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Novel Fullerene-Based Dyes for Solar Cells Applications: Insights from Density Functional Theory and Time Dependent Density Functional Theory Investigations

Ismail Muhammad[1,2] *, Hamisu Ibrahim[2], Muhammad S. Sallau[2], Zaharaddeen N. Garba[2], Şule Erten Ela[3]

[1] Umaru Musa Yar'adua University, Ibrahim Shehu Shema Center for Renewable Energy Research, Katsina, Nigeria
[2] Ahmadu Bello University, Faculty of Physical Sciences, Chemistry Department, Zaria, Nigeria
[3] Ege University, Institute of Solar Energy, Bornova, İzmir, Türkiye

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*Correspondence: ismail.muhammad@umyu.edu.ng

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Abstract

Fullerene-based organic dyes hold significant promise for advancing solar cell technologies due to their exceptional optoelectronic properties. This study investigates two novel fullerene-based dyes, Fullerene Dye 1 and Fullerene Dye 2 (FD1 and FD2), using Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT) to evaluate their potential for solar cell applications. The electronic properties, including the Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO), and HOMO-LUMO (H-L) energy gaps, were analyzed using the B3LYP functional with a 6-31G basis set, incorporating solvation effects with dichloromethane (DCM) in the Polarizable Continuum Model (PCM). FD1 exhibited a HOMO of -5.123 eV, a LUMO of -3.458 eV, and an H-L gap of 1.665 eV, while FD2 showed a slightly larger gap of 1.807 eV with a HOMO of -5.261 eV and a LUMO of -3.454 eV. Time-dependent DFT analysis revealed maximum absorption wavelengths (λmax) of 997.10 nm and 995.16 nm for FD1 and FD2, respectively, with corresponding oscillator strengths of 0.0075 and 0.0048. The light-harvesting efficiencies, LHEs of FD1 and FD2 were 0.018 and 0.012, respectively. Both dyes demonstrated favorable reorganization energy, λ=0.15eV, driving force for charge injection, ΔG_{inj} = 0.542eV for FD1 and 0.546 eV for FD2, and low driving force for charge recombination (ΔG_{CR}), indicating strong potential for efficient charge separation. These findings provide valuable insights into the electronic, optical, and charge transfer properties of fullerene-based dyes, with FD1 exhibiting a more balanced performance. The study highlights the potential of these dyes for enhancing the efficiencies of organic, dye-sensitized solar cells (DSSCs) and provides a foundation for future experimental validation and optimization.

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1. Introduction

The exploration of fullerene-based organic dyes for solar cell applications has garnered significant attention in recent years, primarily due to their unique electronic properties and potential for enhancing photovoltaic efficiency. Fullerenes, a class of carbon allotropes, exhibit remarkable light absorption characteristics and electron-accepting capabilities, making them ideal candidates for use in organic solar cells. The theoretical modeling of these materials, particularly through DFT and TD-DFT, has emerged as a crucial approach in understanding and optimizing their performance in solar energy conversion systems (Babu, 2022). DFT and TD-DFT provide insights into the electronic structure, optical properties, and charge transfer dynamics of fullerene-based dyes, thereby facilitating the design of more efficient organic solar cells. Recent advancements in computational methods have significantly enhanced our ability to model the optoelectronic properties of fullerene derivatives. For instance, studies have demonstrated that DFT can effectively predict the electronic band structure and optical absorption spectra of various fullerene compounds, enabling researchers to identify promising candidates for solar cell applications (Fuhrer et al., 2020). The ability to simulate the interactions between fullerene-based dyes and semiconductor materials further allows for the optimization of charge transfer processes, which are critical for improving the overall efficiency of organic solar cells (Kim and Kim, 2012), (Ku et al., 2011). Moreover, the integration of TD-DFT in these studies provides a dynamic view of excited-state properties, essential for understanding the photophysical behavior of these materials under solar irradiation (Labat et al., 2012).

