

Hetero Junction Based Organic Photovoltaic Cell: Basics, Current Progress and Future Aspects

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Abstract – Although organic solar cells are just the solar cell based on the movement of electron-hole just like amorphous or crystalline silicon semiconductor. We are going to talk about a little bit about that why organic solar cells should be used. As by now we know that we want to reduce cost and what could be less costly compared to then going to a hardware store and buying two cans of paints. If you could buy it, mix them up and can make a solar cell by painting on something. It will be a very-very cheap technology. In practice of course nothing is simple and it turns out that if you go and try to make a cost estimate of organic solar cell it is a then crystalline silicon seems comparably easy and good cell. Its property of semi transparency of OPVs is used in many field and green house is one of them. The recent research shows that hetero junction based organic photovoltaic cells can separate many colour components of sun light. So by making specific compound, special purpose and mostly utilised colour can be separated out from the sun light which can be used in some other process. As in photosynthesis process plants requires mostly only red and yellow colour. So in sun light other colours can be used to generate the electricity whereas the silicon based solar cell completely block the sun light. Excepts this polymer based organic solar cells have some other important benefits in comparison of conventional silicon based solar cell, which will be discussed here in brief.

Key Words- OPVCs (Organic Photovoltaic Cells), HOMO, LUMO, Polymer based organic cells, hetero junction, nano-crystalline silicon and CIGS (copper indium gallium selenide), OPVs material (say P3HT, PTB7, PCMB and ICBA) and Conjugated system in OPVs.

Introduction-

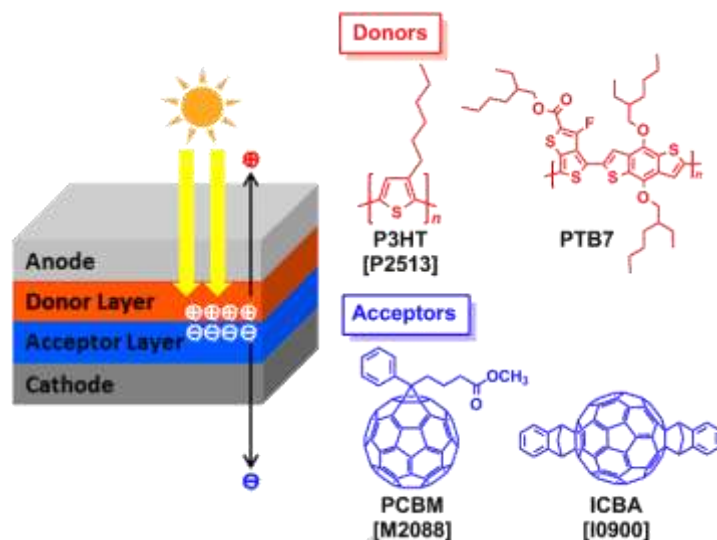
Soon, we are going to leave the solar cell technology based on inorganic semiconductor materials like amorphous, nano-crystalline silicon and CIGS (copper indium gallium selenide). We will discuss the organic solar cell like polymers cell or dye-sensitised solar cell.

The materials used are conducting organic polymer or organic molecules. All these materials can be considered as a large conjugated system. The organic polymer and molecules consist of large compounds based on carbon. Carbon may form cyclic or a-cyclic linear or mixed compound structures. Here we have some examples of materials used for photovoltaic applications like P3HT, PTB7, PCMB and ICBA.

