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Analyzing the Impact of Different Molecular Configurations of Organic Dyes on the Efficiency of Dye-Sensitized Solar Cell

Palwasha Tehseen [1*], **Aafia iftikhar** [2], **Muhammad Ibtihaj Jamil** [3], **Areeba Khalid** [4], **Ammara Naseem** [5], **Mehvish Mushtaq** [6], **Kinza** [7], **Seemab Khanam** [8], **Syeda Azka Sajid** [9]

[1-9] Department of Chemistry, University of Agriculture Faisalabad 38000, Punjab, Pakistan

* Corresponding Author: **Palwasha Tehseen**

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Abstract

Global energy consumption rises each year due to increasing energy demand and population expansion. The main non-renewable energy sources are thermal and hydroelectric power. However, due to increasing consumption rates, these resources are depleting rapidly. Scientists are prioritizing renewable energy technologies like photovoltaic energy, which converts solar radiation into electricity, to meet the demand for abundant energy sources. In recent years, they've developed inorganic, organic, and hybrid photovoltaic systems using diverse techniques to meet various application needs. The most effective organic solar cells are dye-sensitized solar cells (DSSCs), which are inexpensive and easy to use. This review paper emphasizes illustrating the technological significance of the structure of DSSCs, components of DSSC and working mechanism of DSSC, steps towards increasing the efficiency of dyes for DSSC, the effectiveness, and challenges for research and improvement of DSSCs to improve the existing efficiency. The main focus of this paper is to investigate the effect of different molecular configurations of dyes on the efficiency of dye-sensitized solar cells. We have reviewed dyes with various configurations, such as D-π-A, D-π-π-A, D-D-π-A, D-π-A-A, and D-(A-π-A) 2, to show how different donors, pi-spacers, and acceptors affect the photovoltaic characteristics of dye-sensitized solar cells.

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1. Introduction

The worldwide energy consumption has increased yearly by several percentages over the last thirty years. Nowadays, a large amount of energy is provided by fossil fuels on the one hand and by nuclear energy on the other hand. However these sources are insufficient and their consumption has a serious environmental impact, probably extending over several future generations (Brabec, Sariciftci, & Hummelen, 2001) [9]. Pakistan is one of those countries which are deficient in energy with only limited fossil fuel sources. The major sources of energy are gas, coal, and oil. These sources are nonrenewable and inadequate which run out day by day. Due to population increase and the expansion of industries, there is a high energy demand. The burning of fossil fuels is challenging as it is a threat to the environment (Shaikh, Ji, & Fan, 2015) [53]. Therefore, there is a need for an alternative solution to this problem in the form of renewable energy supplies (Eppich, Mullan, Brett-Fleegler, & Cheng, 2016) [23]. The radiant energy coming from the sun is free from any type of contamination and is an endless renewable energy source. Solar energy is adequate to beat out the energy acquired by nonrenewable energy sources like coal petroleum natural gas and will be used in upcoming years as shown in Figure 1(Nijsse *et al.*, 2023) [43].

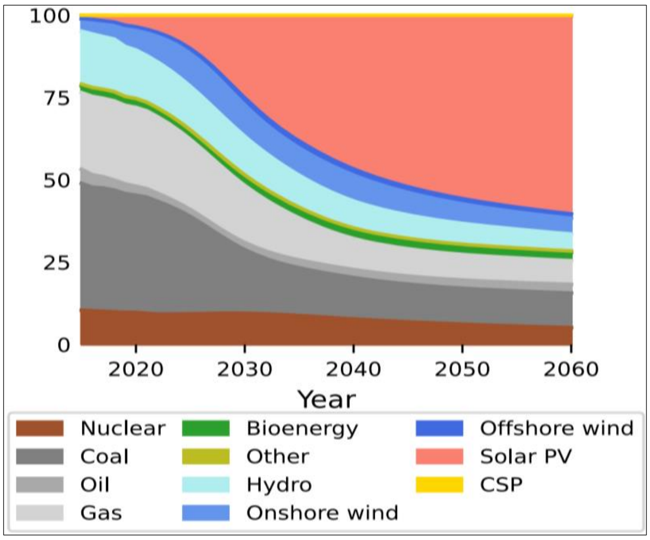

Fig 1: The global distribution of electricity generation from different technologies (Nijsse *et al*., 2023) [43].

Solar power is the best alternative for depleting sources of energy and it is a promising way of producing energy if we want to meet the demands of energy in the current era which is ever increasing (Mwalukuku *et al*., 2023) [42]. New solar cell technologies, which are based on industrially compatible methodological processes and involve using cheap and readily available materials, have been introduced (Gauthier *et al*., 2020) [25]. In this regard, researchers have been focusing their attention on the production of semiconductor devices that switch solar energy into electrical power known as photovoltaics, having sufficiently high value of PCE(Power conversion efficiency), simple design, and cost-appropriate to efficiently satisfy the demands of energy consumption (Ashfaq, Talreja, Singh, & Chauhan, 2023) [7].

Solar cells can be of both types organic and inorganic, but there are some major differences between both types of solar cells. Organic photovoltaics (OPVs) can be made 1000 times thinner than inorganic photovoltaics IPVs, therefore reducing material cost greatly. They (OPVs) have higher absorptivities than IPVs (Bagher, 2014) [8]. They are lightweight (G. Wang, Melkonyan, Facchetti, & Marks, 2019) [67] and cost-effective devices (Duan & Uddin, 2020) [21]. One of the main advantages of OPVs over IPVs is their ability to use solution-processed blend donor and acceptor substances as a dynamic layer (X. Wang *et al*., 2021) [68]. This Solution processing allows the generation of cost-effective solar cells (McDowell, Abdelsamie, Toney, & Bazan, 2018) [41]. Out of various flexible organic photovoltaics (organic solar cells) that are available, ultrathin organic photovoltaics with a thickness of less than 10 µm possess characteristic features i.e. excellent mechanical bending stability and flexibility (Fukuda, Yu, & Someya, 2020) [24]. The two main advantages of organic photovoltaics over inorganic photovoltaics are the ability to generate OPVs on flexible substrates and low-cost manufacturing processes (Ajayan *et al*., 2020) [1].

In photovoltaics (PV), DSSCs are most frequently studied as an accurate substitute for the supply of energy compared with other available PV. DSSCs are considered reliable energy sources due to their safe conversion of light energy into electrical energy, environmentally compatible procedure, and inexpensive and efficient production of energy even in lower light intensity (Rajaramanan, Heidari Gourji, Velauthapillai, Ravirajan, & Senthilnanthanan, 2023) [47]. The reason why DSSCs are considered efficient photovoltaics lies in the fact that materials for them are available easily and at low prices in addition to their simple framework consisting of light, flexible, and smart panels (Hendi *et al*., 2023) [31].

As soon as they were discovered, it was realized that it was quite inexpensive to transform solar energy into electrical power by using them as compared to silicon solar cells. DSSCs (a type of OPVs) have become a piece of attraction as a substitute for silicon-based solar cells (IPVs) (Chung *et al*., 2020) [15] due to lower fabrication costs (Savariraj & Mangalaraja, 2021) [50] and large photovoltaic conversion efficiency (Sutradhar, 2021) [63]. In DSSCs, the process of light absorption by dyes plays a crucial role in energy trapping. By absorbing light, dyes transfer their excited electrons from their high-energy valence band to the conduction band of a semiconductor in an ultrafast manner. This electron transfer process at the interface between the dye and the semiconductor acts as a starting point for the flow of electric current in the solar cell (Seyednoruziyan *et al*., 2021) [52]. Compared to other solar cells, DSSCs perform better when exposed to harsh operating conditions like diffused light and high temperatures (Hagfeldt, Boschloo, Sun, Kloo, & Pettersson, 2010) [30].

Generally, the efficiency of a DSSC relies heavily on some features of the sensitizing dye. These are energy band gap (Chamanzadeh, Ansari, & Zahedifar, 2021) [12], light harvesting efficiency, electronic structure (AL-Temimei & Alkhayatt, 2020) [3], and the method of dye anchoring on the surface of the photoanode (Siddika *et al*., 2022) [56]. One of the key advantages of DSSCs is that they offer the potential to make solar cells with versatilities in shape, color, and clearness (Hagfeldt *et al*., 2010) [30]. The open circuit voltage (V_{oc}) and the short circuit current (I_{sc}) are the two factors that have a significant impact on the overall efficiency of the DSSCs (Damaceanu *et al*., 2019) [18]. The photoelectric conversion efficiency is directly proportional to the open circuit voltage (V_{oc}) and short circuit current (I_{sc}). As the (V_{oc}) and (I_{sc}) increases, the efficiency of DSSC increases (Liu *et al*., 2021) [40]. According to the detailed balance theory, voltage loss in OPVs is due to radiative and non-radiative recombinations. Out of these, non-radiative recombination is related to the intrinsic property of the substances (Wanning Li *et al*., 2018) [38].

