

DFT Studies on the Effects of Functionalization on the Electronic and Optical Properties of 2,7-di-(N,N-diphenylamino)-9,9-dimethyl-9H-fluorene

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Abstract

Density functional theory (DFT) calculations using B3LYP and 6-311+ G(d,p) basis set were performed to investigate the effect of functionalization on the electronic and optical properties of 2,7-di-(N,N-diphenylamino)-9,9-dimethyl-9H-fluorene (DDF). Four derivatives with various combinations of nitro and methoxy functional groups denoted as DDF2o, DDF2n, DDF4o, and DDF4n, were used in the investigation. Conformational studies of the DDF_{2n} molecule revealed only minute energy differences among conformers in the total energy, HOMO, and LUMO energy, however, the different orientation and dipole moments may affect the device performance. Furthermore, the nitro-modified DDF derivatives have absorption spectra in a region of greater solar photon abundance. As the LUMO is located to the nitro moieties, often as strong anchoring groups, the nitro-modified DDF molecules could be excellent dye candidates for dye sensitized solar cells and for organic solar cells.

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1. Introduction

Over the past several decades, concern over the environmental crisis has come increasingly into the public eye, with some even calling it “the defining crisis of our time.”¹ One factor that has garnered particular attention is carbon dioxide emissions, which is largely related to the world energy generation and consumption. As a result, many new methods to harness energy for practical use have been developed. For example, there is currently an international implementation of piezoelectric energy harvesters.^{2, 3} Solar energy is commonly known as “one of the most environmentally benign of any electricity generating source,” and is simultaneously and consistently available worldwide.⁴⁻⁶ However, current levels of solar energy harnessing has yet to produce significant known detriment to the environment.⁷ As such, efforts on converting solar energy to the renewable energy have intensified over the past decade. The currently widely used silicon panels^{8,9} are less aesthetic in appearance¹⁰ and, most importantly, still expensive.¹¹

As an answer to the limitations of silicon solar panels, many new technologies, i.e. dye-sensitized solar cells (DSSCs) and Organic Solar Cells (OSCs), have been developed – each with their own unique merits and problems. Originally developed by O’Regan and Grätzel in 1991,¹² these devices have the potential of replacing inorganic cells with “low cost, abundant material source, easy fabrication, and low energy consumption in the production processes.”^{12, 13} There have been many research and reviews on the developments of DSSCs¹⁴⁻³⁹ as well as OSCs.⁴⁰⁻⁸⁸

Among the many ways of improving solar energy conversion efficiency, investigation of dye molecules is critical and has been one of the major focuses in research.^{36, 74, 89-110} The interest in dye molecules also stimulate their synthesis^{70, 111} and catalysis studies in general.¹¹²⁻¹¹⁴ Synthesis of these small molecules from renewable sources such as ethanol^{115, 116} or others^{117, 118} and development of catalysts¹¹⁹ are all interesting. Furthermore, these dye molecules have also been

used in the development of luminescence sensors,¹²⁰⁻¹²⁶ including the interesting organic long-persistent luminescence sensors.¹²⁷⁻¹⁴⁰ There are other types of sensors¹⁴¹⁻¹⁴⁴ using dye molecules. Additionally, the possibility of transparency and color in DSSC devices allows for the use of these devices as windows, or to fit an existing color scheme of an established business, and would make them more aesthetically pleasing.¹⁴⁵

While most of the research focus has been to functionalize organic dyes to enhance solar cell efficiency,¹⁴⁶⁻¹⁴⁹ there are many studies on the various properties of the dye molecules,^{37, 150-168} including the dynamics effect during photon excitation,¹⁶⁹ the impact of triplet state,^{170, 171} the electron-hole properties.^{172, 173} Despite of these efforts, there are still need to investigate and develop dye molecules in details. In this work, we investigated four molecules denoted as DDF4o, DDF2o, DDF2n, and DDF4n, as shown in Figure 1. Each of these is the parent molecule DDF with varying functional groups on the para-positions of the phenyl rings. Specifically, DDF4o and DDF2o have methoxy groups added, and DDF4n and DDF2n have nitro groups added.

