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## Article

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# Impact of End-Capped Modification on tert-Butyl Carbazole Non-Fused Acceptors for High-Efficiency Solar Cells

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## Abstract

Developing small-molecule-based asymmetric non-fullerene (SM-NFAs) acceptors is highly desirable because they offer significant structural diversity, higher dipole moments, and strong intermolecular interactions. In this study, four new molecules (EE1-EE4) were designed by end-group modification to improve photovoltaic performance. The designed materials show a significant reduction in the energy gap of 1.70-1.88 eV, lower than the reference (2.02 eV). The designed molecules exhibited  $\lambda_{\text{max}}$  values (638.21-682.13 nm) in the gaseous phase, higher than the reference (617.51 nm). In addition,  $\lambda_{\text{max}}$  values were further redshifted in the solvent phase (696.93-769.18 nm) compared to the reference (660.72 nm). The open-circuit voltage ( $V_{\text{oc}}$ ) values (0.64 eV-0.90 eV) were comparable to R (1.25 eV). The lower reorganization energies for electrons ( $\lambda_{\text{e}} = 0.0078$ -0.0115 eV) and holes ( $\lambda_{\text{h}} = 0.0047$ - 0.0069 eV) indicate efficient charge transport and reduced energy losses. This study provides valuable insights into structure-property relationships and offers a rational design strategy for high-performance NFAs in next-generation organic solar cells.

**Keywords:** Band gap, Density of states, End-capped modification, Reorganization energy.

## 1. Introduction

The potential benefits of organic solar cells (OSCs) have attracted a lot of attention. These include lower costs, lower weight, and the possibility of large-scale production <sup>1,2</sup>. Single-junction solar cells incorporate polymers that exhibit p-type behaviour as electron donors with non-fullerene acceptors based on n-type small molecules. The power conversion efficiency of the most effective OSCs has recently reached 19% or more <sup>3,4</sup>. Currently, non-fullerene acceptors (NFAs) with a classical fused-ring structure are the most competitive in high-performance organic solar cell systems. While strategic molecular engineering can adjust the optoelectronic characteristics of Fused-Ring Electron Acceptors (FREAs), synthesizing multiple fused-ring molecular structures is challenging and requires synthesizing and purifying complex molecules. This ultimately leads to a reduction in yield and an increase in the cost associated with organic molecules <sup>5</sup>. Recent research shows that (Power Conversion Efficiencies) PCEs comparable to those of FREAs can be achieved with NFAs consisting of ring structures that are wholly or partially non-fused. Such acceptors are termed NFREAs. A series of high-performance NFREAs has been successfully developed by modifying the end group <sup>6</sup>, changing the side chain <sup>7</sup>, and constructing the backbone configuration <sup>8</sup>. As a result, the PCE reached 16% <sup>6</sup>. This indicates that the system has a Strong capability for attaining high efficiency. Conversely, the ternary mixing strategy has been shown to enhance OSC efficiency. This can be attributed to the simplicity and effectiveness of the methods used <sup>9</sup>. Nonetheless, developing an effective third component to enhance morphology, reduce open-circuit voltage loss, and enhance charge transfer continues to be a significant challenge.

The most effective way to optimize optoelectronic characteristics, molecular alignment in a stacked configuration, and overall device performance is to modify the side chain. A standard technique for optimizing NFAs. It is possible to extend aliphatic side chains to ensure that the resulting molecules are soluble in a variety of solvents. In addition, a small rotational hindrance favours the formation of  $\pi$ - $\pi$  stacks and thus the crystallization of the materials <sup>7</sup>. The second category of modification involves incorporating halogenated side chains, which can precisely adjust the HOMO-LUMO levels, thereby optimising the  $V_{oc}$  (open-circuit voltage). Moreover, the influence of halogenations on the orientation of side groups and the planarity of the backbone is essential, as it allows modulation by adjusting the outward-facing side groups <sup>10</sup>. The third group concerns aromatic side chains, which are a vital research focus in NFREAs.

The 2D chains facilitate both the stacking of solids and orientation, which increases the efficiency of charge transfer within the active layers <sup>11</sup>. Moreover, the three significant categories of side chains described previously, namely N-substituted side chains with diphenylamine, have just been chosen as another characteristic structural unit in NFREAs. This component can donate electrons and exhibits a three-dimensional (3D) conformational profile. These amino substituents play a crucial role in ensuring solubility, suppressing over-aggregation, and increasing the efficiency of intramolecular electron transfer (ICT) <sup>12</sup>. Amino-substituted side chains in NFREAs are associated with power conversion efficiencies above 16% <sup>12</sup>. Tert-butyl carbazole, similar to diphenylamine, acts as an electron donor in two dimensions and has found application in the creation of a range of semiconductor compounds. It possesses a double symmetry axis, a broad conjugated plane, and a high  $\pi$ -electron density <sup>13</sup>. Moreover, the electron-transfer ability of tert-butyl carbazole is remarkable, leading to improved properties, including photoelectric performance, thermal stability, and morphological stability.

The present study describes the design of four novel molecules, comprising modifications to the terminal acceptor units of PCT-4Cl, featuring various electron-accepting groups <sup>14</sup>. Subsequently, six functionals were subjected to computational analysis to evaluate their characteristic properties. Since all molecules were derived from a single core and different electron-acceptor subunits, they were labelled EE1, EE2, EE3, and EE4 according to the core nomenclature and the configuration of the molecule. PCT-4Cl was considered the reference (R) molecule for the aims of this research project. The newly designed molecules differ from one another based on the Various acceptor subunits positioned at their terminal ends. thus, EE1 contains "1-(dicyanomethylene)-2-methylene-3-oxo-2,3-dihydro-1H-indene-5,6-dicarbonitrile", EE2 contains "2-(2-methylene-5,6-dinitro-3-oxo-2,3-dihydro-1H-inden-1-ylidene) malononitrile". EE3 has "(E)-3-(cyano(nitro)methylene)-2-methylene-6-nitro-1-oxo-2,3-dihydro-1H-indene-5 carbonitrile" and EE4 contains "(E)-6-chloro-1-(cyano(nitro)methylene)-2-methylene-3-oxo-2,3-dihydro-1H-indene-5-carbonitrile" acceptor units. The acceptor subunits exhibit exceptional optoelectronic properties, including a reduced bandgap, reduced Ex level, along with a notable oscillator strength.

## 2. Computational methodology

One of the most reliable and commonly utilized theoretical approaches for analyzing how geometric and optoelectronic properties relate in molecules is density functional theory (DFT),

with a special emphasis on time-dependent DFT (TD-DFT)<sup>15,16</sup>. ChemDraw 7.0 software was used to sketch the molecular structures before performing the calculations. Gauss View 6.0<sup>17</sup> software was used to generate an unoptimized structure as input for each molecule. After checking the inputs, computational simulations were performed using Gaussian 09<sup>18</sup>. The Gaussian 09 software uses a variety of functionals to perform DFT calculations. The six most commonly used functionals are B3LYP<sup>19</sup>, CAM-B3LYP<sup>20</sup>, MPW1PW91<sup>21</sup>, WB97XD<sup>22</sup>, M06<sup>23</sup> and M06-2X<sup>24</sup>.

The validity of each functional was determined by comparing the results obtained with R using the 6-31G (d, p) basis set of the DFT. The aim was to determine the optimal functional for use with our molecules. PyMOlyze 1.1<sup>25</sup> software was used to analyse the density of states (DOS). The DOS calculations were performed to validate the consequences of the Frontier Molecular Orbitals (FMO) analysis. Two-dimensional maps of the transition density matrix (TDM) for various molecular areas of the chromophores were generated using MultiWFN 3.8<sup>26</sup> software. From these images, the probabilities of charge localization and delocalization in the chromophores could be easily read. Equations (1) and (2) are used to determine the reorganizational energy for electrons and holes<sup>27</sup>.

$$\lambda_h = (E_o^+ - E_+) + (E_+^o - E_o) \quad (1)$$

$$\lambda_e = (E_o^- - E_-) + (E_-^o - E_o) \quad (2)$$

The energies assigned to optimized molecules with the charges of 0, -1, and +1, are referred to as  $E_o$ ,  $E_o^-$ ,  $E_o^+$  and respectively. Conversely, The energies of the optimized anionic compounds with charges of 0 and -1 are represented by  $E_-^o$  and  $E_-$ , respectively. The energies associated with the optimized cations in the charge states 0 and +1 are referred to as  $E_+^o$  and  $E_+$ , respectively. Furthermore, the energies of positive, negative, and zero charge states are used to determine chemical reactivity parameters, including ionization potential (IP), hardness, softness, and electron affinity (EA).

### 3. Results and discussion

This study determined the electrical and optical features of the reference (R) molecule using six DFT levels: B3LYP, MPW1PW91, CAM-B3LYP, WB97XD, M06-2x, and M06<sup>14</sup>. Different basis sets are employed to evaluate R to determine the suitability of the functionals for use in the simulations. The  $\lambda_{\max}$  value of R for UV-visible (UV-Vis) absorption with the B3LYP, MPW1PW91, CAM-B3LYP, WB97XD, M06-2x, and M06 functionals at the 6-31G (d, p) level of DFT is shown in **Figure 1**. The wavelengths were 660.72 nm, 526.96 nm, 617.42 nm, 510.94 nm,

601.34 nm, and 466.76 nm; the reported R value was 649 nm. Consequently, the B3LYP method yields results that are more consistent with the experimental data. The effect of different basis sets on absorption spectra was investigated.