General description about various OPV materials-

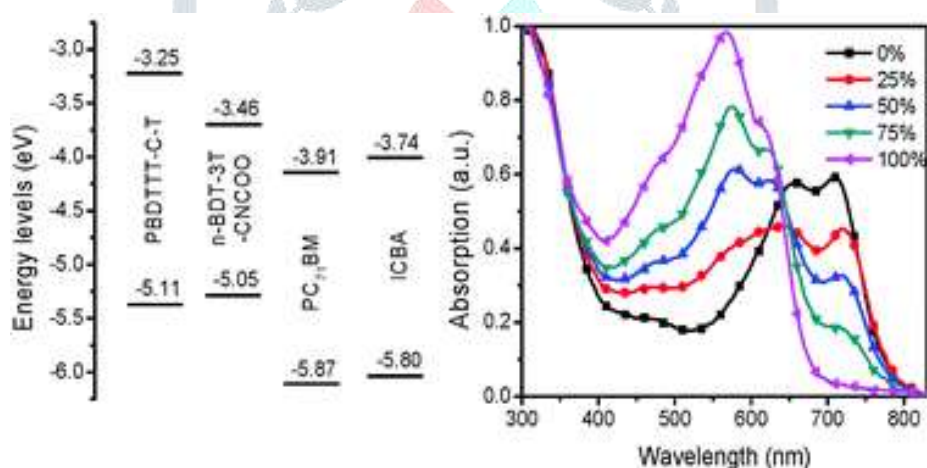
-(LUMO level 3.1 eV) -Poly (3-hexylthiophene) (P3HT) is a regular regular semiconducting polymer. It is used in organic electronics primarily because of its regular end-to-end arrangement of side chain, which allows efficient π - π stacking of the conjugated backbones. On account of the alkyl side group, P3HT is rendered hydrophobic in neutral state.

-PTB7 for high-performance organic photovoltaic. Poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl]], more commonly known as PTB7.



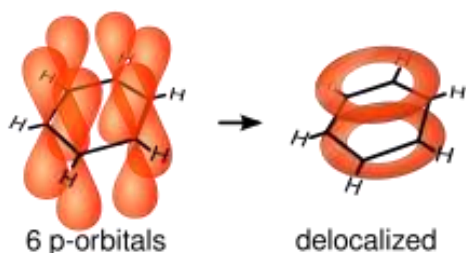
-ICBA Ternary organic solar cells (oscs) are fabricated with indene-C₆₀ bisadduct (ICBA) as an electron acceptor and the low-band-gap polymer PBDTTT-C-T and the highly crystalline small molecule *n*-BDT-3T-CNCOO as electron donors. A high open-circuit voltage of 0.98 V is achieved, which is 0.2 V higher than that of ternary oscs based on phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) as the acceptor. Incorporation of *n*-BDT-3T-CNCOO promotes the power conversion efficiency (PCE) from 5.01% for polymer binary devices to 5.51% for ternary devices. The improved PCE is attributed to the nanofibrous morphology with enhanced crystallinity of the donors and improved aggregation of the ICBA acceptor, which facilitate charge separation and charge transport. This work reveals that the ternary strategy of blending highly crystalline small molecules enhances pces of oscs based on ICBA and other non-fullerene acceptors.

(* The mechanism will be discussed later in this report)



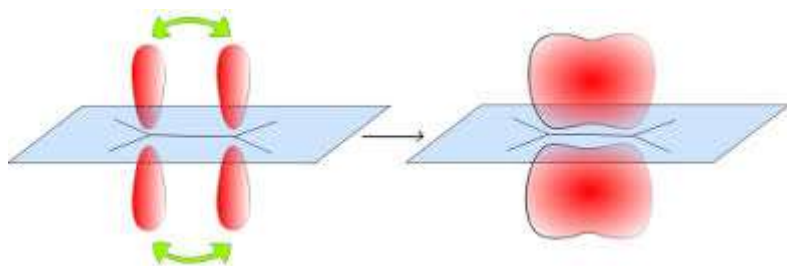
Conjugated system in organic compounds (i.e., in hydrocarbons)-

The conjugated system means that carbon atoms in its chain has an alternative single or double bond and every atom in the chain has p orbital available. The classical example is the benzene molecule which is a cyclic conjugated compound and the P orbital in the conjugated orbital are delocalized. This means that they can form one big mix orbital. The valence electrons of the orbital P orbital is shared over all the orbitals. Here is the example of benzene ring. This molecules has 6 carbon atoms and 6 P orbitals, they mix forming to circle orbitals that are occupied by in total six electrons. These electrons do not belong to one single atom but to a group of atoms.

