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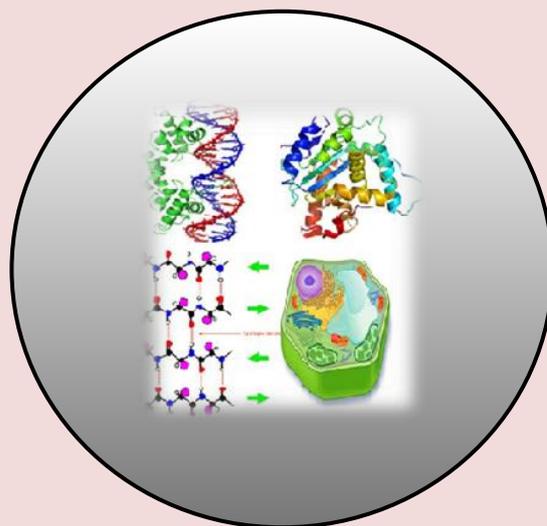
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Theoretical Study of Triphenyl Amine-based Dyes with Different Linker Groups for Dye-sensitised Solar Cells

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ABSTRACT

*A series of metal free triphenyl amine based organic dyes were comprehensively investigated by computational methods, in order to understand the roles of furans (D1), pyrroles(D2), thiophenes(D3), benzothiazoles(D4), benzotriazole(D5) and diketopyrrolopyrrole(D6) as the linker groups in dye-sensitized solar cells (DSSCs). It has been investigated theoretically with density functional theory (DFT) calculation at hybrid functional B3LYP by using 6-311+ G** to evaluate the effects of various linker groups on the optical and electronic properties of the dyes in dye-sensitized solar cells. Optical absorption spectra were obtained using the time-dependent DFT calculations with the B3LYP and coulomb-attenuating method CAM-B3LYP. Optical and electronic properties, UV-Vis absorption spectra, light harvesting efficiency of the dyes have been studied to shed light on how the various linker groups influence the properties of the dyes.*

Key words: Dye-sensitized solar cells, DFT, light harvesting efficiency, UV-Vis absorption spectra and NLO.

INTRODUCTION

The Earth receives an incredible supply of solar energy hence solar energy has become most popular among all the renewable energy forms to meet the increasing global energy consumption without effecting the environment (Z. Ning, et. al. 2008). The most common ways to convert solar energy into electricity is solar cell. The major aim of solar cell research is to increase the solar energy conversion efficiency at low cost to provide a cost-effective sustainable energy source. Silicon-based solar cells were conventionally used but are costly and less efficient. Hence Silicon-based solar cells have been replaced by high efficient and low cost dye-sensitized solar cells (DSSCs) which was first reported by O'Regan and Grätzel (1991) (B. O' Regan et. al. 1991). Different properties of the dyes mainly influence the efficiency of dye-sensitized solar cells (K. Hara, et. al. 2005). These DSSCs are a nano structured high band gap semiconducting electrodes combined with efficient electron injection dyes. The main property of sensitizing dye is the capture of sunlight. The efficiency of dye sensitizer is improved by having a broad absorption spectrum so that large range of photons available in solar energy (S. Jungsuttiwong, et. al. 2009). All over the world Researches on organic dyes are going on as it plays a significant role in the photoelectric conversion efficiency of a DSSCs (M. Grätzel, 2009).

Due to flexibility in molecular design and low production cost, Metal-free dyes are more valuable as compared with other dyes for DSSCs (M. Zhang et. al. 2013). They exhibit high molar extinction coefficients due to intermolecular $\pi - \pi^*$ transitions. In general the organic dyes which are used as sensitizer contain D- π -A structure, where D is donor, π is linker and A is acceptor (S.P. Singh, 2012). The efficiency of organic dyes in DSSCs varies with chemical modification due to the change in redox and absorption properties (Zhang, et. al. 2012).

The prerequisite condition for a Organic dyes to be used as DSSCs is that they must have appropriate levels for the lowest unoccupied molecular orbital(LUMO) and the highest occupied molecular orbital (HOMO) of the dyes. The energy level of the LUMO of the dye must be higher than the CB of the TiO₂ (-4.1 eV), and the energy level of the HOMO of the dye must be lower than the I⁻/I₃⁻ redox potential (-4.80 eV) (O.M. Sarhangi, et. al. 2011). By altering the electron donor, acceptor or π -spacer group of organic dyes, the HOMO and LUMO energy levels and also absorptivities and electronic excitation energies of the dyes can be changed.

