constant, which results in more efficient charge separation.
- SEM examination revealed that the film is very deep, scrubbed, and loosely packed net-like structure. Uniform film thickness and cross-sectional uniformity were found.
- The birefringence (Δn) $K\lambda/t$ was estimated for the material as 1.960, clearly observing that the atomically anisotropic atmosphere of the compound has a non-uniform atomic distribution of optical properties in different subplane directions.
- The open circuit voltage (V_{oc}) was estimated to be 1.067 V at a short circuit current (J_{sc}) of 9.72 (mA/cm²). Therefore, the calculated power conversion efficiency (PCE) was 17%.
- By considering core benzene observations, it was clear that the bond interaction energy of all allied bonds strongly supported the ring, and the core charge accumulation consistently enables exciton voids that hold the exciton energy and reserve steeping photon energy.
- The chemical shift of the cores and allied carbons was estimated to be above δ 125 ppm, implying that the entire core C worked as active nodal zones for the production and disintegration of electron-hole pairs.
- To make good donors of electron clouds, the π -bonding setup was purposively arranged in the HOMO where the π -interaction appeared over the CCC of the center ring and where the highly polarized C-O bond was linked. To achieve adequate acceptor (hole reservoir) σ -bonding interactions over the LUMO, no π -bonding appeared on the LUMO segment. The strangest π -bonding layout appeared on the C-C position of the molecular link, which further terminated the electron trapping pool in the COOH group.
- As the molecule is bisymmetric, the electronic and protonic content can be distinguished clearly, and absolute electrophilic and nucleophilic displacements appeared in the two COOH groups. Although there were highly electronegative atoms present in the central core and there was no significant electrophilic or nucleophilic attack at the molecular site.
- All energy regions were assigned to the $n \rightarrow \pi^*$ transition state in the visible region, and the respective CT complex was C=O, which is the main source of exciton production. In terms of the energy gap of the electronic transition, the binding energy of the exciton was measured at 1.71 and 1.85 eV in dual states. This is very much equal to the band gap energy of the HOMO-LUMO state, and it is also used as the offset energy of the dissociation of the electron-hole.
- The electrophilicity charge transfer (ECT) of the OSC film was -12.01 eV, which proved that the flow of chemical potential was unique and was directed from the ligand to the core.

In summary, the consolidated observations proved that an efficient photoconversion process was taking place in the organic thin film, and they proclaimed that the present organic composite was chosen for the preparation of OSCs.

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Conflict of interest: The authors declare that they have no conflict of interest.
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CRediT authorship contribution statement

Conceptualization: Raman Ananthavalli; Methodology: Raman Ananthavalli; Software: Singaravelu Ramalingam; Validation: Ramadoss Aarthi; Formal Analysis: Jeganathan Karpagam; Investigation: Jeganathan Karpagam; Resources: Jeganathan Karpagam; Data Curation: Raman Ananthavalli; Writing - Original Draft: Singaravelu Ramalingam; Writing - Review and Editing: Jeganathan Karpagam; Visualization: Raman Ananthavalli.

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