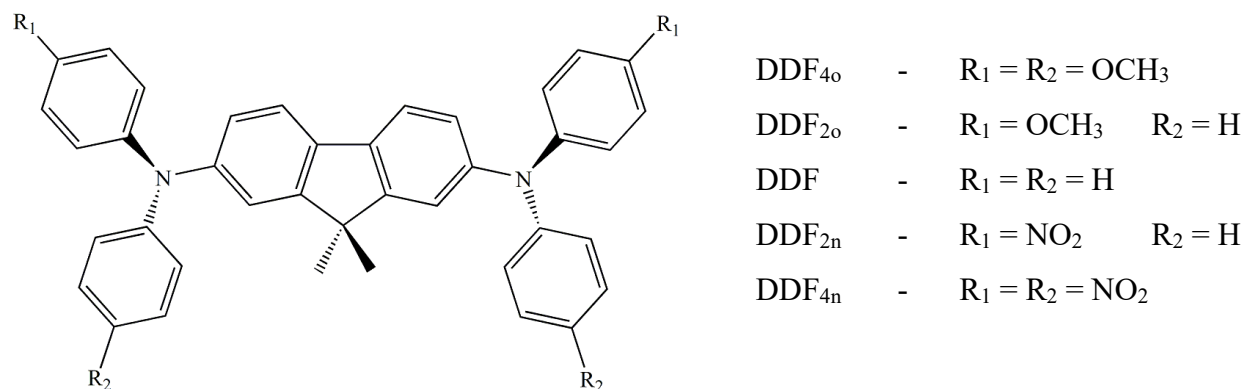


Figure 1. DDF structure and its four derivatives.

2. Computational Details

DFT calculations were performed on the molecules shown in Figure 1. For each molecule, an optimization calculation was performed, followed by frequency and TD-DFT calculations using the optimized structure. These calculations were performed in Gaussian16W software with the GaussView6.0 user-interface, using B3LYP functional,^{174, 175} and a 6-311+G(d,p) basis set. The solvent is toluene, and the solvation was treated via the Polarizable Continuum Model.¹⁷⁶ Default convergency criteria were used in optimizations.

These five molecules shown in Figure 1 were kept in the same geometric conformation (i.e. stereochemistry of phenyl rings and location of functional groups) to ensure consistency in results. No negative frequencies were observed from the frequency calculations, indicating that each of the final geometries are indeed at a minimum configuration.

3. Results

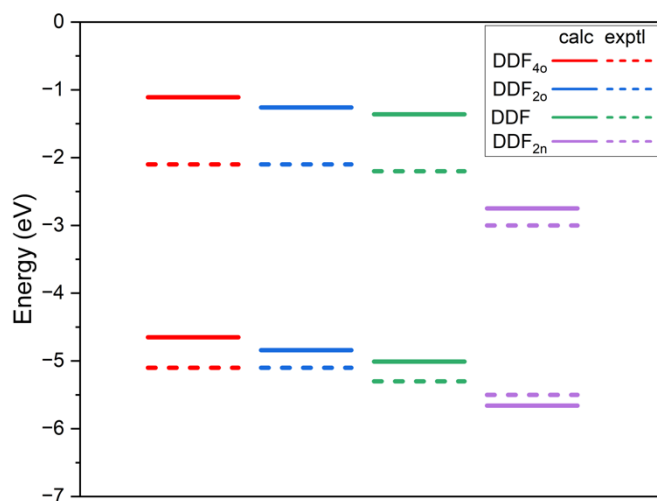
Before we present the DFT results of these five molecules in subsection 3.3, we will first discuss the results of DDF and make comparisons with the previous work, both experimentally and computationally, in subsection 3.1. Then we will discuss the results of conformers of DDF2n in 3.2. In subsection 3.4, we will discuss the potential application of these molecules in solar cell devices.

3.1 A Comparison with Previous Work

DDF was synthesized and studied as an promising organic long-persistent luminescence (OLPL) material previously.¹³⁵ Recently, it was studied using B3LYP/6-31_G(d,p) calculations.¹⁷⁷ Furthermore, DDF2o, DDF2n, and DDF4o were examined for their OLPL performance.^{127, 128} The energies of the HOMO and LUMO of the molecules, along with the maximum absorption wavelengths of the UV-Vis spectrum can be found in Table 1 and Figure 2.

