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Exploring Thiophene Compounds: Pioneering Applications in Organic Electronics

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Abstract: ***This review explores the pivotal role of thiophene compounds in the rapidly advancing field of organic electronics. Due to their unique electronic properties, chemical versatility and structural stability, thiophene derivatives have become essential materials in various applications like organic solar cells (OSCs), organic light emitting diodes (OLEDs) and Organic field effect transistors (OFETs). The review high lights recent progress in the design, synthesis and applications of thiophene based compounds.***

Keywords: Thiophene, Organic electronics, Alternate energy

1. Introduction

Depletion of nonrenewable energy source is a major threat that challenges today's mankind. Solution to this problem is the use of alternate energy resources like solar energy. When materials are exposed to lights a weak electrical current is generated and this effect is termed as photovoltaics. Trapping solar energy and converting it into electrical energy using solar cells is a common phenomenon today. Silicon and other inorganic solar cells are used for this. Even though they have attained maximum efficiency, their high fabrication cost and processing difficulty are its major limitations. Organic solar cells are a good alternative for this. Organic materials having delocalized pi electrons have the capacity to absorb sunlight and convert it into electrical energy. Organic solar cells are better than inorganic cells due to their low manufacturing cost, easy processing methods, light weight and flexible nature.1 But its efficiency has not attained up to the mark. Nowadays research is going on to increase the efficiency of organic solar cells. By controlling the morphology of the active layer and by optimizing the band gap by tuning the energy levels of donor and acceptor molecules scientists are trying to attain maximum efficiency.

Bulk Heterojunction Solar Cells

Current research in organic photovoltaics is based on bulk heterojunction (BHJ) solar cells. BHJ consists of photoactive blend layer with a bicontinuous and interpenetrating network of donor and acceptor molecules sandwiched between two electrodes with different work functions (Indium Tin Oxide electrode and a metal negative electrode).2 Since active layer in BHJ has got large surface area, excitons can easily dissociate into electron - hole pair and make the subsequent charge transportation easier.

Fundamental steps involved in the energy conversion process of organic solar cell is the absorption of light and subsequent generation of excitons, columbicaly attracted electron - hole pair. These excitons get diffused in the donor acceptor interface and under applied electric field they dissociate into free charge carriers and get migrated and collected by the corresponding electrodes.3

When an electron donor absorbs light an electron from the highest occupied molecular orbital (HOMO) of the donor get excited to the lowest unoccupied molecular orbital (LUMO) of the donor. Then theses electrons get transferred in to the LUMO of acceptor. Relative position of LUMO level of donor and LUMO level of acceptor is important for efficient charge transfer. Power conversion efficiency of a solar cell is the ratio of maximum electrical output to the incident energy in the form of sunlight.

$$PCE = \frac{p_{\max}}{\phi_e}$$

$$P_{\max} = I_{sc} \times V_{oc} \times FF$$

Where V_{oc} is the open circuit voltage, I_{sc} is the short circuit current and FF is the fill factor. V_{oc} is the difference between the HOMO of the donor and the LUMO of acceptor. As V_{oc} increases efficiency also increases.

Thiophene Polymers

Thiophene based molecules are very important donor molecules used in BHJ solar cells and has got excellent charge transport properties. This is because of high polarisability of sulphur atoms in thiophene. Polythiophene and its derivatives are important as they are stable in oxidized and normal state. Numerous derivatives of thiophenes are reported since it is easy to derivatise thiophene ring through substitution at three different positions. Poly3hexylthiophene (P_3HT) is a common highly efficient polymer donor used in organic solar cells. By derivatising P_3HT with different conjugated side chains absorbance of system can be increased. Thermal stability of solarcell devices can be enhanced by thermal annealing. Other polyalkyl thiophenes reported are poly (3 - pentylthiophenes), Poly (3 - octylthiophenes), poly (3 - dodecylthiophenes). Longer alkyl chains will lower the mobility and increases the phase separation. Besides the homopolymers of thiophene, copolymers of thiophenes based on different monomers like biphenyl have great potential applications in optoelectronic devices. Copolymerization of diketopyrolopyrole (DPP) with thiophene or benzathiadiazole will result in polymers with ambipolar charge carrier mobilities which can be used in organic field effect transistors (OFETs).

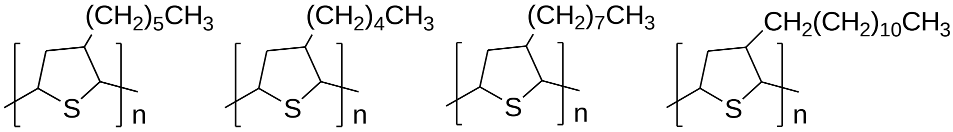

Figure 1: Poly3alkylthiophenes

Thiophene Oligomers

Besides polymers, small molecular donors are used in BHJ solar cells. These molecules have several advantages compared to their polymers. They can be easily synthesized in high purity and the solar cell device can be fabricated by both solution processable and vaccum deposited techniques. Since oligomers have crystalline properties, charge transport properties will also be enhanced. Oligothiophenes with tunable HOMO and LUMO energy levels can be constructed by incorporating electron withdrawing and electron releasing groups on it. Dicyanovinylene (DCV) is a strong electron withdrawing group which can be introduced in to oligothiophene backbone. DCV based oligothiophenes will act as an excellent donor in organic photovoltaics. By replacing vinylic protons in DCV by methyl or phenyl substituents thermal stability of the material can be increased.[4] But introduction of larger subtituents on DCV will decrease Π - Π interaction and results in lower fill factor and shortcircuit current. Benzo [1, 2, 5] thiadiazole (BTDA) is used as an acceptor moiety in oligothiophene based pentamers due to its good optical properties, thermal conductivity, suitable frontier orbital energy levels and strong intermolecular interactions.[5]