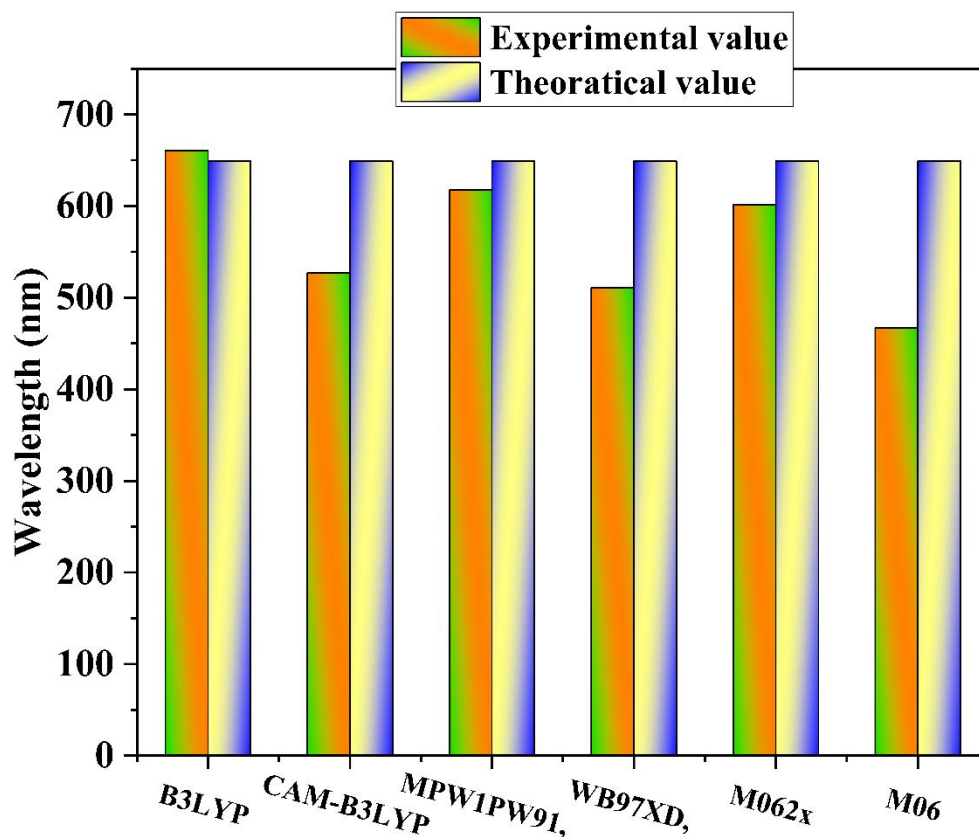


**Figure 1.** Graphical representation of Reference molecule using six different DFT levels in chloroform solvent.

Figure 2 presents the molecular frameworks of the reference and the newly created materials (EE1, EE2, EE3, and EE4).

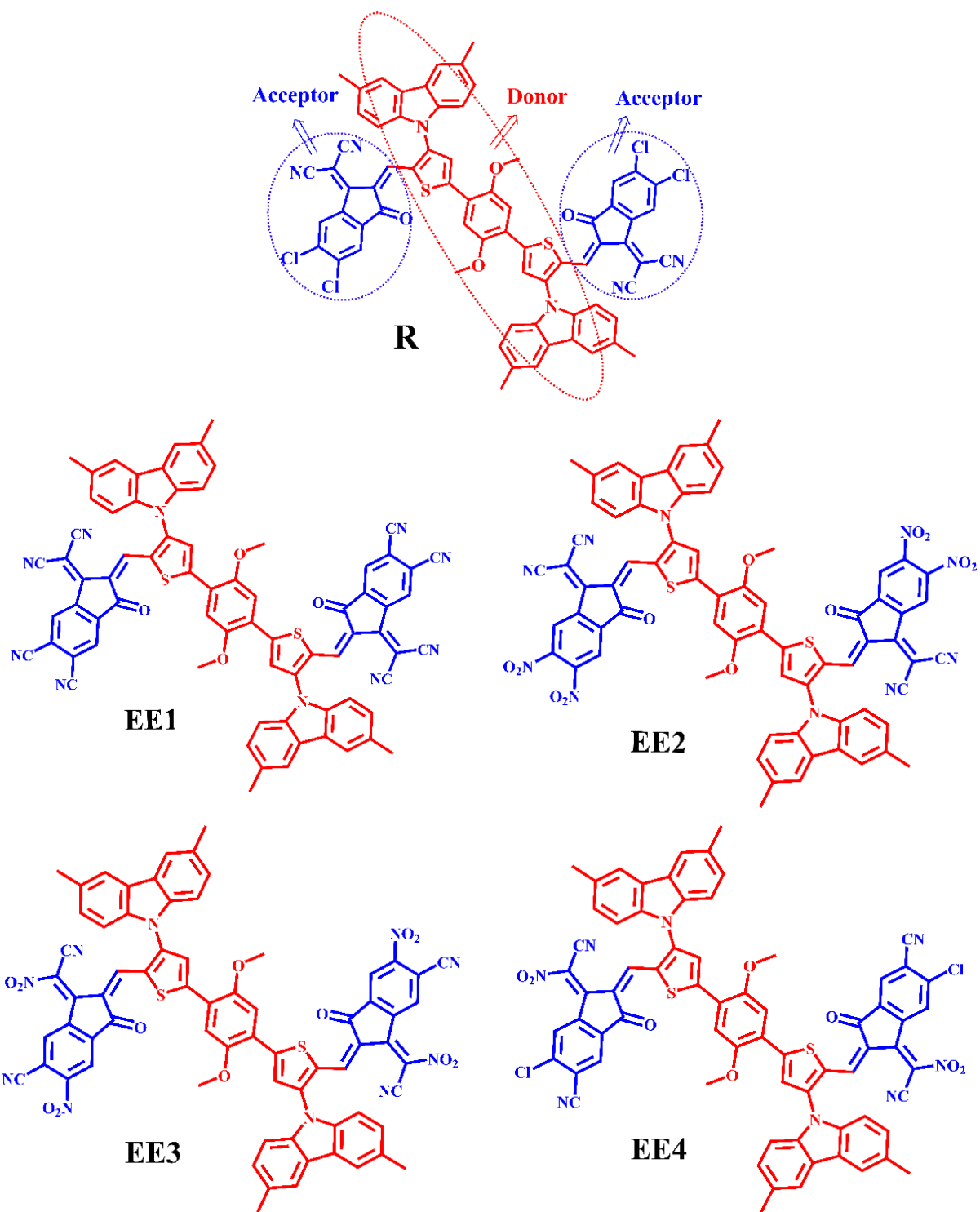
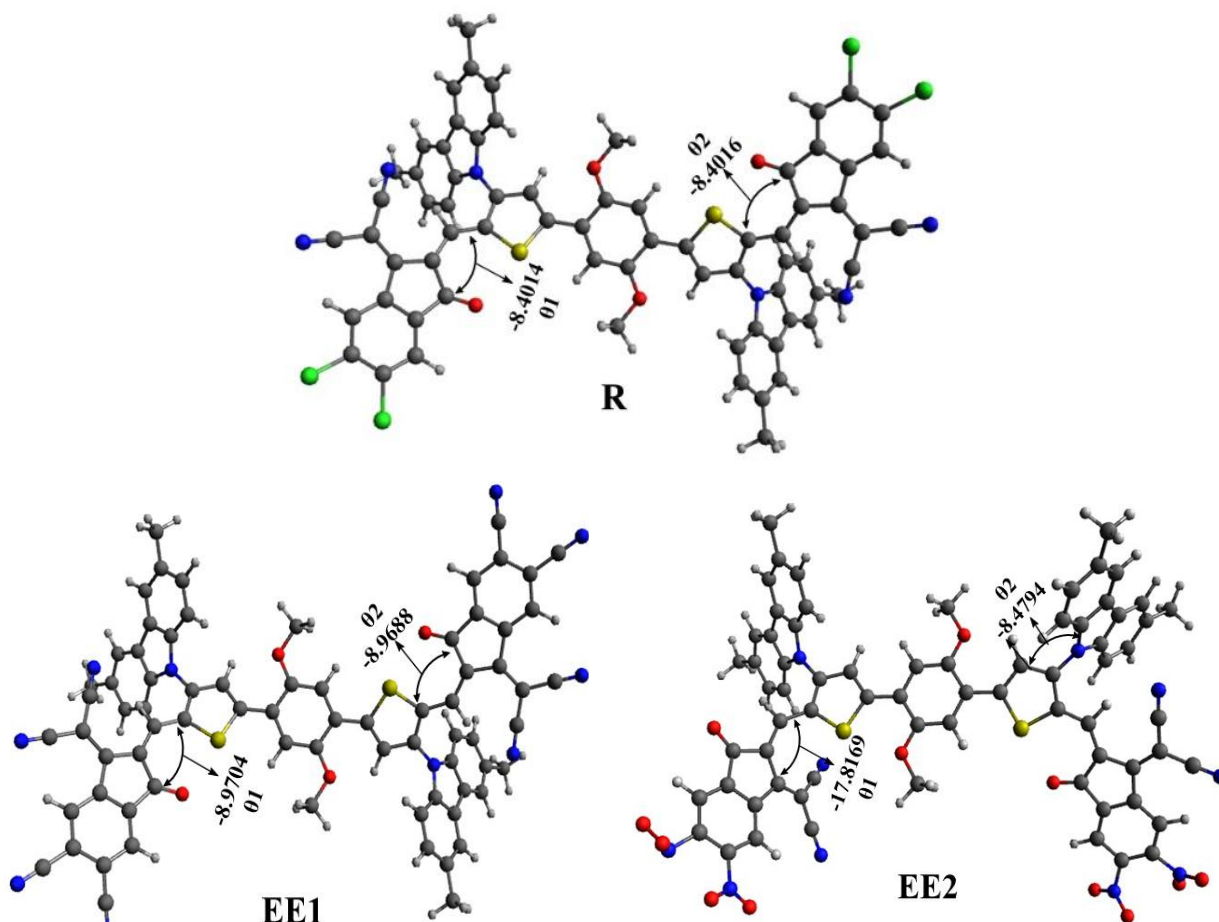


**Figure 2.** Molecular framework of reference **R** and engineered compounds of **EE1**, **EE2**, **EE3**, and **EE4**.

### 3.1. Dihedral angle analysis

Dihedral angle analysis was used to assess the effects of different electron-withdrawing groups on the molecules during the fabrication of the reference (R) molecule to build a series of unique molecules, EE1 to EE4. The dihedral angle greatly enhances conjugation in the molecular structures. Different electron-withdrawing groups induce significant conjugation, thereby enhancing charge-carrier transfer and ultimately increasing short-circuit current and open-circuit voltage ( $V_{OC}$ ). Significant insights into the molecular geometry are revealed by the dihedral angle<sup>28</sup>. Charge-carrier movement and molecular reorganization energy depend on molecular planarity, which is influenced by the dihedral angle. The dihedral angle on both sides of the optimal structure is examined for all newly synthesized molecules, EE1 to EE4. **Figure 3** presents the dihedral angle of the reference and newly proposed EE1 to EE4 molecules.



