



Effect of acceptor on the electronic and optical properties of designed D-A-D molecules for organic solar cells by DFT and TD-DFT method

¹TIGAWA R., ¹ABUBAKARI I., ¹BABU N S

²Department of chemistry, The University of Dodoma, Dodoma, Tanzania

*Corresponding Author: rahmatigawa@gmail.com

Abstract

Searching for new and efficient energy sources to satisfy global energy demand is one of the most inspiring and challenging areas in scientific study in order to replace fossil fuel which is regarded as unsustainable and harmful to the environment. Solar energy through different technologies including organic solar cells (OSCs) seems to be one of the favorable alternatives. However, the efficiency of this category of solar cells needs significant improvements to become one of the best candidates for use as the best alternative energy source in solar cell technology. In this study, four donor molecules (D-A-D) were successfully created using two strong different donor moieties linked together by four different acceptors to form four M1, M2, M3, and M4 molecules to be used in OSCs technology. The density functional theory (DFT) and time-dependent density functional theory (TD-DFT) methods coupled with B3LYP hybrid functional and 6-311G basis set was employed to assess the optoelectronic as well as photophysical properties of four D-A-D designed molecules. All the designed molecules display promising results to be satisfactorily used in organic solar cell applications. However, among the designed molecules, M2 performs better than others due to the lowest energy gap of 1.83 eV and 1.9 eV, open-circuit voltage (VOC) of 1.5151 and 1.4817 and large maximum absorption wavelength (λ_{max}) of 784.96 nm and 821.18 nm in gas and solvent phases, respectively. As a result, the designed molecule is remarkable and highly recommended to researchers for the development of widely effective solar cell system for practical uses.

Keywords: D-A-D; DFT/TD-DFT; Open-circuit voltage; Optoelectronic properties; Organic solar cell; Photophysical properties

Received: 18/06/24
Accepted: 05/12/24
Published: 20/12/24

Cite as, Tigawa *et al.*, (2024). Theoretical investigation on co-sensitization of natural dyes for dye sensitized solar cells (dsscs) applications. *East African Journal of Science, Technology and Innovation* 6 (Special issue 1).

Introduction

Looking for new and efficient energy sources to meet the universal energy demand is one of the most exciting and challenging fields in scientific inquiry (Annam, 2020). The majority of the energy used worldwide today comes from fossil fuels including coal, natural gas, and petroleum (Namivandi *et al.*, 2021; Prajapat, 2023) which are unsustainable and are expected to deplete by

2040 due to an increased energy demand driven by population growth (Mohammadnezhad *et al.*, 2020). Additionally, these energy sources have a finite supply and significantly increase the emission of greenhouse gases to the atmosphere that contribute to global warming. They are also a better candidate for the degradation of the natural environment through extraction processes and their management (Annam *et al.*, 2020). Solar energy appears to be a promising and

preferable alternative to traditional fossil fuels due to its abundance and environmental friendliness (Prajapat *et al.*, 2023).

Solar energy as the best alternative to fossil fuels has been harvested by using a variety of technologies including solar cells which are regarded as the most effective technology for changing solar energy into electrical energy (Jilani *et al.*, 2020). Various types of solar cells (SCs) including dye-sensitized solar cells (DSSCs), hybrid inorganic-organic solar cells, amorphous silicon SCs, perovskite SCs, and organic solar cells (OSCs) (Shehzad *et al.*, 2020), have been successfully invented. Inorganic solar cell devices using silicon-based inorganic materials are frequently used due to their enhanced reliability, stability, and increased power conversion efficiency (PCE) (Khalid *et al.*, 2021). Nevertheless, there are several disadvantages associated with silicon-based solar cells, including their reliance on weather, space requirements, environmental issues, stiffness, and costly fabrication procedures. Owing to these drawbacks, organic solar cells (OSCs), with their low cost, simplicity of manufacture, flexibility, and promising PCE, have attracted attention as a viable solar energy harvesting technique (Ahmed and Kalita, 2018; El-Mhamedi *et al.*, 2023).

Currently, Extensive research is focused on increasing the power conversion efficiency (PCE) of OSCs through techniques such as developing materials with high-performing donor and acceptor components. using tandem device architectures, adding ternary active layers, enhancing carrier transport layers, and improving fabrication techniques. Consequently, significant improvements in PCE have been achieved for single-junction devices as well as ternary and tandem configurations of OSCs (Duan and Uddin, 2020).

However, there are still critical aspects in organic solar cells that require improvement, including increasing light absorption to produce excitons within the active layer, efficiently dividing excitons into free charge carriers at the junction materials that are donor and acceptor, and transferring these charges to the electrodes for collection, where all of this are facilitated by intrinsic electric potential or field (Taouali, 2019).

In organic solar cells, the efficiency is primarily influenced by internal processes such as intramolecular charge transfer (ICT), and intramolecular charge recombination (ICR) at the interface of materials as donor and acceptor (D/A) (Taouali *et al.*, 2019). Absolutely, fast lowering in the intermolecular charge transfer is anticipated to raise the short circuit current (J_{sc}) as well as the recombination mechanism's reaction accordingly (Babu, 2021)

To optimize these properties in OSCs, proper design is crucial to adjust the frontier molecular orbitals (FMOs) and improve cell performance. To increase the open-circuit voltage (V_{oc}), the HOMO energy level must be lowered. Additionally, ensuring that the donor's LUMO energy level is at least 0.3eV higher than the acceptor's LUMO level is necessary to ensure effective charge separation at the interface of donor and acceptor (D/A) (Babu and Vuai, 2021). The energy difference among the HOMO and LUMO levels in organic solar cells (OSCs) directly affects the short-circuit current density (J_{sc}) (Setsoafia *et al.*, 2022).

