

Research Article

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Quantum chemical calculations of phenazine-based organic dyes in dye-sensitized solar cells

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Abstract: In this study, quantum chemical calculations of phenazine-based organic molecules applied in organic dye-sensitized solar cells (DSSCs) have been made and interpreted. Since DSSC molecules work with the electron push–pull system, the sequence of other compounds (2–8) from compound 1 is designed as a donor– π bridge (weak acceptor)–acceptor (D– π –A). Later, the studied molecules were expanded from 2a to 8c by lengthening the conjugation with phenyl, thiophene, and furan to the acceptor parts. Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations are practiced to investigate all structures and absorption spectra of molecules, respectively. It has been observed that the phenazine-based molecule series are good candidates for DSSCs, both with their band gap and their absorption spectrum results. It can be assumed that changing the HOMO and LUMO energy values of all designed structures according to compound 1 can absorb light in the organic dye-sensitized solar cells and transfer electrons to the conductivity band of TiO₂. As a result, it has been resolved that various dyes can be designed for dye-sensitizing solar cells by calculating electronic energies, HOMO–LUMO energies, and absorption wavelengths.

Keywords: organic dyes, phenazine, DSSC, donor, acceptor

1 Introduction

Wide band-gap semiconductors can be made sensitive to the visible area by adsorbing organic dyes on their surface. Previously, Fujihira [1] reported the sensitization of

wide band-gap semiconductors to the visible region using dyes. The organic dye-sensitized solar cell, in other words, the Grätzel battery, is a structure that combines three separate layers such as semiconductor, dye, and electrolyte, which transform photon energy into electrical energy without the need for any chemical transformation [2]. Dye-sensitized solar cells (DSSCs), which are being researched as promising candidates for renewable energy systems, are of great interest in academic and industrial fields [3–11].

A dye-sensitized solar cell consists of the semiconductor film (working electrode) formed by sensitizing the nanocrystalline structure (usually TiO₂) coated on the conductive glass surface with organic dye, platinum-coated conductive glass (counter electrode), and the space that connects the working electrode and the counter electrode and fills the pores of the TiO₂ layer. In liquid electrolyte batteries, the space conducting material consists of iodide/triiodide (I⁻/I³⁻) redox couple in an organic solvent (usually nitriles). Good insulation is required for highly volatile solvent electrolytes. The semiconductor that will be used is directly related to the dye used. Still, TiO₂ has given the best result so far in terms of performance. The reduction (LUMO) and oxidation (HOMO) energy levels of the materials that produce organic DSSCs are selected in a way that the electron migration takes place in the desired direction and voluntarily.

Various dyes are synthesized for use in organic dye-sensitized solar cell production. For these dyes to be efficient in organic solar cells, they must have some basic properties [12]. The absorption spectrum of the dye should cover the entire visible region and the near-infrared (NIR) region. To reduce energy losses and keep the photovoltage at the highest possible level, the excited state energy (LUMO) of the dye should be slightly above the conductivity band of TiO₂ (more negative), and the energy difference should be sufficient to enable electron transfer [13]. Likewise, for the dye to be regenerated, the ground-state energy level (HOMO) must be more positive than the redox potential of the electrolyte [14]. Electron transfer from the excited state of the dye to the conductivity band of TiO₂ must be fast as not to allow quenching reactions such as fluorescence, phosphorescence, or dark process. The dye

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adsorbed on the TiO_2 surface must be stable for 20 years under operating conditions (at the semiconductor–electrolyte interface). It must be capable of solid adsorption to the semiconductor surface. The dye must have high solubility and include a binder group that can adhere to the semiconductor surface. For dye-sensitizing solar cells, there are many parameters to consider in dye designing: The dye should contain a broad absorption spectrum and, if possible, absorb in the IR region. The designed dye should have a high damping coefficient (the dye with this feature provides high photon absorption even in the use of thin semiconductor films). The designed dye must be able to bond strongly to the surface of the metal oxide semiconductor. Therefore, it is necessary to have binding groups such as $-\text{COOH}$, $-\text{H}_2\text{PO}_3$, $-\text{SO}_3\text{H}$ in the designed dye. The energy levels of the dye must be compatible with the conductivity band of the inorganic semiconductor and the redox pair, which additionally acts as a space conduction material. It should possess an easy and understandable synthesis procedure for possible large-scale production. It should be easy to recycle and have low toxicity. The designed dye should not settle on the semiconductor surface. The dye should be electrochemically stable. In order for the dye to be long-lasting, it must be resistant to light and heat.