Among various metal-free organic dyes, the triphenylamine (TPA)-based dyes have been widely investigated for their typical D- π -A structure due to excellent electron-donating capability. Researches are going on to explore the effect of molecular modifications of TPA-based dyes on the performance of DSSC (L.Y. Lin et. al. 2010). Triphenylamine (TPA)-based dyes also have a very good hole-transport properties. Triphenylamine based dyes are extensively used in DSSCs and showed high conversion efficiencies. In this paper, we studied newly designed series of metal free triphenyl amine based organic dyes which were studied by computational methods, in order to understand the roles of furans (D1), pyrroles (D2), thiophenes (D3), benzothiazoles (D4), benzotriazole (D5) and diketopyrrolopyrrole (D6) as the linker groups in dye-sensitized solar cells (DSSCs). The theoretical knowledge of Optical and electronic properties, UV-Vis absorption spectra, light harvesting efficiency, have been calculated and reported. Effect of the various anchoring groups influence the properties of the dyes were studied.

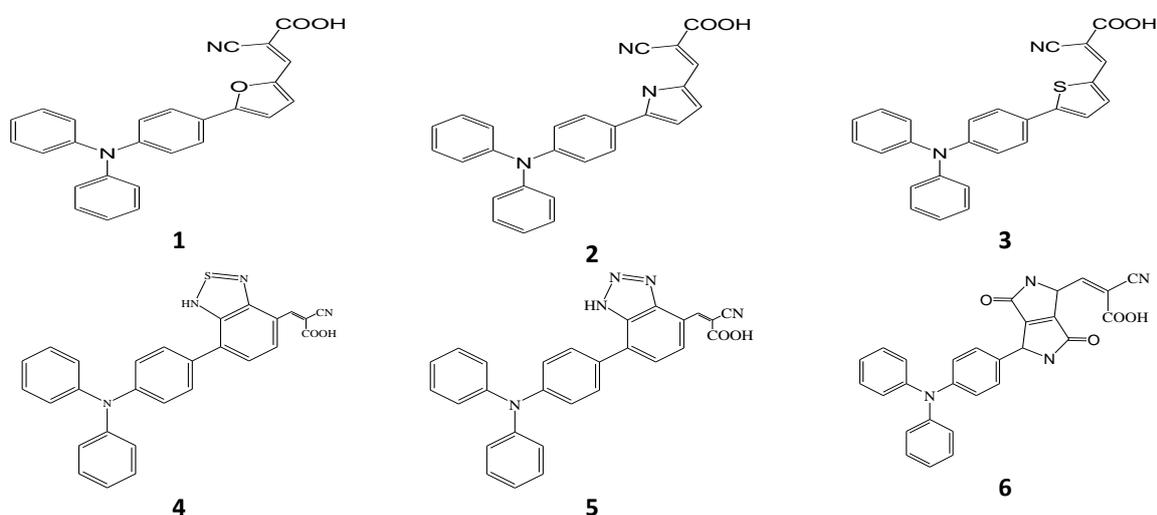


Figure 1. Molecular structure of dyes 1-6.

Computational methods

Computational calculations were obtained by DFT level of theory with the hybrid functional B3LYP (A.D. Becke, 1993) by using 6-311+G** basis set in the gas phase. First the geometry of dyes were optimized then the optimized geometrical parameters are used in the calculation of energy of highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), energy gap, dipole moment (μ), molecular electrostatic potential (MESP) to characterize the stability of molecule and reactive sites in the molecule for the attack of electrophile and nucleophile. For the calculation of non-linear optics, polarisability and hyperpolarisability were calculated from the optimized structure. The optical absorption spectra were obtained using the TD-DFT calculations with the B3LYP and range-separated functional, coulomb-attenuating method CAM-B3LYP (J. Zhang, et. al. 2012), with 6-311+G** basis sets to calculate the excitation energies and oscillator strengths of these dyes for the 20 lowest singlet-singlet transitions. Tetrahydrofuran (THF) was used as solvent to evaluate the effect of solvent on these dyes. Solvation effects were evaluated using the conductor polarisable continuum model (CPCM) (M. Cossi, et. al. 2003).