Table 1. Experimental and calculated data of DDF derivatives

		HOMO (eV)	LUMO (eV)	λ_{\max} (nm)
DDF₄₀	expt ¹²⁸	-5.1	-2.1	381
	calc	-4.65	-1.11	407.2
DDF₂₀	expt ¹²⁸	-5.1	-2.1	382
	calc	-4.84	-1.26	404.8
DDF	expt ¹³⁵	-5.3	-2.2	380
	calc ¹⁷⁷	-5.02	-1.37	397.6
	calc	-5.01	-1.36	397.6
DDF_{2n}	expt ¹²⁸	-5.5	-3.0	410
	calc	-5.66	-2.75	467.2
MAE:		0.29	0.73	31.0

**Figure 2.** Experimental vs. calculated HOMO & LUMO energies of DDF derivatives.

First is a comparison of the molecular orbital energies. In every instance, our calculations have overestimated the energy of the HOMO and LUMO orbitals (i.e. higher energy), except for the

DDF2n HOMO. The mean absolute error (MAE) for the HOMO energies is 0.29eV, with a minimum error of 0.16eV and a maximum error of 0.45eV. Similarly, the LUMO energies had MAE of 0.73eV, with a minimum error of 0.25eV and a maximum error of 0.99eV. We also mention that the results of DDF using two different basis sets are essentially the same. While these errors are significant, the calculations predict the same ordering of energies among the molecules. The calculated energies of the HOMO values are ranked DDF4o > DDF2o > DDF > DDF2n. This trend is similar for the experimental values, with the main difference being that the DDF4o and DDF2o HOMO energies have equal values from experiment. It is interesting that the estimates of both HOMO and LUMO become more accurate as the molecule gains electron-withdrawing functional groups.

For the UV-Vis absorption, the MAE value is 31.0nm with a minimum of 17.6nm and maximum of 57.2nm. The MAE of λ_{\max} from the previous studies of MTPA-type molecules is 89nm,^{178, 179} indicating that these values are reasonable. It is noted that the overestimation of the HOMO-LUMO gap (and subsequently blue-shifted estimates of λ_{\max}) is mostly due to the overestimation of LUMO energies.

3.2 Effect of Conformers on the HOMO, LUMO, and UV-Vis spectra

The DDF2n molecule has four conformers, which are shown in Figure 3. Two things are being altered between these conformations. Firstly, the phenyl rings themselves can be oriented so that the amino bonding planes are parallel with one another (DDF2n^a and DDF2n^b), or so that the amino bonding planes are perpendicular to one another (DDF2n^c and DDF2n^d). Secondly, the nitro groups can be oriented on the same side of the fluorene moiety (DDF2n^a and DDF2n^c), or on opposite sides of the fluorene moiety (DDF2n^b and DDF2n^d).

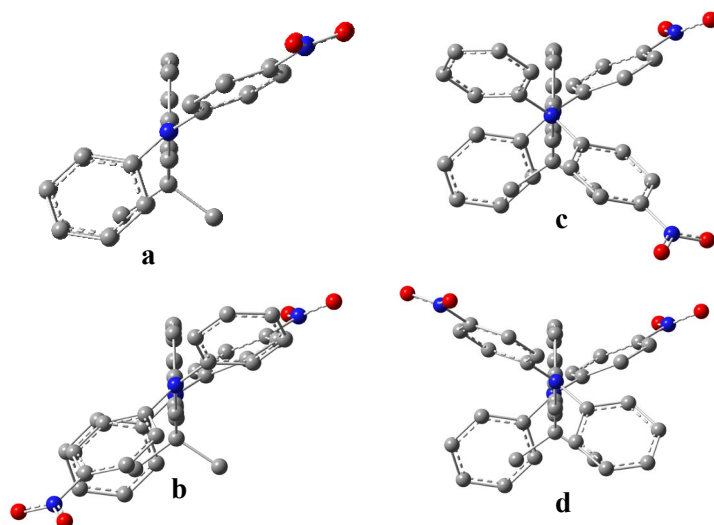


Figure 3. DDF2n conformations showing relative orientations of phenyl rings and nitro groups (H-atoms removed for clarity).

Each of these molecules was optimized, and frequency and TD-DFT calculations were performed, all in toluene. The optimized geometries are depicted in Figure 3, and no imaginary frequencies were found. Table 2 shows some of the calculated properties of these conformations. These data include the molecular total energy difference with respect to the DDF2n^a conformation and the HOMO and LUMO energies, maximum absorption wavelength, and dipole moment for each molecule.