Ruthenium dyes included in organometallic complexes are the dyes with the highest efficiency in organic solar cells so far. As is known, the absorption band expands with the increase of the conjugated system [15]. Although ruthenium polypyridyl dyes are the highest-yielding dyes to date, they are not ideal dyes. The limitations of these dyes are that they are challenging to synthesize, expensive starting materials, low molar absorption coefficients, and absorption in a very narrow range of the solar spectrum. Due to the limitations mentioned regarding metal complexes, interest in metal-free organic chromophores has increased in recent years. Organic dyes have some advantages over ruthenium-based chromophores. Fundamentally, they have a higher molar absorption coefficient and can be modified more easily due to the short synthesis methods (Figure 1).

2 Materials and methods

All calculations were achieved via the Gaussian 09W package [16]. While the density functional theory (DFT) method is used for the ground-state gas-phase optimization, the excited-state calculations are made using the time-dependent DFT (TD-DFT) method. DFT was calculated

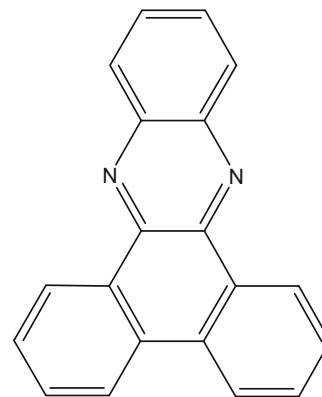


Figure 1: Structure of the parent compound (phenazine).

in hybrid functional B3LYP (Becke3-Lee Yang-Parr hybrid functional) with a 6-311++G(d,p) base set [17]. Excitation energies, oscillator powers, and orbital contribution for the lowest 10 singlet–singlet transitions in the optimized geometry in the ground state were obtained with TD-DFT calculations using the same basis set as geometry minimization.

Calculations were performed on an HP420WS desktop computer with Intel Xeon@CPU E5–1650. Calculations are carried out with high-performance server systems (workstations) over the WINDOWS operating system.

3 Conclusion and discussion

It is possible to synthesize several different chromophores using various donor binding acceptor groups for dye-sensitizing solar cells. Within the scope of the study, it was predicted that the phenazine (weak acceptor) π -bridge-based material will carry out electron transmission with the push–pull system with donor groups attached to one side. First, the pulling force was increased by using cyanoacrylic acid in the acceptor part; studies were conducted to determine the performance parameters of DSSCs of **2–8** molecules. Later, phenyl, thiophene, and furan were modified by cyanoacrylic acid (**2a–8c**). The push–pull system of the synthesized compounds from the donor to the acceptor is a concept that enables electron transmission in molecular dimensions.

Geometry optimizations of all structures (Figure 2) were performed first using the MM2 method, followed by the semi-empirical PM3 coherent molecular orbital (SCFMO) method [18]. Then, further geometry optimizations were achieved using RHF and B3LYP/6-311++G(d,p) levels. Average mode analysis for each structure did not result in any negative frequency in all three calculation