RESULTS AND DISCUSSION

Electronic absorption spectra and energy levels

The ground state geometries of the six dyes were optimised in the gas phase and in solvent THF. The optimised geometries of these dyes in THF are shown in Figure 2.

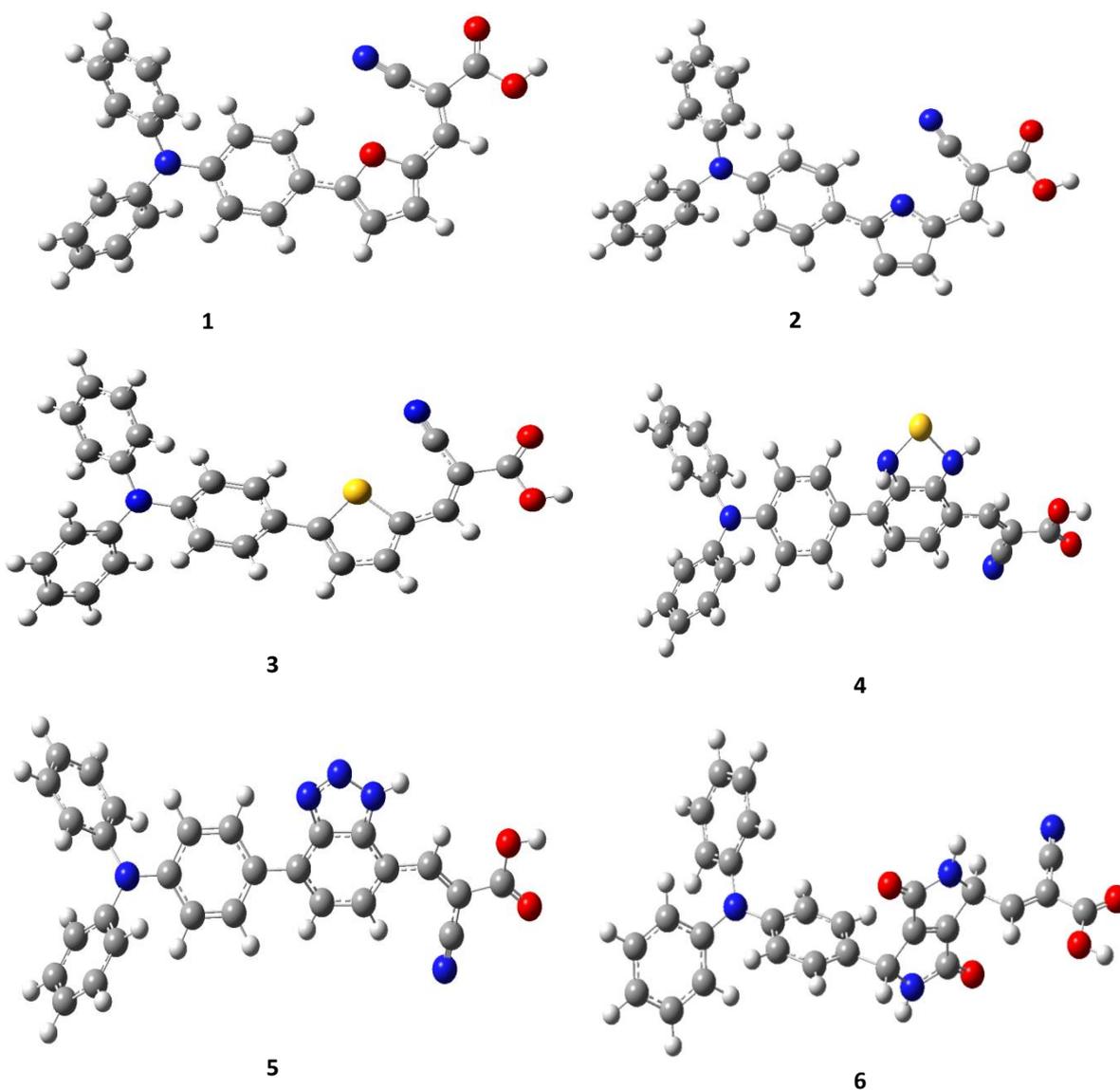


Figure 2. Optimized geometries of dyes 1- 6 in THF with B3LYP/6-311+G**

Table 1. E_{HOMO} (ev), E_{LUMO} (ev) HLG(ev) and maximum wavelength (λ_{max}) of dyes 1-6.

