Donor Functionalized Perylene and Different π-Spacers Based Sensitizers for DSSC Applications - A Theoretical Approach

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Abstract

Perylene based novel organic sensitizers for the Dye sensitized solar cell applications are investigated by using Density functional theory (DFT) and time dependant density functional theory (TD-DFT).The designed sensitizers have perylene and dimethylamine (DM) and N-N-dimethylaniline(DMA) functionalized perylene for the dssc applications.π-spacers are thiophene andcyanovinyl groups and cyanoacrylic acid is chosen as the acceptor for the designed sensitizers. The studied sensitizers were fully optimized by density functional theory at B3LYP/6-311G basis set on gas phase and DMF phase. The electronic absorption of the sensitizers is analyzed by TD-DFT at B3LYP/6-311G basis set in both gas and DMF phase.

1. Introduction

Dye Sensitized Solar Cells are one of the alternative of the silicon and other photovoltaic cells. The efficient DSSC was demonstrated by O'Regan and Gratal reported in 1991[1, 2]. The function of solar cell is absorbedthe photon from solar energy to produce electricity. These devices contain four parts: Oxide semiconductor [3], redox electrolyte[4], dye sensitizers[5] and counter electrode[6].The most promising sensitizers of ruthenium (Ru) complexes such as N3, N719 and black dyesareachieving PCE of 14% [7, 8]. The metal dye like ruthenium complexes are expensive and rare availability. Accordingly, the researchers are focusing todevelop the metal free organic sensitizers for the advantages of easily availability, cost effective and strong light harvesting ability [9]. The metal-free organic sensitizers have the outstanding futures such as high molar extinction coefficient and easily modification of molecular structure[9]. The D-π-A structure consists of Donor -π bridge-acceptor moieties of the dye is more useful for provide charge transfer and higher power conversion efficiency [10]. The strong electron donating ability is the main focus of electron donor and the π-spacers establish the charge transfer (CT) character of the electronic transition. The electron accepting units has accepted the electron from the π-spacers and it is directly anchored to semiconductor surface. The intramolecular charge transfer of the sensitizers is induced by D-π-A structure. These structuresare help to easily modified the donor, π-spacer and acceptor molecules and its help to tune HOMO-LUMO energy gap and redshift of the absorption spectrum of the sensitizers[11]. The addition of donor to the parent donor is increased the donating ability[12–14].These addition donors such as phenoxazine [15], N-N-dimethylaniline [16], tetrahydroquinoline [17, 18], dimethylamine [19], coumarin [20–22] and triphnylamine [23] and they used for dye molecules with higher photovoltaic performance.

Theoreticalapproach to analysis of the sensitizers is the efficient way to analysis and its help to reduce cost, time and error approaches in experimental studies[24, 25]. Theoretical method is based on DFT and TD-DFT calculations. These methods were employed to optimization and photoelectrical properties. Theoretical analysis of sensitizers was used for the studies of electronic structure, absorption spectra, NLO properties and electron injection. The perylene has the planer structure to help the electron donating ability. The N-N-dimethylaniline and dimethylamine molecule has the amine group for electron donating properties. Thiophene andcyanovinyl groups have the better charge transfer ability from the donor to

acceptor. Cyano acrylic acid is the efficient electron withdrawing moiety for the dye sensitized solar cell applications.

In the present study, perylene is the donor molecule and cyanoacrylic acid is electron acceptor groups for all the studied sensitizers and the thiophene and cyanovinyl groups are π-spacers in the different configurations. The six configurations are studied in different positions of thiophene and cyanovinyl groups. Dimethylamine (DM) and N-N-dimethylaniline (DMA) are adding the perylene donor for each six configurations. These sensitizers are investigated by studies of frontier molecular orbital analysis, absorption spectra, light harvesting efficiency, molar extinction coefficient, electron injection and regeneration, natural bonding orbital, Nonlinear optical properties.

2. Theoretical Background

The power conversion efficiency (PCE) of the dye sensitized solar cell were calculated from the following factors: open circuit voltage (V_{oc}),short circuit current (J_{sc}), fill factor (FF) and incident light energy (P_{in}) [26, 27],

$$\eta = \frac{V_{oc} J_{sc} FF}{P_{in}}$$

……1

In dye sensitized solar cell the $V_{oc}$is calculated from disparity between Fermi level of the semiconductor to the redox potential to the redox electrolyte. The short circuit current is depends the factor of photon harvesting ability and injection of electron to the semiconductor. The J_{sc} and V_{oc} should be high possess that the PCE of the solar cell will be high. The short circuit current of the solar cell was calculated to the equation,[28, 29]

$$J_{sc} = \int_{\lambda} LHE(\lambda)\, \varphi_{inject} \eta_{collect} d\lambda$$

……2

Where LHE is the light harvesting efficiency and $\phi_{inject}$is the electron injection efficiency of the sensitizers. for DSSC's the electrode is same and dye sensitizers only differs. So the $\eta_{collect}$ of the DSSC is assumed to be constant.

The LHE of the sensitizers were calculate from the following equation,

$LHE = 1 - 10^{-f}$ …….. (3)

Where, f is the oscillator strength of the sensitizers.

The ϕ_{inject} were calculated from electron driving force ΔG_{inject}. The ΔG_{inject} of the sensitizers were calculated from the equation,[30, 31]

$$\Delta G_{inject} = E^{*}_{OX} - E^{SC}_{CB}$$

……..4

Where, E^{*}_{OX} is the excited state oxidation potential of the sensitizers and E^{SC}_{CB} is the ground state reduction potential of the conduction band edge of the TiO_2. The excited state oxidation potential were calculated from the equation as,

$$E^{*}_{OX} = E_{OX} - \lambda_{max}$$

……..5

Where, E_{ox} is the redox potential of the ground state of the sensitizers and vertical transition energy corresponding to the maximum absorption (λ_{max}).

The elelctron regeneration efficiency of the sensitizers were determined from the driving force for regeneration ΔG_{reg} is given by,[32]

$\Delta G_{reg} = E_{ox} - E_{redox}$ …….. (6)

Where, E_{redox} is the redox potential of the I^{-}/I^{3-} electrolyte (4.8eV).

The Nonlinear optical properties of the sensitizers are determined from dipolemoment and static polarizability to the following equations,[33]

$$\mu_{tot} = \sqrt{(\mu_x^2 + \mu_y^2 + \mu_z^2)}$$

……..7

$$\alpha_0 = \frac{(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}$$

……..8

Where, α_{xx}, α_{yy} and α_{zz} is the polarizability tensor componants.

3. Computational Details

The entire work, the designed sensitizers were ground state optimized on both gas and DMF phase by density functional theory method of B3LYP with 6-311G(d,p)[34–36] basis set using Gaussian 09 program [37] Gauss view visualization program [38] was used for designed the the molecular structure of the sensitizers and Gausssum 3.0 software[39] were to analysis the electronic excitation properties. The solvent effect and projectionof the absorption properties of the sensitizers DMF phase were analyzed from polarizable continuum model (PCM) [40]. The absorption spectrum vertical excitation energy of the sensitizers were investigated by TD-DFT with CAM-B3LYP/6-311G(d,p) basis set [41] in both gas and

DMF phase. During the calculation, the 50 vertical singlet-singlet transitions are considered into the account.