The role of fullerene-based dyes in enhancing the performance of organic solar cells cannot be overstated. Their incorporation into bulk heterojunction (BHJ) architectures has been shown to improve exciton dissociation and charge transport, leading to higher power conversion efficiencies (Paul and Birol, 2019), (Petrus et al., 2017). The unique structural characteristics of fullerenes, such as their spherical shape and conjugated π-systems, contribute to their effectiveness as electron acceptors in DSSCs (Sahoo et al., 2022; Tamighang, 2023). Furthermore, the development of novel fullerene derivatives through synthetic chemistry has opened new avenues for tailoring their electronic properties to meet specific application requirements (Fuhrer et al., 2020), (Sahoo et al., 2022). In addition to their promising optoelectronic properties, the stability and environmental compatibility of fullerene-based organic dyes are critical factors influencing their practical application in solar cells. Recent studies have focused on the stability of these materials under operational conditions, highlighting the importance of molecular design in mitigating degradation pathways (Zhu et al., 2020), (Petrus et al., 2017). The theoretical insights gained from DFT and TD-DFT calculations play a pivotal role in guiding the synthesis of more robust fullerene derivatives that maintain their performance over extended periods (Tamighang, 2023).

The future of fullerene-based organic dyes in solar cell applications appears promising, with ongoing research aimed at further enhancing their efficiency and stability. The integration of advanced computational techniques, such as machine learning and multi-scale modeling, alongside DFT and TD-DFT, is expected to accelerate the discovery of new materials and optimize existing ones (Paul and Birol, 2019). As the demand for renewable energy sources continues to grow, the development of efficient and sustainable solar cell technologies will rely heavily on the insights provided by theoretical modeling of materials like fullerene-based organic dyes.

The advances in theoretical modeling of fullerene-based organic dyes for solar cell applications represent a significant stride towards optimizing photovoltaic technologies. The application of DFT and TD-DFT has proven invaluable in elucidating the electronic and optical properties of these materials, paving the way for the design of high-performance organic solar cells. As research progresses, the continued exploration of fullerene derivatives and their integration into solar cell architectures will be essential for achieving the next generation of efficient and sustainable energy solutions. Conducting DFT and TD-DFT analyses before synthesizing light-absorbing dyes for application in solar cells is essential to ensure the efficient use of resources and minimize chemicals waste. In this study, we explore the key electronic and optical properties of fullerene-based dyes that make them suitable candidates for solar cell applications, as revealed by theoretical modeling using DFT and TD-DFT.

The methodological approach used in this research distinguishes it from existing literatures, which often neglects the impact of solvation on electronic properties. The quantitative insights provided by this study, including the HOMO-LUMO energy levels, absorption wavelengths, oscillator strengths, and light-harvesting efficiencies, are crucial for understanding the performance of FD1 and FD2 in DSSCs. The HOMO-LUMO gap is a vital parameter that influences the light absorption capabilities and charge transfer efficiency of the dyes (Sutradhar and Misra, 2019), (Ji et al., 2022). Additionally, the study discusses critical parameters such as reorganization energy and the driving forces for charge injection and recombination, which are essential for evaluating the operational efficiency of the dyes in solar cells (Wang et al., 2013), (Kavitha et al., 2017). The balance between light absorption, charge transfer, and recombination resistance is particularly emphasized, with FD1 demonstrating superior performance metrics compared to FD2, which aligns with findings in the literature that highlight the importance of optimizing these parameters for enhanced photovoltaic efficiency (Karthikeyan and Lee, 2013), (Ren and Zhang, 2015). Moreover, this research bridges the gap between theoretical insights and practical photovoltaic applications, paving the way for experimental validation and optimization of DSSCs. The direct correlation between computational predictions and experimental outcomes is a significant contribution to the field, as it facilitates the design of more efficient dye sensitizers (Li, 2012). By linking quantum chemistry with renewable energy innovation, the study not only enhances the understanding of dye performance mechanisms but also contributes to the ongoing development of sustainable energy technologies.

2. Materials and Methods

All calculations were performed using the Gaussian 09 software package. DFT and TD-DFT were employed for the electronic structure and optical property investigations.

2.1. Design of organic photosensitizers

The design of two organic photosensitizers, FD1 and FD2, was systematically carried out to incorporate key functional components: fullerene as the acceptor, ethyl hexyl groups for stability, a TPD (triphenylamine derivative) as the π-bridge, and cyanoacrylic acid groups for anchoring to TiO_2. This approach was guided by the design principles outlined by Kim and Kim (2012), emphasizing the specific functional roles of each moiety to enhance the photosensitizer's overall performance. The schematic of the design process is shown in Figure 1, while the resulting photosensitizer dyes are depicted in Figure 2.