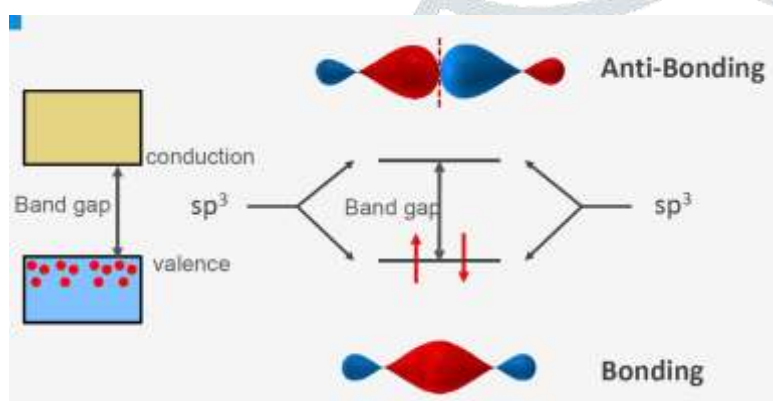


Regions of HOMO and LUMO (hybridisation in atoms)-

A methane molecule with tetrahedral coordinated, has 4 equivalent SP^3 hybrid bond with a bond angle of 109° . Similarly in ethane there is SP^2 hybrid bonds with a bond angle of 120° and an electron in p_z orbital.