Investment in the production of DSSCs has started recently by many companies who believe in the fact that their average life span is 25 to 30 years with a PCE loss of <5%. Newly designed DSSCs are liquid, semi-liquid, or solid-state devices that in addition to a mobile electrolyte contain dyes as sensitizers which decompose when they come in contact with moisture and oxygen. The stability of photovoltaics depends upon its intrinsic and extrinsic factors as well.

2. Components/Parts of Dye-Sensitized Solar cell

A classic DSSC consists of four essential components; the dye molecule (sensitizer), transparent conducting, counter-conducting electrodes, and the electrolyte.

2.1 The dye

Dye is works as a sensitizer in dssc that is present as a single layer in PVs harvests the light incident on it from the sun and creates positive and negative charge carriers in cells similar case to chlorophyll in plants. So, DSSCs provide an excellent substitute concept to PN-junction photovoltaics available today, which is technically and economically credible (Roy *et al*., 2023) [48].

2.2 The electrolyte

In DSSC several types of titanium dioxide nanoparticles are layered with light-sensitive dye and the electrolyte surrounds these nanoparticles. Electrolyte can be I^- /I^-_3, Br^- /Br_2, SCN^- / SCN_2 and Co (II)/Co(III) (Sharma, Sharma, & Sharma, 2018b) [54]. There are five major constituents of an electrolyte, i.e., redox couple, solvent, additives, ionic liquid, and cations.

A suitable electrolyte should have the following properties:

- Redox couples should be proficient in stimulating the oxidized dye powerfully.
- Its strength (chemical, thermal, and electrochemical) should be long-lasting.
- With dssc components electrolyte should be non-corrosive
- Should be capable of allowing rapid distribution of charge carriers, enhancing conductivity, and forming efficient connections between the working and counter electrodes.
- The absorption spectrum of dye and electrolyte should not intersect with each other.

2.3 The photoanodes

The photoanodes in DSSCs are thin semiconductor films that are made of nanomaterials. On the surface of the semiconductor film, the most important component of DSSCs, dye, is present which is capable of the absorption of energy from the sun (Ghosh *et al*., 2011) [27]. Most commonly N719 dyes were used in DSSCs which are ruthenium(II) sensitizers (Roy *et al*., 2023) [48]. To achieve optimum performance in DSSCs, the photoanode must have sufficient surface area allowing effective scattering of photons on its surface, and improved molar absorption coefficient in the absorption region of dye (Selvapriya *et al*., 2023) [51]. Of the many available semiconducting oxide materials, TiO2 is considered best because of its greater surface area, safer nature, environmental compatibility, and chemical and optical stability (Drygała, 2021) [19]. The DSSCs which consists of a photoanode made of semiconductor material TiO2, coated with a layer of light absorbing dye, and a counter electrode dipped in a liquid electrolyte made of redox couple have been commercialized and are a reliable substitute for silicon solar cells (Elmorsy, Badawy, Alzahrani, & El-Rayyes, 2023) [22]. Different types of nanomaterials for TiO_2 photoanode to be used in dssc are available such as; nanofibers, nanocrystals, nanoplates, nanotubes, nanoribbon, nanoflower, nanowires, etc. among them nanofibers is accepted as the best material for photoanode because of its greater surface area, improved efficiency and excellent electrical conductivity (Kuppu *et al*., 2023) [35].

2.4 The counter electrode

In DSSCs, the counter electrode should be stable, highly conductive, and catalytically active for its crucial functions which it performs in DSSCs i.e., transportation of electrons from external circuits and reduction of redox couple in the electrolyte (Peter, Rajamanickam, Ragavendran, Mayandi, & Nithiananthi, 2023) [45].

3. Working of DSSCs

Looking at the mechanism of DSSCs, first dye is photoexcited, then an electron from this excited dye is injected into the conduction band of TiO2, then through this TiO2, electrons are transported to the external circuit, the reducing redox couple of electrolyte regenerate the dye cation, followed by the reduction of redox couple at the counter electrode of DSSCs as illustrated in figure 2.

When the light is incident on the dye, it is photoexcited, and electrons from HOMO orbital jump to LUMO of dye from where they are inserted into the conduction band of the photoanode (Al-Masoodi, Rafiq, El Assyry, & Derouiche, 2021) [2]. For the effective injection of electrons, the conduction band of photoanode should be at an inferior potential than the energy of the lowest unoccupied molecular orbital of the dye. From the photoanode, these electrons are transferred to the external circuit whereby the counter electrode draws these electrons back to the solar cell. To compensate for the dye of its electrons, a redox couple of electrolytes act as a bridge between the counter electrode and dye. For this purpose, the redox couple should be at higher potential than the energy of the HOMO of dye.

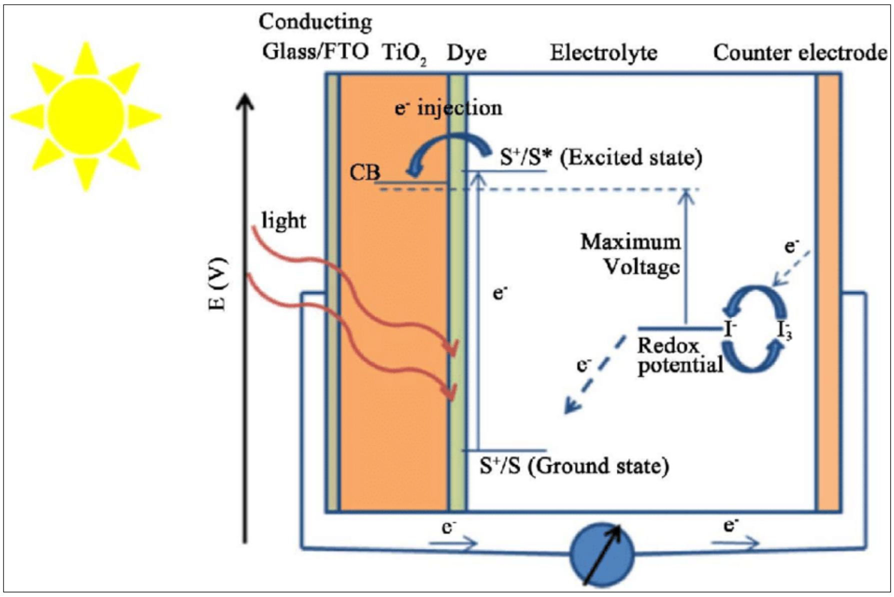

Fig 2: Working of a DSSC (Sharma, Sharma, & Sharma, 2018a) [54].

3.1 DSSCs Power Conversion Efficiency (PCE)

The following equation can be used to calculate the PCE of DSSCs:

$$\mathrm{PCE} = \mathrm{J_{SC}V_{OC}.FF/P_{IN}}$$

While;

Short circuit current density is denoted by J_{SC}, open circuit voltage which can be considered by the variation between the redox potential of redox couple and Fermi level of photoanode is represented by V_{OC}, FF is fill factor and power intensity of incident light is denoted by P_{IN} in the above equation **V_{OC} =** open circuit voltage (can be considered by the variation between redox potential of redox couple and Fermi level of photoanode).

FF = fill factor,

P_{IN} = power intensity of incident light.

Iodide and tri-iodide (I^-/I^{3-}) have been considered as the best redox couple for DSSCs for the last many years because of their redox potential which is adequate when working with dyes.

4. Increasing power conversion efficiency of DSSCs

For the improvement of PCE of DSSCs, several attempts have been made.In this regard, different natural and synthetic dyes have been produced. The functional group of dye is attached to the oxide semiconductor which acts as a component for the insertion of an electron from the valence band of excited dye to the photoanode conduction band (Weldemicheal, Desta, & Mekonnen, 2023) [70]. In order to get improved power conversion efficiency of DSSCs, the design of the photoanode should be such that, maximum dye can be loaded on it, charge carriers can be easily transported and recombination of charge carriers can be minimized to a large extent (Srivastava *et al*., 2023) [60].

4.1 Organic dyes for DSSCs

Among the available dyes, organic dyes are more efficient owing to their ease of transportation of electrons, less toxic nature and higher molar absorption coefficient (Kim, Chung, & Kim, 2013) [34].In comparison to this, natural dyes that are obtained from seeds, stems, flowers, leaves, and roots of plants are considered less efficient due to their slower rate of transfer of electrons, less stability, and lesser absorbance. However these dyes can have higher molar absorption coefficients in the visible region, involve simpler synthetic processes, and are inexpensive, and environmentally compatible in terms of cleanliness (Al Batty, Al-Jubouri, Wali Hakami, Sarief, & Haque, 2022) [4]. Metal-free organic dyes are recognized as efficient, reliable and cost effective component to be used as sensitizer in DSSCs because of their simpler design, higher molar absorption coefficient,, flexibility in structure and their adjustable electrical and optical properties (Dua, Kaya, & Sarkar, 2023) [20].