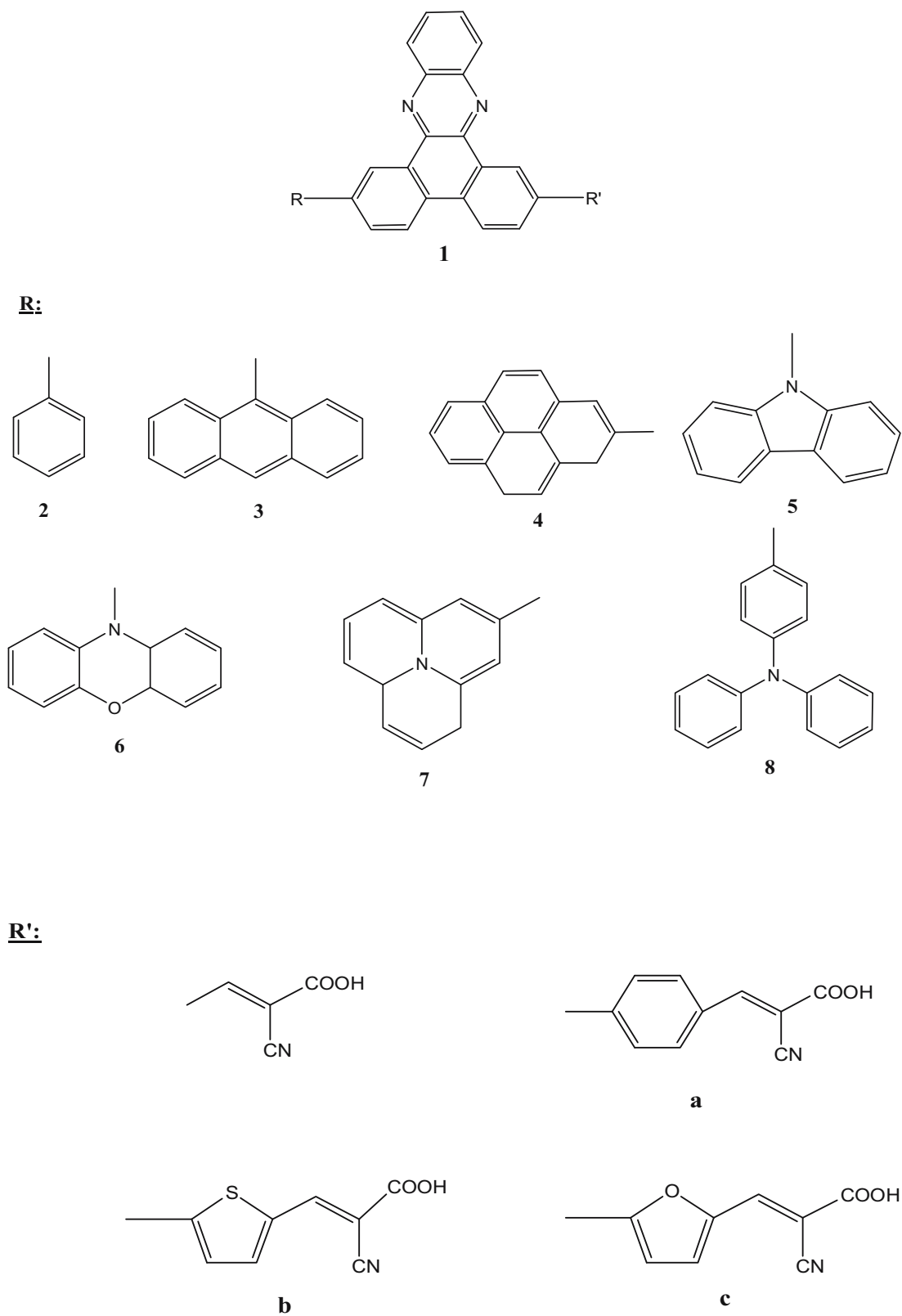


Figure 2: Chemical structures of paints designed on the basis of phenazine.

methods. The results of the analysis are presented in Table 1.

The ground-state geometry (GSG), HOMO, and LUMO diagrams of phenazine-based and dyes calculated in DFT/B3LYP/6-31++(d,p) in the gas phase are given in Table 2.

When examined in Table 2, good separation of HOMO–LUMO did not occur in structures 2a, 2b, and 2c formed by benzene substitution due to the low donor ability of benzene. Also, the HOMO–LUMO energy levels have not changed enough for the structures to have a better semiconducting capability. Deviations from planarity in donor–acceptor dihedral angles allowed good separation of HOMO–LUMO in the system for compounds (3a–8c). From Table 2, for compounds 3a–8c, HOMOs appear to be embedded in the donor part; LUMOs, on the other hand, appear to be embedded in receiver parts, so they can be said to be good semiconductor materials with potential use in devices. These results suggest that

