Theoretical studies of Electronic and Photovoltaic Properties of New Derivatives of Sudan dye by DET and TD-DFT method.

Numbury Surendra Babu, J.J.Makagara and Isaac Onoka

Department of Chemistry, College of Natural and Mathematical Sciences, The University of Dodoma, Post Box: 338, DDODOMA, Tanzania

ABSTRACT

In the present student, Sudan Orange G (SOG) [4-(Phenylazo) resorcinol] derivatives have been studied at Density Functional theory (TD-DFT) at B3LYP level of theory with 6-31G(d) basis set. Different substituent groups were introduced in different position to investigate their effects on the electronic and optical properties. The HOMO and LUMO energies and the energy gap (E_{gap}) between HOMO and LUMO of the studied dyes were calculated. The light harvesting efficiency (LHE), the open-circuit voltage (Voc) and injection driving force (ΔG_{inject}) which are the key parameters related to the solar cell efficiency (η) were computed. The LHE values for the dyes are in different ranges and that all the dyes will give different photocurrent. The D6 dye has highest oscillator strength value 1.1263 and the LHE value is 0.925235. So the D6 dye has more efficiency than other studied dyes. Based on the $\left|V_{RP}\right|$ values, the meta substituent dyes are better sensitizers compare to other dyes.

Introduction

Dye-sensitized solar cells (DSCs) have attracted significant attention because of its potential advantages, such as low cost and highly efficient conversion of sunlight into electricity [1–11]. The DSC is the only photovoltaic device that uses molecules to absorb photons and convert them to electric charges without the need of intermolecular transport of electronic excitation. In particular, these DSSC are composed of a wide band gap semi-conductor (typically TiO2) sensitized with molecular dyes, able to capture light in the visible region of the spectrum, and a redox electrolyte (typically Iodide/triiodide I^-/I^{3-}) [12, 13]. In DSSCs, incoming light causes electronic excitations of the dye sensitizers leading to electron injection to the conduction band of nanocrystalline metal oxide, then, the dyes regain electrons from the redox couple in an electrolyte solution. Many researchers show more interested in synthesizing conjugated molecules because they are not amorphous and can be synthesized as well-defined structures [14]. Moreover, the short conjugated molecules units have attracted much attention, because of their unique electronic properties, to their high photoluminescence quantum efficiency and thermal stability [15]. Many studies have been made recently on the integration of conjugated heterocyclic and the effect on the optoelectronic properties [16].

Theoretical analysis of the electronic structure of conjugated systems can establish the relationships between molecular structure and electronic properties. Theoretical studies on the electronic structures of π-conjugated compounds have given great contributions to the rationalization of the properties of known materials and to the prediction of the yet unknown ones. In this context, quantum chemical methods have been increasingly applied to predict the band gap of conjugated systems [17].

This work will further elucidate geometric and electronic properties with the aim to prove the relationship between molecular structure and electronic properties, and driving towards the next synthesis compounds which are as active materials in optoelectronic. The quantum chemical investigation has been performed to the optical and electronic properties of a series of compounds based on sudan derivatives. The structures of the studied sudan derivates are shown in Fig. 1. Different electron side groups were introduced to investigate their effects on the electronic structure. The theoretical knowledge of the HOMO and LUMO energy levels of the components is basis in studying organic solar cells as the HOMO, LUMO, Gap energy and Voc of the studied compounds have been calculated and reported. Particular attention is paid to electronic structure, absorption and emission properties. Their properties suggest they are good candidates for organic solar cells.
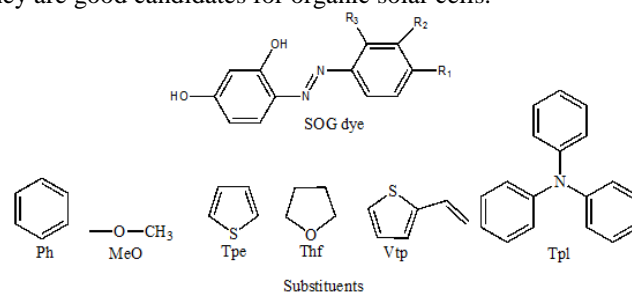
Ph = Phenyl; MeO = Methoxy; Tpe = Thiophene; Thf = tetrahydrofuran; Vtp = 2-vinaylthiophene;
Tpl = triphenyllamine
D1 = R_1 = Ph, R_2 = H, R_3 = H
D2 = R_1 = H, R_2 = Ph, R_3 = H
D3 = R_1 = MeO, R_2 = H, R_3 = H
D4 = R_1 = Ph, R_2 = MeO, R_3 = H