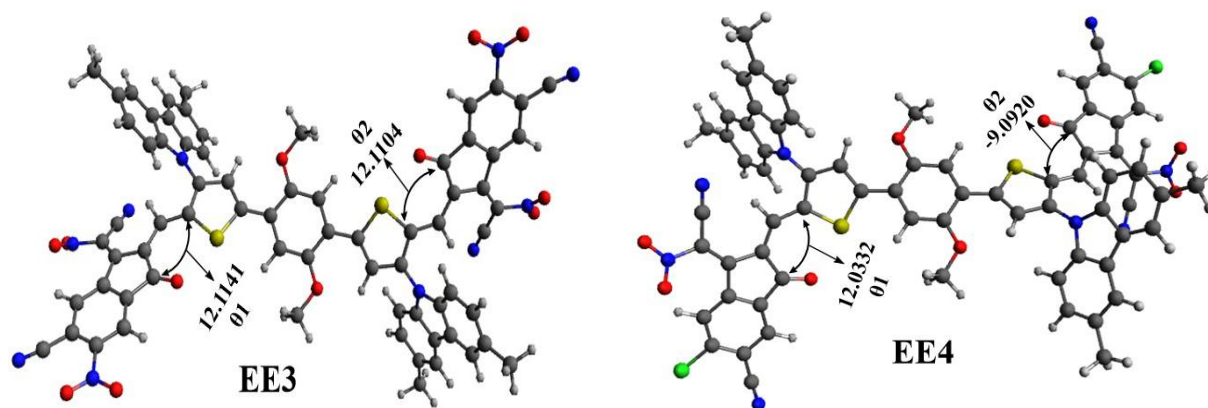


**Figure 3.** Optimized molecular geometric structures of reference (R), EE1, EE2, EE3, and EE4 obtained through a systematic approach.

### 3.2 Frontier molecular orbital (FMO) analysis

FMO is a method for analysing electron-density dispersion based on the Lowest Unoccupied Molecular Orbital (LUMO) and Highest Occupied Molecular Orbital (HOMO) energy levels. The HOMO and LUMO energies for all designed compounds (EE1-EE4), along with R, were examined at the B3LYP/6-31G (d,p) level of DFT. The calculated HOMO and LUMO values for the reference were  $-5.60\text{ eV}$  and  $-3.58\text{ eV}$ , respectively. The HOMO energies of the created compounds EE1, EE2, EE3, and EE4 were estimated as  $-5.85$ ,  $-5.84$ ,  $-5.93$ , and  $-5.74\text{ eV}$ , respectively. The LUMO energy levels are  $-3.97\text{ eV}$ ,  $-3.99\text{ eV}$ ,  $-4.19\text{ eV}$ , and  $-3.93\text{ eV}$ , respectively. **Figure 4** depicts the HOMO - LUMO energies, together with the respective energy gaps. Molecules EE1, EE2, EE3, and EE4 have energy gaps measuring (1.88, 1.85, 1.74, and 1.81) eV, in that order. In contrast, R exhibits an energy gap of 2.02 eV. Compared to R, the engineered molecules possess smaller energy gaps. Of all the designed compounds, EE3 has the lowest  $E_g$  (1.74 eV), which can be attributed to the presence of end-capped, strong electron-withdrawing acceptor groups, namely (E)-3-(cyano(nitro)methylene)-2-methylene-6-nitro-1-oxo-2,3-dihydro-1H-indene-5-carbonitrile.

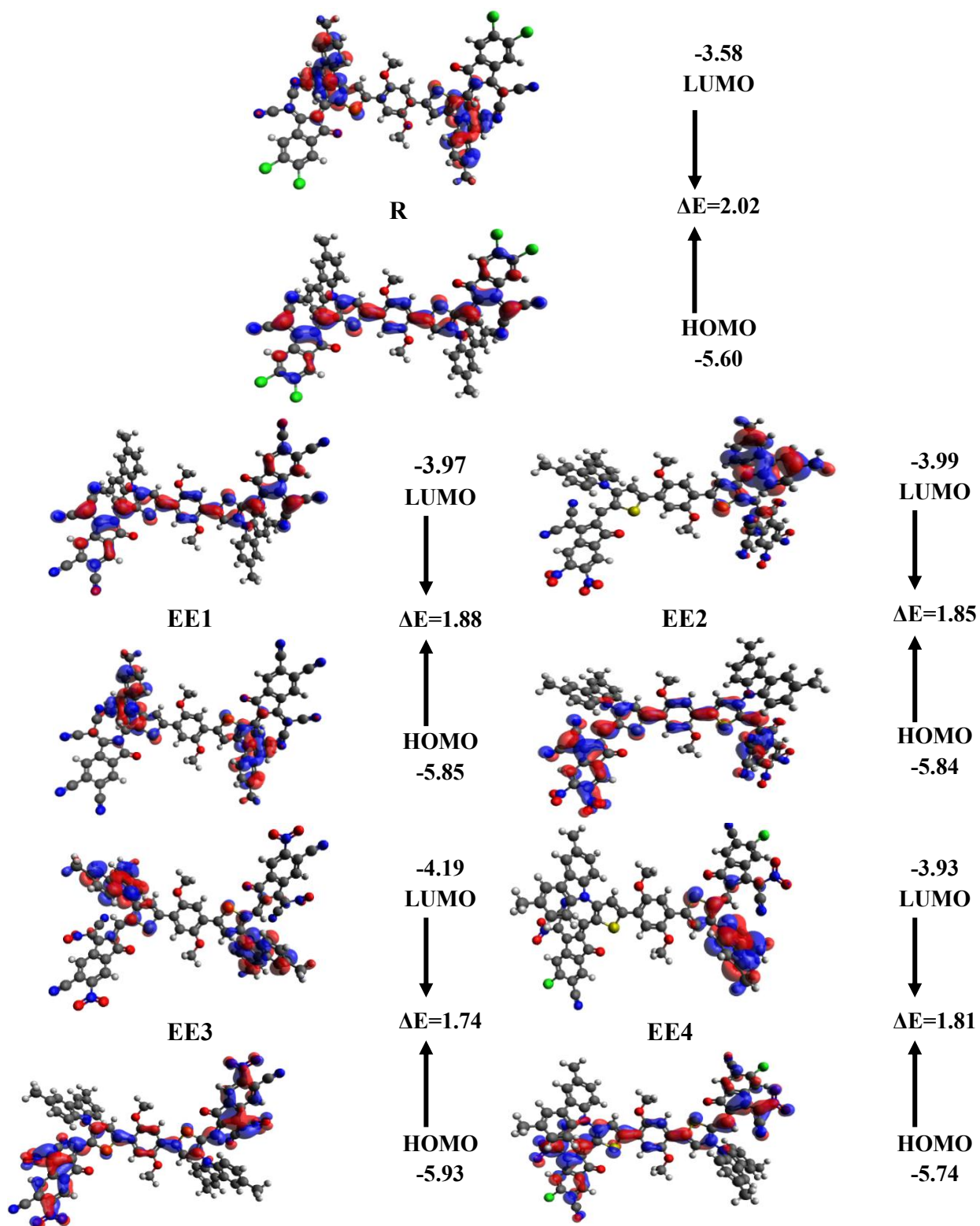


**Figure 4.** The spatial configuration of the HOMO-LUMO distribution of R, EE1, EE2, EE3 and EE4.

### 3.3 Optical properties

The maximum absorption wavelength ( $\lambda_{\max}$ ) was comprehensively analysed and compared together with additional Essential parameters, namely oscillator strength ( $f_{os}$ ), *excitation energy* ( $E_x$ ), *significant contribution and light-harvesting* efficiency. Investigating the absorption properties of OSC materials is of considerable scientific interest, as it provides valuable insight into their potential as Effective light-harvesting materials. Various structural groups, particularly chromophores, shift from the ground to the excited state upon absorbing light, forming excitons that diffuse further and then dissociate at the cathode to conduct electric current. This was performed using the tabulated data presented in **Table 1**, which gives a detailed overview of the results obtained in the gaseous medium and in chloroform solvent, respectively.

**Table 1.** Excitation energy, oscillator strength, theoretical and experimental wavelength, and MO contribution in the gaseous and solvent phases

|               | Molecules  | DFT                  | Exp.                 | $E_x$ | $f_{os}$ | Major contributions<br>MO assignment |
|---------------|------------|----------------------|----------------------|-------|----------|--------------------------------------|
|               |            | $\lambda_{\max}(nm)$ | $\lambda_{\max}(nm)$ | (eV)  |          |                                      |
| Gaseous state | <b>R</b>   | 617.51               | 649                  | 2.01  | 0.8438   | H->L (84%)                           |
|               | <b>EE1</b> | 638.21               |                      | 1.94  | 1.0511   | H->L (87%)                           |
|               | <b>EE2</b> | 645.21               |                      | 1.92  | 0.9353   | H->L (89%)                           |
|               | <b>EE3</b> | 682.13               |                      | 1.82  | 1.0439   | H->L (98%)                           |
|               | <b>EE4</b> | 657.11               |                      | 1.89  | 1.3158   | H->L (92%)                           |
| Chloroform    | <b>R</b>   | 660.72               |                      | 1.88  | 1.5099   | H->L (90%)                           |
|               | <b>EE1</b> | 696.93               |                      | 1.78  | 1.4032   | H->L (92%)                           |
|               | <b>EE2</b> | 712.59               |                      | 1.74  | 0.7753   | H->L (94%)                           |
|               | <b>EE3</b> | 769.18               |                      | 1.61  | 1.0072   | H->L (98%)                           |
|               | <b>EE4</b> | 733.68               |                      | 1.70  | 1.2525   | H->L (96%)                           |

The molecules studied (R & EE1-EE4) showed a significant increase in their  $\lambda_{\max}$ , with EE3 showing the highest value, followed by EE4, EE2, EE1, and R, both in the gaseous and chloroform solvent phase. The addition of acceptors to the designed molecules (EE1-EE4) resulted in an observable shift in  $\lambda_{\max}$ , with this shift occurring in the near-infrared region. Furthermore, this addition also led to a broadening of the absorption spectrum for all four designed molecules.