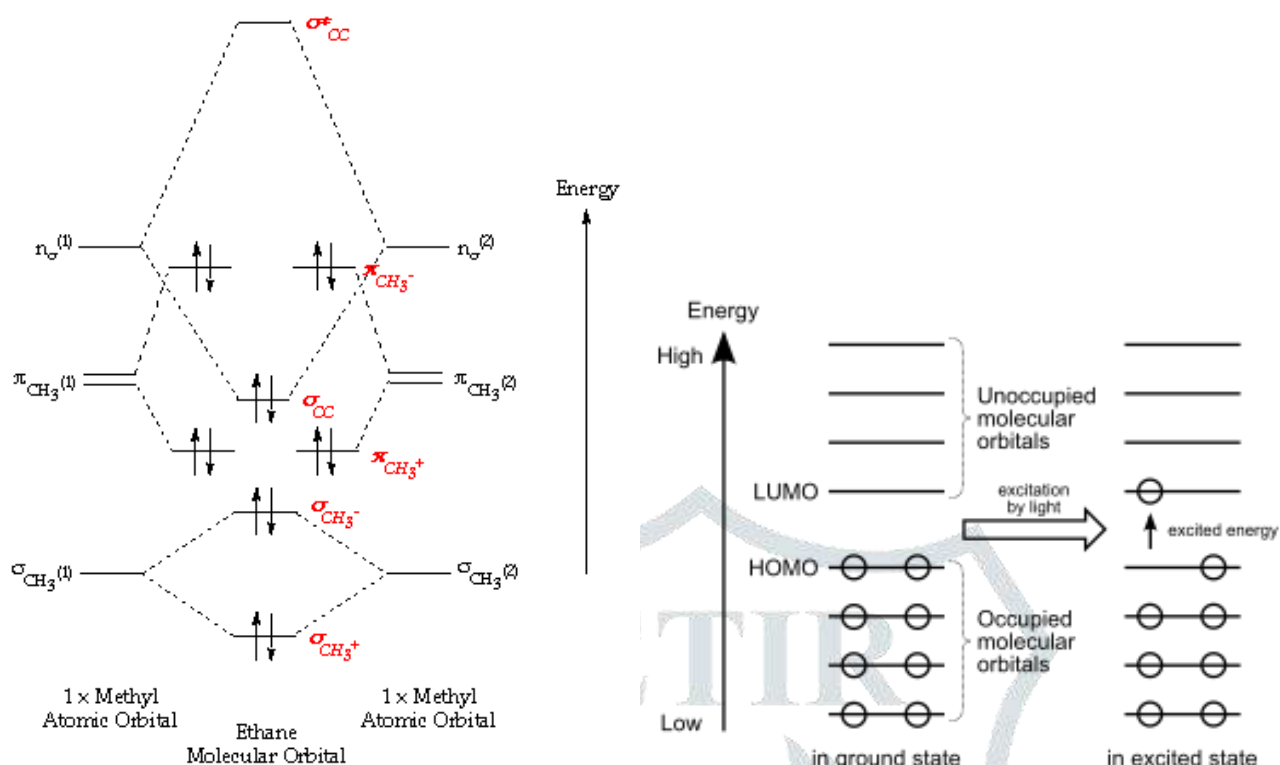


AS two SP^3 hybrid orbitals of a silicon atom can make an antibonding and bonding state. The same is valid for two p_z orbitals making a molecular π orbital. They make a bond and antibonding π State. Conjugated follicular scan have similar properties as semiconductor materials.



Also moving to the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The conjugated molecules are getting longer the HOMO and LUMO created and acts like a kind of valence and conduction band the energy difference between the HOMO and the LUMO that can be considered as the band gap of the polymer material.

The ethane molecule has fourteen valence electrons occupying seven bonding molecular orbitals. As can be seen from the energy diagram - four of the molecular orbitals occur as degenerate pairs. Like in methane - the molecular orbitals of ethane show increasing nodal structure with increasing orbital energy. For the energy diagram and pictorial view of the orbitals. Figure shown.

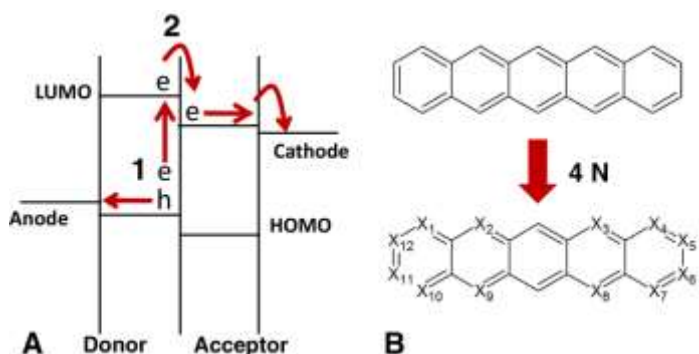


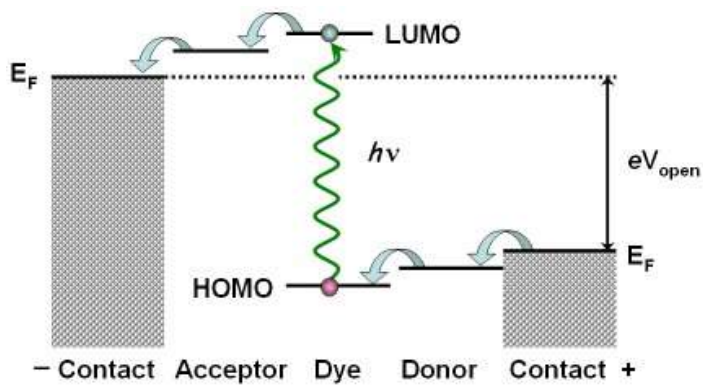
Due to the reason of ionisation energy and electron affinity, lumo attracts electrons from homo. So lumo due to high electron affinity acts as electron acceptor or acts as a conduction band, can easily accept electrons and homo due to low electron affinity, can easily loose the electron and acts as a donor just like semiconductors (say crystalline silicon).