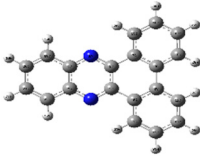
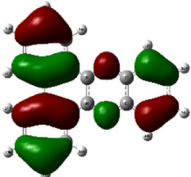
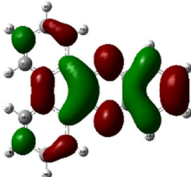
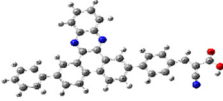
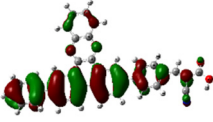
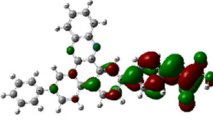
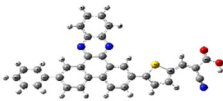
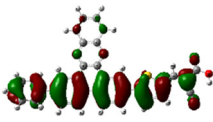
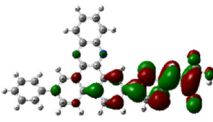
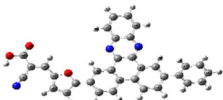
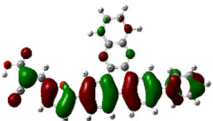
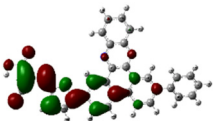
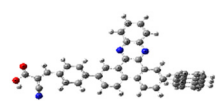
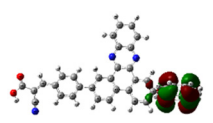
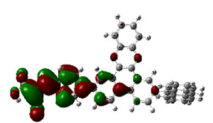
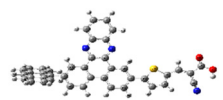
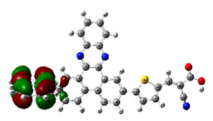
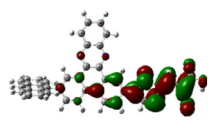
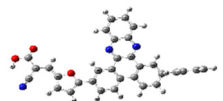

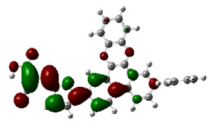
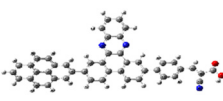
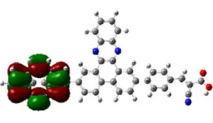
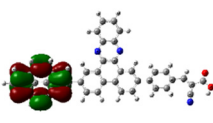
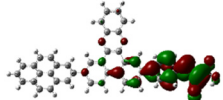
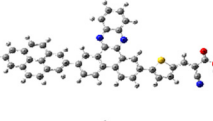
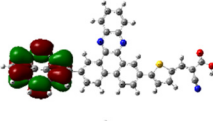
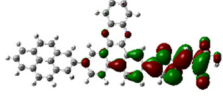
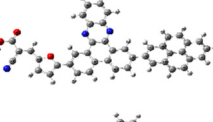
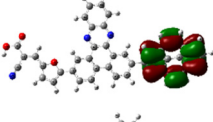
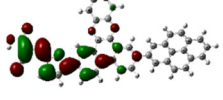
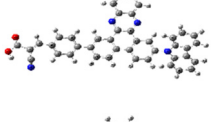
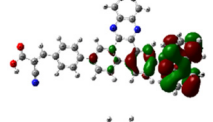
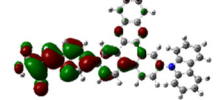
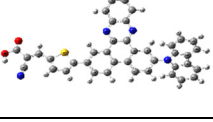
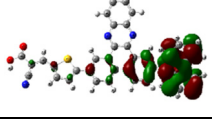
the designed compounds are combinations that might work well.

The frontier MO energies of the optimized compounds were calculated at the DFT/B3LYP/6-31++(d,p) level. Calculation results are shown in Table 1. As is known, the electronic structure of organic semiconductors is based on the conjugation of the electrons they have in their structure. Electrochemical parameters are interpreted with HOMO–LUMO values. From cyanoacrylic acid, which acts as the electron-withdrawing group, in which the LUMO orbitals are delocalized, phenazine in which the electron-donating group HOMO orbitals are delocalized is calculated. In general, as the number of electron-donating groups increases, HOMO and LUMO energy levels also change. The results obtained in Table 1 also support this. The energy band gap is calculated by subtracting the LUMO energy from the HOMO energy. It can be seen from the table that the calculated band gap decreases with increasing conjugation. The band gap of semiconductor

Table 1: Quantum chemical calculation results of dyes designed on the basis of phenazine