Table 2. Comparison of data for DDF2n conformers

Molecule	Rel. Energy (kJ/mol)	HOMO (eV)	LUMO (eV)	λ_{\max} (nm)	μ (D)
a	0	-5.66	-2.75	467.2	14.6
b	-0.16	-5.66	-2.76	482.2	2.2
c	0.02	-5.66	-2.76	471.4	12.1
d	-0.25	-5.67	-2.76	477.1	8.4

The differences in total energy are primarily caused by repulsion between the two nitro groups. Specifically, both DDF2n^d and DDF2n^b have the fluorene moiety buffering the repulsion between the two nitro groups, causing them to have lower total energy. The DDF2n^b molecule then has one nitro group near the methyl group and eclipsed phenyl rings, raising its energy relative to DDF2n^d. Finally, DDF2n^a and DDF2n^c have very similar energies due to the nitro groups' closer proximity to one another. The effects of the eclipsed phenyl rings and closer proximity of nitro groups approximately are present in DDF2n^a and DDF2n^c, respectively. This discussion of the “repulsion of nitro groups” is qualitative. It may more properly be understood that the electron-withdrawing nitro groups cause a large increase of electron density in the surrounding area for many occupied molecular orbitals, with the resulting electron-electron repulsions causing a higher overall molecular energy. It is clearly not feasible to analyze all 162 occupied molecular orbitals of DDF2n, so this is generalized as the “repulsion of nitro groups.” However, it is feasible and useful to analyze the effect on the HOMO and LUMO, which are shown in Figure 4.

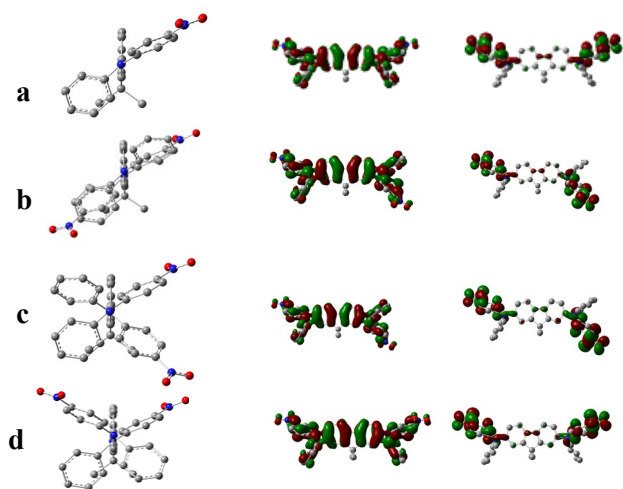


Figure 4. Visualization of HOMO and LUMO of DDF_{2n} conformers.

For each molecules' HOMO, electron density is distributed throughout the entirety of the π -bonding network. The resulting energies are nearly equivalent, with maximum difference of

0.01eV. The only notable difference is that the DDF2n^d conformation has lower energy, presumably for the same reasons as the lower total molecular energy. For each molecule's LUMO, the electron density is concentrated within the nitro groups and attached phenyl ring. It is expected that bringing the nitro groups into closer proximity would increase the energy of the LUMO. Hence, the DDF2n^a molecule has the least stable LUMO, as it has the least separation between nitro groups. This effect is expected to apply to DDF4n as well, with the staggered conformation resulting in a lower LUMO energy. Since all calculations for DDF4n were completed in the eclipsed conformation, this suggests that the LUMO value is slightly overestimated. In contrast, the electron-donating methoxy groups are away from the LUMO, and this effect should be less pronounced for DDF2o and DDF4o. However, the difference for DDF2n is again only 0.01eV, highlighting the similarity of the conformers.

With energy differences on the order of 0.25kJ/mol, these states are very similar in energy, and therefore a mixture of them is expected to be found in solution. Without a more conclusive study of individual use cases – including data like binding energies for the molecules in question, transition state barriers, etc. – it is not possible to state which conformer(s) the DDF molecules would be found in. However, they all have similar properties and should each give reasonable estimates of the physical system. In the rest of the manuscript, the conformer discussed will be denoted via superscript (i.e. DDF2n^a). Note that the “a” configuration is used for calculations of other molecules (with superscript omitted for clarity). It is common and thus complicated when dealing with organic small molecules as many isomers may present.^{96, 180} Further studies on the effect of conformers on the electronic and optical properties will be important.