Dye		E_{HOMO}	E_{LUMO}	HLG	λ_{max}^a	Main transition	λ_{max}^b (Main transition)
Dye 1	Gas	-5.471	-2.818	2.653	510.87	H \rightarrow L(70.38%)	417.11 H \rightarrow L(65.0%)
	THF	-5.477	-2.988	2.921	550.14	H \rightarrow L(70.56%)	442.84 H \rightarrow L(64.24%)
Dye 2	Gas	-5.475	-3.175	2.30	917.37	H \rightarrow L(33.76%)	772.07 H \rightarrow L(15.21%)
	THF	-5.555	-3.542	2.013	1052.81	H \rightarrow L(14.47%)	880.07 H \rightarrow L(15.21%)
Dye 3	Gas	-5.567	-2.915	2.652	513.59	H \rightarrow L(70.4%)	411.99 H \rightarrow L(64.40%)
	THF	-5.506	-2.988	2.517	561.72	H \rightarrow L(70.5%)	438.99 H \rightarrow L(63.59%)
Dye 4	Gas	-5.537	-2.966	2.570	547.60	H \rightarrow L(67.12%)	547.60 H \rightarrow L(67.12%)
	THF	-5.470	-2.995	2.474	582.07	H \rightarrow L(66.31%)	416.68 H \rightarrow L(68.37%)
Dye 5	Gas	-5.601	-3.249	2.351	575.02	H \rightarrow L(70.5%)	419.75 H \rightarrow L(61.88%)
	THF	-5.541	-3.251	2.289	613.32	H \rightarrow L(70.6%)	453.18 H \rightarrow L(64.01%)
Dye 6	Gas	-5.572	-2.946	2.626	534.96	H \rightarrow L(70.21%)	314.07 H \rightarrow L(47.48%)
	THF	-5.495	-2.845	2.636	532.02	H \rightarrow L(70.31%)	310.70 H \rightarrow L(48.77%)

^aB3LYP, ^bCAM-B3LYP

The energy of highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), HOMO-LUMO gap (HLG) ($E_{LUMO} - E_{HOMO}$) of the dyes at DFT level of theory is obtained and given in Table 1. It was found that E_{HOMO} and E_{LUMO} for these dyes in gas phase is less than in THF while the HLG is more in gas phase as compared to THF. The results reveals that the HOMO energy levels of these dyes are lower than the reduction potential energy of the I^-/I_3^- electrolyte (-4.8 eV), i.e. these dyes that lose electrons could be restored by getting electrons from the electrolyte, and, the LUMO energy levels of these dyes are higher than the TiO_2 CB edge (-4.1 eV). This shows that the LUMO levels of all six dyes should be capable of injecting electrons into the CBs of TiO_2 . The electrolytes redox potential energy, CB energy of TiO_2 and The energy level diagram of the HOMO and LUMO of the dyes is show in Figure 3. Table 1 also conclude that the HLG and the λ_{max} are inversely correlated.

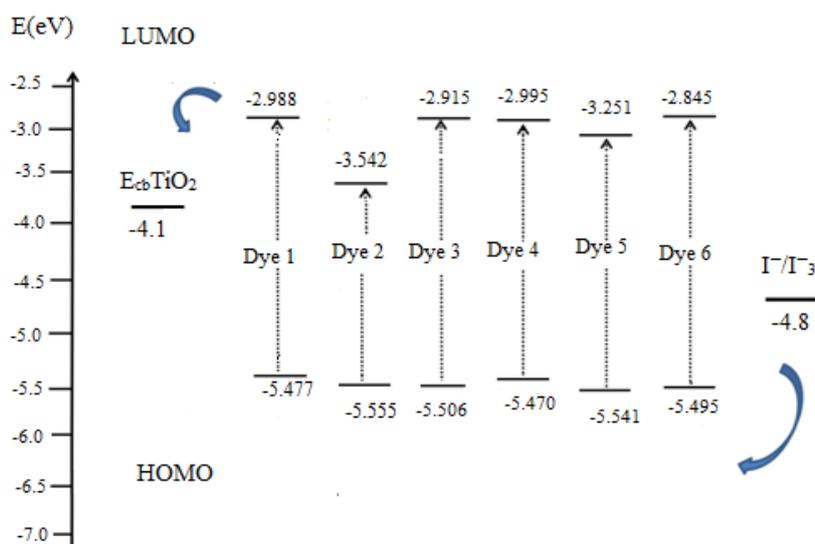


Figure 3. Schematic energy diagram of dyes 1-6, TiO_2 and electrolyte (I^-/I_3^-). E_{HOMO} (eV) and E_{LUMO} (eV) of dyes are in THF.