Several scholars have created electron donor materials with superior solubility, small energy gaps, great mobility, wide absorption, and ideal energy levels (Abram *et al.*, 2018). Donor-acceptor (D-A) architecture is the foundation of the materials employed in most organic solar cells because it promotes internal charge transfer (ICT) nevertheless there are certain restrictions on exciton diffusion, charge separation, and transport for D-A materials. To address these issues, an additional donor can be added to the D-A structure, creating a D-A-D configuration that helps overcome these limitations (Li *et al.*, 2022). Furthermore, the addition of an additional donor to D-A materials is important because it reduces the band gap, improves charge transport and separation, and increases absorption of visible light because donor and acceptor molecular orbitals significantly overlap (Babu and Vuai, 2021). Therefore, this research focuses on designing a novel D-A-D type molecule with two strong donor moieties Triphenylamine and carbazole -9H linked to four different acceptors A1, A2, A3, and A4 to form four different molecules that will enhance the efficacy of organic solar cells.

Materials and Methods

Computational Calculations

The computational parameters that influence the efficacy of organic solar cells to ensure improved conversion efficiency were considered. The open circuit voltage (V_{oc}) which is used to assess the effectiveness of organic solar cells was calculated as shown in equation (1).

$$V_{oc} = \{E_{HOMO}(\text{Donor}) - E_{LUMO}(\text{Acceptor})\} - 0.3 \quad (1)$$

Where E_{HOMO} (Donor) represents the HOMO energy of the donor molecule and E_{LUMO} (Acceptor) represents the energy of the PCBM acceptor. The efficiency and charge separation rate of OSCs are influenced by the exciton binding energy. This energy quantifies the Coulombic interaction between electrons and holes, A higher exciton binding energy indicates a stronger electron-hole interaction and vice versa (Hussain *et al.*, 2020). The exciton energy of molecules was also computed in this study using equation (2).

$$E_b = E_g - E_{pot} \quad (2)$$

Where E_b represents Exciton binding energy, E_g represents energy gap and E_{opt} represents initial singlet excitation energy

Computational Details

The Gaussian 09W package was employed in the computation of all of the designed molecules for

OSC technology. Density functional theory (DFT) with the hybrid Becke's three-parameter and the Lee-Yang-Parr functional (B3LYP) coupled with the 6-311G (d, p) basis set, was utilized to perform structure optimization in the ground state and to examine the optical properties of all molecules. The vertical excitation energy and electronic absorption spectra were studied by time-dependent density functional theory (TD-DFT) coupled also with B3LYP/6-311G(d,p), and the conductor polarization continuum model (CPCM) was employed to examine the designed molecules in solvent phase (Bourass *et al.*, 2017).

In investigating the performance of newly designed (D-A-D) organic molecules, four different acceptors A1, A2, A3, and A4 were substituted to two strong donors namely Triphenylamine (DI) and 9H-carbazole (D2). This resulted in the four different molecules here labeled as M1, M2, M3 and M4. The molecular design strategy for all molecules considered is presented in Figure 1.

Results

The optimized geometrical structure of four designed molecules based on the D-A-D system as presented in Figure 2, was employed to assess the conformation and planarity of proposed molecules where the selected dihedral angle in Table 1 was used to assess those characteristics.

Figure 1

The Structural molecular design used for the designation of the D-A-D framework.