Electron-hole generation (reason of flow of charge in Polymer based OPV) -

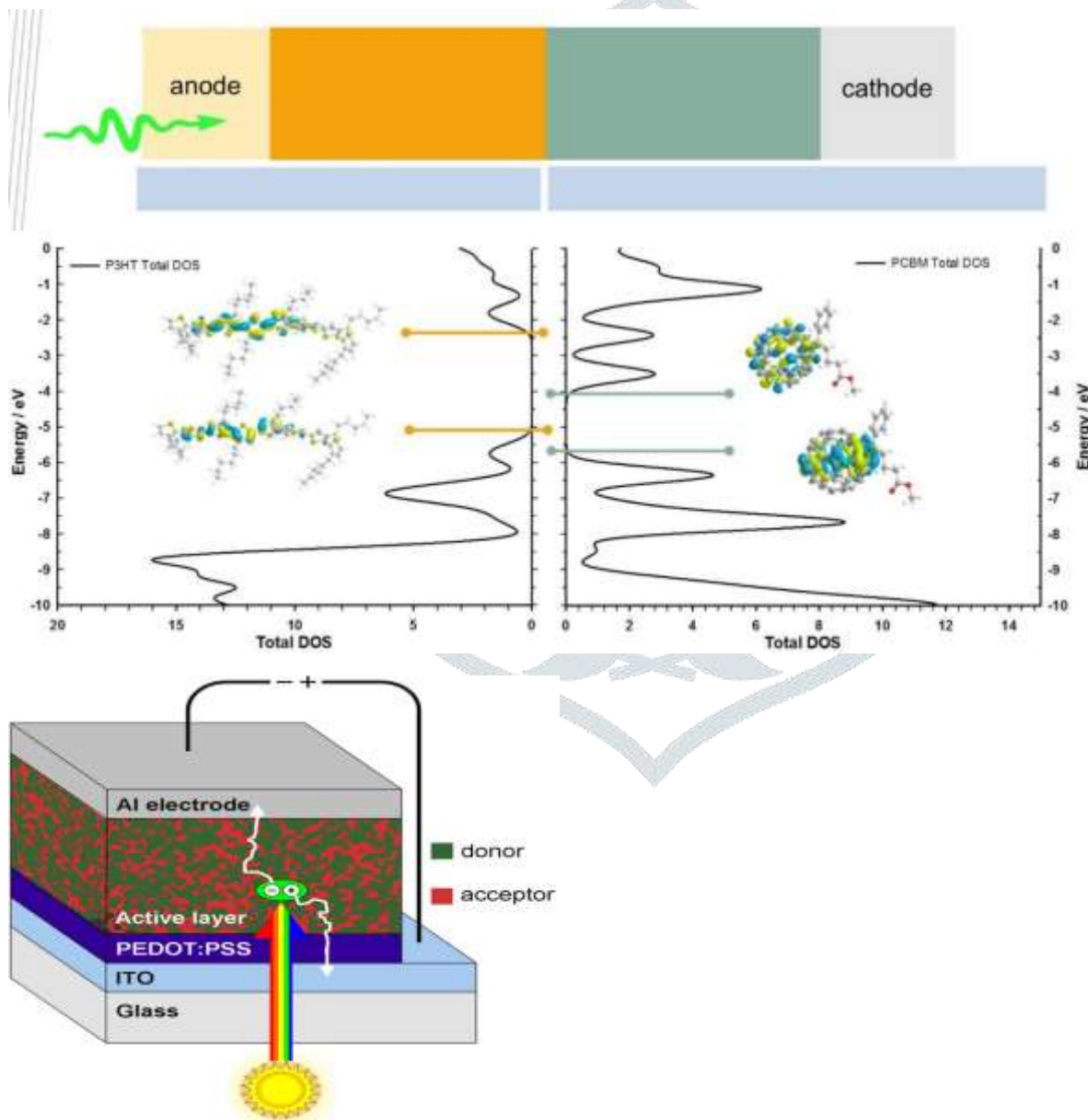
In inorganic semiconductor, electrons can be easily excited to the conduction band from the valence band. Even in silicon semiconductor material the electron and hole pair is weakly bound which can be easily broken up or diffuse away from each other by small energy transfer or adding some impurity. But in organic material excitons are responsible for such case of electron and hole pair releasing. Where the excitons is the balance state of electron and hole pair in organic materials or polymers which is maintained by the coulombic electrostatic attraction force. However these are electrically neutral particles. By getting enough energy from outer source electron can move to upper energy level (say conduction band) and generate some positive in its vacant place. But within few nano-seconds electron is again attracted towards hole or positive charge region due to comparatively large electrostatic attraction force so electron hole remains bound at ground state at every time and called as excitons which can exist in homo and lumo or in electron donor conjugated polymer and electron acceptor conjugated polymer.