4.2 Importance of dyes in solar cells

Dyes have been declared as “exciting area” in many publications due to the properties which they impart to DSSCs. The component which acts as a donor of electrons in DSSCs is the dye, so it should posses’ maximum absorption capacities. An efficient dye should be luminous and should be absorptive in uv-visible and infrared regions (Al Batty *et al*., 2022) [4]. Now-a-days, researches have been conducted on the study of organic dyes; mainly focus on the synthesis of highly efficient and environment friendly dyes. Keeping in the view of above characteristics of dyes, D-π-A sensitizer has been recognized as an effective dye to meet the demands of efficient DSSCs. But still the issues of synthesized organic dyes is that they have weak molar absorption coefficient and very narrow band in the uv-visible and infrared region (Xie, Liu, Li, *et al*., 2019) [73].

4.2 Increasing efficiency of dyes

Modern studies have revealed that the light absorption by dyes and intramolecular charge transfer can be increased by introducing conjugated groups in dyes (Al-Masoodi *et al*., 2021) [2]. The absorption band of dyes can be red-shifted, thus, their light absorbing capacity can be increased by the expansion of π-conjugation in dyes such as the introduction of ethylene groups in them. Despite of this strategy it is not prominent that whether it is universally acceptable or not. However, recent researches are devoted towards the extension of π-conjugation on dyes rather than on donor and acceptor (Park *et al*., 2019) [44].

5. Components of dye

In a DSSCs, dye (sensitizer) consists of three basic components; first one is a **donor (D)** moiety which after photoexcitation, passes the electrons towards the remaining part of the dye, second is a **π-spacer** which acts as a bridge between donor and acceptor part of the dye, carries electrons to the third component of dye that is **acceptor (A)** moiety which accepts the electrons moved by the donor group through π-spacer. These three components are the pillars of D-π-A dye (Dua *et al*., 2023; C.-J. Tan, Yang, Sheng, Amini, & Tsai, 2016) [20, 64]. An anchoring group is connected to the acceptor moiety of dye to bind it with the semiconductor surface. Studies have been conducted on more complex dyes such as D-D-π-A, D-A-π-A etc. which allows the tuning of DSSCs by the introduction of auxiliary donors and acceptors(Tripathi, Kumar, & Chetti, 2022) [66].

5.1 Donors used in dye

Triphenylamine (TPA), carbazole, indoline (Gauthier *et al*., 2020) [25] etc. are most commonly used donors because of their electron-donating abilities and they have shown excellent results in many experiments. Now the focus of modern researches is mainly on introducing new donors or the introduction of extra moieties on the donor group that can increase its electron-donating abilities.

Triphenylamine (TPA) is considered to be an outstanding donor functional group for dyes among the various available donors (Almenningen *et al*., 2021) [5]. The dyes containing triphenylamine functional group as donor moiety are being most frequently used in DSSC (dye-sensitized solar cells) and have been showing excellent photovoltaic performances due to reasons; firstly, it has a non-planar geometry which prohibits aggregation and secondly it possesses excellent hole-transporting properties which make it a good donor(Sangiorgi, Sangiorgi, Sanson, Licchelli, & Orbelli Biroli, 2023) [49].

5.2 Pi-spacers used in dyes

The intramolecular charge transfer efficiency of the cell is affected by the variation of π-spacer between acceptor and donor part of dye and thus play a suitable role in determining the overall efficiency of DSSCs. Keeping in view this consideration, it has been recognized that the introduction of π-spacer in dye causes the red-shift of spectrum and broadens the band of absorption (Gupta *et al*., 2014) [29]. The photophysical properties of cell can be regulated by the nature of π-spacer in the dye. Quite efficient results have been shown by using the thiophene and benzothiadiazole-phenyl heterocycle (Xie, Liu, Bai, & Zhang, 2019) [72] as π-linker. Final dye is largely stabilized by the use of thiophene as π-spacer. Moreover, the recombination rate of dye cation and thus its stability can be increased by the use of unevenπ-conjugated bridge(A-π) in which benzothiadiazole (BTZ), an acceptor group is attached to the thiophene part of triphenylamine and a phenyl ring is present between acceptor (A) unit an anchoring cyanoacrylic acid (Colom *et al*., 2019) [16].

5.3 Acceptors used in dyes

Various electron acceptor moieties are available that can be used in DSSCs for example, **benzotriazole, diketopyrrolopyrrole and benzothiadiazole** etc (Raftani *et al*., 2023) [46]. But **cyanoacrylic-acid** is considered as an effective and has been most commonly used as an acceptor moiety in most of D-π-A organic dyes. The preference of cyanoacrylic acid over other acceptor moieties owes to the electron withdrawing cyano group (Almenningen *et al*., 2021) [5] that is present in a close vicinity to the carboxylic acid group and in addition to increasing, also increases its capacity of injecting electrons its spectral response through intramolecular charge transfer (ICT) (Cowper, Pockett, Kociok-Köhn, Cameron, & Lewis, 2018) [17].

6. Different molecular configurations of dyes

In a comparison to D-π-A dyes, having only one donor moiety, sensitizers having two donor groups **(D2–π–A)** (S. Chen, Pang, & Wu, 2021) [13] are also available which presents following advantages; improves light-absorbing capacity of dye, increases molar absorption coefficient(ε) which is necessary for higher value of short-circuit current density (Jsc), prevents π-π aggregation and decreases recombination ability of dye cation with the injected electrons which is desirable for obtaining a large open circuit voltage (Voc). So, (D2–π–A) sensitizers play an important role in overall increasing the value of power conversion efficiency (PCE) since, PCE is determined by both factors Jsc and Voc at a given incident illumination intensity (Jin *et al*., 2021) [33].

Similarly, dyes with **D-A-π-A** design are also available that contains an auxiliary acceptor unit between donor moiety and π-linker. It results in more efficient photoelectric properties of cell. Moreover, such type of configuration (D-A-π-A) (Wenqin Li, Wu, Zhang, Tian, & Zhu, 2012) [37] acts as a source through which we can accurately regulate the energy level positions so that the transportation of electron become easy from donor to the acceptor moiety (Sharmoukh, Cong, Ali, Allam, & Kloo, 2020) [55].

Furthermore, the auxiliary acceptor A play a significant role in improving the photovoltaic performance of DSSCs because it broadens the absorption wavelength and enhances electron coupling π bridge occupies remarkable importance since it directly affects the absorption spectra. Thus, for the construction of an efficient DSSCs, it is kept at priority to extend the structure as planar-type construction blocks with fused heterocycles using π bridge (Yen, Hsu, Ni, & Lin, 2021) [74].

7. Steps towards increasing efficiency of dyes for DSSCs

Many efforts have been made for the synthesis of novel structured dyes for solar cells, such that their absorption band could be broadened to the infrared region. This can be made possible by using molecular engineering which will lower the energy of lowest occupied orbital of dye. Yet, it is a challenge to construct a dye that can absorb the radiation throughout the region of sunlight spectrum. However, some panchromatic sensitizers are available, but because their LUMO energies are similar to those of the semiconductor oxide (TiO2) conduction band, they have considerably lower PCEs (Wu *et al*., 2020) [71].

7.1 Systematic adsorption of dye on the surface of semiconductor diode

Researchers have shown, based upon their studies that the photovoltaic properties of a cell are greatly affected by the way how sensitizers are adsorbed on the surface of titanium dioxide. On the surface of TiO_2, sensitizers have to face the problems of π–π aggregation due to interaction of pi-electrons which is one of the contributing factors in falling the effectiveness of DSSCs. Furthermore, aggregation will also result in reduced open circuit voltage (V_{OC}) because it will result in the exposure of active points on the surface of titanium oxide, so that redox couple (I^-/I^{3-}) from electrolyte can easily reach its surface and accept electrons (Z.-E. Chen, Zang, Qi, & Zhang, 2020; Colom *et al*., 2019) [14, 16].

By the introduction of bulky groups in dyes or by using different co-adsorbents in dyes, aggregation can be avoided. This will result in prohibition of recombination process to large extent and thus will lead to an increase in the stability of system (Colom *et al*., 2019; Yıldız *et al*., 2021) [16, 75].

7.2 Binding potential of dye on semiconductor diode

Another important factor which affects the stability and PCE of DSSCs is the potency of dye which it binds on the surface of titanium dioxide. Strong binding of dye on the surface of TiO_2 will cause improvement of adsorption and will ultimately result in the facile transfer of electron from dye to the TiO_2 (Chae & Kang, 2011) [11]. Up till yet, the lower efficiency of organic dyes is their weakness of having limited or only one anchoring groups as compared to Ru(II) sensitizers which contain 1 to 4 anchoring groups(Gupta *et al*., 2014) [29].

7.3 Use of multiple anchoring groups in dye

Thus, for improved efficiency and stability of DSSCs various organic dyes with multiple anchoring groups have been designed. This will give better photovoltaic properties to cell in contrast to dye with D-π-A molecular configuration containing a single anchoring group (Grisorio *et al*., 2013) [28].

