Research Article

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Review on Modification of Cyanidin based dyes to improve the performance of Dye- sensitized solar cells (DSSCs)

Vishal Singh

Institute of Chemical Technology, Mumbai

Abstract

Every day, new technologies emerge. The primary environmental danger is the release of greenhouse gases as a result of the burning of fossil fuels [2]. It has an impact on living creatures' survival. Renewable energy is critical for society's survival [3]. Solar energy, the most demanding renewable energy source, is used to replace fossil fuels. Solar energy is the world's inexhaustible energy source [4]. Solar energy is used to power dye sensitized solar cells (DSSC). This review paper focuses on use of modified cyanidin based organic dyes for better efficiency in Dye synthesized solar cells.

Key words - Cyanidin. Solar energy, renewable energy

Introduction -

With depleting non renewable energy resources, mankind's attention has shifted towards finding a renewable energy source which can fulfil the tremendous energy demands and have the least environmental impact. Nobel laureate Richard E. Smalley enforced upon this notion saying that energy will be the top problem for humanity in the next 50 years (R. E. Smalley *Abstr. Paper Am. Chem. Soc.*, 2003, **226** , U24). The energy problems can be effectively tackled by harnessing the potential of the Sun. The Earth receives 174 petawatts(PW) of solar radiation at the upper atmosphere in a year (13). The total solar energy absorbed by the Earth's surface is approximately 3850 zettajoules (ZJ) per year,14 which is more energy in one hour than what the world used in one year15,16. To utilise the solar radiation a solar cell or photovoltaic cell(PV) is used. Solar cells convert the incoming solar radiation into electricity by photoelectric effect. Photovoltaic technology is considered to be the most promising technology among the considered renewable energy sources18–21.

Dye sensitised solar cells have replaced silicon and thin film based solar cells due to their low processing cost and minor environmental impact despite possessing lower efficiency.

Organic dyes are the prime choice for being the constituent of DSSC as they show higher absorption coefficient and stronger exciton generation compared to that of inorganic materials. The structure of the dye plays a significant effect in its overall performance. For effective application in conjunction with new redox mediators or hole conductors, excellent blocking behaviour is required. The electron transport between TiO2 and an oxidised redox mediator or a

hole conductor can be slowed by steric groups (Feldt et al., 2010).

Discussion

The review paper discussed the effect of modifications of donor, acceptor,π - conjugated chain, electron withdrawing group and electron donating group on cyanidin based dyes.

1.1 Effect of variation in π- conjugated chain

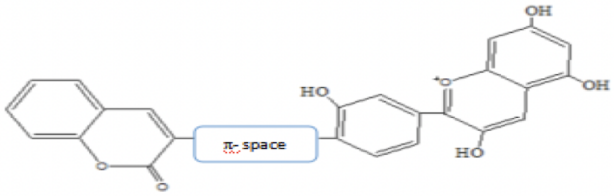
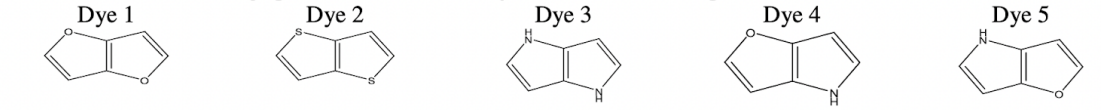


Fig.-1: The D-π-A Structure of an Organic Dye Molecule

The structure of π- conjugated chains for the dye can be seen in Fig.-2 below:



Furo [3,2-b] furan | Thieno [3,2-b] thiophene | 1,4-dihydro-pyrrolo [3,2-b] Pyrrole | 4H-Furo [3,2-b] Pyrrole | 4H-Furo [3,2-b] Pyrrole

Fig.-2: The Molecular Structure of π-conjugated Chains

With a band gap of 1.5344 eV, dye 3 has the lowest band gap and hence has the best light absorption efficiency. The N atom, which has an electronegativity value of 3.04, is responsible for dye 3's efficiency. This value is lower than that of the O atoms (3.44) but greater than that of the S atom (2.58). Due to the electronegative atoms imagined by the acceptor chain, a more electronegative atom at the chain will make it more difficult for the acceptor chain to withdraw electrons. Electrons from less electronegative atoms are simpler to extract from electronegative atoms. As a result, dye 3 is thought to be able to absorb light with a wavelength of 809.7 nm.

Dye 2, which has a S atom in its -conjugated chain, has the second lowest bandgap. This situation arises from the fact that the S atom is more electropositive, making it simpler for the acceptor chain, which is more electronegative, to take electrons from the -conjugated chain. However, because the pore of the S atom is bigger than that of the N atom, withdrawing electrons with the acceptor chain is more difficult. Dye 1 has an O atom in its chain, which has a large number of O atoms in both the acceptor and donor chains. As a result, electron resonance from donor to acceptor necessitates a significant quantity of energy.

The sole variation between dyes 4 and 5 is the location of the O and N atoms inside the -conjugated chain. The band gap of dye 5 is lower than that of dye 4. The O atom is closer to the acceptor chain in dye 5 than the N atom is to the donor chain. The proximity of the O atom to the acceptor chain makes the extraction of electrons from N atom more simpler than it is for N atom to withdraw electrons from O atom.