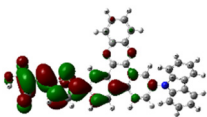

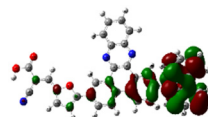
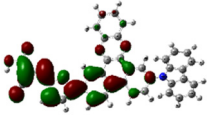
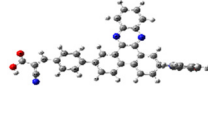
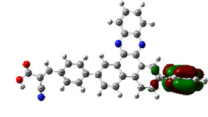
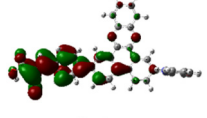
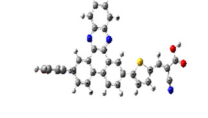
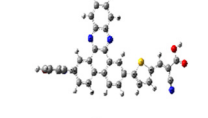
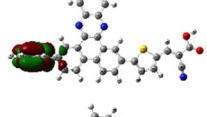
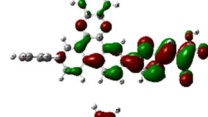
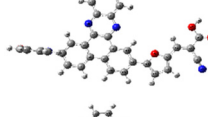
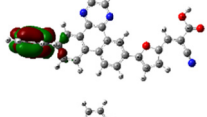
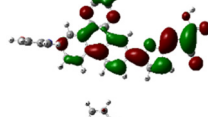
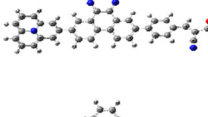
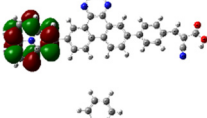
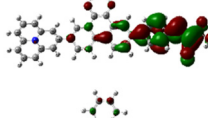
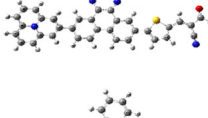
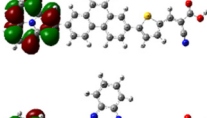
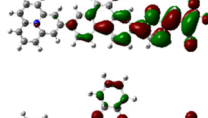
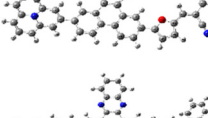
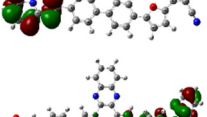
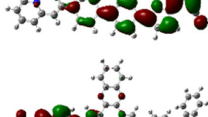
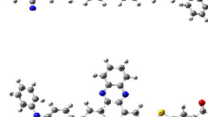
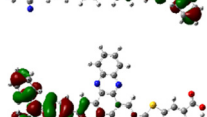
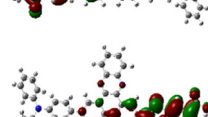
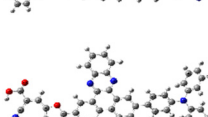
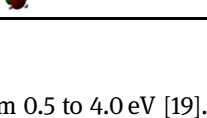