4. Result And Discussion

4.1 Structure of the sensitizers.

Perylene based D-π-A structured sensitizers are investigated by DFT/ B3LYP-6-311G basis set. All configurations of π-spacers and acceptor is reported at pounraj et al.[42] These sensitizes have 6 configurations of π-spacers positions and mono anchoring group with cyano acrylic acid. Thiophene and cyanovinyl groups are π-spacers in the different configurationsand configurations of the sensitizers have different positions of same groups. Thiophene and cyanovinyl group already provide good PCE of the DSSC applications. Especially thiophene based sensitizers have lower energy gap and broad absorption spectrum. In the present work, mainly focused the perylene donor and dimethylamine and N-N-dimethylaniline functionalized perylene combined with above π-spacers and acceptor configuration. Perylene is the polycyclic aromatic hydrocarbon and their intrinsic π – conjugation and chargew delocalization properties exhibits there is used for optoelectronocapplications Perylene and its derivatives with huge absorption coefficient, high fluorescence quantum yield and outstanding photo chemical stability have been widely employed as luminous probes in cytochemistry, dopants in organic light emitting diodes[43]. Perylene structure is shown in Fig. 1.

Perylene have twelve functionalizable positions in which 3,4,9,10 positions are known as peri, the 1,6,7,12 positions are known as bay and the 2,5,8,11 are ortho positions. The π-spacers are connected to the 10th positions of the perylene donor. The π-spacers are transfer electron from donor to acceptor.Moveable π-bonds is the key constraint for π-bridge .More number of π-spacers is minimizing the band gap and improves absorption spectrum. The six configurations of the spacer are substituted in the perylene and donor functionalized perylene. The donor modified perylene donor has dimethylamine and N-N-dimethylaniline donor group.In the study dimethylamine andN-N-dimethylaniline are indicates that DM and DMA andperylene donor sensitizer are indicates that PER and donor functionalized perylene sensitizers are indicates DM-PER and DMA-PER. DM and DMA groups are connected to the 2nd, 5th position of each perylene sensitizers.The chemical structure of the sensitizers is illustrated in Fig. 2(a-c) andstructural arrangement is summarized in Table 1. Configurations 2 and 3 have similar molecular formula and different π-spacer setup and also, configurations 4, 5 and 6 have similar molecular formula and different π-spacer setup. The geometrical structure of the PER, DM-PER, and DMA-PER sensitizers are in illustrated in Fig. 3.

Table 1
Structural arrangement of PER, DM-PER and DMA-PER dye molecules.

Configurations	Perylene based	Additional donor group	
		Dimethylamine	N-N-dimetylaniline
Configurations – 1	PER-1	DM-PER-1	DMA-PER-1
Configurations – 2	PER-2	DM-PER-2	DMA-PER-2
Configurations – 3	PER-3	DM-PER-3	DMA-PER-3
Configurations – 4	PER-4	DM-PER-4	DMA-PER-4
Configurations – 5	PER-5	DM-PER-5	DMA-PER-5
Configurations – 6	PER-6	DM-PER-6	DMA-PER-6

PER sensitizers:

The PER sensitizers have perylene as a donor. The six π-spacers configurations are connected to the perylenering in the 10th position and due to this connection, the sensitizers are named as PER-1,PER-2, PER-3,PER-4,PER-5 and PER-6.The optimized structure of the PER sensitizers is shown in Fig. 3.

DM-PER sensitizers:

The DM-PER donors have perylene and dimethylamine molecules. The dimethylamine molecule is attached the perylene in the positions of 2nd and 5th. The DM molecule has the planer structure and higher electron donating ability. The planer structures of the molecules were help to effective electron transfer process. Due to the substitution, the sensitizers were named as, DM-PER-1,DM-PER-2, DM-PER-3,DM-PER-4,DM-PER-5 and DM-PER-6. The optimized structure of the PER sensitizers is shown in Fig. 3.

DMA-PER sensitizers:

The DMA-PER donors have the perylene substituted with theN-N-dimethylanilinemolecule. N-N-dimethylaniline (DMA) molecule was dimethyl amino group connected to a phenyl group. The DMA dyes have simpler structures and are strong electron donating ability compared to coumarin(r). Due to the substitution, the sensitizers were named as, DMA-PER-1,DMA-PER-2, DMA-PER-3,DMA-PER-4,DMA-PER-5 and DMA-PER-6. The optimized structure of the PER sensitizers is shown in Fig. 3.

4.2 NBO analysis:

Natural Bonding Orbital values are determining the population of charges on the molecules and intramolecular charge transfer to the acceptor from donor through π-spacers[44–48]. NBO values are positive and negative, which is indicating that electron donating ability and accepting ability. q^{donnor} values are positive indicates that, donor molecules areelectron donating groups. A negative value of the $q^{acceptor}$ represents that, electron accepting from π-spacers effectively. Positive $q^{\pi-spacers}$ values are

illustrated by electron donating ability and π-spacers acts as donor molecules. Cyano acrylic acid has more negative values are indicating that strong electron acceptor. Charge variation between natural charges of the donor and acceptor molecules represented as q^{D-A}. The higher values of q^{D-A} are illustrated as stronger charge separation.The charge population values of dye molecules are listed in Table 2. All the molecules have positive q^{D-A} values and the configuration 2 has the maximum values of the alldonor groups. From Table 2, configuration 5 of the all donor groups and DM-PER-2 has the negative value of $q^{\pi-spacers}$ values indicates that, the π-spacers are acting as an acceptor. Configurations 2 and 3 have different spacers configuration and same molecular formula but different q^{D-A} values. Similarly configuration 4, 5 and 6 has the same. The above results show that, the configuration 2 of the dimethylamine and N-N-dimethylaniline functionalized donors based sensitizers have the higher q^{donnor} values comparatively other dye sensitizers and more donating ability then others.

Table 2
NBO analysis of PER, DM-PER and DMA-PER dye molecules.

Dye	q^{Donor}	$q^{\pi-spacers}$	$q^{Acceptor}$	Δq^{D-A}
PER – 1	0.11723	-	-0.1173	0.23456
PER – 2	0.11675	0.0296	-0.14632	0.26307
PER – 3	0.05063	0.04084	-0.09147	0.1421
PER – 4	0.11135	0.03235	-0.14369	0.25504
PER – 5	0.09466	-0.00367	-0.09101	0.18567
PER – 6	0.0284	0.05019	-0.07856	0.10696
DM-PER-1	0.13154	-	-0.13152	0.26306
DM-PER-2	0.13734	0.01809	-0.15542	0.29276
DM-PER-3	0.13734	-0.03252	-0.10481	0.24215
DM-PER-4	0.1303	0.01802	-0.14831	0.27861
DM-PER-5	0.11069	-0.01532	-0.09535	0.20604
DM-PER-6	0.03652	0.04548	-0.08202	0.11854
DMA-PER-1	0.13076	-	-0.13081	0.26157
DMA-PER-2	0.13708	0.01845	-0.15557	0.29265
DMA-PER-3	0.06455	0.03501	-0.09958	0.16413
DMA-PER-4	0.13409	0.01568	-0.14976	0.28385
DMA-PER-5	0.11437	-0.01754	-0.09684	0.21121
DMA-PER-6	0.03886	0.0445	-0.08339	0.12225