3.3 Effect of Functional Groups

Table 3 showcases the effect of the varying functional groups on the molecules' HOMO and LUMO energies. The trends are rather clear: addition of electron-donating groups increases the energy of the HOMO and LUMO (DDF4o & DDF2o), and addition of electron-withdrawing groups decreases their energies (DDF4n & DDF2n). These differences have unequal size, as the nitro groups appear much more stabilizing than the methoxy groups are destabilizing. This is attributed to the fact that the nitro group is a stronger electron-withdrawing group than the methoxy group is electron donating, as evidenced by the magnitude of their Hammett constants.¹⁸¹

Table 3. Calculated HOMO, LUMO, and absorption wavelength of the DDF derivatives

	HOMO (eV)	LUMO (eV)	ΔE_{gap} (eV)	λ_{max} (nm)
DDF_{4o}	-4.65	-1.11	3.54	407.2
DDF_{2o}	-4.84	-1.26	3.58	404.8
DDF	-5.01	-1.36	3.65	397.6
DDF_{2n}	-5.66	-2.75	2.91	467.2
DDF_{4n}	-6.09	-3.19	2.9	462.6

In addition to affecting the absolute values of the HOMO and LUMO energies, the addition of functional groups affects the energy difference between these orbitals. While DDF4o and DDF2o have an overall higher HOMO and LUMO both, their difference is smaller. This is even more pronounced with the nitro-modified molecules, having an even smaller HOMO-LUMO gap. This is corroborated by a red-shifting of the absorption maxima. Furthermore, the molecules' absorption spectra will be discussed in subsection 3.4.

3.4 Application in Solar Cell Devices

Figure 5 shows the HOMO and LUMO energy values of each of the DDF derivatives along with the energy levels of the TiO₂ conduction band (-4.94eV) and the iodide/triiodide redox level (-4.04eV).³³ While all five molecules have their LUMO energy above the TiO₂ conduction band value, only the DDF4n, DDF2n, and DDF molecules have HOMO energy below the iodide/triiodide redox level. Further, the difference between the DDF HOMO and iodide/triiodide energy is not significant enough to promote feasible reaction rates (>0.2eV).³⁴ Hence, only the DDF4n and DDF2n molecules are predicted to be useful for a DSSC. It is noted that the literature values of the DDF4o, DDF2o, and DDF HOMOs are below the iodide/ triiodide redox level.^{127, 128} In other words, the MAE values for HOMO prediction was 0.29eV; any molecule with HOMO close to the energy of the iodide/triiodide redox level must be considered carefully to try and account for this error. In such cases it is useful to compare the ordering of energy levels with known molecules, as ordering is generally preserved. Here this is not necessary, as none of DDF4o, DDF2o, nor DDF have strong anchoring groups to adsorb onto the TiO₂ surface.

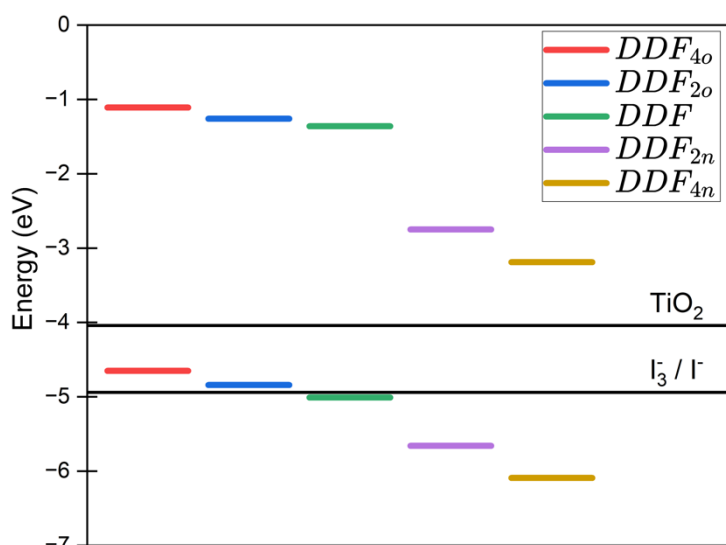


Figure 5. HOMO and LUMO energies for DDF derivatives.