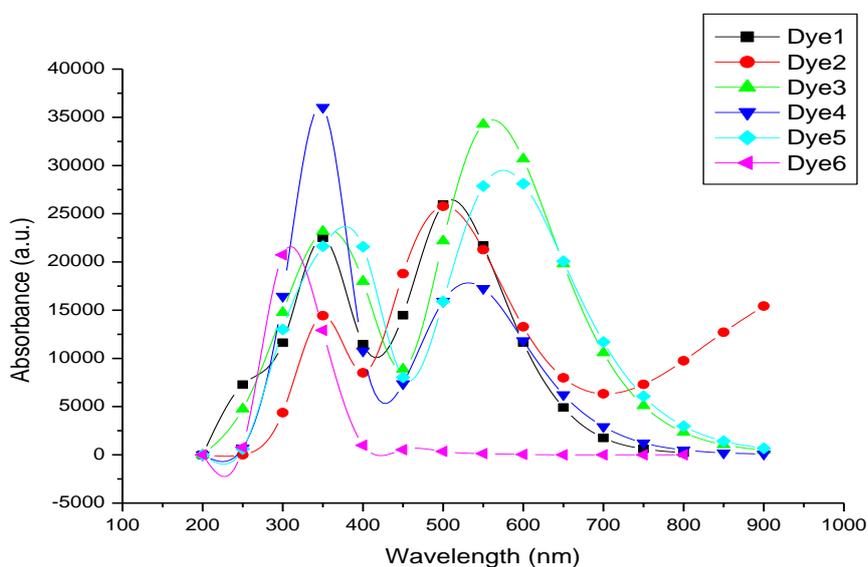


Figure 4. Electronic absorption spectra of dyes 1-6 in the solvent (THF) with B3LYP/6-311+G**

Optical properties

The distribution patterns of FMOs for the different dyes are plotted in Figure 5. The examination of distribution pattern of frontier molecular orbitals (FMOs) are useful for determining optical electronic properties.