The observed shifts ranged from 638 nm to 769 nm. This significantly enhanced conjugation, enabling absorption across a broad wavelength range and inducing electronic excitations. The estimated  $\lambda_{\text{max}}$  of R is 617 nm, while the considered molecules (EE1-EE4) have  $\lambda_{\text{max}}$  values of 638.21 nm, 645.21 nm, 682.13 nm, and 657.11 nm, respectively. The  $\lambda_{\text{max}}$  of R was observed at 660 nm, while the designed molecules (EE1-EE4) exhibited  $\lambda_{\text{max}}$  values of 696.93 nm, 712.59 nm, 769.18 nm, and 733.68 nm, respectively.

$E_x$  holds significant importance in this process. Reduced  $E_x$  values suggest that, due to a smaller bandgap, a minimal amount of energy is sufficient to excite electrons from the ground to the excited state (transition of HOMO to LUMO). This subsequent transition allows further processes to use the absorbed light to generate an electrical current. The calculations were performed in solvent and gas phases using the IEFPCM solvation model. The objective was to elucidate the electronic properties of the studied molecules.  $E_x$  of the considered molecules (EE1-EE4) displayed a significant reduction, which contributed significantly to the broadening of the absorption band and allowed the excitation of larger light intensities. It was assumed that this would improve the optical properties of the OSC material. The  $E_x$  of R and EE1-EE4 in the gas phase and in chloroform were found to be (2.01, 1.94, 1.92, 1.82, and 1.89 eV) and (1.88, 1.78, 1.74, 1.61, and 1.70 eV), respectively. The  $E_x$  value in the solvent phase is lower than in the gas phase due to solvent stabilization. **Figure 5** shows the absorption spectra in both the gas and solvent phases.

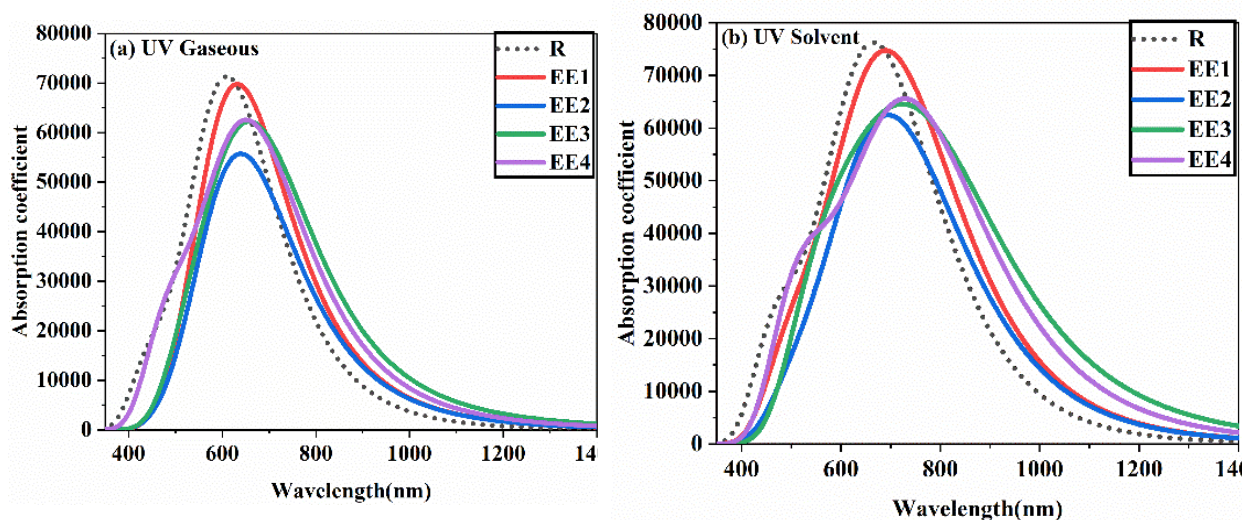
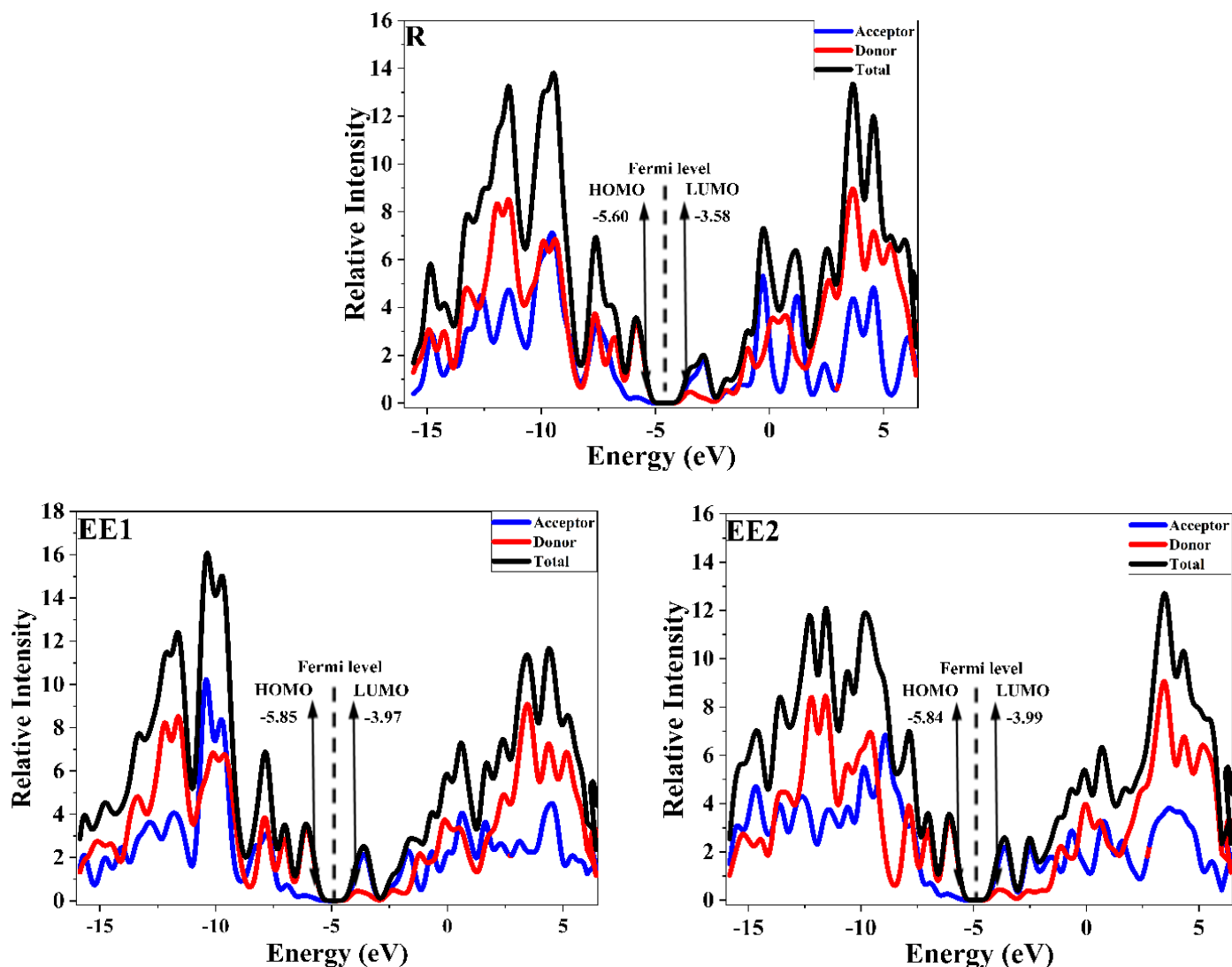


**Figure 5.** UV-Vis profiles of R and EE1–EE4 in gas phase and in chloroform solution.

### 3.4 Density of state analysis

The validity of the FMOs diagram was evaluated by a DOS investigation using the B3LYP/6-31G (d, p) functional for R and the engineered compounds (EE1-EE4). **Figure 6** illustrates how changes in the terminal groups affect the dispersion of electron density near the valence and conduction bands. R shows a dominance of electrons in the molecular core region in the HOMO, while electrons from the terminal acceptor groups mainly populate the LUMO. Similarly, the DOS graphs for EE1-EE4 show that most of the overall electron-density distribution (black lines) is occupied by core electrons, notably those in the HOMO.