Tele: +255 672221238
E-mail address: nsbabusk@gmail.com

D5 = R₁ = Ph,   R₂ = H,   R₃ = MeO
D6 = R₁ = Tpe,   R₂ = H,   R₃ = H
D7 = R₁ = Ph,   R₂ = Tpe,   R₃ = H
D8 = R₁ = Ph,   R₂ = H,   R₃ = Tpe
D9 = R₁ = Thf,   R₂ = H,   R₃ = H
D10 = R₁ = Ph,   R₂ = Thf,   R₃ = H
D11 = R₁ = Ph,   R₂ = H,   R₃ = Thf
D12 = R₁ = Vtp,   R₂ = H,   R₃ = H
D13 = R₁ = Ph,   R₂ = Vtp,   R₃ = H
D14 = R₁ = Ph,   R₂ = H,   R₃ = Vtp
D15 = R₁ = Ph,   R₂ = Tpl,   R₃ = H
D16 = R₁ = Ph,   R₂ = H,   R₃ = Tpl
D17 = R₁ = Ph,   R₂ = MeO,   R₃ = Tpe
D18 = R₁ = Ph,   R₂ = Thf,   R₃ = Tpl
D19 = R₁ = MeO,   R₂ = Tpe,   R₃ = Vtp
D20 = R₁ = H,   R₂ = H,   R₃ = Ph

Figure 1. The structures of studied SOG dyes derivates.

In this research article, for new molecular structures based on Sudan Red G (SRG) [1-(2-Methoxyphenylazo)-2-naphthol] dye were designed. The SOG is a yellowish red lysochrome azo dye and it has the appearance of an odorless reddish-orange powder with melting point 225 °C. It is soluble in fats and used for coloring of fats, oils, and waxes, including the waxes used in turpentine-based polishes [18]. Sudan Orange G (SOG) [4(Phenylazo)resorcinol] is useful for staining triglycerides in animal tissues (frozen sections) [19].To the best of our knowledge a systematic theoretical study of such compounds has not been reported. Fundamental understanding of structural and optical and electronic properties of this kind of materials could be useful so as design new molecules.

Computational methods

The optimized structures of all studied SOG derivates have been calculated by DFT with the hybrid B3LYP functional theory combined with 6-31G (d) basis sets using Gaussian 09 program[20] with Becke's three parameter gradient-corrected exchange potential and the Lee-Yang-Parr gradient-corrected correlation potential (B3LYP) [21-23]. All calculations were performed without any symmetry constraints by using polarized split-valence 6-31G (d) basis set in gas phase. The electronic absorption spectrum, oscillator strengths and the vertical excitation energy were simulated using TD-DFT with B3LYP/6-31G (d) level in gas phase on the entirely DFT optimized geometries. The power conversion efficiency of each molecule was determined by the position of the band gap depending on the difference [LUMO (molecule) – LUMO (acceptor)].

In the present research work, to make an effort to determine and evaluate the the absorption peaks (λ_{max}) in the UV spectra of the studied dyes. In addition to analyze electro- optical properties, electron injection, electronic copling constants, light harvesting efficiencies, open circuit voltages (V_{oc}) and Quantum chemical parameters.

Results and discussion

Electronic properties

The optimized structures of all studied SOG dye derivates dyes are shown in figure 2. All the molecular geometries have been calculated by DFT with the hybrid B3LYP functional theory combined with 6-31G (d) basis sets using Gaussian 09 program. Electronic properties of the HOMO and LUMO energy levels of the dyes are crucial in studying