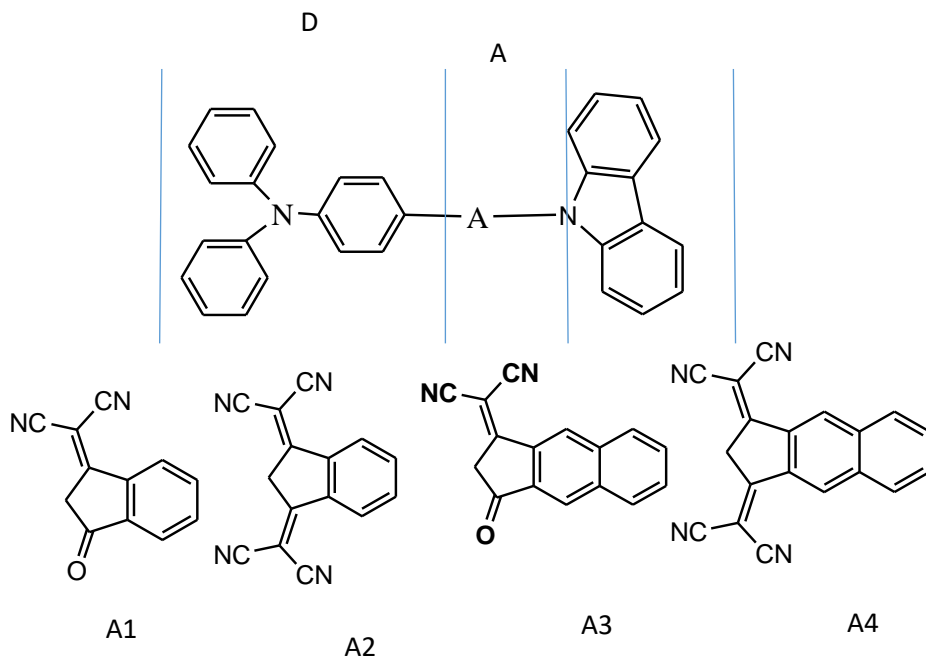


Figure 2

The optimized structure of designed molecule M1 -M4

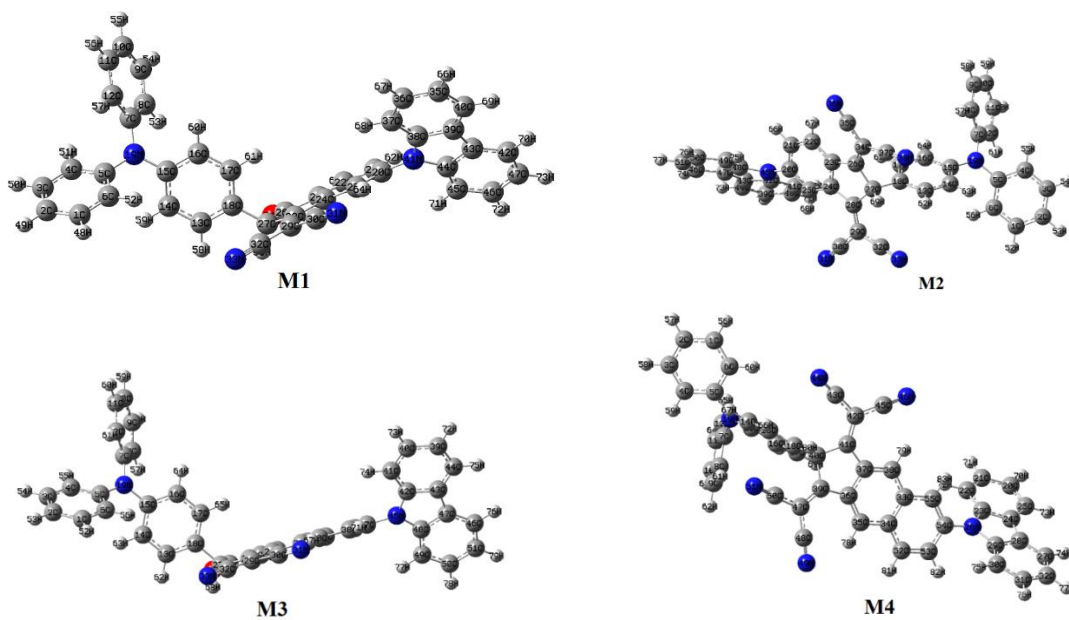


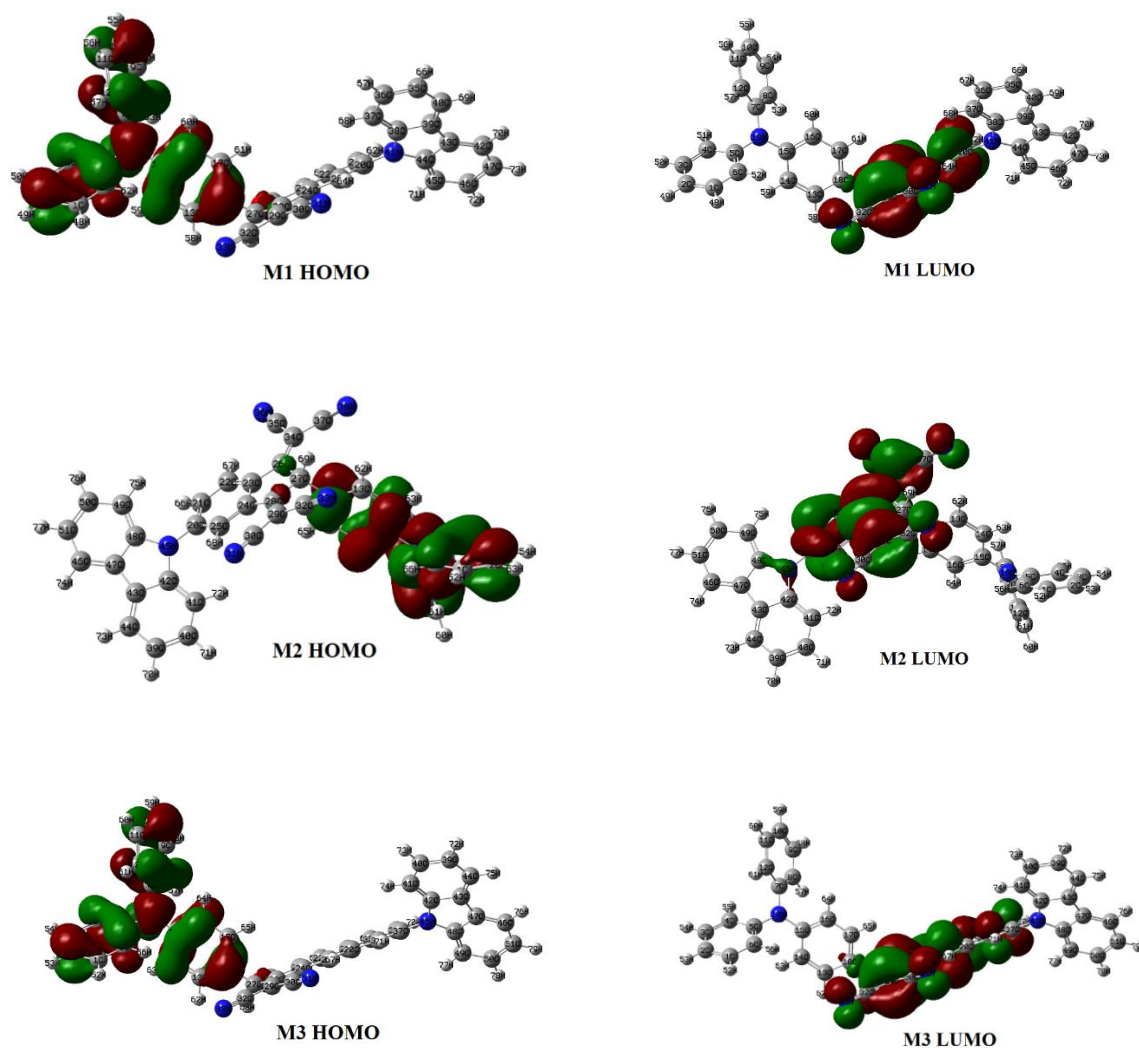
Table 1

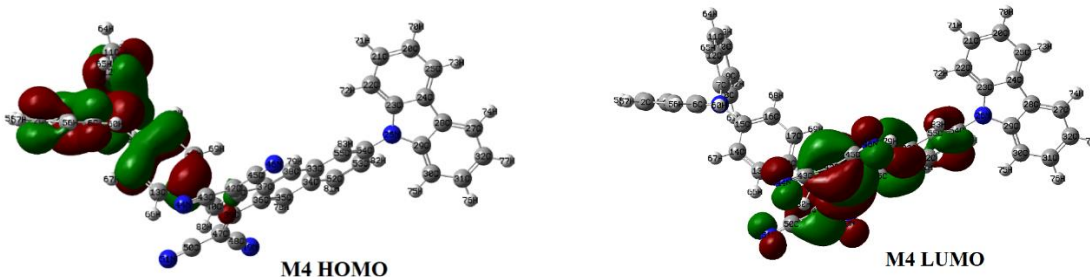
Selected dihedral angle of all investigated molecules in the solvent phase

Molecules	D-A		A-D	
	ANGLE	DEGREE	ANGLE	DEGREE
M1	C13-C18-C27-C28	142	C25-C20-N41-C44	129
M2	C13-C18-C27-C28	119	C21-C20-N45-C48	130
M3	C13-C18-C27-C28	142	C38-C37-N45-C48	126
M4	C13-C18-C40-C41	122	C53-C54-N26-C23	128

Figure 3

The HOMO and LUMO diagram of designed M1-M4 molecules in the solvent phase





The HOMO and LUMO diagrams of four designed molecules based on D-A-D are presented in Figure 3. The presented diagrams

provide insight into the molecular orbitals' distribution throughout the molecules during intramolecular charge transfer.

Table 2

The Computed absorption properties of the designed molecules M1-M4 in the solvent phase

Molecules	$E_{ex}(ev)$	$\lambda_{max} (nm)$	F	Mo contribution
M1	1.6459	753.27	0.0097	HOMO→LUMO + 1 (99.35%)
M2	1.5098	821.18	0.026	HOMO→LUMO + 1 (98.56%)
M3	1.751	708.06	0.005	HOMO→LUMO + 1 (99.37%)
M4	1.6969	730.66	0.0301	HOMO→LUMO + 1 (99.54%)

This study involves also the investigation of absorption properties. Figures 4 and 5 present the absorption properties of molecules M1-M4 as investigated through maximum wavelength and absorption intensity.