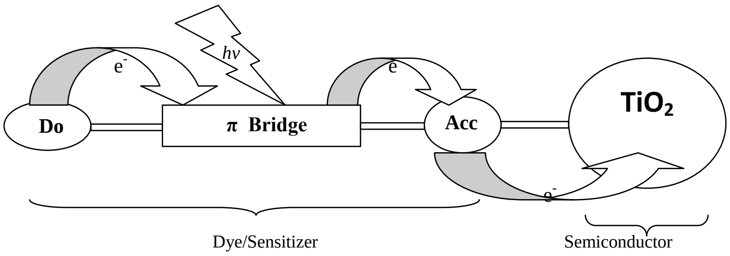
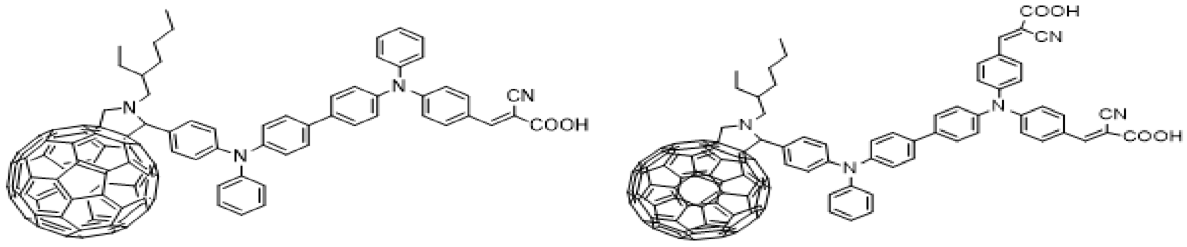


Figure 1. Design principle of photosensitizer dye



FD1 FD2

Figure 2. Design fullerene dyes

2.2. Computational details

The methodology used for studying the two fullerene-based dyes (FD1 and FD2) involved a step-by-step approach to ensure accurate analysis of their structural and electronic properties. First, the ground-state geometries of the dyes were optimized using the B3LYP functional, which combines Becke's three-parameter nonlocal-exchange functional with the Lee–Yang–Parr correlation method, along with a 6-31G (d) basis set for all atoms (Mennucci, 2012). To verify that these optimized geometries represented true energy minima, frequency calculations were performed at the same level of theory, ensuring the absence of imaginary frequencies and confirming the stability of the structures (Skora et al., 2014). Next, the solvent effects were considered by analyzing the geometries in DCM using the PCM at the same B3LYP/6-31G (d) level, which accounts for the influence of the solvent environment (Mennucci, 2012). Finally, the UV-visible absorption properties of the dyes were investigated using TD-DFT with the CAM-B3LYP functional. This approach provided more accurate predictions of excitation energies and absorption spectra (Guido et al., 2015).

3. Results and Discussions

3.1. Photosensitizer design

Figure 1 displays the structures of a novel category of dyes FD1 and FD2. These dyes were designed with specific molecular components to enhance their functionality. Fullerene was introduced as an electron acceptor due to its excellent electron mobility and ability to stabilize charge-separated states. Its incorporation aimed to enhance the electron transport and overall efficiency of the dye-sensitized system. (Paul et al., 2020). The introduction of ethyl hexyl groups improves solubility and film-forming properties while minimizing dye aggregation, thus promoting stability and performance (Majid et al., 2020). TPD serves as the electron donor, characterized by high hole mobility, facilitating charge transfer and ensuring robust interactions with both the fullerene acceptor and the anchoring group (Saccone et al., 2016). Cyanoacrylic acid acts as an anchoring group, providing strong binding to semiconductor surfaces like TiO_2, while its electron-withdrawing nature enhances charge injection efficiency (Movahedi et al., 2019). This structural design optimizes light absorption, charge transport, and dye-semiconductor interactions, which are crucial for maximizing the performance of organic photosensitizers in photovoltaic applications (Xie et al., 2022). Figure 3 shows the optimized 3D structures of the dyes prior to DFT and TD-DFT.

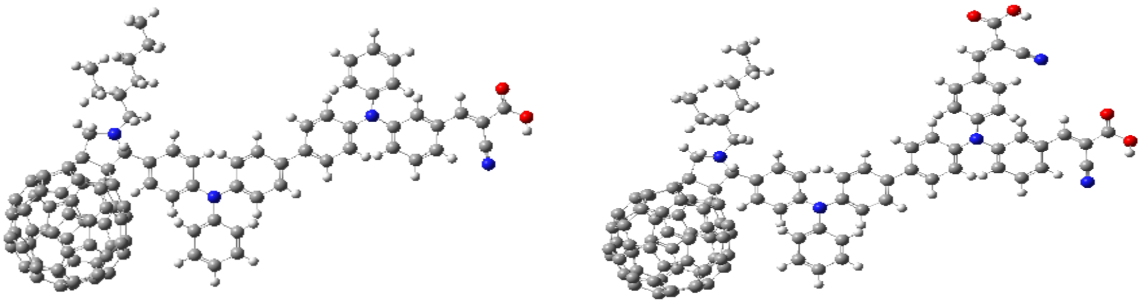


Figure 3. Optimized geometries of dyes FD1 and FD2. Gray, white, blue, red, colors represents carbon atom, hydrogen atom, nitrogen atom and, oxygen atom, respectively.