organic solar cells. The HOMO and LUMO energy levels of the donor and of the acceptor dyes for photovoltaic devices are key important factors to determine whether the effective charge transfer will happen between donor and acceptor. In general, a power conversion efficiency dye sensitizer has the following characteristics: the highest occupied molecular orbital (HOMO) energy must be located below the HOMO energy of electrolyte to accept the electron from a redox electrolyte pair (I^-/I^{3-}), the lowest unoccupied molecular orbital (LUMO) should have a higher energy than that of the conduction band of semi-conductor (TiO_2).
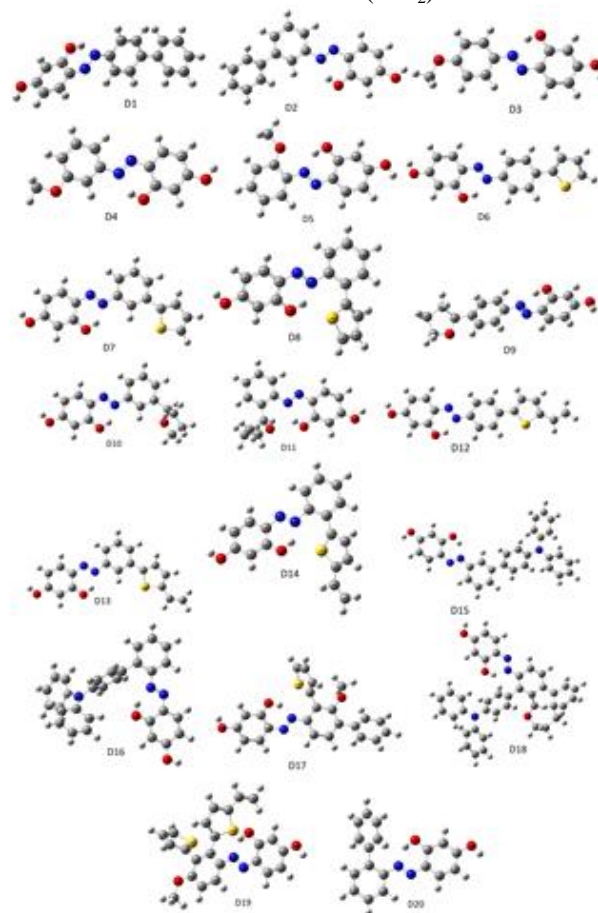

Figure 2. Optimized geometry molecular structure of studied dyes with B3LYP/-6-31G (d) basis set.

The HOMO and LUMO energies of the studied dyes are computed in Table 1 and Figure 2 shows the frontier molecular orbitals for all the SOG derivates. As shown in table I, The HOMO and LUMO energies of D1 to D20 change significantly, the HOMOs for D1, D2, D3, D4, D5, D6, D7, D8, D9, D10, D11, D12, D13, D14, D15, D16, D17,D18, D19 and D20 are located at -4.9791, -5.7490, -5.4379, -5.6997, -5.4668,-5.4910, 5.7141,-5.6061,-5.6262, -5.6730, -5.5977, -5.3326, -5.4834, -5.4069, -4.9628, -4.8956,-5.5582,-4.4714, -5.3685   and   -5.6548   eV, respectively. The LUMOs for D1, D2, D3, D4, D5, D6, D7, D8, D9, D10, D11, D12, D13, D14, D15, D16, D17,D18, D19 and D20 are located at -2.3279, -2.2055, -2.0158, -2.1211, -2.0409, -2.3032, -2.2373, -2.1973, -2.1138, -2.1070, -2.0591, -2.3500, -2.2512, -2.2270, -2.1696, -2.1777, -2.2169, -2.1051, -2.0455 and -2.1524 eV, respectively.

Table 1. Energy values of E_{LUMO} (eV), E_{HOMO} (eV), ΔE_{gap}, and dipole moment (μ) of the studied dyes obtained by DFT at B3LYP/6-31G (d).

Dye	HOMO Ev	LUMO Ev	ΔE_{gap}	μ
D1	-5.6090	-1.8317	3.7773	2.4579
D2	-5.7490	-2.2055	3.5435	3.9413
D3	-5.4379	-2.0158	3.4221	3.9413
D4	-5.6997	-2.1211	3.5786	2.9238
D5	-5.4668	-2.0409	3.4259	1.6788
D6	-5.4910	-2.3032	3.1878	3.0211
D7	-5.7141	-2.2373	3.4768	2.5523
D8	-5.6061	-2.1973	3.4088	1.7944
D9	-5.6262	-2.1138	3.5125	2.8281
D10	-5.6730	-2.1070	3.5661	2.5978
D11	-5.5977	-2.0591	3.5386	1.9522
D12	-5.3326	-2.3500	2.9826	3.0216
D13	-5.4834	-2.2512	3.2322	2.6469
D14	-5.4069	-2.2270	3.1799	1.9219
D15	-4.9628	-2.1696	2.7933	1.7429
D16	-4.8956	-2.1777	2.7179	2.4922
D17	-5.5582	-2.2169	3.3413	1.2556
D18	-4.4714	-2.1051	2.3663	3.2221
D19	-5.3685	-2.0455	3.3231	3.6562
D20	-5.6548	-2.1524	3.5024	1.9617