Figure 4

The simulated absorption spectra of all studied molecules in the gas phase

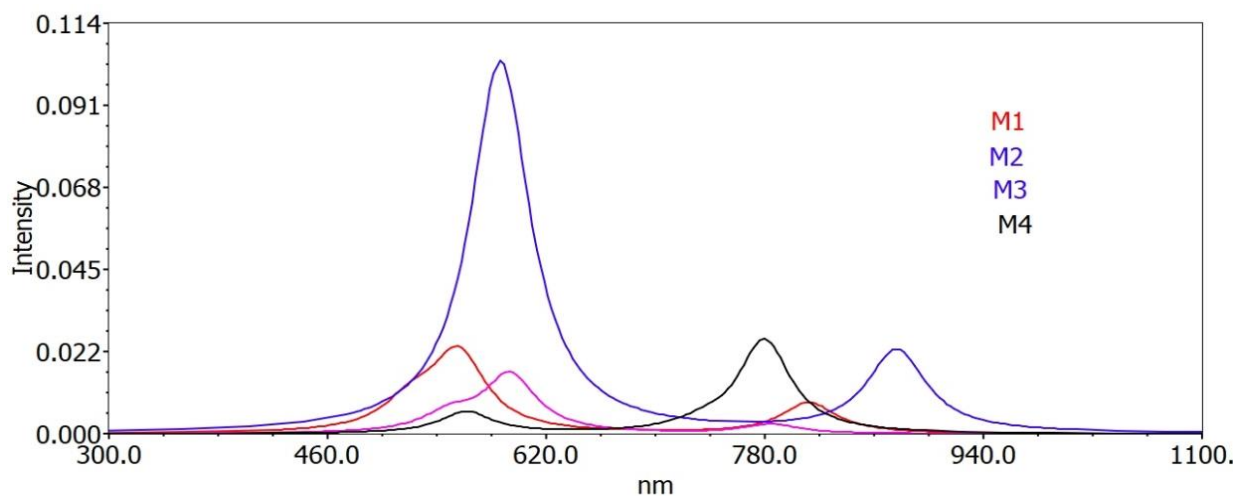
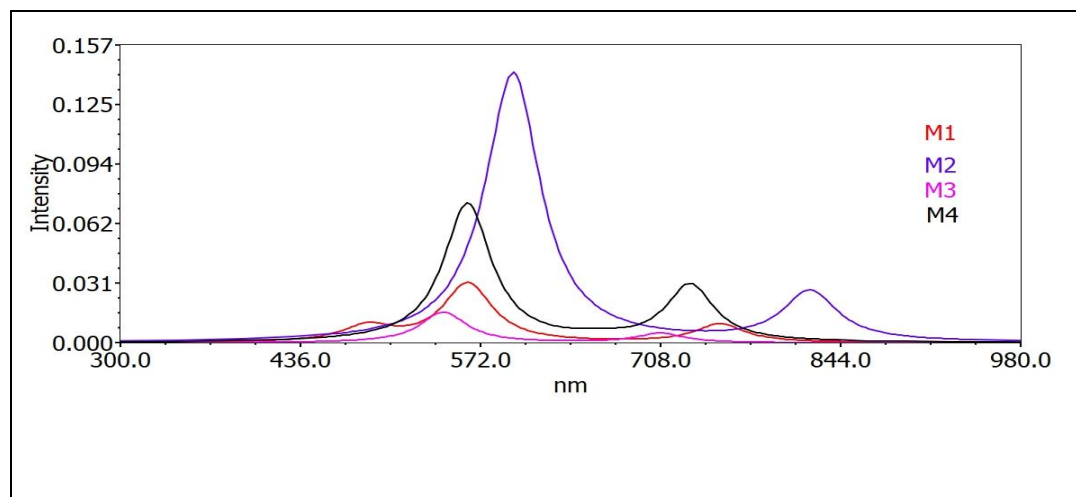


Figure 5

The simulated absorption spectra of all investigated molecules in the solvent phase.



The detailed absorption properties of the designed M1-M4 molecules which include maximum wavelength (λ_{\max}) in nm, vertical excitation energy E_{ex} in eV, oscillator strength (f), and molecular orbital (MO) contributions are presented in Table 2 and Table 3 as computed in gas phase and solvent phase, respectively.

The other properties considered in the investigation of the designed molecules were electronic and photophysical. The properties are presented in Tables 4 and 5 as they were computed in the gas phase and solvent phase, respectively. The properties were used to assess the efficiency of molecules in OSC technology.

Table 3

The electronic and photophysical properties of all investigated molecules in the gas phase.

Molecules	HOMO (ev)	LUMO (ev)	E_g (ev)	E_{opt} (ev)	E_b (ev)	V_{oc}	μ (Debye)
M1	-5.3367	-3.3747	1.96	1.5258	0.4342	1.3367	4.2347
M2	-5.5154	-3.6809	1.83	1.4139	0.4161	1.5154	5.8415
M3	-5.3037	-3.3059	1.99	1.5995	0.3905	1.3037	5.3051
M4	-5.4806	-3.4752	2.00	1.5895	0.4105	1.4806	6.679

Table 4

The electronic and photophysical properties of all investigated molecules in solvent phase

Molecules	HOMO (eV)	LUMO (ev)	E_g (ev)	E_{opt} (ev)	E_b (eV)	V_{oc}	μ (Debye)
M1	-5.4199	-3.301	2	1.6459	0.3541	1.4199	5.6516
M2	-5.4817	-3.5416	1.9	1.5098	0.3902	1.4817	7.3471
M3	-5.4115	-3.2359	2.17	1.751	0.419	1.4115	7.0804
M4	-5.4724	-3.3497	2.1	1.6969	0.4031	1.4724	8.6471

Discussion

Geometry Optimization

Through DFT/B3LYP/6-311G level optimization computations, the proposed organic molecules were optimized down to their lowest energy with no imaginary frequency emerging. The minimal energy-optimized molecular structure of all molecules was obtained and is presented in Figure 2. The planarity of the molecules plays a vital role in determining their optoelectronic characteristics and eventually their efficiency in solar cell performance. It is also useful for molecules to absorb a wide range of solar radiation since they regularly have lower energy, lower band gap, and broad absorption spectra. In this study, dihedral angles from two bonding sites (D-A and A-D) were investigated to examine the state of planar molecules by connecting three distinct units. The investigated dihedral angle reveals whether the donor unit and acceptor are oriented in the same plane within the molecules (Lyakurwa and Babu, 2023) where initial and subsequent dihedral angles are D-A and A-D, respectively. The dihedral angle between D-A and A-D was investigated after optimization and the results are shown in Table 1. The optimized molecules have the dihedral angle between 120° to 145° which is nearly 180° hence suggesting the planar conformation for the designed molecules. This assures that the molecules have the ability for light absorption and are capable of OSC application.