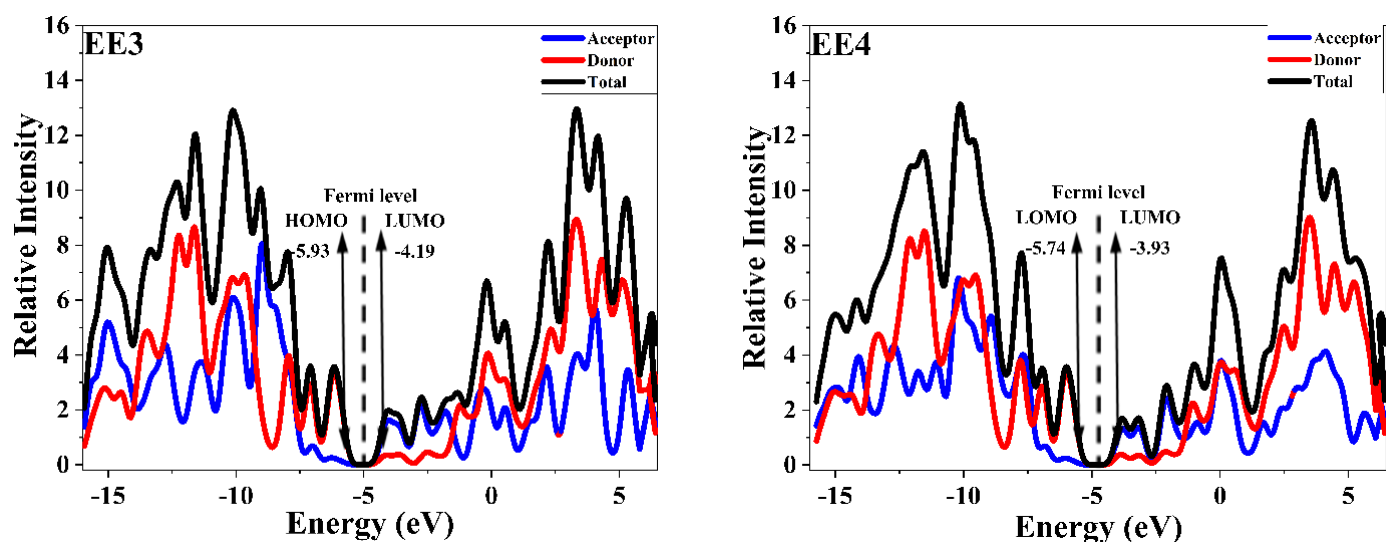


**Figure 6.** The DOS analysis of standard R and the engineered (EE1-EE4) compounds.

**Table 2** shows the impact of individual components on HOMO and LUMO and illustrates electron transfer from the core to the terminal section of the electron acceptors. The terminal electron acceptors of EE3 were identified as the main contributors to the LUMO, accounting for 74.1%. The ability of acceptor molecules to conduct electricity is influenced by the precise arrangement of their molecular framework. A molecule positioned closer to the LUMO enables more electronic states and therefore greater participation of the acceptors in the conduction process. The modified terminal groups increased LUMO peaks in EE1-EE4, confirming that terminal-group modification can enhance the conductivity of acceptor molecules when paired with a suitable donor.

**Table 2.** DFT-based analysis of the relative contributions of acceptor and in elevating the HOMO-LUMO levels of R and EE1-EE4

| Molecule   | Excitation energy state | %age contribution |               |
|------------|-------------------------|-------------------|---------------|
|            |                         | Donor (eV)        | Acceptor (eV) |
| <b>R</b>   | HOMO                    | 90.6              | 9.4           |
|            | LUMO                    | 39.1              | 60.9          |
| <b>EE1</b> | HOMO                    | 91.6              | 8.4           |
|            | LUMO                    | 35.7              | 64.3          |
| <b>EE2</b> | HOMO                    | 94.4              | 5.6           |
|            | LUMO                    | 33.9              | 66.1          |

|            |      |      |      |
|------------|------|------|------|
| <b>EE3</b> | HOMO | 93.6 | 6.4  |
|            | LUMO | 25.9 | 74.1 |
| <b>EE4</b> | HOMO | 94.6 | 5.4  |
|            | LUMO | 29.3 | 70.7 |

### 3.5 Global reactivity parameters

The chemical reactivity of compounds is predicted using global chemical reactivity factors, which are computed through a quantum approach. Included among these parameters are chemical potential ( $\mu$ ), electron affinity (EA), hardness ( $\eta$ ), softness ( $s$ ), and ionization potential (IP). Table 3 shows how these properties are influenced by frontier orbital energies. The corresponding parameters are calculated using Equations (3-10). These descriptors provide insight into the chemical reactivity, molecular stability, and polarity of the compounds <sup>29</sup>.

$$IP = (E_o^+ - E_o^-) \quad (3)$$

$$EA = (E_o - E_o^-) \quad (4)$$

$$\mu = \frac{(E_{HOMO} + E_{LUMO})}{2} \quad (5)$$

$$\eta = \frac{(E_{LUMO} - E_{HOMO})}{2} \quad (6)$$

$$\sigma = \frac{1}{\eta} \quad (7)$$

$$\chi = -\frac{(E_{HOMO} + E_{LUMO})}{2} \quad (8)$$

$$\omega = \frac{\chi^2}{2(\eta)} \quad (9)$$

$$\Delta N = \frac{\mu}{\eta_{max}} \quad (10)$$

**Table 3.** The electron affinity, ionization potential, chemical potential, softness and hardness of R and EE1–EE4.

| Molecules | I.P<br>(eV) | E.A<br>(eV) | $\mu$<br>(eV) | ( $\eta$ )<br>(eV) | s<br>(eV) | $\chi$<br>(eV) | $\omega$<br>(eV) | $\Delta N_{\max}$<br>(eV) |
|-----------|-------------|-------------|---------------|--------------------|-----------|----------------|------------------|---------------------------|
| R         | 6.76        | 0.80        | -4.59         | 1.01               | 0.99      | 3.77           | 4.59             | 4.55                      |
| EE1       | 6.96        | 2.75        | -4.91         | 0.94               | 1.06      | 4.89           | 4.91             | 5.22                      |
| EE2       | 6.89        | 2.65        | -4.91         | 0.93               | 1.08      | 4.81           | 4.91             | 5.31                      |
| EE3       | 6.24        | 2.95        | -5.06         | 0.87               | 1.15      | 5.03           | 5.06             | 5.83                      |
| EE4       | 6.68        | 2.06        | -4.84         | 0.90               | 1.11      | 4.42           | 4.84             | 5.35                      |

The IP of materials incorporated within the active layer can affect their ability to promote charge transfer. Lower IP in materials often leads to higher charge mobility, as it facilitates electron extraction and charge-carrier formation. As a result, these molecules can improve solar cell performance. The IP values of EE1-EE4 molecules and R are 6.76, 6.96, 6.89, 6.24, and 6.68, respectively. According to the data, EE3 has the lowest IP among the molecules. This suggests superior charge-transport ability, since it has a greater tendency to donate electrons than R.

Higher EA in materials often increases charge mobility, as electron addition and charge-carrier formation occur more readily. This may improve device performance. In intramolecular charge transfer, a high electron affinity in the acceptor segment strengthens its attraction to charges, driving transfer within the molecule from the donor (D) to the acceptor (A) segment. Enhanced charge movement improves charge transport, resulting in better OSC device performance. The electron affinity measurements for R and the newly engineered molecules EE1 to EE4 are 0.80, 2.75, 2.65, 2.95, and 2.06 eV, respectively. This shows that all engineered molecules have a greater ability to attract electric charges because they have higher electron affinity than R.

The chemical potential measures the tendency of electrons to escape and can be associated with electronegativity, where a more negative chemical potential makes electron loss harder but facilitates electron gain. All designed molecules (EE1-EE4) have a more negative chemical potential than R, indicating their ability to accept electrons.

The parameters of  $\eta$  and S provide deeper insight into the behaviour of chemical systems. Chemical hardness represents stability, whereas softness signifies reactivity. Among the structures

created, EE3 shows the most exceptional softness and hardness values, indicating the highest reactivity among the engineered materials. Electrophilicity ( $\omega$ ) denotes a molecule's tendency to attract electrons as an electrophile, whereas lower levels indicate electron-donating capacity and nucleophilic character. Because the designed molecules (EE1-EE4) function as acceptors, they all show higher electrophilicity than R, which is significant.

### 3.6 Transition density matrix

The TDM analysis elucidates the behaviour of the acceptor and donor components within the framework, with a particular focus on the excitons' ability to escape electrostatic forces. TDM analysis provides a way to elucidate electron transitions between the D and A fragments in a molecule. These graphs are important for determining the nature of charge localization and delocalization in the molecule under study. The TDM investigation allows the characterisation of the excitation density at different points within the molecule. It was decided that hydrogen atoms would be excluded by default, using these TDM graph settings, given that they have minimal impact on transition characteristics. For a more straightforward interpretation of electronic excitations, the atoms within each molecule were partitioned into distinct components for these plots, namely donor (D) and acceptor (A). As shown in **Figure 7**, most of the molecules studied exhibited a uniform distribution of excitons from the donor to the acceptor groups, suggesting effective Electron transfer occurring between the donor and acceptor units.

Furthermore, the presence of several luminescent spots in the acceptor and donor regions of the studied molecules suggests significant charge density in these regions. As a result, both the fused donor and the end-capped acceptor contribute significantly to efficient exciton transfer from the donor to the acceptor region. A comprehensive analysis of the TDM graphs indicates remarkable exciton migration through the designed structures. Transfer of holes and electrons to the donor-acceptor interface facilitates efficient charge transfer. A comprehensive analysis of the TDM diagrams shows a remarkable migration of excitons through the investigated structures due to dissociation at the interface, where the excitons separate into their constituent electrons and holes. Notably, exciton migration is particularly evident in the designed structures EE1-EE4.