The injection of electron from dye to semiconductor is depends on the HOMO and the LUMO energy levels of the dye (donor) and semiconductor (acceptor). For effective injection of the electron from the excited dye into the acceptor (metal oxide semiconductor e.g. TiO$_2$,) the LUMO level of the dye needs to be higher than the conduction band edge of the acceptor. The band edge of TiO$_2$ is approximately at - 4.2 eV (relative to vacuum) and the LUMO energy level of all dye derivates indicating that the LUMO levels of all four dyes are higher than the conduction band edge of TiO$_2$. The HOMO level of the dye needs to be sufficiently lower than the redox couple to ensure the efficient regeneration of the dye. The most widely used redox couple in the electrolyte of DSSC is the I^-/I^{-3} pairs where the estimated energy level is at   - 4.8 eV (relative to vacuum). The HOMO energy of all SOG dye derivates are less than the redox couple. In addition, energy (E_{gap}) of the studied molecules differs slightly from 2.5066 to 3.952 eV depending on the different substituent and position. They are in the following order: D18 > D16 > D15 > D12 > D14 > D6 > D13 > D19 > D17 > D8 > D3 > D5 > D7 > D20 > D9 > D11 > D2 > D10 > D4 > D1.

Photovoltaic properties

The power conversion efficiency (η) of solar cell devices is determined generally by the open-circuit photovoltage (V_{OC}), short-circuit current density (J_{SC}), and the fill factor (FF), as compared to incident solar power (P_{inc}).The power conversion efficiency (η) was calculated according to the Eq. 5:

$$\eta = \frac{FFV_{oc}J_{sc}}{P_{inc}} \qquad (1)$$

where P_{inc} is the incident power density, J_{sc} is the short-circuit current, V_{oc} is the open-circuit voltage, and FF denotes the fill factor. The J_{SC} is estimated by the maximum current which flows in the device under illumination when no voltage is applied, in which dependent on the morphology of the device and on the lifetime and the mobility of the charge carriers [24].

The J_{SC} in DSSCs is determined by the following equation [25]

$$J_{sc} = \int LHE(\lambda)\Phi_{inject}\eta_{collect}d\lambda \qquad (2)$$

where LHE(λ) is the light harvesting efficiency at a given wavelength, Φ_{inject} evinces the electron injection efficiency, and $\eta_{collect}$ denotes the charge collection efficiency. In the systems which are only different in sensitizers, $\eta_{collect}$ can be reasonably assumed to be constant. LHE (λ) can be calculated from the following equation

$$LHE = 1 - 10^{-f} \qquad (3)$$

where f represents the oscillator strength of adsorbed dye molecules. Φ_{inject} is related to the driving force ΔG_{inject} of electrons injecting from the excited states of dye molecules to the semiconductor substrate. It can be estimated as [26]

$$\Delta G_{inject} = E_{OX}^{dye*} - E_{CB}^{TiO_2} = E_{OX}^{dye} + E_{0-0}^{dye} - E_{CB}^{TiO_2} \qquad (4)$$

From the equations 1−4, we could roughly predict the efficiency of novel dyes without intensive calculations.

Where E_{OX}^{dye*} is the oxidation potential of the excited dye, E_{OX}^{dye} is the redox potential of the ground state of the dye, E_{0-0}^{dye} is the vertical transition energy, and $E_{CB}^{TiO_2}$ is the conduction band edge of the TiO$_2$ semiconductor. So J_{SC} can be well estimated through f and ΔG_{inject}. Two models can be used for the evaluation of E_{OX}^{dye*}[27]. The first implies that the electron injection occurs from the un relaxed excited state. For this reaction path, the excited state oxidation potential can be extracted from the redox potential of the ground state, E_{OX}^{dye} which has been calculated at the B3LYP-6-31G(d) approach and the vertical transition energy corresponding to the photoinduced intermolecular CT (ICT),

$$E_{OX}^{dye*} = E_{OX}^{dye} - \lambda_{max}^{ICT} \qquad (5)$$

where λ_{max}^{ICT} is the energy of the ICT. Note that this relation is only valid if the entropy change during the light absorption process can be neglected. For the second model, one assumes that electron injection occurs after relaxation. Given this condition, E_{OX}^{dye} is expressed as [28]:

$$E_{OX}^{dye*} = E_{OX}^{dye} - E_{0-0}^{dye} \qquad (6)$$

To analyze the relationship between V_{OC} and E_{LUMO} of the dyes based on electron injection (in DSSCs) from LUMO to the conduction band of semiconductor TiO$_2$ (E_{CB}), the energy relationship can be expressed [29]:

$$V_{oc} = E_{LUMO} - E_{CB} \qquad (7)$$

The Photovoltaic properties λ_{max}, ΔG_{inject}, E_{OX}^{dye} , E_{OX}^{dye*} , λ_{max}^{ICT} , and LHE, we have presented in Table 2. The short-circuit current (J_{sc}) depends on two main influencing factors; light harvesting ability (LHE) and the electronic injection free energy (ΔG_{inject}) (Eq. 4).

Table 2. Calculated absorption spectra λ_{max}, λ_{max}^{ICT}, E_{OX}^{dye*} ΔG_{inject}, $\left|V_{RP}\right|$ and V_{OC} of dyes at TDDFT/B3LYP/6-31G (d) level of theory.

Dye	λ_{max}	λ_{max}^{ICT}	f	LHE	E_{OX}^{dye*}	ΔG_{inject}	$\left|V_{RP}\right|$	V_{oc}
D1	394.91	3.1395	1.1462	0.908652	2.4695	1.5305	0.7653	2.1683
D2	376.09	3.2966	0.5531	0.720166	2.4524	1.5477	0.7738	1.7945
D3	383.56	3.2324	0.7871	0.836732	2.2055	1.7945	0.8973	1.9842
D4	330.28	3.7539	0.4465	0.642316	1.9458	2.0542	1.0271	1.8789
D5	388.98	3.1874	0.6012	0.749504	2.2794	1.7206	0.8603	1.9591
D6	414.37	2.9921	1.1263	0.925235	2.4989	1.5011	0.7506	1.6968
D7	372.24	3.3307	0.4900	0.676406	2.3834	1.6166	0.8083	1.7627
D8	410.65	3.0192	0.3106	0.510897	2.5869	1.4131	0.7066	1.8027
D9	377.79	3.2818	0.7349	0.815880	2.3444	1.6556	0.8278	1.8862
D10	372.86	3.3253	0.5554	0.721640	2.3477	1.6523	0.8262	1.8930
D11	374.87	3.3074	0.4444	0.640582	2.2903	1.7097	0.8549	1.9409
D12	344.00	3.6042	0.3107	0.511011	1.7284	2.2716	1.1358	1.6500
D13	376.23	3.2954	0.6990	0.800011	2.1880	1.8120	0.9060	1.7488
D14	316.75	3.9143	0.2611	0.451849	1.4926	2.5074	1.2537	1.7730
D15	376.99	3.2888	0.8459	0.857406	1.6740	2.3260	1.1630	1.8304
D16	380.26	3.2605	0.4288	0.627437	1.6351	2.3649	1.1825	1.8223
D17	405.82	3.0551	0.7048	0.802667	2.5031	1.4969	0.7485	1.7831
D18	494.64	2.5066	0.2328	0.414941	1.9648	2.0352	1.0176	1.8949
D19	393.41	3.1515	0.4617	0.654618	2.2170	1.7830	0.8915	1.9545
D20	387.28	3.2014	0.4828	0.329008	2.4534	1.5466	0.7733	1.8476

The LHE is considered as a very important factor for the organic dyes in which we could appreciate the role of dyes in the DSSC, i.e. absorbing photons and injecting photo-excited electrons to the conduction band of the semi–conductor (TiO$_2$). In the order to know that to give an intuitional impression to how the influencing of donor spacer of the LHE, we simulated the UV/Vis absorption spectra of dyes. We remark that as the different dyes the oscillator strengths were changed. As shown in Table 2, the LHE of the dyes fall within the range: 0.1462–1.1263. The LHE values for the dyes are in different ranges and that all the dyes will give different photocurrent. But the D6 dye has highest oscillator strength value i.e 1.1263 and the LHE value is 0.925235. So the D6 dye has more efficiency than other studied dyes. The influencing factor as mentioned above, for enhancing the value of J_{sc}, which is the electronic injection free energy ΔG_{inject}. From the table 2, for all studied dyes, ΔG_{inject} is negative; this reveal that the electron injection process is spontaneous, and showing that dye's excited state would lies above the conduction band edge of TiO$_2$ resulting favorable condition for electron injection. The obtained values Voc of the studied dyes calculated according to the Eq. 7 range from 1.6500 eV to 1.9842 eV of TiO$_2$ (Tab. 2) these values are sufficient for a possible efficient electron injection.