3.2. Electronic properties

Figures 4 and 5 illustrate the distributions of the HOMO and the LUMO for fullerene dyes FD1 and FD2, where fullerene acts as a strong electron acceptor. In both systems, the HOMO is predominantly localized on the donor group, while the LUMO is primarily concentrated on the fullerene. This spatial arrangement indicates effective charge separation, as electrons move from the donor to the fullerene upon excitation. The presence of cyanoacrylic acid as the anchoring group enhances this electron transfer by withdrawing electron density from the donor and facilitating its flow toward the fullerene. The electron-withdrawing nature of cyanoacrylic acid improves the coupling between the donor and fullerene, enabling efficient charge transfer. Fullerene's high electron affinity and ability to stabilize delocalized electrons further contribute to its role as a strong acceptor. Regardless of whether one (FD1) or two (FD2) cyanoacrylic acid groups are used, the LUMO remains primarily localized on the fullerene, indicating that nearly all transferred electrons are stabilized there. This highlights fullerene's dominant role in driving electron transfer and maintaining charge separation, making it an excellent component in donor-acceptor systems.

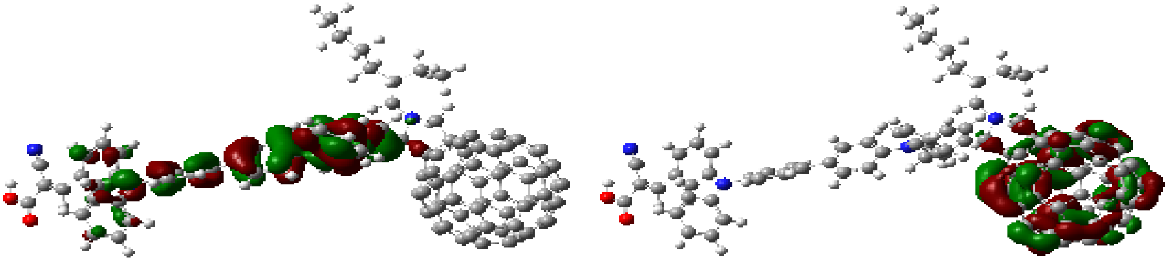


Figure 4. FD1 HOMO (Left) and LUMO (Right)

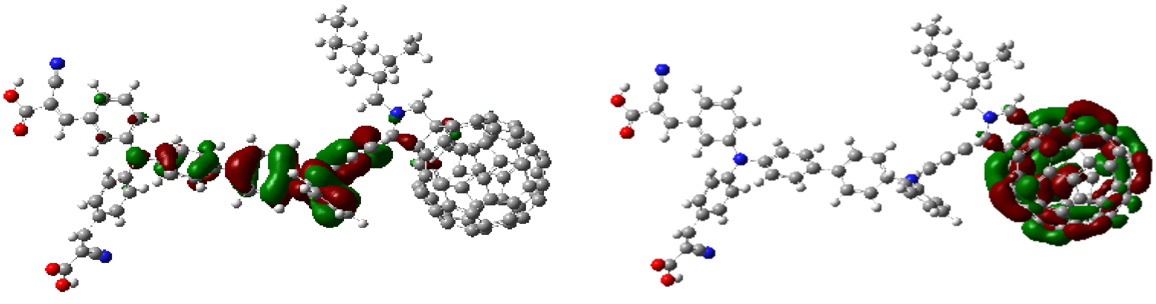


Figure 5. FD2-HOMO (Left) and LUMO (Right)