7.4 Use of multiple molecular configurations of dyes

For commercial applications and without compromising with the stability and efficiency of DSSCs, many organic dyes, with different pattern such as **D-D-π-A** having additional donor, **D-π-π-A** with additional π-spacer, **D-π-A-A** having extra acceptor moiety and(Sun, He, Chaitanya, & Ju, 2020) [62] **D-(A-π-A)**$_2$ with extra acceptor and pi spacer at low cost and by using simple fabrication processes, have been synthesized (Wazzan, Soliman & Jha, 2023) [69].

8. Historical background of dyes with variable modifications based on different molecular configurations

8.1 Dyes based on D-A-π-A molecular pattern

Based on **D-A-π-A** molecular configuration, three novel dyes were constructed with improved efficiency of DSSCs. These dyes used arylamine as donor, cyanoacrylic acid as acceptor and thiophene and furan-based moieties as π-linker as illustrated in figure 3 because thiophene and furan both have lower resonance energies 29Kcal/mol and 16Kcal/mol respectively as compared to benzene (36Kcal/mol).

WS6 Dye

WS6 dye was designed using 4, 7-di (thiophen-2-yl)benzo[c][1, 2, 5]thiadiazole as π-spacer with a PCE of 3.5%.

WS5 Dye

WS5 dyes was designed by using 4, 7-di(furan-2-yl)benzo[c][1, 2, 5]thiadiazole as π-linker with a PCE of 5.5%.

WS7 Dye

WS7 dyes with 4-(thiophen-2yl)benzo[c][1, 2, 5]thiadiazole as π-spacer having a PCE of 4.3%.

These dyes displayeda superior molar absorption coefficient of (>21800$M^{-1}cm^{-1}$) in the visible region (Sharmoukh *et al*., 2020) [55]. Various calculations of dyes have been shown in table 1.

Table 1: The obtained energy values of investigated dyes **$\lambda_{abs, max}$ (ε) [nm (m^{-1} cm^{-1})]** highest absorption in CH_2Cl_2 solution (10^{-5} M) at 25 °C **$\Lambda_{em, max}$** highest emission in CH_2Cl_2 solution (10^{-5} M) at 25 °C **E_{gap}** energy gap between the E_{red} of sensitizer (dye) and the conductive band (CB) of TiO_2 (Sharmoukh *et al*., 2020) [55].

Dyes	Pi-spacers	$\lambda_{abs, max}$ (ε) [nm (m^{-1} cm^{-1})]	$\Lambda_{em, max}$	E_{gap}	PCE%
WS6	4, 7-di(thiophen-2-yl)benzo[c][1, 2, 5]thiadiazole	532 (21800) 419 (29530)	716	0.56	3.5
WS5	4, 7-di(furan-2-yl)benzo[c][1, 2, 5]thiadiazole	497 (16690) 348 (50900)	710	0.64	5.5
WS7	4-(thiophen-2yl)benzo[c][1, 2, 5]thiadiazole	499 (18980) 354 (45780)	710	0.63	4.3

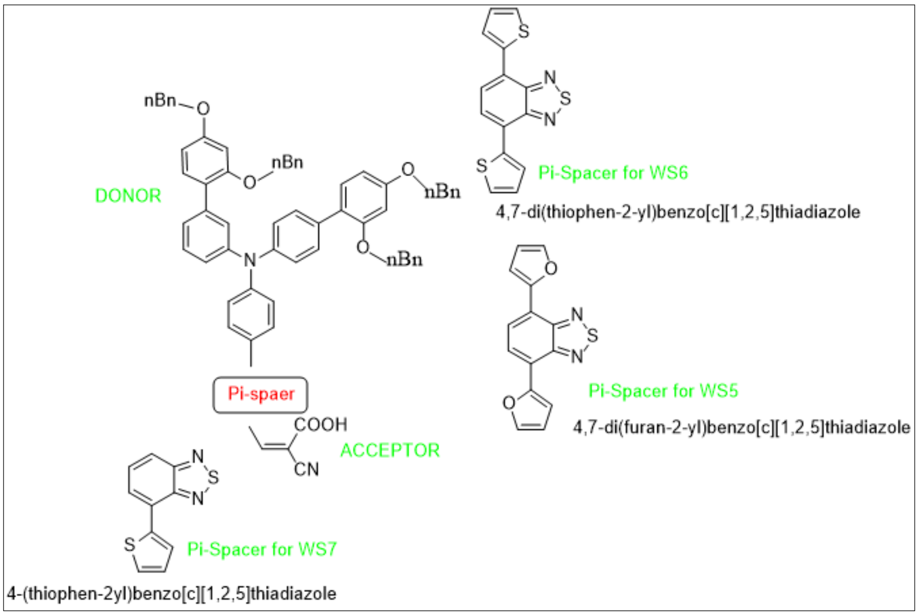

Fig 3: The chemical structures of investigated compounds (Sharmoukh *et al*., 2020) [55].

8.2 Dyes with D-π-D-A design

As presence of auxillary donor improves the photovoltaic properties of cells, due to enhancement in facile electron transportation, a significant increase in photoelectric current and longer term stability of DSSCs (Slodek *et al*., 2019; Wazzan *et al*., 2023) [57, 69], so, three new dyes based on **D-π-D-A** pattern bearing an auxillary donor with phenothiazine scaffold were synthesized as shown in figure 4. These dyes contained three different donors in addition to phenothiazine, acetylene as pi-spacer and acceptor is cyanoacrylic acid group.

9, 9'-dibutylfluorenyl as auxillary donor

2c dye was designed, used 9, 9'-dibutylfluorenyl as auxillary donor with phenothiazine and showed different values of power conversion efficiency, open ciruit voltage, short circuit current and fill factor in contrast to normal N719 dye.

Bithienyl as auxillary donor

2b dye contained bithienyl as auxillary donor.

Dibenzothiophene as auxillary donor:

2a dye contained dibenzothiophene donor. with Hence, auxillary donor has a significant effect on efficiency of cell as compare to normal N719 dye with a PCE of 3.56% as results illustrated in table 2(Slodek *et al*., 2020) [58].

Table 2: Calculated results of investigated dyes **ΔE (eV)** = E_{LUMO}-E_{HOMO} (Slodek *et al*., 2020) [58].

Dyes	Auxiliary donors	ΔE (eV)	Jsc (mA/cm^2)	Voc (mV)	FF	PCE%
2c	9, 9'-dibutylfluorenyl	1.89	12.80	703	0.56	4.80
2b	Bithienyl	1.80	11.87	631	0.54	4.22
2a	Dibenzothiophene	1.95	17.96	700	0.48	6.22

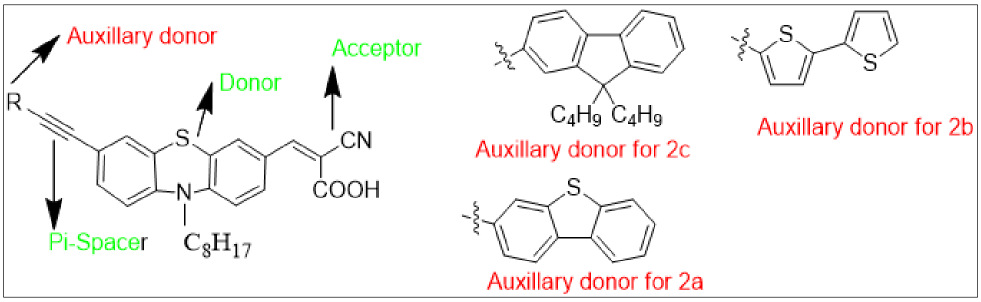

Fig 4: The chemical structures of investigated compounds (Slodek *et al*., 2020) [58].

8.3 Dyes base on D-π-A configuration (showing relationship between aromaticity and resonance energy)

The **aromaticity of π-linker** has a considerable effect on the photovoltaic properties of cells, which is directly linked with their resonance energies (Geng *et al*., 2015) [26]. So, in order to illustrate the relationship between aromaticity and resonance energy, seven dyes were synthesized by taking a standard **D-π-A, D2** dye shown in figure 5.

Anthanthrene as pi-spacer

D2 containing anthanthrene as pi-spacer substituted with nonane alkyl group at positions 6-12, triphenylamine as donor group and cyanoacrylic acid group linked with thiophene unit as acceptor moiety.D2 had a total efficiency of 4.20%, resonance energy of 694KJ/mol and a band gap energy of 4.03eV as shown in table 3.New seven D-π-A dyes constructed by just replacing the pi-spacer of **D2** with other heterocyclic spacers of lower resonance energies substituted with nonane alkyl groups.