Frontier Molecular Orbitals

The frontier molecular orbitals studies are utilized to examine how charge moves, where HOMO levels clarify the particular bonding nature of the molecule, facilitating electron transformation, whereas the LUMO provides insight into the molecule's anti-bonding characteristics. In OSCs, electrical charge is transferred when electrons move from the HOMO of the donor to the LUMO of the acceptors and vice versa which in turn facilitates current generation. It is necessary to increase the LUMO energy to maximize sunlight capture and device performance (Deogratias *et al.*, 2020). Enhanced sunlight absorption occurs when highly stable LUMOs effectively hold a greater amount of electrons in the acceptor area of the cell for a long time, in turn, it facilitates the

conversion of sunlight to electricity thereby enhancing the functioning of the device, As presented in table 4, the value of HOMO and LUMO in the gas phase are -5.3367, -5.5154, -5.3037, -5.4806 eV and -3.3747, -3.6809, -3.3059, -3.4752 eV respectively, whereas table 5 display the value of HOMO and LUMO in acetonitrile solvent which is -5.4199, -5.4817, -5.4115, -5.4724 eV and -3.301, -3.4116, -3.2359, -3.3497 eV respectively, it implies that HOMO is lower than LUMO, therefore, all molecules have greater electronic excitation and enhanced light absorption. The inclusion of acceptor A2 in molecule M2 resulted in a lower HOMO value of -5.5154 eV in the gas phase and -5.4817 eV in the acetonitrile solvent and a higher LUMO value of -3.6809 eV in the gas phase and -3.4116 eV in acetonitrile solvent compared to other. So, this molecule has greater excitation and enhanced light absorption since it can capture more sunlight than others therefore useful in solar cell applications.

The distribution pattern or Frontier molecular orbitals (FMOs) as determined by DFT/B3LYP/6-311G calculations provides insight into the molecular orbitals' distribution throughout the molecules. During intramolecular charge transfer, the HOMO distribution show where the electrons will originate while LUMO shows where the electrons will end up. As shown in Figure 3, It shows that HOMO is extensively concentrated in the ATP unity of the donor in all molecules, this implies that the ATP donor is more effective compare to CZ. LUMO is more confined and densely packed on the acceptor of the molecules so at the acceptor it's where electrons will end up.

The energy values for the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) of the M1, M2, M3, and M4 molecules are displayed in Tables 4 and 5 for gas and solvent phases respectively. Also, all the designed compound has an energy gap range from 1.83 eV to 2eV in the gas phase as shown in table 4, and 1.9 eV to 2.17 eV in the solvent presented in Table 5. Organic solar cells will exhibit superior photovoltaic performance if the E_g is lower also the most notable charge transfer behavior is

evidenced by a narrow energy gap of the molecule as illustrated in Table 4 for gas and 5 solvent phases, from the result molecule M2 has a small energy gap of 1.83 eV in gas phase and 1.9 eV in acetonitrile solvent, which is narrow as compared to other molecules. Therefore, this signifies that it has a more pronounced charge transfer than other molecules.

Absorption properties

Tables 2 and 3 illustrate the values for the maximum absorption wavelength (λ_{max}), excitation energy (E_{ex}), oscillator strength (f), and significant MO contribution in the gas phase and acetonitrile solvent. The absorption spectra of developed molecules (M1-M4) have the maximum absorption wavelength ranging from 780.03 to 812.51 nm and 708.06 nm to 821.18 nm in both gas and solvent phases, respectively. The maximum absorption wavelength value of molecules M1-M4 was estimated by substitution of acceptors, where Molecules M2 display a broad absorption peak in spectra of 821.18 nm in the solvent phase as shown in Figure 4. Our newly created molecules have small excitation energy, hence making them perfect for use in OSCs. In organic solar cells, higher power conversion efficiency (PCE) and improved charge transfer are seen in the developed molecules with lower excitation energy, and vice versa. The increasing order of excitation energy for all suggested molecules is $M2 < M1 < M3 < M4$ and $M2 < M1 < M4 < M3$ in gas phase and acetonitrile solvent respectively, from the result M2 have lower excitation energy of 1.5098 eV compared to others. Therefore, it will absorb light in a broad range compared to other molecules.

Open circuit voltage (V_{oc})

The performance of OSCs is also measured using the open-circuit voltage (V_{oc}). The amount of V_{oc} produced is directly related to the effectiveness of organic solar cell devices. The V_{oc} indicates the maximum voltage or current reached by photovoltaic devices when no current is flowing. A high V_{oc} enhances the fill factor (FF) of organic solar cell devices, which is a crucial component in determining their efficiency (Zhao, 2015). The saturation voltage and the photo-generated current in photovoltaic devices affect the V_{oc} , which promotes recombination. The open-circuit voltage (V_{oc}) is directly influenced by the HOMO

energy of the donor and the LUMO energy of the acceptor molecules which is computed using equation 1. PC71BM ([6,6]- phenyl-C71-butyric acid methyl ester) is a highly effective acceptor due to its high electron affinity, as evidenced by its LUMO energy of -3.7eV. Since the acceptor used in this study is PC71BM, Table 4 presents the value of V_{oc} in the gas phase whereas in acetonitrile solvent the value is presented in Table 5. From the result molecule M2 has good performance compared to others with a value of 1.5154 eV in gas and 1.4817 eV in acetonitrile solvent, therefore this molecule shows high efficiency to be used in OSCs.