3.3. Energy levels

The data presented in Table 1 and Figure 6 illustrates the energy levels of the HOMO and LUMO for the two different dyes. The energy levels of the HOMO and the LUMO are critical in determining the charge transfer capabilities of DSSCs. The HOMO energy levels of FD1 (-5.123 eV) and FD2 (-5.261 eV) indicate that FD1 has a higher oxidation potential, suggesting a better capacity for charge donation during regeneration by the redox mediator. Both dyes exhibit LUMO levels (-3.458 eV for FD1 and -3.454 eV for FD2) that are favorable for electron injection into the conduction band of titanium dioxide (TiO_2), which is positioned at approximately -4.0 eV (Yang et al., 2015). The smaller HOMO-LUMO gap (H-Lgap) of FD1 (1.665 eV) compared to FD2 (1.807 eV) implies enhanced light absorption and electron transfer efficiency, making FD1 more advantageous for DSSC applications (Wei et al., 2015). The structural variations, particularly the number of cyanoacrylic acid groups, significantly influence the electronic properties, highlighting the importance of chemical design in optimizing dye performance (Ji et al., 2012).

Table 1. Simulated and calculated parameters of the dyes

Dyes	HOMO (eV)	LUMO (eV)	H-L gap (eV)	λ_{max} (nm)	f	LHE	λ (eV)	ΔG_{inj} (eV)	ΔG_{CR} (eV)
FD1	-5.123	-3.458	1.665	997.10	0.0075	0.018	0.15	0.542	1.665
FD2	-5.261	-3.454	1.807	995.16	0.0048	0.012	0.15	0.546	1.807

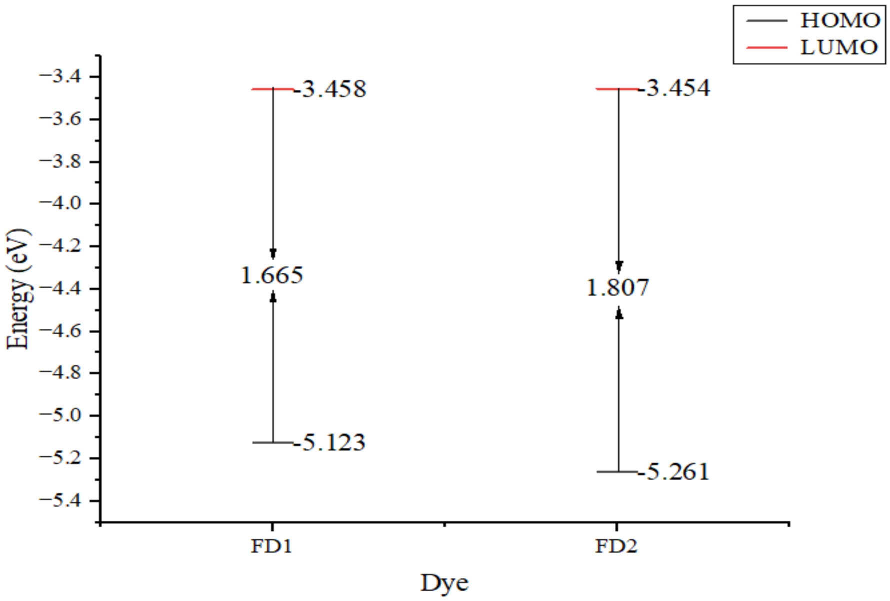


Figure 6. Energy band gaps of the dyes

3.4. Absorption spectra

The UV-Vis spectra of fullerene dyes FD1 and FD2 in Table 1 and Figure 7 reveal absorption peaks in the near-infrared (NIR) region, specifically at 997 nm for FD1 and 995 nm for FD2. Notably, FD1 demonstrates a higher absorption intensity compared to FD2, correlating with their respective molar extinction coefficients (f-values) of 0.0075 for FD1 and 0.0048 for FD2. These low f-values indicate that both dyes exhibit relatively weak electronic transitions, which is characteristic of fullerene-based compounds (Chen et al., 2012). The absorption peaks in the NIR region suggest potential applications in optoelectronic devices and photovoltaic systems, particularly for solar energy harvesting, where strong electron-accepting properties are advantageous (Zhang et al., 2017). The slight difference in peak wavelengths may be attributed to minor structural variations affecting electronic transitions (Vitnik et al., 2017). Overall, the UV-Vis data indicate that FD1 and FD2 are promising candidates for applications requiring efficient light absorption and electron transfer, with FD1 showing slightly superior performance (Zatsikha et al., 2019).