4.3 Frontier Molecular Orbital analysis

The electron density charge distribution of the sensitizers is the vital parameter of the photo excitation process. The photo excitation is the fundamental process of the mechanism of DSSC. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels, energy gap (E_g) of sensitizers crucial factor for the charge separation process. During the charge separation process the energy gap of the HOMO and LUMO energy levels should be minimum and it's provide better efficiency of the solar cell[10]. The HOMO and LUMO energy values and energy gap of the PER, DM-PER and DMA-PER sensitizers in gas phase and DMF phase is summarized in the Table 3 and energy gap of the sensitizers is illustrated in Fig. 4. The HOMO values of all the sensitizers are above the CBE of semiconductor (-4.0 eV) and LUMO values are below the redox electrolyte (-4.8eV)[49, 50]. The π-spacer of the sensitizers is extended due to inclusion of thiophene and cyanovinyl group and change the configuration of the π- spacer is decrease the energy gap. The configuration 2 and 3 has the similar molecular formula and differentpositions and configuration 4,5 and 6 also same. PER, DM-PER and DMA-PER sensitizers are optimized in DMF phase in using polarizable continuum model (PCM). The energy gap of the sensitizers is minimum as compared to Gas phase due solvent polarization. The solvent polarization is stabilizes the energy levels so$E_g$has been reduced. The energy gap of the PER sensitizers in gas phase in the decreasing order: PER-1 > PER-2 > PER-3 > PER-4 > PER-5 > PER-6. The PER-6 has the minimum$E_g$value of 1.830eVin the six configurations. The $E_g$values of the PER sensitizers in DMF phase in the decreasing order as same as gas phase. The energy gap of the DM-PER sensitizers in gas phase in the decreasing order: DM-PER-1 > DM-PER-2 > DM-PER-3 > DM-PER-4 > DM-PER-5 > DM-PER-6. The PER-6 has theminimum $E_g$value of 1.582eV in the six configurations. The energy gap values of the DM-PER sensitizers in DMF phase in the decreasing order as same as gas phase. The energy gap of the DM-PER sensitizers in gas phase in the decreasing order : DMA-PER-1 > DMA-PER-2 > DMA-PER-3 > DMA-PER-4 > DMA-PER-5 > DMA-PER-6. The DMA-PER-6 has the lowest energy gap value of 1.534eV in the six configurations. The energy gap values of the PER sensitizers in DMF phase in the decreasing order as same as gas phase. The HOMO and LUMO charge distribution of the studied sensitizers are localized in the Donor and acceptor part. The HOMO-LUMO charge distribution of the studied sensitizers is illustrated in Fig. 5 (a-c). From Fig. 5 (a-c), the electron density of HOMO is localized in donor and LUMO is localized in π-spacer and acceptor. HOMO is localized in the entire molecule of configuration-1 of the all donors. The LUMO of the all sensitizers are localized in the acceptor part this is help to electron injection of the Cyanoacrylic acid effectively. From results shows that, the N-N-dimethylaniline functionalized DMA-PER sensitizers have minimum energy gap compared the other donor groups and Configuration-6 better than others of the all donorsespecially DMA-PER-6 have the lowest Eg value and more suitable for the DSSC applications.

Table 3
HOMO-LUMO values of PER sensitizers in Gas phase and DMF phase

Dyes	Gas phase (eV)		E_{H-L}	DMF phase (eV)		E_{H-L}
	HOMO	LUMO		HOMO	LUMO	
PER-1	-5.647	-3.089	2.559	-5.585	-3.106	2.478
PER-2	-5.545	-3.374	2.170	-5.488	-3.359	2.129
PER-3	-5.532	-3.363	2.168	-5.452	-3.360	2.093
PER-4	-5.524	-3.561	1.963	-5.444	-3.502	1.942
PER-5	-5.569	-3.607	1.962	-5.425	-3.524	1.901
PER-6	-5.560	-3.730	1.830	-5.396	-3.639	1.757

4.4 Optical properties.

Absorption spectra of the sensitizers have the extensive spectrum of absorption in the visible to Near IR. Intramolecular charge transfer process of the sensitizer take place while during photo excitation process. The ICT process is crucial parameter for improve the J_{sc}. The studied sensitizers is calculated by TD-DFT with B3LYP-6-311G basis set in gas phase and DMF phase. The absorption spectra of the sensitizers are illustrated as Fig. 6 and absorption maximum (λ_{max}), Molar extinction coefficient(ε) of the sensitizers are encapsulated in Tables6,7,8and also oscillator strength (f), transition assignment of the sensitizers are summarized in Table 4. Absorption maximum wavelengths of parent configuration perylene based sensitizers are in the range of 454nm to 541nm. The maximum value of 541nm having configuration-4. The configuration 2 and 3 have similar molecular formula and configuration disparate from the π-spacers the maximum absorption is decreased. The configuration 4, 5 and 6 has also same as above. These above results are same as dimethylamine and N-N-dimethylaniline functionalized donors. The configuration 2 and 4 has bathochromic shift of the absorption maximum values compared the configuration 1 and 3 due to addition of thiophene and cyanovinyl groups. All the designed sensitizers are calculated in DMF phase and the sensitizers are bathochromic shift due to the solvent effect. The absorption maximum values of the sensitizers are same as bathochromic and hypsochromic shift in the gas phase. Molar extinction coefficient (ε) is another important parameter of absorb the photon to inject the electron to the semiconductor. The ε values of the sensitizers of are in the range of 5.3 x 10^4 to 16.4 x 10^4. The molar extinction coefficient of the PER sensitizers in gas phase are in the decreasing order: PER-6 > PER-5 > PER-4 > PER-2 > PER-3 > PER-1. The PER-6 has the high value of (ε) compared to the other sensitizers. The (ε) values of the PER sensitizers in DMF phase in the decreasing order as same as gas phase.The (ε) value of the DM-PER sensitizers are in the decreasing order:DM-PER-5 > DM-PER-6 > DM-PER-4 > DM-PER-2 > DM-PER-3 > DM-PER-1.The (ε) values of the PER sensitizers in DMF phase in the decreasing order: DM-PER-6 > DM-PER-5 > DM-PER-4 > DM-PER-2 > DM-PER-3 > DM-PER-1. The molar

extinction coefficient of the DMA-PER sensitizers are in the decreasing order : DMA-PER-5 > DMA-PER-6 > DMA-PER-4 > DMA-PER-2 > DMA-PER-3 > DMA-PER-1.The ε values of the PER sensitizers in DMF phase in the decreasing order: DMA-PER-6 > DMA-PER-5 > DMA-PER-4 > DMA-PER-2 > DMA-PER-3 > DMA-PER-1. All the designed sensitizers have higher value of (ε) in DMF phase compared to gas phase since of due to solvent effect. The configuration 6 has the higherε of the all the sensitizers and more efficient to DSSC applications.