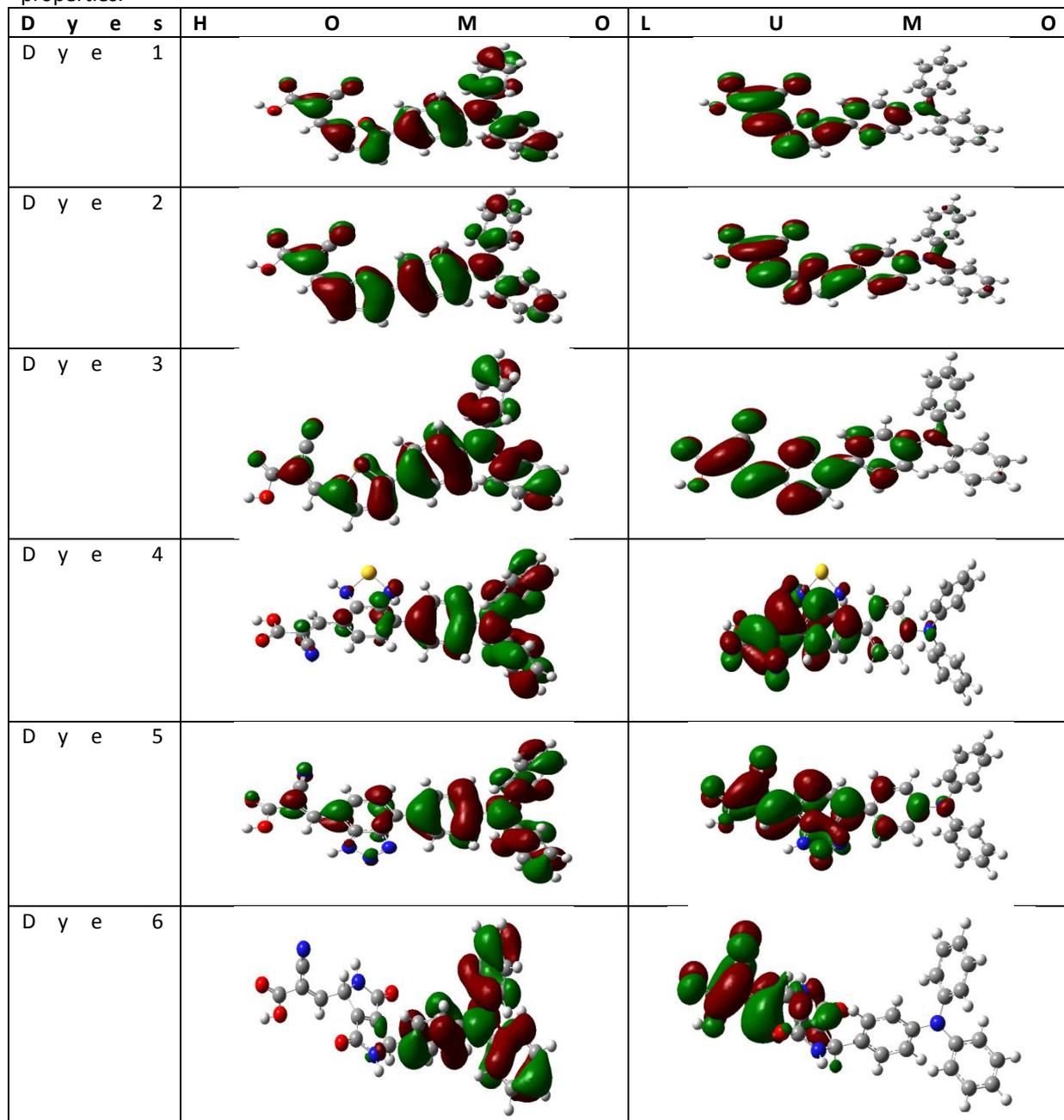


Figure 5. The distribution patterns of FMOs of Dye 1-6.

From the results of table 1 we can conclude that in the presence of solvent the absorption bands of these dyes shifts towards the longer wavelength. By increasing solvent polarity the energy of the excited state is lowered more than that of the ground state, and this produces a red shift due to which π^* shows relatively better stability in comparison to π on the inclusion of solvent will result in a red shift. The simulated absorptionspectra by B3LYP in THF for all the six dyes are shown in Figure 4.

TD-DFT results based on the B3LYP method show that maximum absorbance (λ_{max}) for the dyes are in the order of 2>5>3>4>1>6. Also, CAM-B3LYP results show that the order of λ_{max} is 2>1>5>3>4>6. For these dyes, the HOMOs are π orbitals whereas LUMOs are π^* orbitals. Due to which these absorption bands are assigned to the $\pi \rightarrow \pi^*$ transitions and the Solvent stabilises the π^* relative to the π with the observed red shift of the maximum absorbance. It was found that dye 2 containing pyrrole π spacers shows the best absorption properties in UV-Vis range, i.e. redshifted λ_{max} and broader absorption spectrum, while the dye with diketopyrrolopyrrole in dye 6 as anchoring group shows the smallest λ_{max} and more narrow spectrum. The better properties of dye 2 with the pyrrole π spacer as the anchoring group may be attributed a great influence on the DSSC performance.

The intrinsic property of the anchoring group is the electronic coupling between the dye and the semiconductor which could affect the electron injection. The efficiency of electron injection could influence the short-circuit photocurrent density (J_{sc}) that is a vital feature which affects the efficiency of DSSCs. We can conclude that when the amount of charge injection into the TiO_2 surface increases, the short-circuit photocurrent density (J_{sc}) also increases (P.S. Kumar, et. al. 2010). Improving the J_{sc} is a potent way to enhance the efficiency of DSSCs. Light-harvesting efficiency LHE (λ) of a dye which is a factor related to J_{sc} , can be obtained from this equation,

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

Where $A(f)$ is the absorption (oscillator strength) of the dye corresponding to λ_{max} . It has been found that higher the value of LHE due to the larger f , increases the light capturing capability. Improving the LHE could enhance the J_{sc} . In order to give an account of how the different anchoring groups affect the electronic properties of the dyes, maximum absorption wavelengths (λ_{max}), oscillator strengths (f) and light-harvesting efficiency (LHE) computed with B3LYP/6-311+G** basic set in THF, are summarised in Table 2.