Naphthalene as pi-spacer

D5 was synthesized by using naphthalene as pi-spacer which gives the dye an efficiency of 4.45%, resonance energy of 255KJ/mol and band gap energy of 4.10eV

Antharecene as Pi-Spacer

D6 (pi-spacer = antharecene, PCE = 4.44%, E_R = 347KJ/mol, E_g = 4.01eV)

Phenanthrene as pi-spacer

D7 (pi-spacer = phenanthrene, PCE = 4.46%, E_R = 381KJ/mol, E_g = 4.16eV)

Pyrene as pi-spacer

D8 (pi-spacer = Pyrene, PCE = 4.45%, E_R = 356KJ/mol, E_g = 4.12eV)

Naphthacene as pi-spacer

D9 (pi-spacer = Naphthacene, PCE = 4.77%, E_R = 460KJ/mol, E_g = 3.86eV)

Chrysene as pi-spacer

D10 (pi-spacer = chrysene, PCE = 4.45%, E_R = 487KJ/mol, E_g = 4.17eV)

Perylene as pi-spacer

D11 (pi-spacer = perylene, PCE = 4.43%, E_R = 529KJ/mol, E_g = 4.05eV). So from table 3 it can be demonstrated that all these dyes have lower resonance energies and higher efficiencies than standard dye **D2** (Wazzan *et al*., 2023) [69].

Table 3: Energy calculations of dyes, **E_R** = Resonance energy, **E_g** = E_{LUMO}-E_{HOMO} (Wazzan *et al*., 2023) [69].

Dyes	Pi-spacer	E_R (KJ/mol)	E_g(eV)	PCE%
D2	Anthanthrene	694	4.03	4.20
D5	Naphthalene	255	4.10	4.45
D6	Antharecene	347	4.01	4.44
D7	Phenanthrene	381	4.16	4.46
D8	Pyrene	356	4.12	4.45
D9	Naphthacene	460	3.86	4.77
D10	Chrysene	487	4.17	4.45
D11	Perylene	529	4.05	4.43

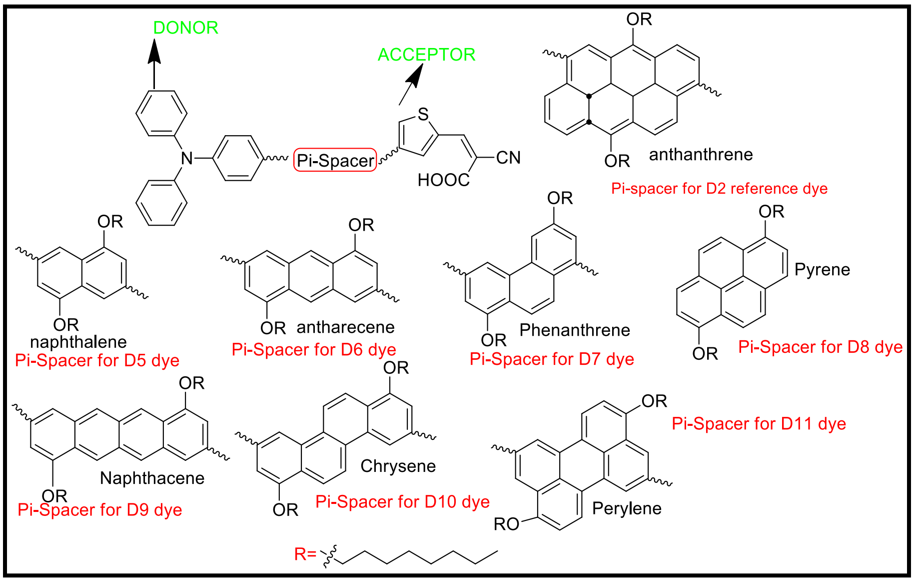

Fig 5: The chemical structures of investigated compounds (Wazzan *et al*., 2023) [69].

8.4 Dyes with D-A-π-A arrangement

To adjust the photovoltaic properties of DSSCs, **improved intramolecular charge transfer**, red shift the absorption maximum and overall PCEof cell new organic dyes havingD-A-π-A pattern withauxillary acceptor naphtho[2, 3-d] [1–3]triazole (NTz), different dithienoheterocycles as pi-spacer and cyanoacrylic acid as acceptor moiety as shown in figure 6 were synthesized(Yen *et al*., 2021) [74].

Cyclopentadithiophene (CPDT) as pi-spacer

When Cyclopentadithiophene(CPDT)(C.-T. Li, Wu, Lee, Yeh, & Lin, 2017; Song *et al*., 2016) [59] was used as pi-spacer **HJL-1**dyewith a PCE of 5.85% was synthesized(Yen *et al*., 2021) [74].

Dithieno [3, 2-b: 2′, 3′-d] silole (DTS) as pi-spacer

when dithieno[3, 2-b:2′, 3′-d] silole(DTS) (Capodaglio, Callegari, Cecconet, & Molognoni, 2017; Y. Tan *et al*., 2014) [10] was used as pi-spacer **HJL**-2dye was synthesized with a PCE of 5.28%(Yen *et al*., 2021) [74].

Dithieno [3, 2-b: 2′, 3′-d] pyrrole (DTP) as pi-spacer

when dithieno[3, 2-b:2′, 3′-d]pyrrole(DTP) (Song *et al*., 2016) [59] was used as pi-spacer

HJL-3dyewas synthesizedwith a highest PCE of 6.91% due to efficient injection of electrons.

HJL-2 had lowest efficiency of all, as shown in table 4 because its highest occupied molecular orbital is at high potential, so regeneration of sensitizer becomes difficult. Furthermore, the efficiency of DSSCS with **HJL-3** was further increased to 7.17%when CDCA (chenodeoxycholic acid) as a co-adsorbent was used which is 95% efficiency of normal N719 dye solar cell(Yen *et al*., 2021) [74].

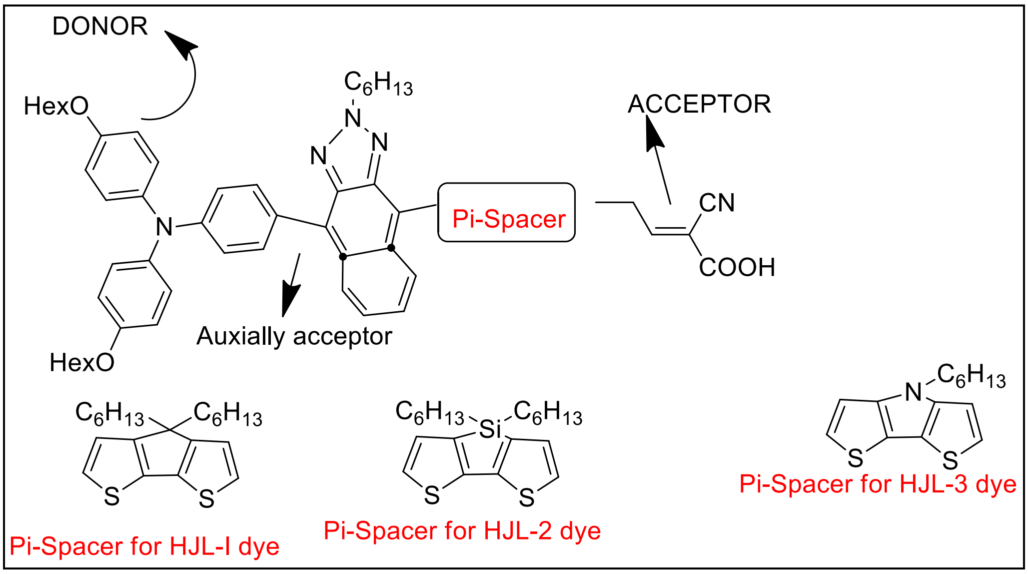

Fig 6: The chemical structures of investigated compounds (Yen *et al*., 2021) [74].

Table 4: Various calculations of dyes **CDCA** chenodeoxycholic acid (co-adsorbent) (Yen *et al.*, 2021) [74].

Dyes	Pi-spacers	λ_{abs} ($\varepsilon \times 10^{-4}$ M^{-1} cm^{-1}) nm	CDCA (mM)	V_{oc} (V)	FF	J_{SC}(mA/cm^2)	PCE%
HJL-1	Cyclopentadithiophene	510 (4.64)	0	0.617±0.008	0.67±0.01	14.21±0.28	5.85±0.20
			5	0.622±0.002	0.68±0.01	13.57±0.03	5.73±0.02
HJL-2	Dithieno[3, 2-b:2′, 3′-d]silole	507 (4.01)	0	0.612±0.002	0.67±0.01	12.82±0.12	5.28±0.07
			5	0.628±0.004	0.67±0.01	13.53±0.18	5.67±0.08
HJL-3	Dithieno[3, 2-b:2′, 3′-d]pyrrole	486 (4.36)	0	0.639±0.006	0.62±0.01	17.51±0.03	6.91±0.11
			5	0.645±0.003	0.61±0.01	18.35±0.15	7.17±0.08

8.5 Dyes based on D-π-A configuration showing efficient charge transfer

In order to maximize photoelectric current generation and minimize charge recombination, an effective intramolecular charge separation relies on the energy of the acceptor's LUMO and the donor's highest occupied molecular orbital. (Dua *et al.*, 2023) [20].Thus, three **D-π-A** organic dyes, shown in figure 7, were synthesized based on arylmine donor, conjugated spacer and cyanoacrylic acid acceptor group.