Table 4
HOMO-LUMO values of DM-PER sensitizers in Gas phase and DMF phase

Dyes	Gas phase (eV)		E_{H-L}	DMF phase (eV)		E_{H-L}
	HOMO	LUMO		HOMO	LUMO	
DM-PER-1	-5.206	-2.870	2.336	-5.137	-3.031	2.106
DM-PER-2	-5.166	-3.233	1.933	-5.098	-3.323	1.775
DM-PER-3	-5.223	-3.272	1.951	-5.058	-3.342	1.716
DM-PER-4	-5.253	-3.473	1.780	-5.082	-3.478	1.604
DM-PER-5	-5.293	-3.532	1.761	-5.071	-3.510	1.561
DM-PER-6	-5.255	-3.674	1.582	-5.027	-3.630	1.398

Table 6
Absorption maximum (λ_{max}), molar extinction coefficient (ε) of the PER sensitizers

Dye	λ_{max}		ε x10^4	
	Gas phase	DMF phase	Gas phase	DMF phase
PER – 1	454	484	5.297	6.339
PER – 2	509	536	8.436	9.630
PER – 3	476	494	8.038	9.752
PER – 4	541	565	13.338	14.628
PER – 5	528	552	15.873	17.647
PER – 6	510	535	16.409	18.334

Table 7
Absorption maximum (λ_{max}), molar extinction coefficient (ε) of the DM-PER sensitizers

Dye	λ_{max}		ε x10^4	
	Gas phase	DMF phase	Gas phase	DMF phase
DM-PER-1	474	504	4.949	5.816
DM-PER-2	531	553	8.069	9.137
DM-PER-3	494	506	7.663	9.481
DM-PER-4	557	575	13.069	14.443
DM-PER-5	540	559	15.470	17.457
DM-PER-6	520	538	15.159	18.135

Light harvesting efficiency is anothervitalconstraint for intensity of the absorption spectra of the sensitizers. The LHE values of the sensitizers are calculated by Eq. 3 and tabulated in Table 5. From the Table 5, the LHE values are functionalized perylene sensitizers are higher compared to perylene donor. The configuration 1 has the minimum LHE value of the designed sensitizers. The configuration 2 and 3 has the similar molecular formula and different π-spacer positions, but different LHE values. The results of Configuration 4,5,6 as same as configuration 2 and 3. The configuration 6 has the maximum value of LHE, it seen that it is better candidate for DSSC applications. Dimethylamine and N-N-dimethylaniline functionalized DM-PER-6 and DMA-PER-6 has the higher LHE values which indicates, these are better candidate compare to other sensitizers.

Table 5
HOMO-LUMO values of DMA-PER sensitizers in Gas phase and DMF phase

Dyes	Gas phase (eV)		E_{H-L}	DMF phase (eV)		E_{H-L}
	HOMO	LUMO		HOMO	LUMO	
DMA-PER-1	-5.198	-2.866	2.331	-5.234	-3.086	2.148
DMA-PER-2	-5.168	-3.218	1.950	-5.208	-3.343	1.865
DMA-PER-3	-5.142	-3.243	1.900	-5.185	-3.354	1.832
DMA-PER-4	-5.177	-3.444	1.733	-5.198	-3.494	1.705
DMA-PER-5	-5.213	-3.506	1.707	-5.192	-3.519	1.672
DMA-PER-6	-5.183	-3.649	1.534	-5.169	-3.635	1.534

Table 8
Absorption maximum (λ_{max}), molar extinction coefficient (ε) of the DMA-PER sensitizers

Dye	λ_{max}		ε x10^4	
	Gas phase	DMF phase	Gas phase	DMF phase
DMA-PER-1	469	495	5.692	6.558
DMA-PER-2	531	548	9.145	10.210
DMA-PER-3	499	506	8.225	10.219
DMA-PER-4	563	576	13.867	15.229
DMA-PER-5	547	561	16.270	18.268
DMA-PER-6	527	540	15.639	18.976

Table 9
Oscillator strength (f), Light harvesting efficiency of the PER, DM-PER and DMA-PER sensitizers

Dye	f	LHE	TRANSITION ASSIGNMENT	
			Major	Minor
PER – 1	0.732	0.815	H->L (97%)	
PER – 2	1.166	0.932	H->L (88%)	H-1->L (3%), H-1->L + 1 (2%), H->L + 1 (5%)
PER – 3	1.109	0.922	H->L (79%), H->L + 1 (10%)	H-1->L (6%)
PER – 4	1.841	0.986	H-1->L (10%), H->L (72%), H->L + 1 (11%)	H-1->L + 1 (3%)
PER – 5	2.193	0.994	H-1->L (15%), H->L (61%), H->L + 1 (18%)	-
PER – 6	2.267	0.995	H-1->L (39%), H->L (48%)	H->L + 1 (9%)

Table 10
Oscillator strength (f), Light harvesting efficiency of the PER, DM-PER and DMA-PER sensitizers

Dye	f	LHE	TRANSITION ASSIGNMENT	
			Major	Minor
DM-PER-1	0.682	0.792	H->L (94%)	H-2->L (3%)
DM-PER-2	1.113	0.923	H->L (81%)	H-2->L (8%), H->L + 1 (7%)
DM-PER-3	1.058	0.912	H-2->L (10%), H->L (76%), H->L + 1 (10%)	-
DM-PER-4	1.804	0.984	H-2->L (16%), H->L (65%), H->L + 1 (14%)	H-3->L + 1 (2%)
DM-PER-5	2.135	0.993	H-2->L (20%), H->L (53%), H->L + 1 (20%)	H-3->L + 1 (2%)
DM-PER-6	2.088	0.992	H-2->L (39%), H->L (47%)	H->L + 1 (8%)

Table 11
Oscillator strength (f), Light harvesting efficiency of the PER, DM-PER and DMA-PER sensitizers

Dye	f	LHE	TRANSITION ASSIGNMENT	
			Major	Minor
DMA-PER-1	0.786	0.836	H-2->L (16%), H->L (82%)	-
DMA-PER-2	1.262	0.945	H-2->L (13%), H->L (75%)	H-3->L (2%), H->L + 1 (5%)
DMA-PER-3	1.136	0.927	H-2->L (13%), H->L (68%)	H-3->L (5%), H->L + 1 (9%)
DMA-PER-4	1.914	0.988	H-2->L (14%), H->L (59%), H->L + 1 (13%)	H-3->L (7%), H-3->L + 1 (2%)
DMA-PER-5	2.245	0.994	H-3->L (11%), H-2->L (14%), H->L (48%), H->L + 1 (19%)	H-2->L + 1 (2%)
DMA-PER-6	2.154	0.993	H-3->L (27%), H-2->L (15%), H->L (45%)	H->L + 1 (8%)

Table 12
Electron injection (ΔG_{inject}), electron regeneration (ΔG_{reg}) of the PER sensitizers

Dyes	E_{Ox}	λ_{max}	E^*_{Ox}	ΔG_{inject}	ΔG_{reg}
PER-1	5.647	2.731	2.917	-1.083	0.847
PER-2	5.545	2.434	3.111	-0.889	0.745
PER-3	5.532	2.606	2.926	-1.074	0.732
PER-4	5.524	2.291	3.234	-0.766	0.724
PER-5	5.569	2.349	3.220	-0.780	0.769
PER-6	5.560	2.433	3.128	-0.872	0.760