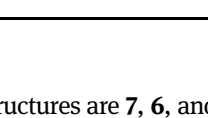
	$E_{(B3LYP)} (au)$	$E_{HOMO} (eV)$	$E_{LUMO} (eV)$	$E_{gap} (eV)$	$\mu (Debye)$	Wavelength (nm)	
						EST1	EST2
1	-879.1134	-6.36	-2.59	3.77	0.3487	386.33	380.42
2	-1468.5436	-6.39	-3.08	3.31	6.4683	416.60	394.01
2a	-1699.6535	-6.29	-3.18	3.11	7.5680	442.86	421.00
2b	-2020.4218	-6.26	-3.27	2.99	8.4398	458.61	433.00
2c	-1697.4459	-6.18	-3.21	2.97	7.9350	456.55	434.23
3	-1775.8642	-5.58	-2.94	2.64	5.7510	540.99	473.57
3a	-2006.9720	-5.57	-3.04	2.53	6.7191	542.56	499.29
3b	-2327.7391	-5.59	-3.13	2.46	7.4852	561.37	506.07
3c	-2004.7633	-5.59	-3.07	2.52	6.9881	550.87	496.79
4	-1852.1264	-5.76	-2.94	2.82	6.2643	489.42	432.35
4a	-2083.2341	-5.75	-3.03	2.72	7.2572	494.23	455.06
4b	-2404.0011	-5.78	-3.12	2.66	8.1106	509.12	460.19
4c	-2081.0255	-5.77	-3.06	2.71	7.5782	500.73	457.56
5	-1753.8007	-5.75	-3.02	2.73	4.6738	518.97	466.58
5a	-1984.9085	-5.71	-3.09	2.62	5.0692	527.71	494.66
5b	-2305.6754	-5.74	-3.18	2.56	5.8156	541.05	501.77
5c	-1982.6997	-5.73	-3.12	2.61	5.4221	534.34	494.40
6	-1829.0136	-5.01	-3.09	1.92	4.0095	801.02	657.09
6a	-2060.1217	-4.99	-3.13	1.86	3.8323	779.90	698.68
6b	-2380.8925	-5.01	-3.11	1.89	5.2960	786.98	697.88
6c	-2057.9171	-5.01	-3.07	1.94	4.8185	775.89	679.80
7	-1753.7627	-4.19	-2.99	1.20	5.7289	1484.38	1012.83
7a	-1984.8705	-4.17	-3.06	1.11	6.6205	1433.03	1128.01
7b	-2305.6438	-4.17	-3.02	1.15	5.3487	1436.35	1110.70
7c	-1982.6683	-4.17	-2.97	1.20	5.2072	1396.37	1070.53
8	-1986.0946	-5.33	-2.89	2.44	7.1119	566.72	500.87
8a	-2217.2022	-5.31	-3.01	2.30	8.1615	589.63	536.07
8b	-2537.9692	-5.34	-3.09	2.25	9.0984	608.02	542.53
8c	-2214.9936	-5.33	-3.03	2.30	8.5296	593.83	533.75

Table 2: GSG, HOMO, and LUMO diagrams of phenazine-based designed dyes calculated in DFT/B3LYP/6-311++g(d,p) in the gas phase

	GSG	HOMO	LUMO
1			
2a			
2b			
2c			
3a			
3b			
3c			
4a			
4b			
4c			
5a			
5b			

(Continued)

Table 2: Continued

	GSG	HOMO	LUMO
5c			
6a			
6b			
6c			
7a			
7b			
7c			
8a			
8b			
8c			

molecules ranges from 0.5 to 4.0 eV [19]. From Table 1, it is seen that the ΔE values, including the main compound (1), are below 4 eV. This band gap has narrowed with the addition of donor and acceptor units. The most significant reason for this is that the conjugation in the structure is prolonged with the combination made precisely as expected. As a result, it can be assumed that all compounds have the potential to be semiconductor materials. The three molecules with

the narrowest band gap among all structures are 7, 6, and 8 and their derivatives.

Regarding the addition of donor groups to one side of the parent compound (1) and the acceptor group on the other side, considering the compounds numbered 2–8 obtained by keeping the acceptor group constant and changing the donor groups, it was discovered that the three molecules with the lowest band energy were 7, 6,

and **8**. From Table 1, it can be observed that the HOMO–LUMO energy levels did not change enough for the structures to have better semiconductivities due to the two structures formed by benzene substitution and the low donor ability of benzene. Anthracene (**3**) [20], pyrene (**4**) [21], carbazole (**5**) [22], pheoxazine (**6**) [23], quinolizine (**7**) [24], and triphenylamine (**8**) [25] based systems have been well researched in the literature. Therefore, combining each of these donors with the parent compound resulted in potential candidate compounds working well for semiconductivity. When examining the **2a–8c** structures in terms of energy (Table 1), ΔE of the HOMO–LUMO ranges from 3.11 to 1.11 eV. These results reveal that the designed compounds are combinations that can work well. The potential utilization of compound **1** as a semiconductor material has been successfully increased by modification with strong donor groups and strong acceptor groups.

Substituents added to the structure in the synthesis of phenazine-based dyes cause changes in the absorption spectrum. The photophysical properties of the gas phase were calculated using TD-DFT calculations to obtain and interpret phenazine derivatives with high absorption in a wide range in the red/NIR region. From Table 1, EST_1 gives the first transition state wavelength and EST_2 gives the second single pass wavelength. The incoming peaks are due to the π – π^* transitions and the second peaks are due to the intramolecular charge transfer (ICT) between the donor and acceptor.