Table 2. Calculated λ_{max} (nm), oscillator strengths (f), light-harvesting efficiency (LHE) of the dyes at the B3LYP/6-311+G level.**

D y e s	$\lambda_{m a x} (n m)$	f	L H E
D y e 1	5 5 0 . 1 4	0 . 7 7 1	0 . 8 3 0
D y e 2	1 0 5 2 . 8 1	0 . 4 5 6	0 . 6 5 0
D y e 3	5 6 1 . 7 2	0 . 8 5 7	0 . 8 6 1
D y e 4	5 8 2 . 0 7	0 . 3 0 3	0 . 5 0 2
D y e 5	6 1 3 . 3 2	0 . 8 7 5	0 . 8 6 6
D y e 6	5 3 2 . 0 2	0 . 0 3 4	0 . 0 7 5

Comparing figure 3 and table 2 we find that the different anchoring groups in the molecular structures could influence the maximum absorption wavelength (λ_{max}) and oscillator strength (f). As can be seen in Table 3, the λ_{max} of dyes 1–6 obtained via B3LYP method is in the order: 6<1<3<4<5<2 and the LHE is 3<6<1<4<5<2. Dye 2 has the larger oscillator strength (f) than that of the other dyes, and has achieved an improved LHE. Indeed, comparing the LHE of these dyes indicates that the dye with pyrrole π - spacer has a higher LHE and broader absorption spectra than that of the other dyes.

Molecular electrostatic potential

The molecular electrostatic potential (MESP) depicts the electronic density and gives the information regarding electrophilic, nucleophilic attack as well as hydrogen-bonding interactions (S. Fatma, et. al. 2015). Molecular electrostatic potential counter map are made by B3LYP/6-311G** (d,p) method using Gauss view 9.0 program. The molecular electrostatic potential contour surface of dyes 1-6 is given in the Fig 6. Different colours in MESP represents different values of the electrostatic potential at the surface. Potential increases in the order red < yellow < green < light blue < blue (D. Glossman-Mitnik, 2013). The colour pattern on MESP surface represents electron rich region (partially negative charge) by red which shows nucleophilic reactivity and electron deficient region (partially positive charge) is represented by blue which shows electrophilic reactivity. The yellow, green and light blue colours indicating slightly electron rich, neutral and slightly electron deficient regions respectively.

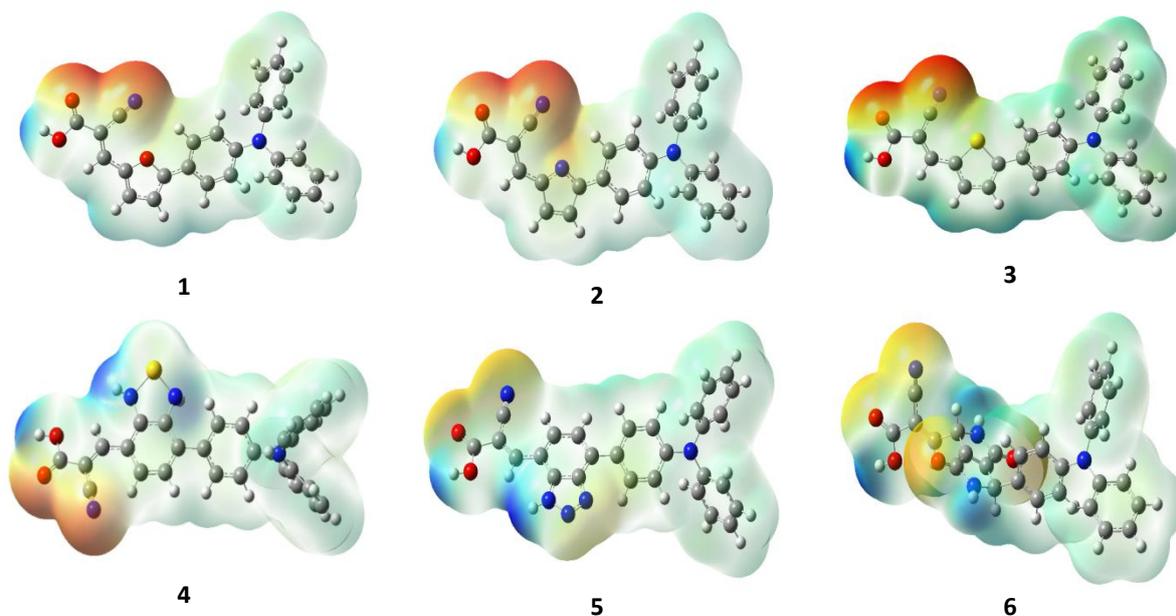


Figure 6. 3-D plots of the molecular electrostatic potential of dyes 1-6.