Exciton binding energy (E_b)

The exciton binding energy in OSCs influences the rate and effectiveness of charge separation. It quantifies the coulombic forces of interaction between electrons and holes. A higher exciton binding energy indicates a stronger coulombic interaction between electron and hole, while a lower binding energy signifies a weaker interaction. Table 5. display the exciton binding energy of the designed compound. If the exciton binding energy is lower, charge separation becomes more pronounced. From the result, all designed molecules have the exciton binding energy ranging from 0.3541 eV to 0.6392 eV in the solvent phase, where $M3 > M4 > M2 > M1$ are arranged in the order of decreasing, from the result molecule M1 has the lowest exciton binding energy (0.3541 eV) than other so this implies that it has greater charge separation rate than other donor molecules. Therefore, exciton binding energy has a significant effect on the current charge density (J_{sc}) where the lower the exciton binding energy the greater the current charge density.

Dipole moment

The polarity of the created molecules (M1-M4) in solvent acetonitrile is assessed by determining their dipole moments. The solubility of organic solar cell materials is directly related to their dipole moments, meaning that as the dipole moment increases, the solubility of the organic solar cell materials also rises (Qiu *et al.*, 2017). The charge transfer behavior of organic solar cell molecules is also affected by their dipole moment in other words a higher dipole moment enhances

electron flow between the ground and excited states. As a result, the polarity of the created molecules tends to increase at their excited states. The dipole moment (in Debye) of all studied molecules is displayed in Tables 4 and 5 in the gas and solvent phase. It was observed that the dipole moment for all molecules studied is lower in the gas phase and higher in the solvent phase (in acetonitrile). Therefore, acetonitrile has a significant effect on the solubility of all molecules since the dipole moment increased with solvent where the dipole moment for all molecules ranges from 4.2347 to 6.679 Debye in gas and 5.6516 to 8.6471 Debye in solvent phase. The acetonitrile solvent displays a significant effect on the dipole moment of all molecules from the result in table 4 and 5 all studied molecules have promising dipole moments since electrons can flow between the ground state and excited states, hence to be used in OSCs, however, molecule M4 has higher dipole moment 6.679 Debye and 8.6471 Debye the former in gas and the later in the solvent phase.

Conclusion

Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TDDFT) methods were employed to theoretically investigate the electronic structures, electronic transition characteristics, and absorption spectra of the newly developed TPA and CZ-based on D-A-D system for M1, M2, M3 and M4 molecules. Global descriptors such as band gap and FMOs were discussed as well as open circuit voltage which is an important factor that influences the efficacy and performance of organic solar cells. The result display that all the studied molecules have higher values of V_{oc} ranging from 1.4115-1.4817 eV with broader absorption spectra values ranging from 780.03 to 812.51nm in gas phase and

References

- Abram, T., Kacimi, R., Bouachrine, M., & Bejjit, L. (2018). New Molecules Based On Thiophene and Oxathiazole for Solar, Organic Application, Cells. *RHAZES: Green and Applied Chemistry*, 1(1), 31–37.
- Ahmed, S., & Kalita, D. J. (2018). Charge transport in isoindigo-dithiophenepyrrole based D-A

708.06 nm to 821.18 nm in acetonitrile solvent. Consequently, all the examined molecules have potent applications on organic solar cells. The M2 molecules which are designed with ATP and CZ linked to acceptor A2 display good performance in both studied properties including electronic, photovoltaic, and absorption properties. Since it has the maximum absorption spectra of 821.18nm, the least excitation energy of 1.5098 eV, an exciton binding energy of 0.3902 eV, a reduced energy gap of 1.9eV, and a V_{oc} value of 1.4817eV. Therefore, the design will reveal improved charge transfer and higher power conversion efficiency, hence strongly suggested for experimental studies aiming to develop highly efficient organic solar cells.

Recommendation

This work is based on computational investigations, in which the optoelectronic properties of the suggested donor molecules are theoretically calculated and predicted without doing any tests using the Gaussian 09 computer software. Verifying the optical and optical properties of the M2 as suggested to be a good performer than the other organic compounds, depends heavily on the experiment. Ultimately, the usage of artificial components is required to verify the theory that donor molecules intended for organic solar cells can be employed.

Acknowledgment

The writers express their gratitude to the College of Natural and Mathematical Science specifically at the Computational Chemistry laboratory at the University of Dodoma for supplying the computational resources used in this study.

type oligomers: A DFT/TD-DFT study for the fabrication of fullerene-free organic solar cells. *Journal of Chemical Physics*, 149(23).

<https://doi.org/10.1063/1.5055306>

- Annam, S. C., Padmavathi, K. V., Krishna, N. M., & Mannam, S. (2020). Computational Designing of Low Energy Band Gap of New Donor-Acceptor (D-A) Copolymer Monomers for Organic Solar Cells: DFT and TD-DFT Study. *Science and Technology*