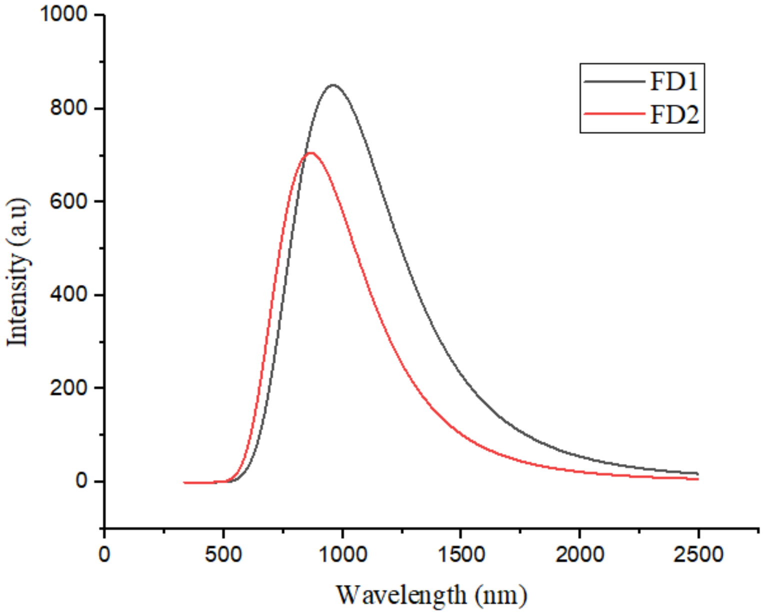


Figure 7. Theoretical UV- Vis of Dyes

3.5. Light Harvesting Efficiency (LHE), Reorganization Energy (λ), Driving Force for Charge Injection (ΔG_{inj}) and Recombination (ΔG_{CR})

LHE was calculated using the formula:

$$LHE = 1 - 10^{-f} \quad (1)$$

where f is the oscillator strength of the dye.

The FD1 outperforms FD2 in LHE, with values of 0.018 and 0.012, respectively. While these values are low due to small oscillator strengths, FD1's higher LHE suggests better light absorption (Griffith et al., 2012).

λ was typically calculated using:

$$\lambda = \lambda_{internal} + \lambda_{external} \quad (2)$$

We assume that $\lambda_{\mathrm{external}}$ is negligible, and the internal component depends on molecular-level calculations of geometry and energy. We can assume a plausible range based on literature values for fullerene-based dyes, $\lambda_{\mathrm{internal}}$~0.1−0.2eV (Selim and Mohamed, 2017).Both dyes demonstrate low reorganization energy λ=0.15eV, which is favorable for efficient charge transfer, minimizing energy losses during electron injection into the TiO_2 conduction band (Brauer et al., 2015).

ΔG_{inj} was calculated as:

$$\Delta Ginj = E_{LUMO}^{Dye} - E_{CB}^{TiO2} \tag{3}$$

Here, conduction band edge of TiO_2 is typically around −4.0eV.

In terms of charge injection; both dyes exhibit thermodynamically favorable values, with FD1 at 0.542 eV and FD2 slightly higher at 0.546 eV, indicating efficient electron transfer (Imahori et al., 2010).

ΔG_{CR} was calculated as:

$$\Delta GCR = E_{LUMO}^{Dye} - E_{HOMO}^{Dye} \tag{4}$$

However, FD1 has a lower driving force for charge recombination ΔG_{CR}=1.665 eV compared to FD2, 1.807eV. This suggests FD1 is less prone to back-electron transfer, a critical factor for maintaining high photocurrents and overall device efficiency (Selim and Mohamed, 2017).

4. Conclusions

This study explores the potential of two novel fullerene-based dyes, FD1 and FD2, for application in DSSCs through comprehensive computational analysis using DFT and TD-DFT methodologies. The findings underscore the exceptional optoelectronic properties of these dyes, particularly their efficient charge separation and favorable energy parameters. FD1, with its balanced H-L gap, strong light-harvesting efficiency, and optimal driving forces for charge injection and recombination, demonstrates slightly superior performance metrics compared to FD2. These insights not only affirm the viability of fullerene-based dyes in advancing solar cell technologies but also establish a robust foundation for further experimental validation and material optimization. By addressing the intricate interplay between electronic, optical, and charge transfer properties, this work contributes significantly to the design and development of next-generation organic and dye sensitized solar cells materials. Future studies should focus on experimental synthesis and testing to validate and refine these computational predictions, paving the way for real-world applications.

Authorship Contribution Statement

Each author contributed significantly to the study. IM and ŞEE: study conception and design; IM, HI, MSS and ZNG analysis and interpretation of results. All authors reviewed the results and approved the final version of the manuscript.

Conflict of Interest

The authors declare no conflict of interest.

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