Electron injection

The description of the electron transfer from a dye to a semiconductor, the rate of the charge transfer process can be derived from the general classical Marcus theory, [43-45].

$$k_{inject} = \left|V_{RP}\right|(2/h(\pi/\lambda k_B T)1/2\exp[-(\Delta G^{inject}+\lambda)2/4\lambda k_B T] \quad (8)$$

In eq. (8), k_{inject} is the rate constant (in s-1) of the electron injection from dye to TiO2, kB is the Boltzmann thermal energy, h the Planck constant, G^{inject} is the free energy of injection, $\left|V_{RP}\right|$ is the coupling constant between the reagent and the product potential curves. The use of the Generalized Mulliken-Hush formalism (GMH) allows evaluating |VRP| for a photoinduced charge transfer [30, 31]. Hsu et al. explained that |VRP| can be evaluated as [31]

$$\left|V_{RP}\right| = \frac{\Delta E_{RP}}{2} \quad (9)$$

The injection driving force can be formally expressed within Koopmans approximation as

$$\Delta E_{RP} = \left[E_{LUMO}^{dye} + 2E_{HOMO}^{dye}\right] - \left[E_{LUMO}^{dye} + E_{HOMO}^{dye} + E_{CBO}^{TiO_2}\right] \quad (10)$$

where $E_{CBO}^{TiO_2}$ is the conduction band edge. It is difficult to accurately determine $E_{CBO}^{TiO_2}$, because it is highly sensitive to the conditions (e.g. the pH of the solution) thus we have used $E_{CBO}^{TiO_2} = $ -4.0 eV [32] which is experimental value corresponding to conditions where the semiconductor is in contact with aqueous redox electrolytes of fixed pH 7.0 [46,47].

More quantitatively for a closed-shell system E_{LUMO}^{dye} corresponds to the reduction potential of the dye E_{RED}^{dye}, whereas the HOMO energy is related to the potential of first oxidation (i. e., - $E_{HOMO}^{dye} = E_{OX}^{dye}$). As a result, Eq. (11) becomes,

$$\Delta E_{RP} = \left[E_{OX}^{dye} + E_{OX}^{TiO_2}\right] \quad (11)$$

The $\left|V_{RP}\right|$ values were calculated from eq: 9-11 and the values presented in Table 2. The larger $\left|V_{RP}\right|$ leads to higher rate constant which would result better sensitizer according to eq (8). In all studied dyes the substituents phenyl; methoxy; thiophene; tetrahydrofuran; 2-vinaylthiophene and triphenyllamine are substituted at para, meta and ortho positions. From the table revealing the meta substituent dye s have high vales of $\left|V_{RP}\right|$ and para positions have low values in all the dyes because of that the o-otho and meta positions improve while the p-para position reduce them. So the ortho position substitutes of dyes are better sensitizer than other substituent's dyes. The order of studied dyes in terms better sensitizer are: m-meta > o-ortho > p-para position.

The absorption spectra of studied dyes have been computed at TD-DFT/BLYP with 6-31G (d) level of theory in gas phase. The transition character of the absorption bands in UV–Vis region for all dyes computed at the TD-DFT/B3LYP/6-31G (d) level are listed in Table 3 and Fig. 3. Electronic transitions up to 6 states were studied for all new designed sensitizers. According to the transition character, most of the dyes show the HOMO→LUMO transition as the first singlet excitation.

Table 3. The vertical singlet states, transition character of the absorption bands in UV–Vis region for all dyes computed at the TD-DFT/B3LYP/6-31G (d) level.