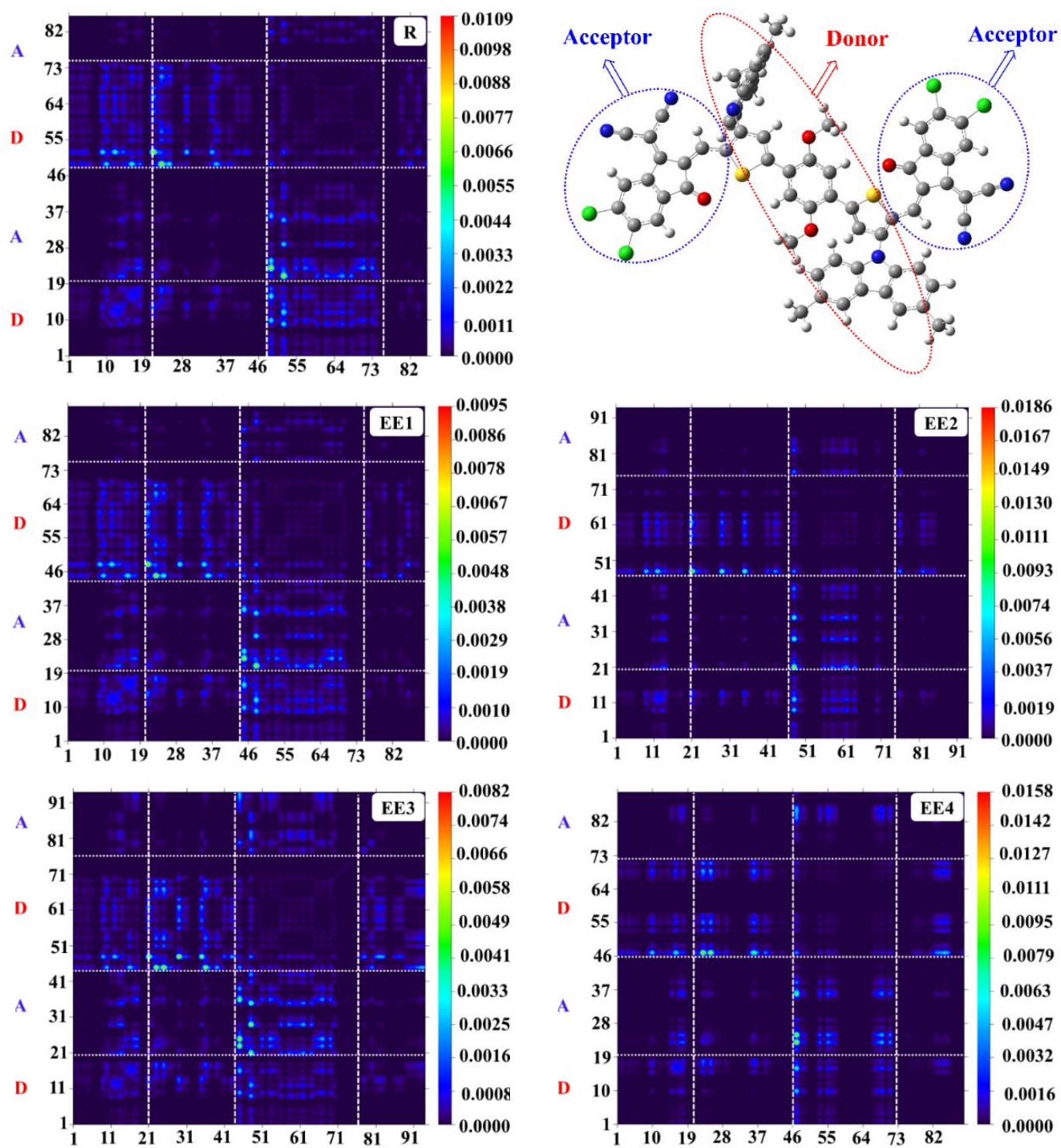


**Figure 7.** TDM plots of reference and engineered (EE1–EE4) molecules.

### 3.7 Heat map

Hole-electron contribution maps provide an excellent method for predicting charge transfer across diverse regions of a molecule. The heat maps show the atoms involved in the electron-hole formation. They also reveal where holes and electrons overlap. The influence of hydrogen atoms is not considered in the construction of heat maps, since no electronic transitions involving these atoms are present, which are essential for the analysis and therefore do not contribute to the resulting findings. To enhance the visual representation of the contributions of individual fragments, each molecule is divided into two distinct units: the acceptor and the donor.

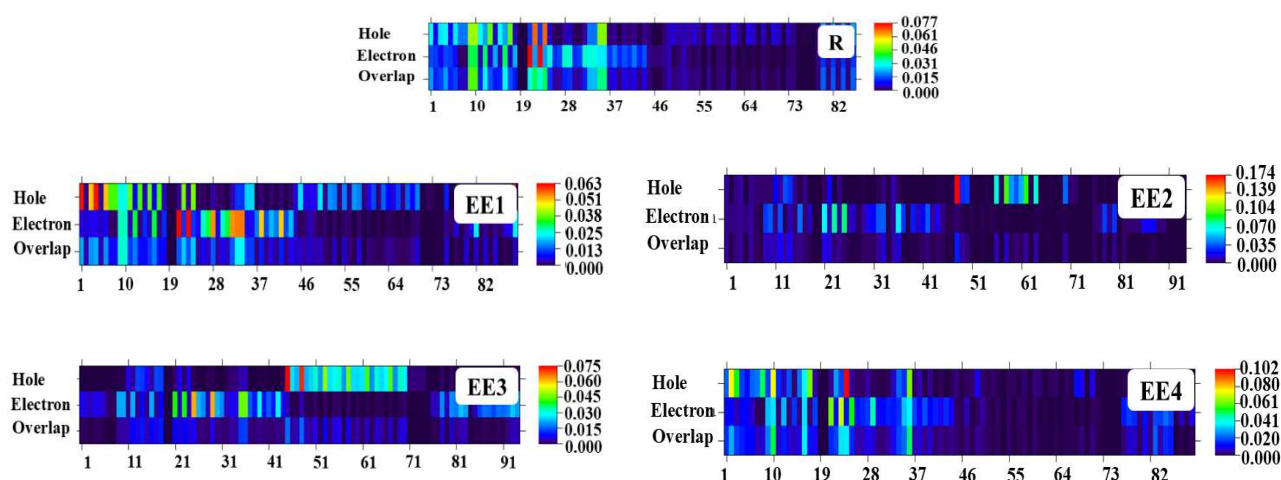


**Figure 8.** Hole-electron distribution heat maps for R, along with EE1 to EE4

**Figure 8** illustrates the iso-surface maps generated by the MultiWFN program. Table 2 presents the number of atomic units included in each fragment. The heat maps of each molecule exhibit a considerable number of atoms, excluding hydrogen, distributed along the x-axis. Conversely, a colour scale with corresponding values is displayed along the y-axis, indicating involvement in Hole-electron interaction and the associated contribution. The red regions depicted in these iso-surface maps indicate the extent to which the holes contribute to the overall result. It can be surmised that the most significant structural contribution comes from the carbon atoms in the acceptor parts, which facilitate the connection between the donor and acceptor moieties.

### 3.8 Reorganization energy

Reorganization energy strongly influences OSC efficiency by affecting charge-carrier movement within molecules. Electron-hole motion decreases as molecular reorganization energy increases. Consequently, a molecule with low reorganization energy can achieve greater electron ( $\lambda_e$ ) and hole

( $\lambda_h$ ) movement<sup>30</sup>. The reorganizational energy of the molecules serves a crucial role in determining the activation energy for charge transport. Other factors, such as thermal activation energy, molecular packing, and electronic coupling, can also influence the charge-transfer rate. **Table 4** presents the computed RE values for all analysed molecules.

**Table 4.** Calculated reorganization energies for the electron ( $\lambda_e$ ) and hole ( $\lambda_h$ ) for R and studied (EE1-EE4) molecules.

| Compounds | $\lambda_e$ (eV) | $\lambda_h$ (eV) |
|-----------|------------------|------------------|
| R         | 0.0095           | 0.0040           |
| EE1       | 0.0078           | 0.0047           |
| EE2       | 0.0085           | 0.0052           |
| EE3       | 0.0102           | 0.0069           |
| EE4       | 0.0115           | 0.0055           |

The data presented in **Table 4** indicate that  $\lambda_e$  decreases in the following sequence: EE4 > EE3 > R > EE2 > EE1. This shows that EE1 and EE2 act more effectively as electron-transport components than the others, as their  $\lambda_e$  values are lower than R. EE3 and EE4 values are comparable to the reference molecule.

### 3.9 Open circuit voltage

Another tool utilized to identify an OSC's maximum operational capacity is the open-circuit voltage ( $V_{oc}$ ). Calculating the open-circuit voltage ( $V_{oc}$ ) can assess an OSC's efficiency.  $V_{oc}$  represents the maximum voltage that can be drawn from a given optical apparatus. In this study, the following equation was used to estimate the  $V_{oc}$  values of R and EE1-EE4.

$$V_{oc} = (\text{HOMO}_{(\text{PM6})} - \text{LUMO}_{(\text{acceptor})}) - 0.3 \quad (11)$$

To meet the conditions of the equation above, this study used the well-established donor polymer PM6, with HOMO and LUMO levels of -5.13 and -3.28 eV, respectively. The HOMO energy of PM6 was compared to the LUMO energies of the acceptor materials, which include reference and EE1-EE4. Figure 9 shows the results from Equation 11, computed using the HOMO level of PM6 and the LUMO levels of the acceptor molecules. The  $V_{oc}$  value for R concerning the HOMOPM6-LUMO acceptor is calculated to be 1.25 eV.  $V_{oc}$  values of 0.86, 0.84, 0.64, and 0.90 eV were observed for EE1 to EE4, showing comparability with the reference material R. Electron

transfer from the  $E_{\text{HOMO}}$  of the donor molecules is enhanced by a low-lying  $E_{\text{LUMO}}$  in the acceptor molecule, thereby increasing the  $V_{\text{oc}}$  and directly enhancing the optoelectronic characteristics.

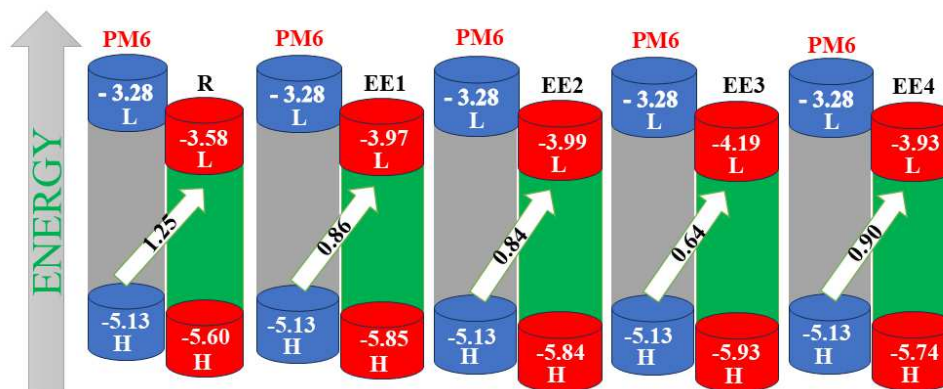


**Figure 9.**  $V_{\text{oc}}$  values of R and the designed molecules EE1–EE4 relative to PM6.

### 3.10 Natural population analysis (NPA)

The electronic structures and other calculated parameters can be obtained using Mulliken and natural charges, and quantum chemical calculations can also be performed. The negative and positive charges for the Oxygen (negative) and hydrogen (positive) can be revealed by performing the Mulliken and natural charge analysis for the complexes, while the carbon atoms exhibit either positive or negative charges (shown in **Figure 10**). A positively charged nitrogen atom is attached to an oxygen atom in molecules EE2, EE3, and EE4. Similarly, all oxygen atoms are negatively charged and found near nitrogen and hydrogen. As shown by the Mulliken charge analysis, the molecules EE and EE1 to EE4 carry charge in different regions because of the negatively charged elements carbon, nitrogen, and oxygen.