Now to utilise this concept and to make organic polymer solar cell, two different layer of polymer (with two different properties) are combined to make an interface of conjugated polymer (say electron acceptor and electron donor conjugated polymer).





Because of two different materials, an electrostatic force and hence an electric field is set up between the two layers. The conjugated polymers are selected in such a way such that they can create maximum possible electric field and electron-hole pair can be easily broken up by a small energy from external sources (say most of the time solar energy). Electron moves towards electron acceptor conjugated polymer and vacancy of electron (say hole) remains in electron donor conjugated polymer.



Mechanism of flow of electron and hole-

To remove electron and hole pair efficiently and effectively, the gap between the two layer should in the order of few nanometre but the gap must be even more than 10 nanometre to make proper absorption of light. To solve this problem, the conjugated

polymers are combined in bulk and many times the acceptor and donor are directly mixed to achieve the required diffusion length. The electron-hole pair (say excitons are generated due to the light absorption and due to the strong electrostatic force setup between the two conjugated layers, electrons starts to move towards acceptor side and finally to electrode and hole are collected at another electrode (most of the time transparent conducting thin film).

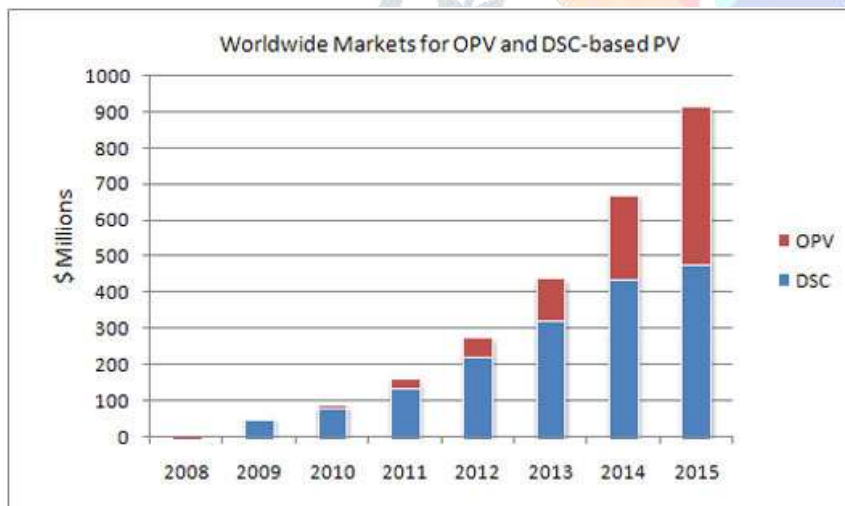
And hence by getting small energy from external source electrons and holes release and start to move in above said direction, which results in flow of electric charge and hence generation of electrical energy.