As seen in Table 1, the **2–8** molecules gave absorption spectra at 416.60, 540.99, 489.42, 518.97, 801.02, 1484.38, and 566.72 nm, respectively; thus, a redshift, that is, bathochromic effect, was observed by changing the 386.33 nm wavelength donor groups of compound **1**. Similarly, a bathochromic effect was observed in the absorption spectra due to increased conjugation with the addition of phenyl (**a**), thiophene (**b**), and furan (**c**) groups to the acceptor site of the phenazine-based molecule. Again, a considerable increase in redshift is observed with the effect of substances added to phenazine. It can be assumed that it can be applied in photovoltaic applications as it absorbs the solar spectrum in the visible region and the NIR region, among the other molecules studied. The best candidates are molecule **7**.

The molecule with the lowest bandgap (**7a**) gave a longer wavelength in the gas phase than other structures. The provided structures made it even more stable by adding π -bridge, donor, and acceptor groups. As a result, it can be assumed that both increasing the conjugation and heteroatoms have made the structure more stable by shifting the oxidation potential to the right; oxidation

potential means the HOMO energy of the molecule. To provide effective regeneration in the solar cell, the HOMO potential of the dye should be lower than that of the electrolyte. The energy level in the I^-/I^{3-} system is -4.8 eV [26]. Increased conjugation and the addition of different substitution groups also affect the reduction potential in a molecule. With the increase of conjugation, the reduction potential, namely the LUMO value, shifts to a more negative region. The LUMO value must be higher than the conductivity band of TiO_2 (-4.0 eV for TiO_2) to ensure electron transfer from the organic molecule to the conductivity band (CB) of TiO_2 . Thus, the dyes synthesized can absorb light and transfer electrons to the conductivity band of TiO_2 in organic DSSCs [27]. When looking at the result table, the HOMO values of all molecules, including molecule number **1**, are lower than -4.8 eV, and all LUMO values are higher than -4.0 eV. This reveals that the energy levels and band gaps of the designed and studied molecules can be applied in DSSCs. As a result, many different dyes can be designed for dye-sensitizing solar cells by calculating electronic energy, HOMO–LUMO energies, and absorption wavelengths.

4 Results

In this study, the group is the highly soluble derivative of the structure known in the literature as phenazine or quinoxaline. This group has a weak acceptor feature and attracts the electrons given to the structure by the donor at a specific rate and provides transmission to the strong acceptor group on the other side. In this study, the properties of organic dyes that contain different donor groups to phenazine-based molecules and that can be used in organic solar cells by adding other π -linker groups to the system on the acceptor side have been quantum chemically studied. Therefore, it was assumed that various dyes could be a guide for a rational design. Using cyanoacrylic acid and then the derivatives of cyanoacrylic acid with phenyl, thiophene, and furan as the acceptor, the transmission of the electron along the molecule has been tried to be achieved most efficiently.

The phenazine derivative π -bridge group in the structure has a very high conjugation. Molar absorption coefficients that increase with conjugation are a factor that increases light absorption and charge separation. The π -bridge-group length decreases the possibility of reunifying the loads with its structure, providing structural rigidity and high conjugation and all these effects. Thiophene has lower transition energy and lower equilibration energy

than those of phenyl and furan by adding the free electron pair in its structure to conjugation. As a result, the absorption redshifts, and the molar absorption coefficient is increased, with a relatively narrow bandgap and more photons have been absorbed.

One of the most critical parameters in dye-sensitizing solar cells is the movement of the electron from the dye to the anode in the opposite direction, namely the cathode, which is called recombination. Although there are multiple factors such as the use of materials that do not have suitable band values, the use of unsuitable electrolytes, and the conductivity band values of the selected electrodes, the synthesis and the use of materials with appropriate band gaps are the most important. The HOMO value has increased in all of the designed molecules and the LUMO value has also been brought to a more negative value than the vacuum.

Phenazine-based molecule series are good candidates for DSSCs, both with band gap and absorption spectrum results. It can be assumed that by changing the HOMO and LUMO energy values of all designed structures according to compound **1**, it can absorb light in the organic dye-sensitized solar cell and transfer electrons to the conductivity band of TiO₂. As a result, many different dyes can be designed for dye-sensitizing solar cells by calculating electronic energy, HOMO–LUMO energies, and absorption wavelengths.

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