Diphenylamine as donor, biphenyl as pi-conjugated spacer

Dye **A**(E)-2-Cyano-3-(4′-(diphenylamino)biphenyl-4yl)acrylic Acid was synthesized using diphenylamine donor, biphenyl as pi-conjugated spacer (E_{HOMO} = -5.490eV, E_{LUMO} = -2.575eV, E_{gap} = 2.915eV, V_{OC} = 0.898eV).

1-nephthylamine as donor, biphenyl as conjugated spacer

Dye **B**((E)-2-Cyano-3-(4′-(naphthalen-1-yl(phenyl)amino)biphenyl-4-yl)acrylic Acid was synthesized using 1-nephthylamine as donor, biphenyl as conjugated spacer (E_{HOMO} = -5.513eV, E_{LUMO} = -2.562eV, E_{gap} = 2.950eV, V_{OC} = 0.887eV).

Biphenylamine donor, -9, 9-diethyl-9H-fluorene as pi-spacer

Dye **C** ((E)-2-Cyano-3-(7-(diphenylamino)-9, 9-diethyl-9H-fluoren-2-yl)acrylic Acid was synthesized using biphenylamine donor, -9, 9-diethyl-9H-fluorene as pi-spacer (E_{HOMO} = -5.465eV, E_{LUMO} = -2.479eV, E_{gap} = 2.986eV, V_{OC} = 0.986eV).

1-nephthylamine donor, -9, 9-diethyl-9H-fluorene as pi-spacer

Dye **D** (-2- Cyano-3(9, 9-diethyl-7-(naphthalen-1-yl(phenyl)amino)-9H-fluoren-2-yl)acrylic Acid was synthesized using 1-nephthylamine donor, -9, 9-diethyl-9H-fluorene as pi-spacer (E_{HOMO} = -5.340eV, E_{LUMO} = -2.402eV, E_{gap} = 2.938eV, V_{OC} = 0.999eV).

As it is clear from table 5 that D has highest HOMO energy and lowest band gap energy so it has highest electron donating ability and due to highest V_{OC} it is most efficient of other synthesized dyes. As the LUMO energy of TiO_2 IS -4.0eV which is lower than HOMO energies of all dyes and HOMO energy of $I^{-1}\backslash I^{3-}$ is -4.8eV(X. Li, AN, Xia, & Ju, 2020) which is higher than LUMO energies of all dyes, so these dyes fulfill all requirements of efficient charge transfer (Al-Masoodi *et al.*, 2021) [2].

Table 5: Calculated energy values of dyes $\Delta E_{gap}(eV) = E_{LUMO}-E_{HOMO}$ (Al-Masoodi *et al.*, 2021) [2].

Dyes	Donors	Pi-spacers	$E_{HOMO}(eV)$	$E_{LUMO}(eV)$	$\Delta E_{gap}(eV)$	Λ_{max}(nm)	V_{OC}(eV)
A	Diphenylamine	Biphenyl	-5.490	-2.575	2.915	369.98	0.898
B	1-nephthylamine	Biphenyl	-5.513	-2.562	2.950	526.45	0.887
C	Biphenylamine	9, 9-diethyl-9H-fluorene	-5.465	-2.479	2.986	386.53	0.986
D	1-nephthylamine	9, 9-diethyl-9H-fluorene	-5.340	-2.402	2.938	379.84	0.999

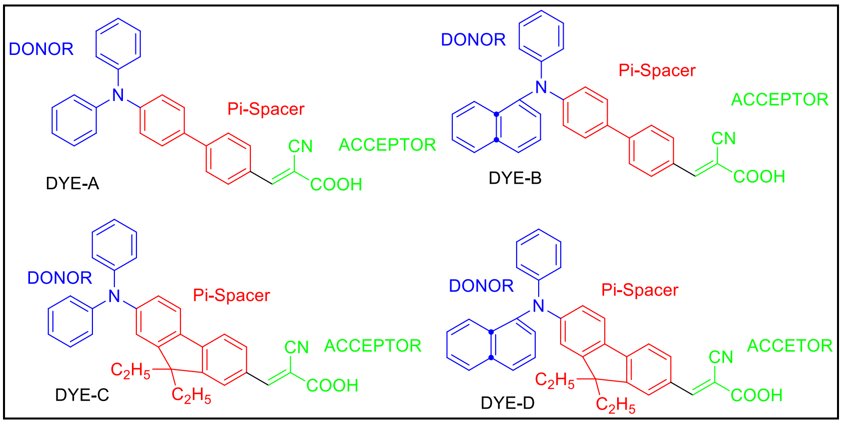

Fig 7: The chemical compositionof investigated dyes (Al-Masoodi *et al.*, 2021) [2].

8.6 Dyes that followD-π-A and D–(π–A)$_2$ arrangement (Effect of substituents on donor and anchoring groups on photovoltaic properties of cell)

As the anchoring group has a major effect on the binding strength of dye on TiO_2(Ambrosio, Martsinovich, & Troisi, 2012), in order to improve the light absorbing capacity of dye and to prevent charge recombination various dyes were synthesized with**D-π-A** and **D–(π–A)$_2$** molecular arrangement using substituted pyranylidene as donor, thienyl π-conjugated spacer and cyanoacrylic acid as acceptor moiety shown in figure 9. The purpose of this study to checks the effect of various substituents on donor pyranylidene and to check the effect of number of anchoring groups towards the photovoltaic properties of cell.

8.6.1 D–(π–A)$_2$ Sensitizers (dyes)

Three D–(π–A)$_2$ dyes were synthesized by using double(cyanoacrylic acid) acceptor and one differently substituted pyranylidene donor illustrated in figure 9.

T-butylated pyranylidene as donor
10a dye (donor = t-butylated pyranylidene, V_{OC} = 565mV, J_{SC} = 8.26mA/cm^2, PCE = 3.35%)

Phenyl substituted pyranylidene as donor
10b dye (donor = phenyl substituted pyranylidene, V_{OC} = 532mV, J_{SC} = 8.52mA/cm^2, PCE = 3.25%)

Thienyl substituted pyranylidene as donor
10c dye (donor = thienyl substituted pyranylidene, V_{OC} = 538mV, J_{SC} = 9.74mA/cm^2, PCE = 3.57%).

Out of these **10a** is highly efficient because of its bulky ter-butyl group which prevents charge recombination on the surface of TiO_2 as illustrated in table 6.

Table 6: The obtained results for investigated D–(π–A)$_2$ dyes (Gauthier *et al*., 2020) [25]

Dyes	Donors	V_{OC}(mV)	FF%	J_{SC}(mA/cm^2)	PCE%
10a	t-butylated pyranylidene	565	72(±1)	8.26	3.35
10b	Phenyl substituted pyranylidene	532	72(±1)	8.52	3.25
10c	Thienyl substituted pyranylidene	538	68(±2)	9.74	3.57

8.6.2 D-π-A Sensitizer (dyes)

Three dyes with monoachoring groups D-π-A were designed using ter-butylated pyranylidene donor, cyanoacrylic acid anchoring group and pi-spacer with different number of thienyl units as shown in figure 8.

One thienyl unit as pi-spacer
17a (spacer = one thienyl unit, V_{OC} = 652mV, J_{SC} = 11.43mA/cm^2, PCE = 5.23%)

Two thienyl unit as pi-spacer
18a (spacer = two thienyl unit, V_{OC} = 612mV, J_{SC} = 9.84mA/cm^2, PCE = 4.32%)

Three thienyl unit as pi-spacer
19a (spacer = three thienyl unit, V_{OC} = 574mV, mJ_{SC} = 9.73mA/cm^2, PCE = 3.90%). As it is obvious from table 7, **17a** dye with mono-anchoring group and with one thienyl unit as pi-spacer is highly efficient than all other dyes because of its efficient shielding on TiO_2 due to high loading because of being less bulky.so, it was concluded that mono-anchoring dyes are more efficient for DSSCs than di-anchoring dyes (Gauthier *et al*., 2020) [25].

Table 7: The obtained results for investigated D-π-A dyes (Gauthier *et al*., 2020) [25].