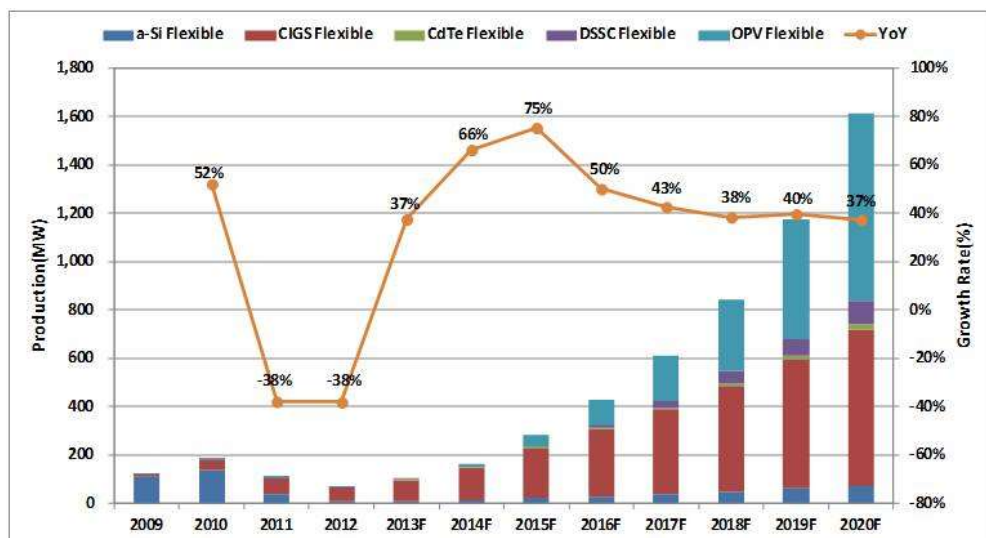
Advantages of OPVs -

The main advantages of an organic polymer solar cell are flexibility, production efficiency, low material cost, less prone to damage and failure. Also the main disadvantage of organic polymer photovoltaic cell is less durable and efficiency. The traditional solar cell last for 15 to 25 year whereas the organic solar cell cannot even last for single year. The efficiency is also less as of 5 to 6% only whereas the efficiency of convention silicon solar cell is about 15%.

Reason of Organic solar cell instead of conventional solar cell, future aspects and possibilities for hetero junction based Organic (Polymer) solar cell-

As it is the main power source technology that converts the abundant power source of energy on earth that is sun into current and into the flow of electrons. But the discussion is, why another new technology is required as already silicon based solar cells are available that are quit cheaper and very successful which also show good efficiency now a days. But something are there, these technologies cannot do. These are current control and semi transparency. These reason provides the platform to the Polymer based organic polymer cell. Even these OPVs are best suited with green house effects. Silicon cell would block all the light but OPV utilise the light at the same time allows the light to enter or pass through the OPV film. OPV can be designed as according to the building architectures whereas the buildings must be designed according to the silicon solar cell to properly utilise the energy. Even as does not require all the components of sun light which can be controlled by specific OPV films. OPV can be designed in such a way that they will harvest only some specific colours as plants mostly required red colour light to generate energy in the process of Photosynthesis. OPVs are also under research to make them a climate controller for the southern US, southern Arabia, Southern Africa.





Acknowledgement- This report consist of small discussion and research about the basics of Polymer based Organic Photovoltaic Solar Cell, recent devolvement and future aspects. This project, entitled as *Hetero Junction Based Organic Photovoltaic Cell: Basics, Current Progress and Future Aspects*, is done by Aakash Chaudhary in the partial fulfilment of Masters in Physics (M.Sc.) degree under the supervision of Prof (Dr.) Shailesh Kumar Singh.

Reference-

1. PV materials - <http://www.tcichemicals.com/pdf/F2033E.pdf>
2. <https://www.sigmaaldrich.com/catalog/product/aldrich/698997?Lang=en®ion=IN>
3. www.1-material.com › Category By Function › Organic Photoconductors
4. <http://pubs.rsc.org/en/content/articlelanding/2017/qm/c6qm00308g>
5. http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/
6. Lectures by Dr. Harald Ade @ NC State University

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