Excitingly, the molecular orbital visualizations of the molecules' HOMOs and LUMOs corroborate the suggestion that the nitro-modified DDF molecules would make good dyes (Figure 6). Specifically, the HOMO of both DDF_{2n} and DDF_{4n} is distributed throughout the conjugated portion of the molecule, while the LUMO is concentrated on the nitro groups and connected phenyl rings. This means that the high-energy LUMO electron would be located close to the TiO₂ surface which the NO₂ moiety is bound to. Thus, it is expected that dye injection will be more likely, increasing device efficiency.

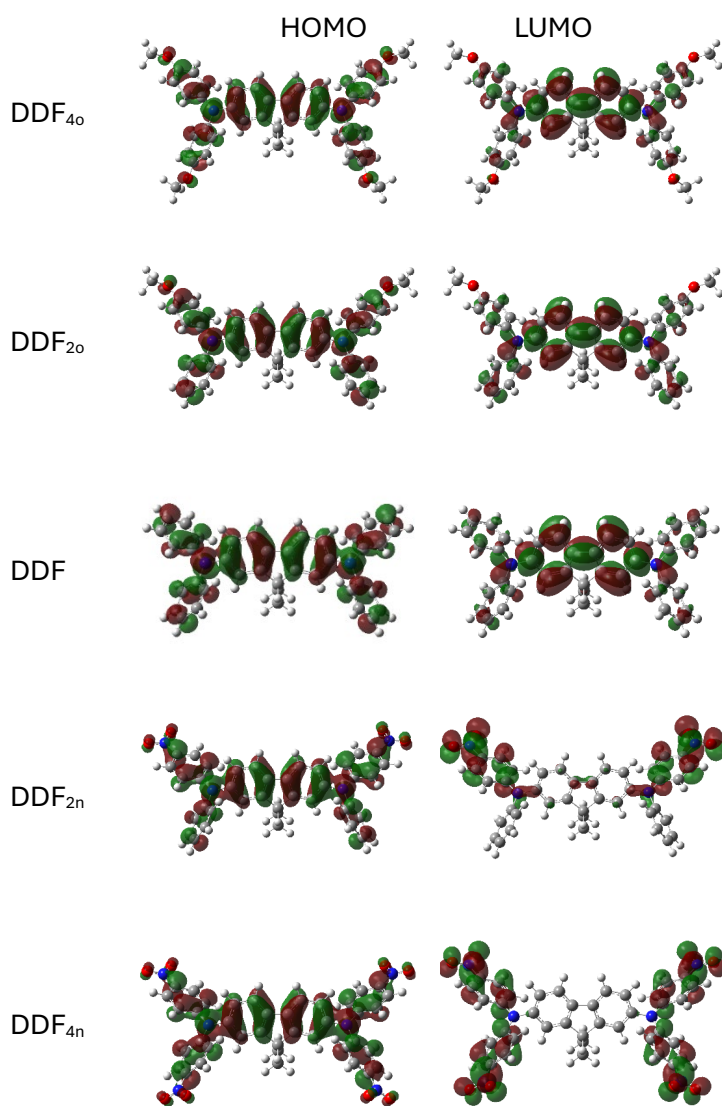


Figure 6. HOMO and LUMO visualizations for DDF derivatives.

We note that Zhang and Cole have also reported the opposite effect in literature for a molecule with dispersed LUMO.³³ This effect is expected to be less pronounced in the DDF4n molecule than for DDF2n, as the four separate nitro groups cause the LUMO orbital to be less centralized. Additionally, the HOMO distribution throughout the molecule is expected to facilitate dye regeneration by the electrolyte.

One major consideration for DSSC dye usage has been neglected up to this point: the dye must absorb visible light. Figure 7 shows the absorption spectra of each of the DDF derivatives. Additionally, the standard AM 1.5 Solar Spectra is included in Figure 7 for reference.⁸ Each of these molecules does absorb within the UV-visible region. However, the DDF4o, DDF2o, and DDF molecules have greatly blue-shifted absorption spectra, nearly into the UV region. Consequently, this is an area of lower photon abundance. The simple argument here is that “if there are fewer photons which can be absorbed, then fewer photons will be absorbed,” especially considering the similar molar absorptivity. In contrast, the DDF2n and DDF4n molecules have peak absorption near the region of maximal solar emission, suggesting further gains in efficiency for these molecules in a DSSC.