Dyes	Pi-spacers	V_{OC}(mV)	FF%	J_{SC}(mA/cm^2)	PCE%
17a	one thienyl unit	652	70(±1)	11.43	5.23
18a	Two thienyl unit	612	72(±1)	9.84	4.32
19a	Three thienyl unit	574	70(±1)	9.73	3.90

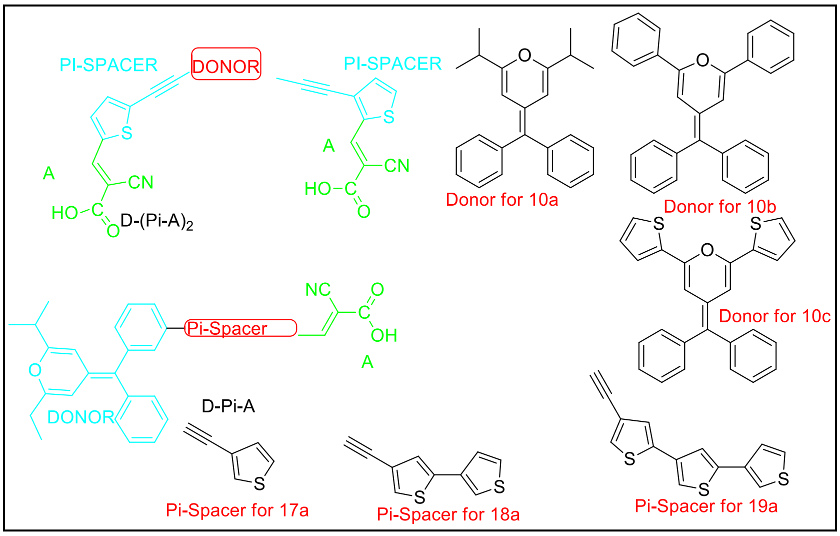

Fig 8: The chemical structures of investigated dyes (Gauthier *et al*., 2020) [25].

8.7 Dyes that follow D-π-A layout (effect of different π-linkers)

To study the effect of different π-linkers on p-type triphenylamine dye and thus to enhance the photovoltaic properties of DSSC, five organic dyes with **D-π-A** configuration as shown in figure 9, were synthesized. Triphenylamine was used as donor, formic acid as an anchor and 2-methylenemalononitrile as acceptor moiety with varying π-linkers. Dyes were synthesized using a reference dye **O2** which used thiophene as pi-spacer (λ_{max} = 428nm).

O2-A Dye: O2-A (π-spacer = 1-ethyl-4-methyl-2, 5-dihydro-1H-1, 2, 3-triazole, λmax = 345nm)

O2-B Dye: O2-B dye (π-spacer = 1, 3, 4-oxadiazole, λmax = 407nm)

O2-C Dye:
O2-C dye (π-spacer = benzo[c][1, 2, 5] thiadiazole, $_{\lambda max}$ = 524nm)

O2-D Dye:
O2-D dye (π-spacer = 4-(thiophen-2- yl) benzo[c][1, 2, 5]thiadiazole, $_{\lambda max}$ = 559nm)

O2-E Dye: O2-Edye (π-spacer = 4-(1, 3, 4-oxadiazol-2-yl) benzo[c][1, 2, 5]thiadiazole, $_{\lambda max}$ = 473nm).

From the table 8 it is clear that all these synthesized dyes had the values of LUMO energies which are larger than conduction band of semiconductor NiO(E_{CB} = –4.98 eV) which made the injection easy, similarly the values of energies of HOMO for all these dyes were at lower potential than that of electrolyte (E(I^{3-}/I^{-1}) = –4.80 eV)(Al-Masoodi *et al*., 2021) [2] which gave the confirmation of fast regeneration of dye, which are necessary conditions for efficient working of solar cell(Dua *et al*., 2023) [20]. Looking at the HOMO and LUMO energies of the dyes from the table 8, it was observed that **O2-A** is further in the favour of hole injection than other dyes because HOMO and LUMO for this dye were almost in overlapping with each other, but looking at maximum absorption wavelength and their comparison with that of reference dye **O2** it can be concluded that **O2-C** and **O2-D** dyes are more efficient for DSSCs (X. Li *et al*., 2020) [39].

Table 8: Energy calculations of investigated dyes (X. Li *et al*., 2020) [39].

Dyes	Pi-spacers	E(eV)	Λ_{max}(nm)
O2-A	1-ethyl-4-methyl-2, 5-dihydro-1H-1, 2, 3-triazole	1.27	345
O2-B	1, 3, 4-oxadiazole	2.31	407
O2-C	Benzo[c][1, 2, 5] thiadiazole	2.14	524
O2-D	4-(thiophen-2- yl)benzo[c][1, 2, 5]thiadiazole	1.92	559
O2-E	4-(1, 3, 4-oxadiazol-2-yl)benzo[c][1, 2, 5]thiadiazole	1.84	473

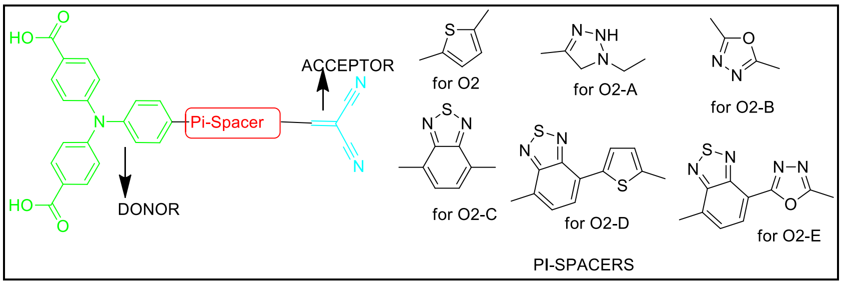

Fig 9: The chemical structures of investigated compounds (X. Li *et al*., 2020) [39].

8.8 Dyes havingD-D-π-A configuration

The effect of π-spacer on the workingof dye sensitized solar cells, five novel dyes based on **D-D-π-A** configuration having auxillary donor, as shown in figure 10, were synthesized. All these dyes used phenothiazine as donor, 2, 4-dipropoxyphenyl as auxillary donor, cyanoacrylic acid acceptor moiety and thiophene with varying units as π-spacer illustrated in figure 11. To prevent aggregation of the dye, phenothiazine is substituted with hexyloxyphenyl moiety(Hua *et al*., 2015). **DMA-0** is a reference dye which is without any π-spacer and a **DMA-5** dye used somewhat different π-spacer than all other dyes.

When no pi-spacer is used
DMA-0 dye (spacer = no spacer, V_{OC} = 0.83V, J_{SC} = 10.1mA/cm^2, PCE = 5.7%)

Monothiophene as pi-spacer
DMA-1dye (spacer = Monothiophene, V_{OC} = 0.77V, J_{SC} = 10.6mA/cm^2, PCE = 5.6%),

Dithiophene as pi-spacer
DMA-2 dye (spacer = dithiophene, V_{OC} = 0.772V, J_{SC} = 10.9mA/cm^2, PCE = 5.6%)

Trithiophene as pi-spacer:
DMA-3 dye (spacer = Trithiophene, V_{OC} = 0.70V, J_{SC} = 11.0mA/cm^2, PCE = 5.2%)

Quaterthiophene as pi-spacer
DMA-4 dye (spacer = Quaterthiophene, V_{OC} = 0.628V, J_{SC} = 7.3mA/cm^2, PCE = 3.1%)

Thieno [3, 2-b]thiophene as pi-spacer
DMA-5 dye(spacer = thieno[3, 2-b]thiophene, V_{OC} = 0.74V, J_{SC} = 10.3mA/cm^2, PCE = 5.3%).

Looking at the table 9, from these results it was concluded that there is approximately no effect of increasing thiophene units up to three units because PCE% from **DMA-0** to **DMA-3** is almost same while lowest for Quarter thiophene (Almenningen *et al*., 2021) [5].

Table 9: Calculated results for investigated dyes (Almenningen *et al*., 2021) [5].

Dyes	Pi-spacers	V_{OC} (V)	J_{SC} (mA/cm^2)	FF	PCE%
DMA-0	No spacer	0.83±0.01	10.1±0.2	0.68±0.01	5.7±0.2
DMA-1	Monothiophene	0.77±0.01	10.6±0.2	0.69±0.02	5.6±0.2
DMA-2	Dithiophene	0.772±0.002	10.9±0.1	0.67±0.01	5.6±0.1
DMA-3	Trithiophene	0.70±0.01	11.0±0.1	0.68±0.01	5.2±0.1
DMA-4	Quaterthiophene	0.628±0.002	7.3±0.1	0.68±0.04	3.1±0.2
DMA-5	Thieno[3, 2-b]thiophene	0.74±0.01	10.3±0.1	0.69±0.01	5.3±0.1

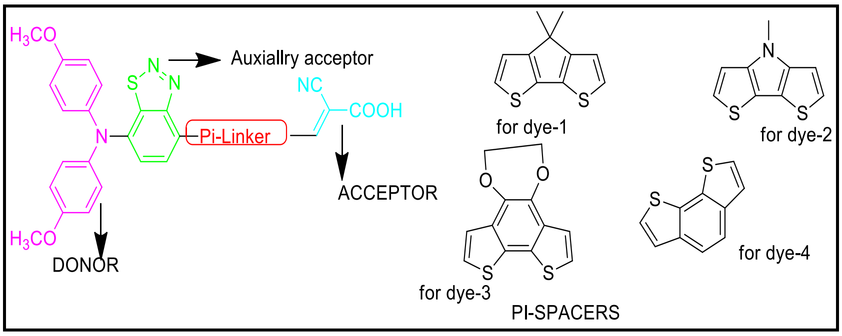

Fig 10: The chemical structures of investigated dyes (Almenningen *et al*., 2021) [5].