Table 13
Electron injection (ΔG_{inject}), electron regeneration (ΔG_{reg}) of the DM- PER sensitizers

Dyes	E_{Ox}	λ_{max}	E^*_{Ox}	ΔG_{inject}	ΔG_{reg}
DM-PER-1	5.206	2.618	2.588	-1.412	0.406
DM-PER-2	5.166	2.336	2.830	-1.170	0.366
DM-PER-3	5.223	2.511	2.711	-1.289	0.423
DM-PER-4	5.253	2.228	3.026	-0.974	0.453
DM-PER-5	5.293	2.295	2.998	-1.002	0.493
DM-PER-6	5.255	2.385	2.870	-1.130	0.455

Table 14
Electron injection (ΔG_{inject}), electron regeneration (ΔG_{reg}) of the DMA-PER sensitizers

Dyes	E_{Ox}	λ_{max}	E^*_{Ox}	ΔG_{inject}	ΔG_{reg}
DMA-PER-1	5.198	2.643	2.555	-1.445	0.398
DMA-PER-2	5.168	2.337	2.831	-1.169	0.368
DMA-PER-3	5.142	2.485	2.658	-1.342	0.342
DMA-PER-4	5.177	2.201	2.976	-1.024	0.377
DMA-PER-5	5.213	2.267	2.946	-1.054	0.413
DMA-PER-6	5.183	2.354	2.829	-1.171	0.383

Table 15
NLO properties of the PER, DM-PER and DMA-PER sensitizers

Dye	Dipole moment	Polarizability	
		(au)	x10^{-23}esu
PER – 1	7.577	153.416	2.273
PER – 2	3.757	200.557	2.972
PER – 3	11.464	211.478	3.134
PER – 4	8.139	262.808	3.894
PER – 5	15.807	292.203	4.330
PER – 6	17.774	303.495	4.497
DM-PER-1	9.044	187.698	2.781
DM-PER-2	6.546	229.655	3.403
DM-PER-3	13.262	244.680	3.626
DM-PER-4	10.516	292.604	4.336
DM-PER-5	18.003	328.258	4.864
DM-PER-6	19.762	342.537	5.076
DMA-PER-1	10.555	240.960	3.571
DMA-PER-2	8.009	280.599	4.158
DMA-PER-3	13.897	298.076	4.417
DMA-PER-4	11.958	345.635	5.122
DMA-PER-5	19.491	389.651	5.774
DMA-PER-6	21.451	407.471	6.038

4.5 Electron injection and electron regeneration

Electron injection and electron regeneration of the sensitizers is the important parameter to understood the inject the electron to TiO_2 from sensitizer and regeneration of electron from redox electrolyte[48].The electron injection (φ_{inject}) is relation to the thermodynamics driving force (ΔG_{inject}).Enhanced the ΔG_{inject} process of the DSSC is needs for maximize the PCE of the solar cell. The better performance to the dye sensitizer has lower negative value of the electron injection and less positive value of the electron regeneration.The lower value of electron regeneration has suppress the recombination process and degeneration process has minimized.

The electron injection and electron regeneration of the perylene based donor and donar functionalized perylene donor based sensitizers were analyzed from DFT and TDDFT functions and calculated using Eq. 4,6 and tabulated at Table 6.From the Table 6, all the perylene and donor functionalized perylene sensitizers have ΔG_{inject}values are negative and ΔG_{reg}values are positive. All the value of electron injection and electron regeneration indicates that the excited state of the sensitizers above the TiO_2 conduction band and ground state has below the redox electrolyte.This combination of sensitizers are make the spontaneously inject the electron at the time of the photo excitation process. This results shows that the perylene based sensitizer has the lower negative value of electron injection and lower positive value of the electron regeneration compared to donor functionalized perylene sensitizers.

The values of electron injection are show that the donor functionalized perylene sensitizers have negatively increased the compared perylene donor. The all configurations of the perylene donors has lower value of ΔG_{inject}compared to all configuration donor functionalized perylene, such as PER-1 < DM-PER-1 < DMA-PER-1, it is seen that the modification of the donors are affect the injection and regeneration efficiency.The configuration 4 to the studied sensitizers such as PER-4,DM-PER-4 and DMA-PER-4 has lower negative value of electron injection value in comparison to other configuration, the electron injection and electron regeneration studies of perylene and donor functionalized perylene show that the perylene based donor are more efficient the DSSC applications.

4.6 NLO properties:

Nonlinear optical properties of the sensitizers are one of crucial parameter for effective DSSC performance. NLO property response are depends on minimum energy gap of the sensitizers. The dipolemoment (μ) express that, electronic charge distribution of the sensitizers. the maximum values of dipolemoment and static polarizability is exhibit the active NLO performance. The dipolemomentvalues of designed sensitizers are calculated from the Eq. 7 and values are summarized in Table.7. From Table.7, the dipolemoment of the parent configurations of the sensitizers in the descending order: PER-6 > PER-5 > PER-3 > PER-4 > PER-1 > PER-2. The PER-6 has the maximum μ value of 17.7739 debye. The DM and DMA functionalized donor molecules has the same manner for parent configurations. The dipolemoment values of the all designed donor groups in decreasing order: DMA-PER > DM-PER > PER. The DMA functionalized donor has the maximum μ values in other donor groups for the six configurations.

The static polarizability of the sensitizers is directly proportional to the dipolemoment. The static polarizability values of the studied sensitizers are calculated from the Eq. 8 and values are summarized in Table 7. From the Table 7, the static polarizability values of parent configurations in decreasing order: PER-6 > PER-5 > PER-3 > PER-4 > PER-1 > PER-2. The PER-6 has maximum value of static polarizability of 303.495 au and4.497×10^{-23}esu. The DM and DMA functionalized perylene donors has same decreasing order for six configurations. The static polarizability values of studied sensitizers are exhibits the DMA functionalized perylene donor has the maximum values for six configurations compared to other donor groups. From the results, the dipolemoment and static polarizability values are illustrated that, DMA

functionalized donor has maximum μ and static polarizability values, especially DMA-PER-6 possess better NLO performance in comparison with other sensitizers.

5. Conclusion

The designed sensitizers have optimized through DFT with B3LYP/6-311G basis set in both gas and DMF phase. Absorption spectra and molar extinction coefficient of the sensitizer analyzed through TD-DFT with B3LYP/6-311G basis set in both gas and DMF phase. From NBO analysis of the designed dye sensitizers, Configuration 2 of DM and DMA functionalized perylene donors has maximum q^{donnor} values indicated that, more electron donating ability compared to other studied sensitizers. The FMO analysis results shows that, the DMA functionalized perylene donor molecules have minimum energy gap of the sensitizers compared to the other sensitizers. The configuration 6 is better than other configurations, especially DMA-PER- 6 have low energy gap and more suitable for DSSC applications. In absorption spectrum, LHE and molar extinction coefficient results is illustrated DMA functionalizedperylene donor have maximum LHE and ε values compared to the other sensitizers and especially DMA-PER- 6 have the higher LHE and ε values for efficient sensitizers to the PCE performance. The electron injection and electron regeneration properties of the sensitizers are investigated that, configuration 4 for DMA functionalizedperylene donor have lower negative ΔG_{inject}value and lower positive ΔG_{reg} values. For NLO properties, the DMA-PER sensitizers especially configuration 6 have the maximum dipolemoment and static polarizability. From the results, the DMA-PER- 6 exhibit the active NLO performance compared to the other studied sensitizers. the Frontier molecular orbitals, light harvesting efficiency, molar extinction coefficient and NLO performance results are indicated that, the DMA functionalized perylene donor is the better performer, especially DMA-PER-6 is the better candidate for the DSSC applications.