Linear oligothiophenes can be used as semiconductors for P - channel organic field effect transistors.[6] Unsubstituted oligothiophenes are difficult to be solution processed. By changing their molecular shape to more three dimensional one it can be easily processed. Thus star shaped hybrid molecules consisting of benzene, truxene or triphenylamine cores in which oligothiophene groups are radialy attached exhibits improved solution processability.[7] Compounds with central part consisting of fused thiophene rings are also easily solution processed and has air stability.[8] Coplanar heteroacenes with aromatic central ring and solubilising alkyl end groups has excellent electrical transport properties. Introduction of vinylene spacer between fused rings results in reduction of aromatic character of planar structure and thus increases Π - electron localization. Branched V - shaped benzothiophenes based structures are also used as acceptor materials in blended photovoltaics.

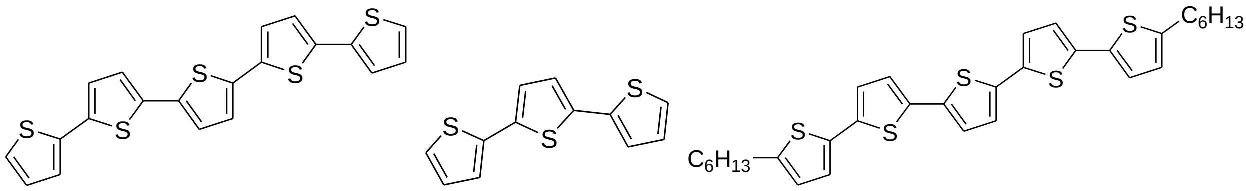

Figure 2: Linear oligothiophenes

Dendrimers

Dendrimers are a class of compounds having the properties of both polymers and small molecules. They have the features like synthetic reproducibility, monodispersion and high processable purity. They have got versatile applications in organic field effect transistors (OFET), organic light emitting devices (OLEDS) and in organic photovoltaics (OPVs).9 Thiophene based dendrimers are good p - type semiconductors. Similar to dendrimers cyclic oligothiophenes are also promising materials in organoelectronics due to their unique self- assembling properties.[10]

Fullerenes

Fullerenes are the widely used acceptor materials in organic solar cells. Recently a copolymer molecule made of fluorene, benzothiadiazole and dicyanovinyl moieties is reported as an acceptor in organic solar cells. Thiophene s, s - dioxide rings can also be used as acceptor materials due to their strong electron affinity.[11] Thiophene based compounds like [bis (9, 9 - dimethyl fluoren - 2 - yl) amino]benzothiophene (electron donor) and cyanoacrylic acid (electron acceptor) bridged by a thiophene or vinylene thiophene is used as push - pull organic dyes in dye sensitized solar cells.[12]

Phenylene (P) –Thiophene (T) Oligomers

Unsubstituted Phenylene (P) –Thiophene (T) oligomers with various P: T ratios are a promising class of semiconductors used in light emitting diodes as well as in p - chanels in OFET.1[3] They offer high carrier mobility and good environmental stability. If P - T oligomers are functionalized with terminal n - hexyl group solubilising effect will increase and so it can be used in solution processable FET's. Incorporation of phenylene units into thiophene backbone results in lowering of HOMO energy and thereby reduction in the off current thus increasing the device on/off ratio.

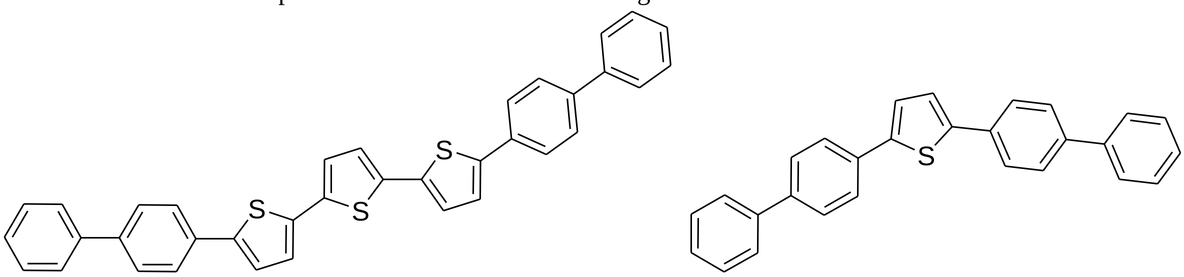

Figure 3: Phenylene - Thiophene Oligomers

2. Conclusion

Understanding how molecular geometry influences the optoelectronic properties is crucial for fine tuning materials for organic electronic devices. Researchers around the globe are dedicated to designing and synthesizing novel oligomeric molecules to unlock their potential in various applications such as OLEDs, OFETs and OPVs. Ongoing research into novel thiophene derivatives continues to unlock new possibilities, expanding their applications into areas of organic electronics. As the demand for sustainable and versatile electronic materials grows, thiophene based compounds are poised to play a critical role in the future of organic electronics.

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