- Journal*, 8(2).
<https://doi.org/10.36771/ijre.44.2>.
- Babu, N. (2022). DFT and TD-DFT studies of new triphenylamine-based (D-A-D) donor materials for high-efficiency organic solar cells. 3526–3535.
<https://doi.org/10.1039/d2ma00048b>
- Babu, N. S., & Vuai, S. A. H. (2021). Theoretical studies of optoelectronic and photovoltaic properties of D-A polymer monomers by Density Functional Theory (DFT). *Designed Monomers and Polymers*, 24(1), 224–237.
<https://doi.org/10.1080/15685551.2021.1956209>
- Bilal, M., Siddique, A., Hussain, R., Siddique, A., Mehboob, M. Y., Irshad, Z., Iqbal, J., & Adnan, M. (2020). Designing Triphenylamine-Configured Donor Materials with Promising Photovoltaic Properties for Highly Efficient Organic Solar Cells. 7358–7369.
<https://doi.org/10.1002/slct.202001989>
- Bourass, M., Touimi Benjelloun, A., Benzakour, M., Mcharfi, M., Jhilal, F., Serein-Spirau, F., Marc Sotiropoulos, J., & Bouachrine, M. (2017). DFT/TD-DFT characterization of conjugational electronic structures and spectral properties of materials based on thieno[3,2-b][1]benzothiophene for organic photovoltaic and solar cell applications. *Journal of Saudi Chemical Society*, 21(5), 563–574.
<https://doi.org/10.1016/j.jscs.2017.01.001>
- Deogratias, G., Seriani, N., Pogrebnaya, T., & Pogrebnoi, A. (2020). Journal of Molecular Graphics and Modelling Tuning optoelectronic properties of triphenylamine based dyes through variation of pi-conjugated units and anchoring groups : A DFT / TD-DFT investigation. *Journal of Molecular Graphics and Modelling*, 94, 107480.
<https://doi.org/10.1016/j.jmglm.2019.107480>
- Duan, L., & Uddin, A. (2020). *Progress in Stability of Organic Solar Cells*. 1903259.
<https://doi.org/10.1002/advs.201903259>
- El-Mhamedi, I., El-Karkri, A., El-Malki, Z., & Bouachrine, M. (2023). *Theoretical Study on New Conjugated Compounds of Organic Solar Cell : DFT , TD-DFT and AMPS1D*. 11(D), 1221–1235.
- Jilani, F., Iqbal, J., Shahid, I., Yaseen, M., Shabir Mahr, M., Khalid, M., & Ayub, K. (2020). Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. *Computational and Theoretical Chemistry*, 1187(March), 112916.
<https://doi.org/10.1016/j.comptc.2020.112916>
- Khalid, A., Khera, R. A., Saeed, A., Khalid, M., Iqbal, S., & Iqbal, J. (2021). Designing benzothiadiazole based non-fullerene acceptors with high open circuit voltage and higher LUMO level to increase the efficiency of organic solar cells. *Optik*, 228(July 2020), 1–11.
<https://doi.org/10.1016/j.jjleo.2020.166138>
- Li, Y., Huang, W., Zhao, D., Wang, L., Jiao, Z., Huang, Q., Wang, P., & Sun, M. (2022). *Recent Progress in Organic Solar Cells: A Review on Materials from Acceptor to Donor*.
- Lyakurwa, M., & Babu, S. (2023). DFT and TD-DFT study of Optical and Electronic Properties of new donor – acceptor – donor (D – A – D 0) monomers for polymer solar cells. 3(March).
- Mohammadnezhad, M., Selopal, G. S., Wang, Z. M., Stans, B., Zhao, H., & Rosei, F. (2020). *Role of Carbon Nanotubes to Enhance the Long-Term Stability of Dye-Sensitized Solar Cells*.
<https://doi.org/10.1021/acsp Photonics.9b01431>
- Namivandi, M. N., Taherpour, A. A., Ghadermazi, M., & Jamshidi, M. (2021). Novel donor-acceptor non-fullerene metal-organic solar cells based on open edge Sc@BN: a DFT and TD-DFT study. *Journal of the Iranian Chemical Society*, 18(9), 2271–2282.
<https://doi.org/10.1007/s13738-021-02188-x>
- Prajapat, K., Dhonde, M., Sahu, K., Bhojane, P., Murty, V. V. S., & Shirage, P. M. (2023). The evolution of organic materials for efficient dye-sensitized solar cells. *Journal of Photochemistry and Photobiology C: Photochemistry Reviews*, 55(April), 100586.
<https://doi.org/10.1016/j.jphotochemrev.2023.100586>
- Qiu, N., Zhang, H., Wan, X., Li, C., Ke, X., Feng, H., Kan, B., Zhang, H., Zhang, Q., Lu, Y., & Chen, Y. (2017). *A New Nonfullerene Electron Acceptor with a Ladder Type Backbone for High-Performance Organic Solar Cells*. 1–5.
<https://doi.org/10.1002/adma.201604964>
- Setsoafia, D. D. Y., Ram, K. S., Mehdizadeh-Rad, H., Ompong, D., Murthy, V., & Singh, J.

- (2022). DFT and TD-DFT Calculations of Orbital Energies and Photovoltaic Properties of Small Molecule Donor and Acceptor Materials Used in Organic Solar Cells. *Journal of Renewable Materials*, 10(10), 2553–2567.
<https://doi.org/10.32604/jrm.2022.020967>
- Shehzad, R. A., Iqbal, J., Khan, M. U., Hussain, R., Javed, H. M. A., Rehman, A. U., Alvi, M. U., & Khalid, M. (2020). Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. *Computational and Theoretical Chemistry*, 1181(January), 112833.
<https://doi.org/10.1016/j.comptc.2020.112833>
- Taouali, W., Casida, M. E., Znaidia, S., & Alimi, K. (2019). Rational design of (D-A) copolymers towards high efficiency organic solar cells: DFT and TD-DFT study. *Journal of Molecular Graphics and Modelling*, 89, 139–146.
<https://doi.org/10.1016/j.jmgm.2019.03.014>
- Zhao, J. (2015). High-efficiency non-fullerene organic solar cells enabled by a difluorobenzothiadiazole-based donor polymer combined with a properly matched small molecule acceptor. *Energy & Environmental Science*, 8, 520–525.
<https://doi.org/10.1039/C4EE02990A>