Declarations

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Conflicts of interest/Competing interests:

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Availability of data and material: Not Applicable

Code availability: Not Applicable

Authors' contributions:

D.Nicksonsebastin - Conceived of the presented idea,

Developed the theory and performed the computations

Carried out the experiments and performed the calculations

P. Pounraj - Conceived of the presented idea

Developed the theory and performed the computations

M.Prasath - Conceived of the presented idea

Supervised the findings of this work

All authors discussed the results and contributed to the final manuscript.

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Figures

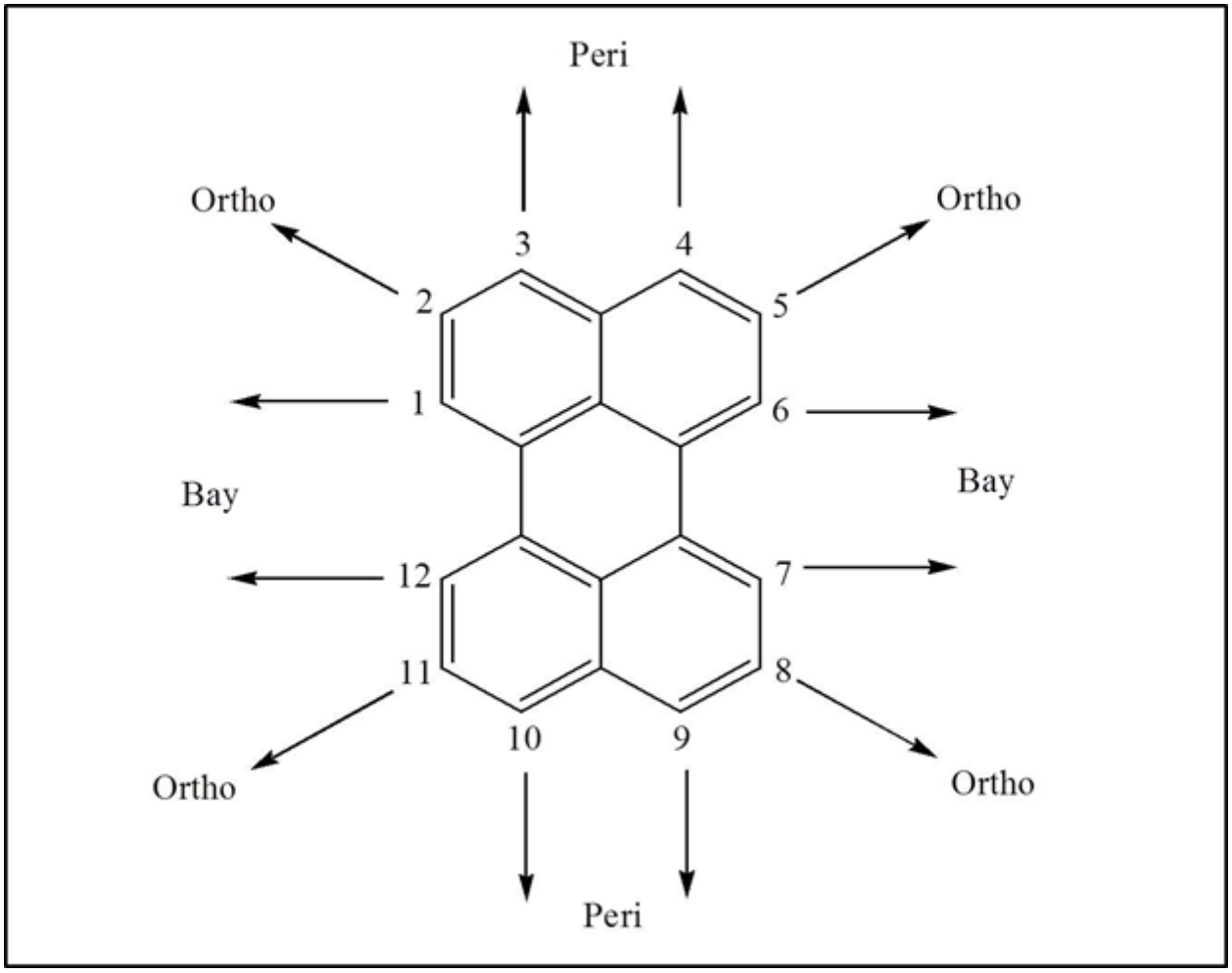

Figure 1

chemical structure of the perylene molecule

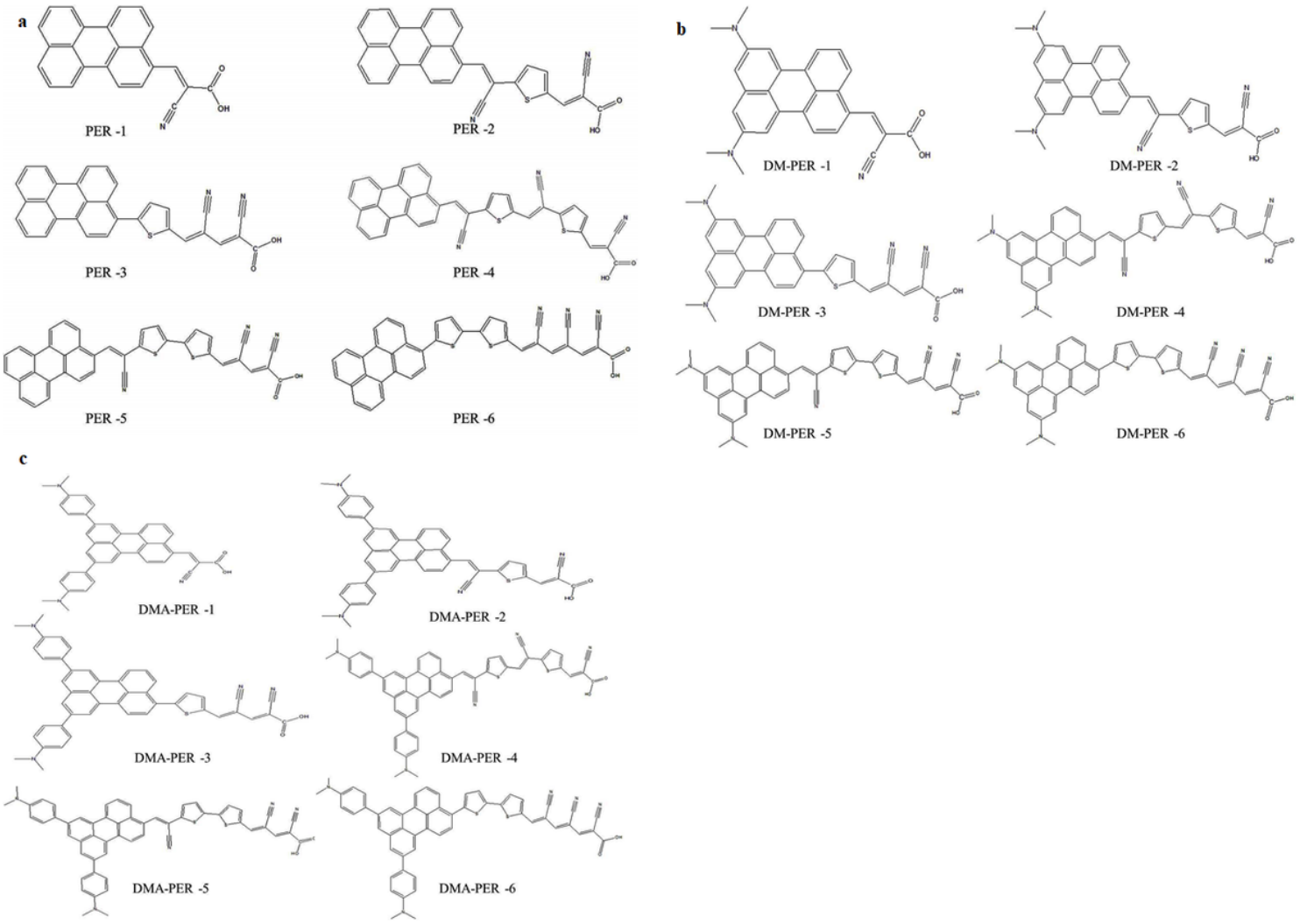

Figure 2

a. the chemical structure of the PER sensitizers. b. the chemical structure of the DM-PER sensitizers. c. the chemical structure of the DMA-PER sensitizers.

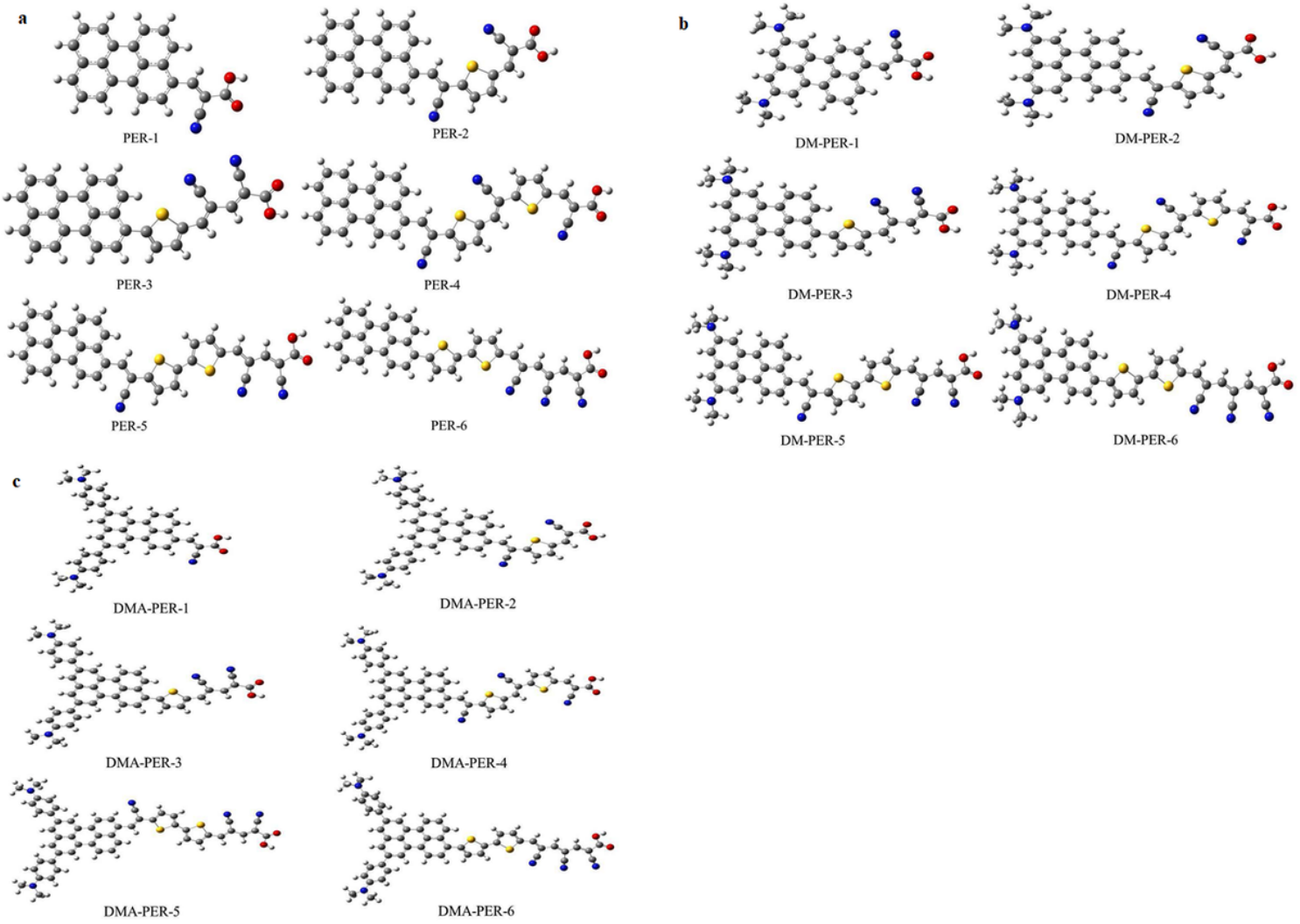

Figure 3

a. the geometrical structure of the PER sensitizers. b. the geometrical structure of the DM-PER sensitizers. c. the geometrical structure of the DMA-PER sensitizers.