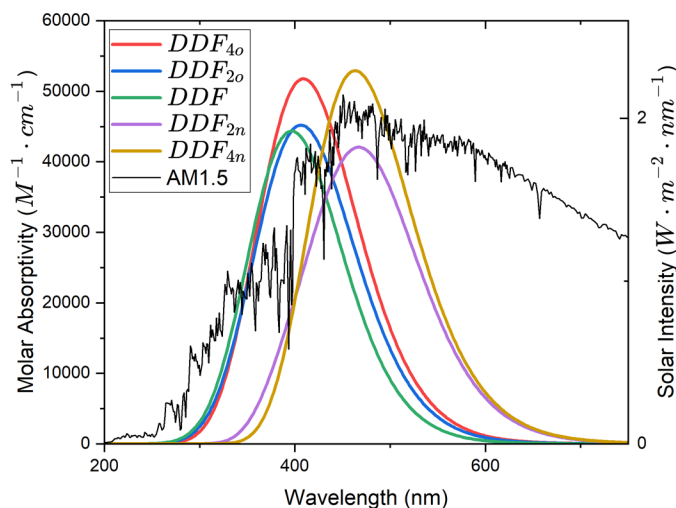


Figure 7. Absorption spectra of DDF derivatives vs. AM 1.5 Solar Spectra.⁸

The expected red-shifting (especially for DDF4n and DDF2n) is clearly present in Figure 7. In terms of absorption peak height, the DDF2n, DDF, and DDF2o molecules have approximately equal peak height, and DDF4n and DDF4o approximately equal peak height. As shown in Figure 7, dyes are needed for utilizing low energy photons of sunlight.¹⁸² For the nitro-modified molecules, many of the positive traits discussed for DSSCs carry over into the OSC case. For example, the absorption spectra of the molecules indicate that the nitro-modified DDF molecules could be an excellent light-absorbing material, regardless of which device they are used in. Similarly, the concentration of the DDF4n and DDF2n LUMO at the nitro groups will likely boost the efficiency of exciton separation and intermolecular charge transfer. One slight difference is that the DDF4n molecule having all four nitro groups with electron density may be a benefit in an OSC, in that the strictly greater number of nitro groups causes a greater chance of acceptor molecules being near a nitro group. Further, the delocalized HOMO orbitals could now facilitate intermolecular hole transport. Especially for the methoxy-modified molecules, the obvious similarities to spiro-OMeTAD suggests high potential for use as hole transport materials. The delocalization of the LUMO for DDF4o, DDF2o, and DDF may also allow them to work well as traditional OSC acceptor materials. However, their high-energy absorption spectra preclude them from being an efficient light-absorbing material.

4. Conclusions

To study functionalization effect to DDF, functional groups were added to the *para*-positions of the external phenyl rings of DDF. These functional groups included electron-donating methoxy groups and electron-withdrawing nitro groups at either two or four of the *para*-positions. DFT calculations were performed with B3LYP functional and 6-311+ G(d,p) basis set in toluene. The HOMO, LUMO, and λ_{max} values predicted from calculations were in good agreement with those

obtained experimentally for DDF_{4o}, DDF_{2o}, DDF, and DDF_{2n}. Furthermore, configurational studies of the DDF_{2n} molecule – based on the relative orientation of the phenyl rings and attached nitro groups – revealed only minute differences in energy between these states, suggesting that each could be found in solution. Different configurations of these conformers may affect the device performance as dipole moments of these conformers are different. For optical properties, it was found that the red-shifting caused by the nitro groups of DDF_{2n} and DDF_{4n} put these molecules' absorption spectra into a region of greater solar photon abundance. The LUMO of molecules with nitro groups was also found to be concentrated on the nitro groups. In a DSSC setup, the nitro groups provide potential anchoring units, which – combined with their increased LUMO density – could help to facilitate electron injection into the TiO₂ conduction band. Furthermore, in an OSC setup, this would allow the nitro-modified DDF molecules to act as superior donor molecules. Conversely, the DDF_{4o}, DDF_{2o}, and DDF molecules have a highly delocalized LUMO throughout the entire molecule, promoting their use as a hole transport material in conjunction with a donor molecule with higher HOMO and LUMO energies. However, their low absorption within the visible region of light hinders their usage as a dye or donor molecule. It is hypothesized that other electron-withdrawing functional groups, such as cyano- or 2-carboxy-2-cyanovinyl groups, would also perform well as dye or donor molecules.

Acknowledgements

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