| Dye	transition	% contribution	Dye	transition	% contribution
D1	H -1->L	1.5276	D14	H ->L	28.6207
	H ->L	47.8573		H -3->L	8.3273
D2	H-3->L	11.5123		H-1 ->L	5.5458
	H->L	87.8661		H-1 ->L+1	10.6417
D3	H- ->L	5.0708		H ->L+1	44.1800
	H->L	94.9222	D15	H -4->L	4.0664
D4	H -3 ->L	77.7529		H-2->L	4.3767
	H -1 ->L	4.6769		H-1->L	83.8046
	H ->L	14.3487		H ->L+1	6.2382
D5	H-3->L	4.4480	D16	H -3->L	6.9147
	H-2->L	2.8370		H-2->L	2.8393
	H ->L	92.7549		H-1->L	86.1801
D6	H ->L	98.2073		H ->L+1	2.6102
D7	H-1 ->L	13.8044	D17	H-4->L	2.1541
	H-2 ->L	62.4671		H-1->L	8.0641
	H->L	22.3660		H ->L	88.9164
D8	H-1->L	11.4328	D18	H-1->L	2.2770
	H ->L	85.5013		H-2->L	11.3869
D9	H-2->L	8.1527		H ->L	4.0453
	H ->L	90.4943		H ->L+1	79.5615
D10	H-2->L	12.4012	D19	H -3->L	12.6635
	H->L	86.4954		H-2->L	4.0413
D11	H-2->L	13.0469		H-1->L	63.3735
	H-->L	13.7047		H ->L	17.2896
	H->L	72.7435	D20	H -3->L	6.0371
D12	H -3 ->L	65.0667		H-2->L	2.0693
	H-1->L	8.3673		H ->L	90.3141
	H->L+1	23.4832	H=HOMO; H-1= HOMO-1;H-2=HOMO-2; H-3=HOMO-3; L=LUMO;L+1=LUMO+1		
D13	H->L	11.8682			
	H-1->L	82.0942			
	H->L	2.2676			
	H->L+1	2.6376			
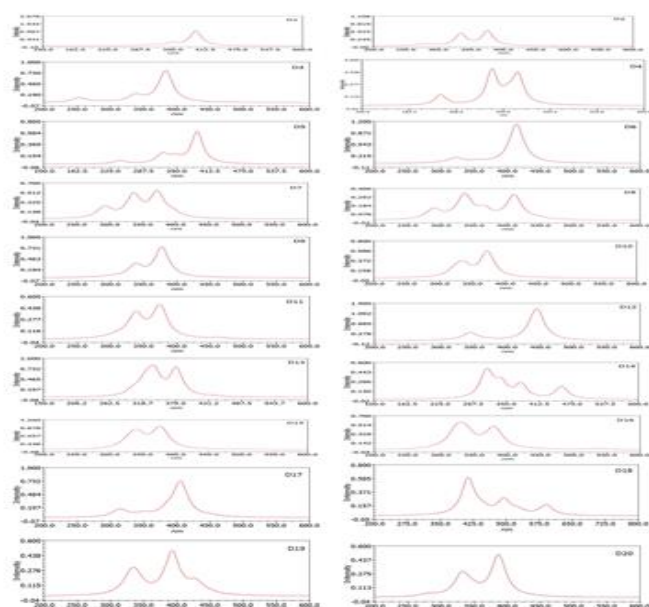
Figure 3. Calculated absorption spectra of studied dyes with B3LYP/6-31G9d) basis set in gas phase.

Conclusion

In the present study the effect of substituted groups and different position on structural and optoelectronic properties of the studied dyes by using 6-31G (d, p) basis set at a density functional B3LYP level. The studied molecules can be used in organic-sensitized solar cell because the electron injection process from the studied dyes to the conduction band of TiO_2 and the subsequent regeneration is possible LUMO (Dyes)> LUMO (TiO_2). The HOMO energy of all SOG dye derivates are less than the redox couple but expect the D1 and D17 is very slightly less than and D17 is approximately equal and D19 is greater than the redox couple. The LHE values for the dyes are in different ranges and that all the dyes will give different photocurrent. But the D6 dye has highest oscillator strength value i.e 1.1263 and the LHE value is 0.925235. So the D6 dye has more efficiency than other studied dyes. The $|V_{RP}|$ values shows that the meta substituent dyes are better sensitizers compare to other position substituent. Finally, the procedures of theoretical calculations can be employed to predict the electronic properties on the other compounds, and further to design novel materials for sensitizers for solar cells.

References

[1] M. Grätzel, Nature. 414 (2001) 338.

[2] M.Grätzel, J. Photochem. Photobiol. C 4 (2003) 145.

[3] M. K. Nazeeruddin, G. M.Festschrift, Coord. Chem. Rev, 248 (2004) 1161.

[4]N. Robertson, Angew. Chem. Int. Ed, 45, (2006) 2338.

[5]T.W. Hamann, R.A. Jensen, A.B.F. Martinson, H.V. Ryswyk, J.T.Hupp, Energy Environ. Sci, 1 (2008) 66.