8.9 Dyes with D-A-π-A configuration (altering π-spacer effect on the performance of photovoltaic cell)

D-A-π-A sensitizer having benzothiadiazole as auxillary acceptor were synthesized as shown in figure 12 to study the effect of varying π-spacer on the performance of photovoltaic cell, by using two reference dyes named as **1** and **2**. These dyes used diphenylamine as donor moiety and 2-cyanoacrylic acid group as acceptor moiety. The synthesized dyes **3** and **4** were different on the basis of pi-spacers, illustrated in figure 11.

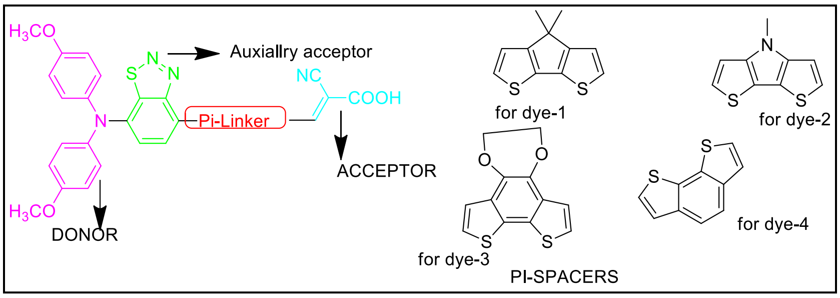

Fig 11: The chemical structures of dyes (K. Sun *et al*., 2020) [61].

Dye1: Dye**1** (spacer = -4, 4-dimethyl-4H-cyclopenta [2, 1-b:3, 4-b']dithiophene, ΔE^a = -2.62eV, ΔE^b = 0.25eV, V_{OC} = 1619mV, J_{SC} = 37.92mA/cm^2, PCE = 45.54%)

Dye2: Dye**2**(spacer = --4-methyl-4H-dithieno[3, 2-b:2′, 3′-d]pyrrole, ΔE^a = -1.47eV, ΔE^b = 0.26eV, V_{OC} = 1575mV, J_{SC} = 37.77mA/cm^2, PCE = 44.14%)

Dye3: Dye**3** (spacer = benzo [2, 1-b:3, 4-b']dithiophene-, ΔE^a = -1.78eV, ΔE^b = 0.23eV, V_{OC} = 1588mV, J_{SC} = 35.85mA/cm^2, PCE = 42.26%).

Dye4: Dye**4**(spacer = --2, 3-dihydrodithieno[3′, 2':3, 4; 2″, 3":5, 6]benzo[1, 2-b] [1, 4]dioxine, ΔE^a = -1.83eV, ΔE^b = 0.23eV, V_{OC} = 1647mV, J_{SC} = 36.82mA/cm^2, PCE = 44.33%).where ΔE^a showsenergy variation between LUMO of dye and conduction band of TiO_2 when dye is isolated and ΔE^b represents energy gapbetween LUMO of dye and conduction band of TiO_2 when dye is adsorbed.

Table 10: Various energy calculations of investigated dyes **ΔE^a**, **ΔE^b** when dye is adsorbed) (K. Sun *et al*., 2020).

Dyes	Pi-spacers	ΔE^a(eV)	ΔE^b(eV)	V_{OC}(mV)	J_{SC}(mA/cm^2)	PCE%
A	4, 4-dimethyl-4H-cyclopenta[2, 1-b:3, 4-b']dithiophene	-2.62	0.25	1619	37.92	45.54
B	4-methyl-4H-dithieno[3, 2-b:2′, 3′-d]pyrrole	-1.47	0.26	1575	37.77	44.14
C	Benzo [2, 1-b:3, 4-b']dithiophene	-1.78	0.23	1588	35.85	42.26
D	2, 3-dihydrodithieno[3′, 2':3, 4; 2″, 3":5, 6]benzo[1, 2-b] [1, 4]dioxine	-1.83	0.23	1647	36.82	44.33

9. Conclusion

Graphical Abstract:

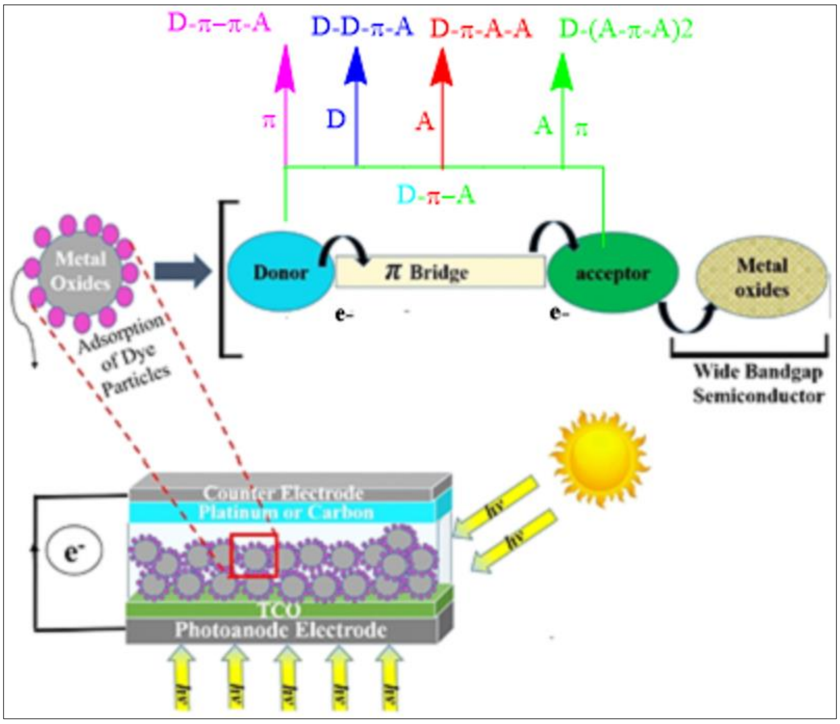

Fig 12: Multiple molecular configurations of dyes

This study examined a variety of dyes with various chemical structures and noted how each affected the dye-sensitized solar cell's overall efficiency. Three new dyes, designated WS5, WS6, and WS7, have been reviewed. They have distinct pi-spacers, arylamine as the donor, and cyanoacrylic acid as the acceptor, all based on the D-A-π-A chemical arrangement. In a similar manner, three new dyes have been studied: 2a, 2b, and 2c. These dyes are based on the D-π-D-A configuration and have an auxiliary donor with a scaffold made of phenothiazine. Together with phenothiazine, these dyes also comprised acetylene as a pi-spacer and cyanoacrylic acid group as an acceptor moiety.

Furthermore, in order to illustrate the relationship between aromaticity and resonance energy, seven dyes have been reviewed by taking a standard D-π-A. Another review has been made on three organic dyes named as HJL-1, HJL-2 and HJL-3, with D-A-π-A pattern having axiallry acceptor naphtho (2, 3-d) [1–3]triazole (NTz), different dithienoheterocycles as pi-spacer and cyanoacrylic acid as acceptor moiety. A review has been made on four organic dyes named as dye A-dye D base on D-π-A configuration having arylamine donor, conjugated spacer and cyanoacrylic acid as acceptor group. Similarly, to check the effect of substituents on donor and anchoring groups on photovoltaic properties of cell, six dyes have been reviewed, three dyes named as 10a-10c were based on $D–(π–A)_2$ configuration were investigated containing double (cyanoacrylic acid) acceptor and one differently substituted pyranylidene donor. Other set of three dyes, named as 17a-19a, with monoachoring groups D-π-A has been investigated containing ter-butylated pyranylidene donor, cyanoacrylic acid anchoring group and pi-spacer with different number of thienyl units.

Review of five organic dyes with the D-π-A configuration called O2A-O2E was conducted to examine the impact of various π-linkers on p-type triphenylamine dye. Triphenylamine was used as the donor, formic acid as an anchor, and 2-methylenemalononitrile as the acceptor moiety with different π-linkers. Thiophene was utilized as a pi-spacer in the synthesis of dyes by means of the reference dye O2. DMA1-DMA5, five new dyes with a D-D-π-A configuration have been reviewed again. They have thiophene with different units acting as π-spacer, cyanoacrylic acid acceptor moiety, 2, 4-dipropoxyphenyl as auxiliary donor, and phenothiazine as donor. DMA-0 was utilized as a reference dye without a pi-spacer. The D-A-π-A configuration of dyes 3 and 4 has undergone a final assessment. Two dyes were used as reference dyes named as 1 and 2. These dyes used diphenylamine as donor moiety and 2-cyanoacrylic acid group as acceptor moiety. Thus, all the reviewed data provides important information about suitable donors, acceptors and pi-spacers which are efficient to be used in dye sensitized solar cells. It also demonstrates the effect of auxillary donor, acceptor extra pi-spacers and substituents on the efficiency of DSCS. From these results, one can make a clear idea which results will be obtained if a particular donor, acceptor and pi-spacer is used in dye and which modifications can be made to meet the desired results.

10. References

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