1.2 Effect of variation of donor chain

The lowest bandgap may be found in dye 10, which has a value of 1.1153 eV. This finding demonstrates that organic dye 10 with penantrokarbazol as the donor has a higher light absorption efficiency. The electron resonance of a dye is longer from donor chain to acceptor chain due to its molecular structure; the longer the resonance of a dye, the longer the wavelength of the light.

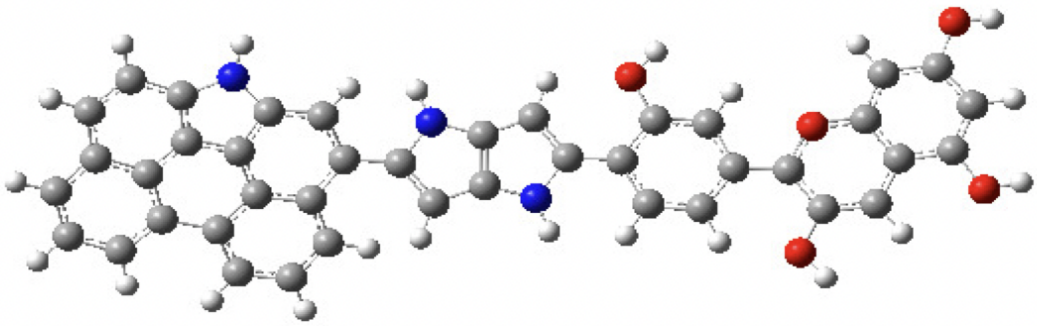


Fig.-8: The Structure of Dye 10 after being Optimized with A B3LYP / 6-31G Basis Set

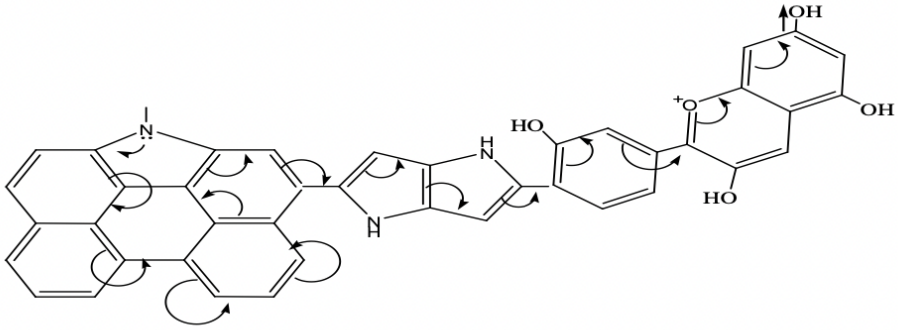


Fig.-9: Mechanism of Electron Resonance of Dye 10

Dyes that have a longer wavelength are expected to be able to perform absorption within the IR region.

1.3 Effect of Electron Withdrawing and Donating Chains

Electron-withdrawing Group (EWG)

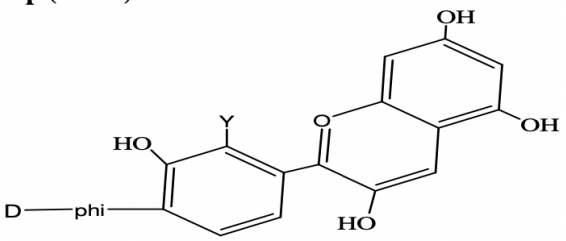


Fig.-13: The Structure of Dye 6 by the Addition of Electron Withdrawing Molecule (Y) to the Acceptor Chain

Table-4: The Effect of The Addition of Electron Withdrawing Group To Dye 6

Dyes	Electron withdrawing molecule (Y)	$E_{HOMO\ (eV)}$	$E_{LUMO\ (eV)}$	$\Delta E_{(eV)}$	$\lambda_{excitation}$(nm)
14	Cl	-6,6384	-5,4418	1,1966	1036,5
15	**NO_2**	**-6.8115**	**-5.7010**	**1.1105**	**1118.9**
16	OH	-6.6156	-5.4123	1.2032	1032.6
6	Unavailable	-6.5407	-5.4254	1.1153	1114.0

Table-4 shows that adding a NO2 molecule can reduce Dye 6's band gap. Because NO2 contains more electronegative atoms than other EWG, the band gap is 1.1104 eV, and it is projected to absorb light at 1118.9 nm wavelength.

EDG and EWG additions can reduce the band gap more effectively than just adding EDG or EWG. At a wavelength of 1400 nm, the band gap was 0.8873 eV. Because electrons are substantially provided by EDG toward the acceptor chain and forcefully removed by NO2 from the donor chain, the EDG and EWG clusters facilitate electron resonance inside the organic dye. It may be inferred that combining EDG and EWG with organic dye improves light absorption.

Conclusions-

With a variant of -conjugated chain, dye 3 has the shortest band gap, whereas dye 10 has a lower band gap than other donor variations. The dye's band gap was reduced when C4H5 was added as an EDG and NO2 was added as an EWG. Dye 17 is a mixture of EWG and EDG additives with the lowest band gap. As a result, dye 17 has a greater potential as a sensitizer in DSSCs.

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