[6]A. Hagfeldt, G.Boschloo, L.Sun, L.Kloo, H.Pettersson, Chem. Rev. 110 (2010) 6595.

[7] T.A.Heimer, E.J.Heilweil E.J, C.A.Bignozzi, G.Meyer, Phys J. Chem. A 104 (2000) 4256.

[8] M.K. Nazeeruddin , Coord. Chem. Rev, 248 (2004) 1161.

[9] P.V. Kamat, M. Haria, S. Hotchandani, J. Phys. Chem. B, 108 (2004) 5166.

[10] J. Bisquert, D. Cahen, G. Hodes, S. Ruehle, A. Zaban, Phys J. Chem. B, 108 (2004) 8106.

[11]A. Furube, R. Katoh, T.Yoshihara, K. Hara, S. Murata, H.Arakawa, et. al., J. Phys. Chem. B 108 (2004) 12583.

[12]G. Wang, S. Qian, J.Xu, W.Wang, X. Liu, X. Lu, F. Li, Physica Part B, 279 (2000) 116.

[13]S.Ando, J.Nishida, E.Fujiwara, H.Tada, Y.Inoue, S. Tokito, Y.Yamashita, Synth. Met, 156 (2006) 327.

[14]Y. Lei, Q. Niu, H. Mi, Y. Wang, I. Nurulla, W. Shi, J. Dyes and Pigments, 96 (2012) 138.

[15]P. Morvillo, E. Bobeico, J. Solar Energy Materials & Solar Cells, 92 (2008) 1192.

[16]C.L.Chochos, S.A.Choulis, J.Progressin PolymerScience, 36 (2011) 1326.

[17]A.S.Shalabi, S.Abdel Aal, M.M. Assem, J. Nano Energy, 1 (2012) 608.

[18] http://en.wikipedia.org/wiki/Sudan_Red_G.

[19]E.C.Vilarinho, O.A.Fernandes, E.Omoto, and etal., Journal of Economic Entomology, 99 (6) (2006) 2110.

[20] M.J. Frisch, G.W.Trucks, H.B Schlegal, G.E.Scuseria, M.A. Robb, J.R. Cheesman, et.al, Gaussian 09W, Revision A 11.4, Gaussian, Inc, Pittsburgh PA, 2002.

[21]S.Ando, J.Nishida, Y.Inohue, S.Tokito, Y.Yamashita, Idem. Synth. Met, 156 (2006) 327.

[22]Q. Shi, H. Fan, Y. Liu, W. Hu, Y. Li, X. Zhan, J. Phys. Chem. C, 114 (2010) 16843.

[23]M.Zhang, X.Guo, Y.Li, Adv. Energy Mater, 1(2011) 557.

[24]S.E.Shaheen, C.J.Brabec, N.S.Sariciftci, F.Padinger, T.Fromherz, J.C. Hummelen Appl Phys Lett, 78(6) (2001) 841.

[25]J. Zhang, H.B.Li, S.L.Sun, Y.Geng, Y. Wu, Z.M.Su, J. Mater. Chem, 22(2) (2012) 568.

[26] R.Katoh, A.Furube, T.Yoshihara, K.Hara, G. Fujihashi, S.Takano, et.a al, J. Phys. Chem. B, 108 (15) (2004) 4818.

[27] P.F. Barbara, T.J. Meyer, M.A. Ratner, J Phys Chem, 100 (1996) 13148.

[28] F.De Angelis, S.Fntacci, A.Selloni, Nanotechnology, 19 (2008) 424002.

[29]T. Marinado, K. Nonomura, J. Nissfolk, M.K. Karlsson, D.P. Hagberg,VL. Sun, et.al, Langmuir, 26 (4) (2009) 2592.

[30]G. Pourtois, J. Beljonne, M.A. Ratner, J.L. Bredas, J Am Chem Soc, 124, 4436 (2002).

[31]C.Hsu , Acc Chem Res, 42 (2009) 509.

[32]J.B. Asbury J, Y.Q. Wang , E. Hao, H. Ghosh, T. Lian , Res Chem Intermed, 27 (2001) 393.

[33]R. Katoh, A. Furube, T. Yoshihara, K. Hara. et al, J Phys Chem B, 108 (2004) 4818.

[34]A. Hagfeldt, M. Grätzel, Chem Rev, 95 (1995) 49.