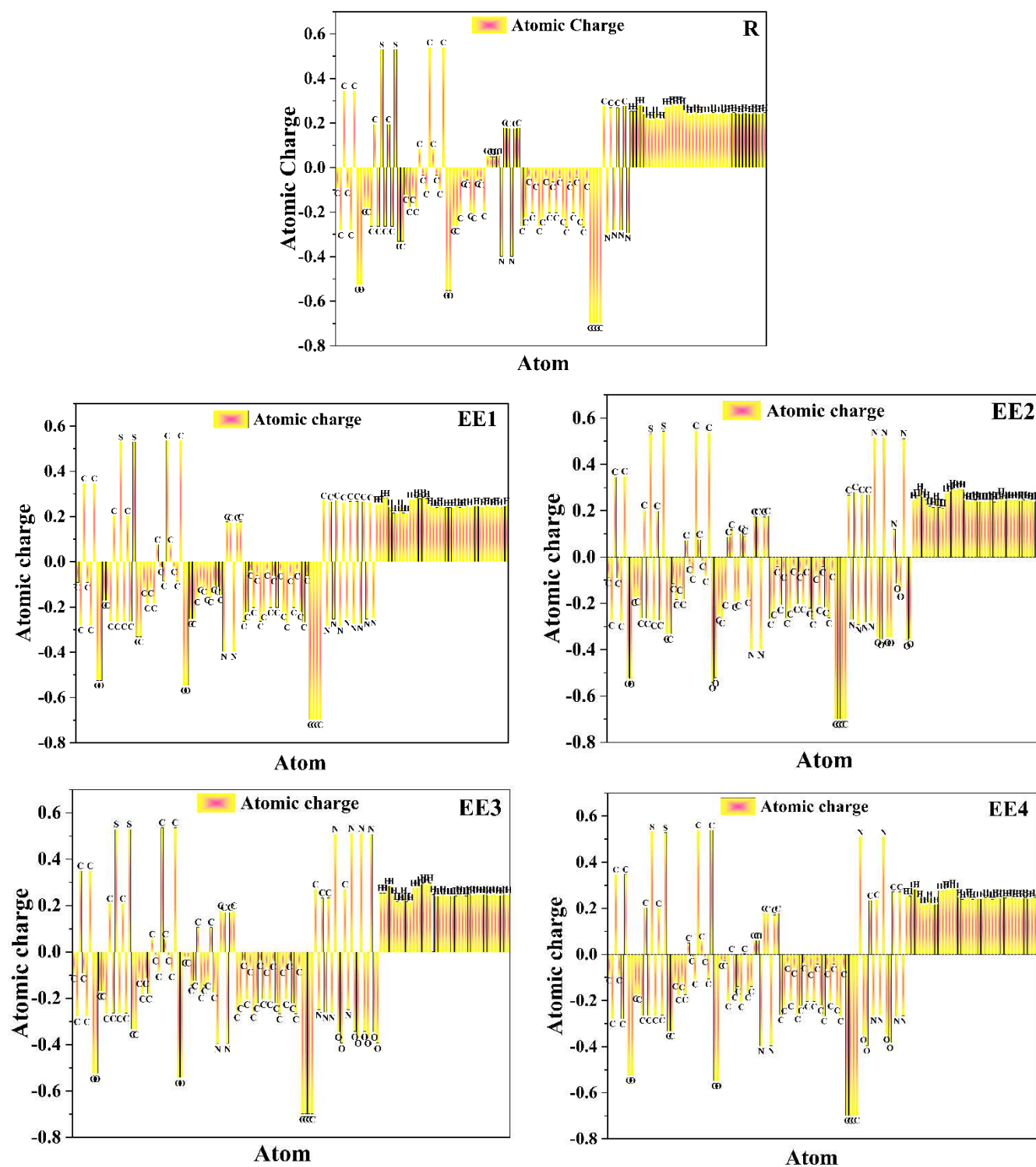


**Figure 10.** Atomic charge and electron density distributions shown by a Natural Population Analysis (NPA) of molecules R and EE1-EE4.

### 3.11 Electron density difference (EDD)

EDD maps play a key role in understanding how molecules change as they transition between states or as their nuclei move. These methods work particularly well when atomic densities offset each other, like when subtracting one molecular density from another. The electronic structures of synthetic molecules were analyzed using MultiWFN, and EDD maps were created to gain deeper insight into charge separation resulting from electronic excitation. **Figure 11** shows the EDD maps for the specified molecules R and (EE1-EE4). The blue region indicates a reduction in electron density upon excitation, whereas the green region indicates an increase in electron density. The acceptor unit demonstrates the highest electron density, whereas the donor unit possesses the lowest among all analyzed substances. **Table 5** outlines the features of intermolecular charge transfer (ICT), including parameters for both e/h transitions. The CDD plots indicate that the incorporation of end caps on both sides improves e/h mobility by raising the H index <sup>31</sup>.

**Table 5:** Outcomes from the electron density difference study of the reference (R) and designed molecules (EE1-EE4).

| Molecule   | HDI<br>(eV) | EDI<br>(eV) | Integral<br>of Hole<br>(amu) | Integral<br>of<br>electron<br>(amu) | Integral<br>of TD<br>(amu) | t<br>Index<br>(Å) | H<br>Index<br>(Å) | D<br>Index<br>(Å) | H.CT<br>(eV) |
|------------|-------------|-------------|------------------------------|-------------------------------------|----------------------------|-------------------|-------------------|-------------------|--------------|
| <b>R</b>   | 5.19        | 4.14        | 0.984023                     | 0.986014                            | -<br>0.000101              | 0.585             | 7.761             | 2.007             | 1.421        |
| <b>EE1</b> | 5.14        | 4.03        | 0.981459                     | 0.982364                            | 0.000524                   | 0.706             | 7.954             | 2.154             | 1.448        |
| <b>EE2</b> | 7.24        | 4.61        | 0.963794                     | 0.961585                            | 0.001160                   | 2.669             | 4.884             | 5.282             | 2.613        |
| <b>EE3</b> | 5.21        | 4.13        | 0.987680                     | 0.989984                            | 0.001117                   | 0.948             | 8.478             | 1.012             | 1.960        |
| <b>EE4</b> | 7.18        | 5.09        | 0.975683                     | 0.976595                            | -<br>0.000489              | 2.098             | 5.107             | 4.436             | 2.338        |

The t-index values for all of the suggested compounds are positive. This changes how well the excitation charge moves from (HOMO to LUMO) donor to acceptor. This gradually makes the device less useful <sup>32</sup>. The t index is used to measure the distance between electrons and holes in the CT direction. If the t index is less than zero, CT does not differentiate the hole and electron. A positive t-index must correspond with a clear distinction between the electron and hole

distributions. The H index shows the typical distance between holes and electrons, as shown in **Table 5**. The HDI and EDI indices correctly measured the homogeneity of the spatial distribution, which reflects hole and electron delocalization, respectively. The less HDI (EDI), the more uniformly spread out the hole (electron) is across the system. HDI and EDI are useful for figuring out how wide spatial distributions is not good when electrons or holes are spread out in changed places <sup>28</sup>.