Dipole moment, Polarisability and Hyperpolarisability analysis

By changing molecular structure, important physical quantities i.e. Dipole moment, polarisability and hyperpolarisability of dye sensitizer that could be affected (M.P. Balanay, 2011). Determination of intramolecular charge delocalisation in π -electron-conjugated dyes are done by polarisability which is a nonlinear optical (NLO) property. Higher the NLO property of dyes higher will be the high photoelectric conversion efficiency. In order to investigate the relationships among dipole moment and NLO properties of the dyes with different anchoring groups, the following equations were adopted to calculate these parameters.

The dipole moment could be calculated from the following formula:

$$\mu = \sqrt{\mu_x^2 + \mu_y^2 + \mu_z^2} \quad (2)$$

where μ_x , μ_y , μ_z are defined as the vector components of the dipole moment.

$$\alpha = \frac{(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})}{3} \quad (3)$$

The anisotropy of polarisability $\Delta\alpha$ could be calculated from the following formula:

$$\Delta\alpha = \sqrt{\frac{(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{xx} - \alpha_{zz})^2 + (\alpha_{yy} - \alpha_{zz})^2}{2}} \quad (4)$$

In equations 3 and 4, α_{xx} , α_{yy} , α_{zz} are the tensor components of polarisability.

The total first-order hyperpolarisability, β_{tot} , is defined as:

$$\beta_{tot} = \sqrt{\left[(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{xzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2 \right]} \quad (5)$$

where β_{xxx} , β_{xyy} , β_{xzz} , β_{yyy} , β_{yzz} , β_{yxx} , β_{zzz} , β_{zxx} and β_{zyy} are the tensor components of hyperpolarisability [29,30,31].

Table 3. Calculated dipole moment μ (Debye), isotropic polarisability α , anisotropy of polarisability $\Delta\alpha$, total first-order hyperpolarisability β_{tot} .

D y e s	μ	α (10^{-22} esu)	$\Delta\alpha$ (10^{-22} esu)	β_{tot} (10^{-28} esu)
D y e 1	7 . 2 8	0 . 6 2	0 . 7 3 0	2 . 1 6
D y e 2	9 . 4 3	0 . 7 7	1 . 0 1 5	7 . 8 2
D y e 3	8 . 6 4	0 . 6 7	0 . 7 1 5	2 . 8 3
D y e 4	7 . 5 9	0 . 7 1	0 . 9 2 7	2 . 4 4
D y e 5	5 . 9 2	0 . 7 5	0 . 8 6 3	2 . 0 1
D y e 6	6 . 1 9	0 . 5 7	0 . 3 2 5	1 . 2 3

As seen in table 4 Dipole moment (μ) is in order: 2>3>4>1>6>5, isotropic polarisability (α) is in order 2>5>4>3>1>6, anisotropic polarisability($\Delta\alpha$) is in order 2>4>5>1>3>6 and frst-order hyperpolarisability (β_{tot}) is in order 2>3>4>1>5>6. From the above results we could find a general trend that the dyes with larger polarisabilities usually have larger dipole moment.

CONCLUSIONS

Computational approach have been applied in the present work, which combines DFT and TDDFT techniques to study six triphenyl amine based organic dyes with different anchoring groups to evaluate the effects of various anchoring groups on the electronic and optical properties, electron injection efficiency. Major factors that has been calculated includes maximum absorption wavelength (λ_{max}), light-harvesting efficiency (LHE), dipole moment (μ), the NLO properties (polarisability (α), anisotropy of polarisability ($\Delta\alpha$) and hyperpolarisability (β)) of all the dyes by computational methods. The influences of different anchoring groups on these factors demonstrate that dyes 2 and 5 with pyrrole and benzotriazole as the linker groups in dye-sensitized solar cells (DSSCs), respectively, have the best absorption properties, i.e. the largest λ_{max} and the widest absorption spectrum, the largest LHE. Also, these dyes have a higher dipole moment, larger NLO properties. We hope this study will be useful for the design of organic dyes with target properties to increase the efficiency of DSSCs.

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