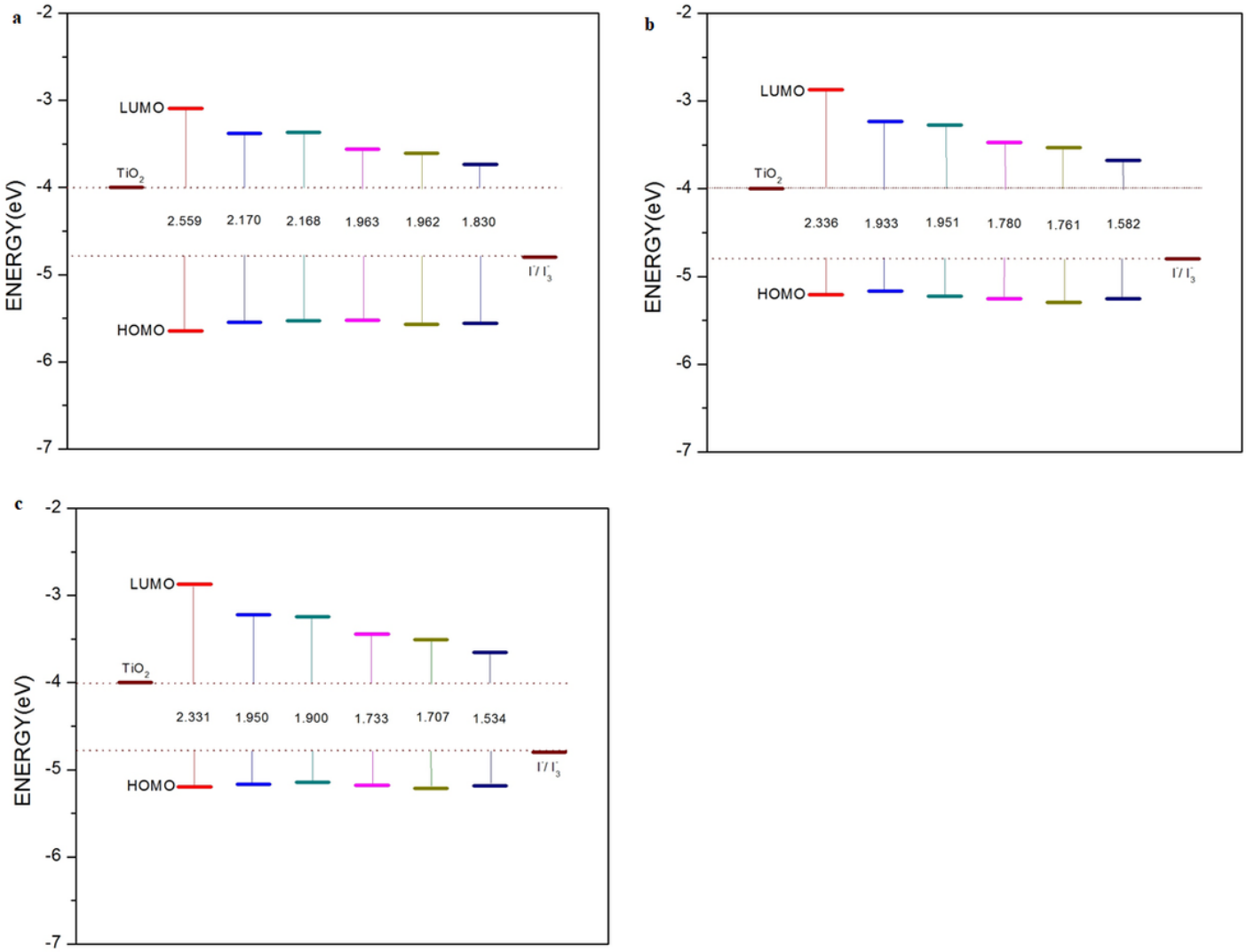

Figure 4

a. the HOMO-LUMO energy level of the PER sensitizers in gas phase. b. the HOMO-LUMO energy level of the DM-PER sensitizers in gas phase. c. the HOMO-LUMO energy level of the DMA-PER sensitizers in gas phase.

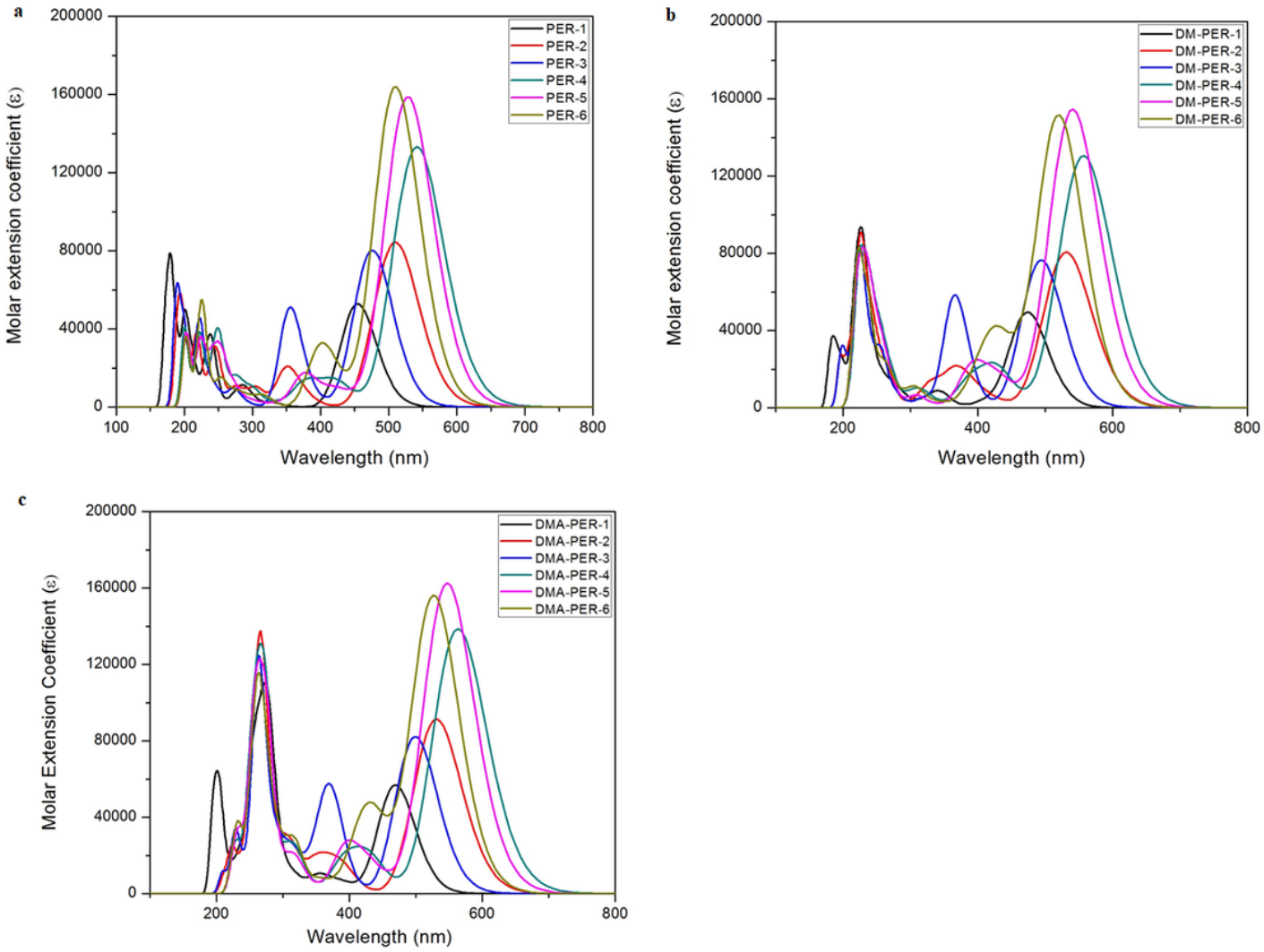

Figure 5

a. electronic absorption spectra of PER sensitizers in gas phase. b. electronic absorption spectra of DM-PER sensitizers in gas phase. c. electronic absorption spectra of DMA-PER sensitizers in gas phase.

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