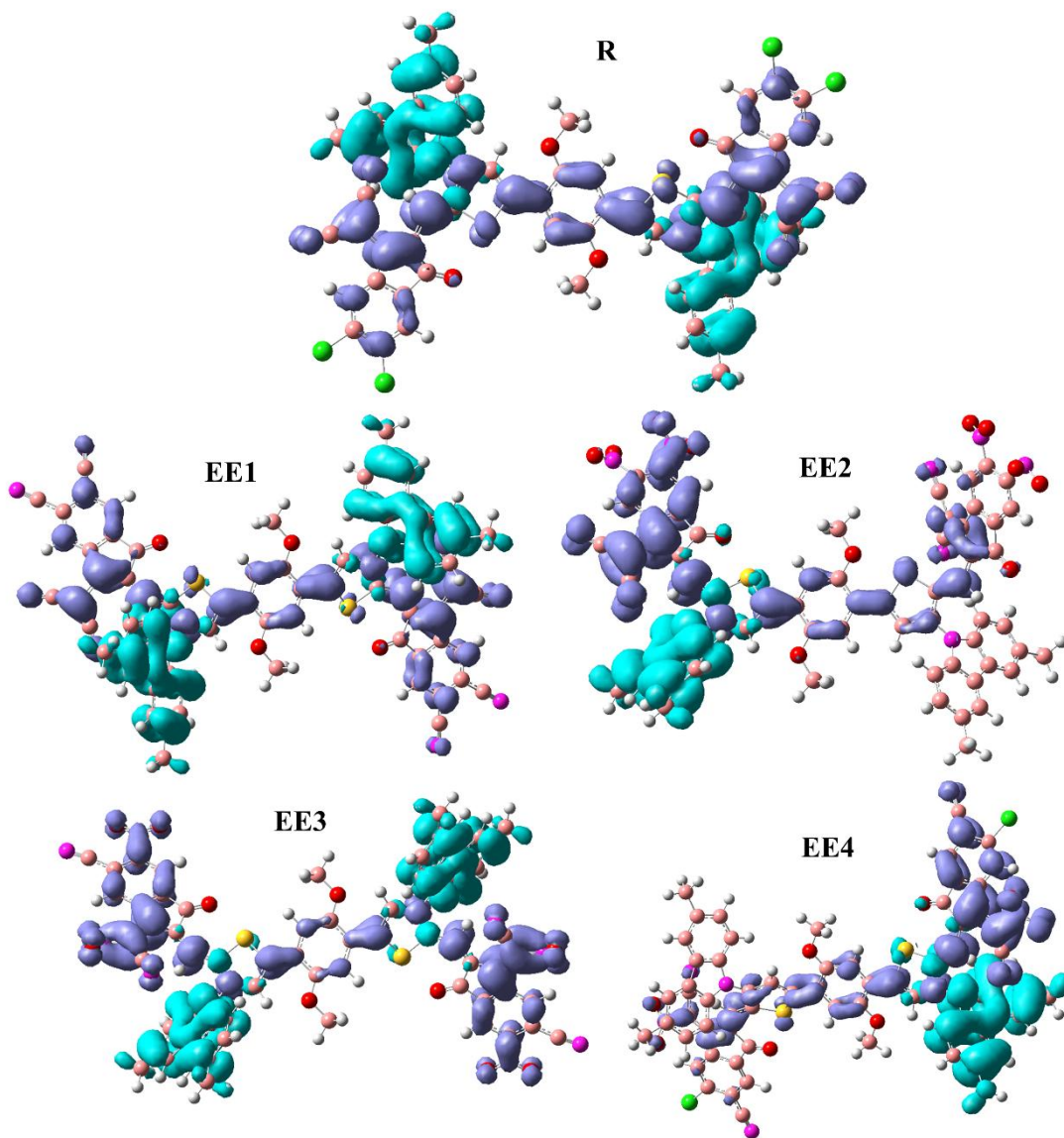


**Figure 11:** Electron density difference map of the standard reference and the studied EE1-EE4 molecules.

### 3.12 Quadrupole Analysis

A key part of determining interfacial energies in NFA-based OSCs is the quadrupole moment of the donor compounds. The H-L energy gap within the molecular architecture decreases with stronger acceptors, especially those with electron-withdrawing moieties<sup>33</sup>. This lowers the energy of the interfacial charge transfer state and affects the device's open-circuit voltage ( $V_{oc}$ ). The determined quadrupole moment is perpendicular to the  $\pi$ -system ( $Q_{20}$ ) for each of the NFAs examined and compared it to the  $V_{oc}$  data, as illustrated in **Figure 12a**. The comparison was done with experimental data since the calculated  $V_{oc}$  values were higher than the experimental observations<sup>34</sup>. Discovered an inverse association between  $V_{oc}$  and  $Q_{20}$ , as predicted. This connection is particularly applicable to the several donor chemicals examined in our study<sup>35</sup>. **Figure 12b** shows that the computed  $Q_{20}$  values were also compared with each molecule's highest-occupied and lowest-unoccupied molecular orbitals. It is obvious from the graph that a greater H-L gap results to a bigger  $Q_{20}$ <sup>36</sup>. Furthermore, these acceptors exhibit the largest  $\lambda_{max}$  within the near infrared. This can help donor photons absorb light in the visible range, leading to an effective mix for photon harvesting.

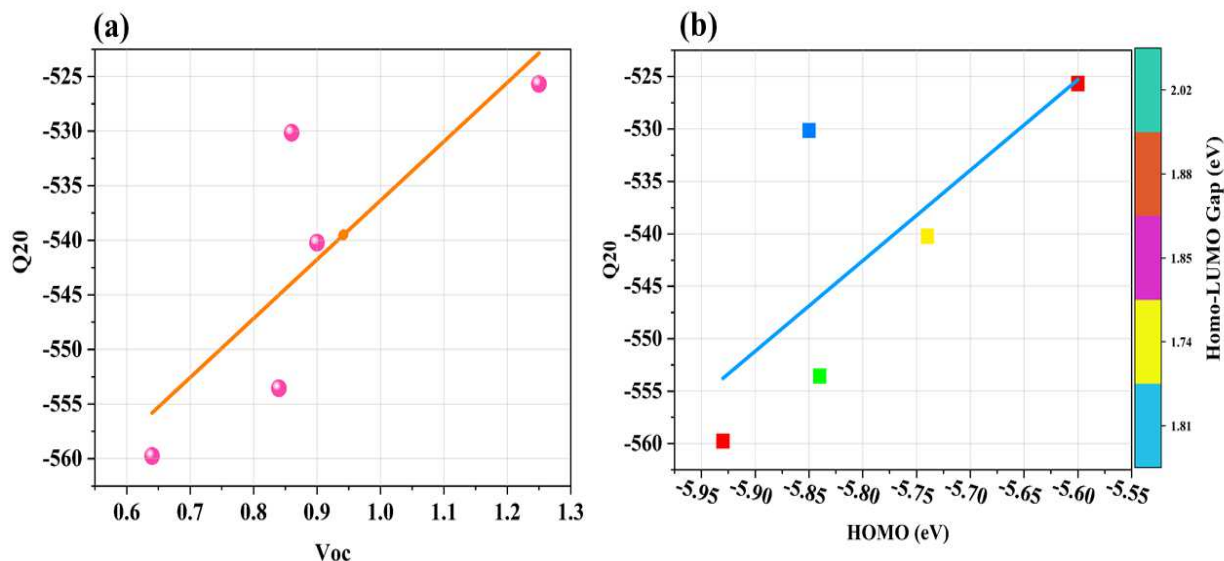


**Figure 12:** a) The quadrupole moment in reference to the  $V_{oc}$  b) Plot shows the correlation between  $Q$  and the NFA complexes, with colors that show the magnitude of the HOMO-LUMO gap.

### 3.13 Charge transfer analysis

This investigation of the donor-acceptor (D-A) complex examined the charge transfer (CT) mechanism between the donor polymer PM6 and the acceptor molecule EE3. EE3 was chosen for

this investigation due to its promising optoelectronic and photovoltaic capabilities. EE3 was selected for its narrow  $E_g$ , low  $E_x$ , low  $E_b$ , red-shifted absorption spectra, good charge transport properties, and promising photovoltaic metrics such as open-circuit voltage ( $V_{oc}$ ). Hence, the PM6:EE3 blend was chosen as an effective donor-acceptor system to analyze charge-transfer behavior.

The frontier molecular orbital analysis shows that the electron density of the HOMO is mostly dispersed on the donor unit of PM6, while the electron density of the LUMO is mainly localized on the acceptor unit <sup>35</sup>. The large separation of electron density between donor and acceptor parts reflects the effective intramolecular charge transfer after photoexcitation. Upon light absorption by the molecule, the electrons may readily jump from the HOMO of PM6 to the LUMO of the acceptor, leading to efficient charge separation. These charge-transfer properties are desirable for solar applications, as they reduce charge recombination and enhance charge transport. Moreover, the molecular orbital (MO) analysis shows substantial electronic interaction between donor and acceptor units, emphasizing the importance of PM6 in the charge-transfer process, as shown in **Figure 13**. These results imply that the PM6-based system has good electrical characteristics and may improve solar cell performance.

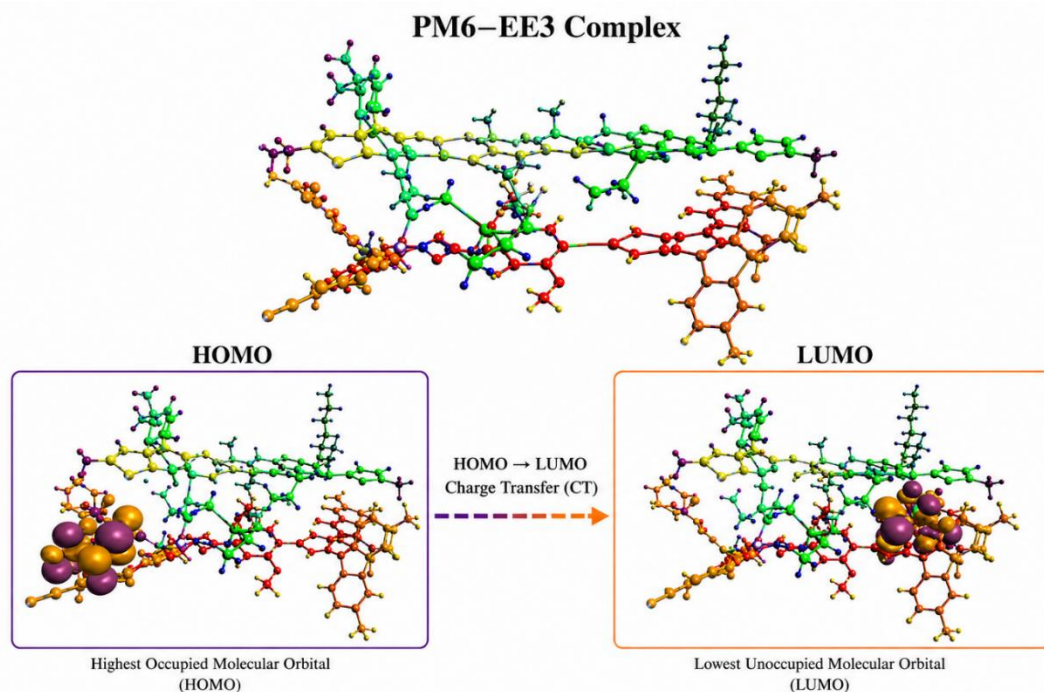


**Figure 13:** Electronic charge distribution of the EE3 donor-acceptor complex with polymer PM6 HOMO and LUMO of complex molecule.

## Conclusion

The optoelectronic properties of a series of newly designed NFAs molecules for EE1-EE4 were investigated using quantum-chemical calculations and compared with those of a reference molecule. Structural modification systematically reduced the frontier-orbital energy gaps and enhanced the optical response of the designed molecules. Among the investigated compounds, EE3 exhibited the smallest energy gap (1.74 eV), compared with 2.02 eV for the reference, together with pronounced, red-shifted absorption maxima of 682.13 nm in the gas phase and 769.18 nm in solvent. Its corresponding excitation energies were reduced to 1.82 and 1.61 eV, respectively, indicating favourable electronic excitation and extended light absorption. The calculated open-circuit voltages remained comparable to those of the reference molecule, suggesting that the structural modifications do not substantially compromise the energetic driving force for charge separation. EE3 also showed the lowest electron and hole reorganization energies ( $\lambda_e = 0.0102$  eV and  $\lambda_h = 0.0069$  eV) among the designed molecules, consistent with reduced structural relaxation during charge transfer and potentially favourable charge-transport characteristics. These results identify EE1-EE4 as computationally interesting NFA candidates for further investigation in organic photovoltaic systems, with EE3 showing a particularly favourable combination of electronic, optical, and charge-transport descriptors. Experimental synthesis, morphological characterization and device-level measurements will be necessary to establish the practical photovoltaic performance of these materials and to determine how the calculated molecular properties translate into solar-cell efficiency.

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