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Review: Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications

Ramasamy Ganesamoorthy[a], Govindasamy Sathiyan[a], Pachagounder Sakthivel[a,b,*]

[a] Department of Chemistry, School of Advanced Sciences, VIT University, Vellore- 632014, India
[b] Department of Nano Science and Technology, Bharathiar University, Coimbatore- 641046, Tamilnadu, India

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ABSTRACT

Bulk hetro-junction organic solar cells (BHJ-OSCs) which made by coating the blend of highly electron rich, poly-3-hexylthiophene (P3HT) as a donor and extremely electron deficient, soluble C_{60} derivative, [6,6]-phenyl-C_{61}-butyric acid methyl ester ($PC_{61}BM$) as an acceptor between the high work function positive electrode, ITO and low work function metal negative electrode Al, showed exciting results than the bilayer counterpart in the last two decades, thus the scientific circle and solar cell manufacturing groups are focusing on this treasured field. Fullerene derivative based BHJ-OSCs showed astonishing efficiencies due the high donor-acceptor (D-A) interface, high open-circuit voltage (V_{oc}), easy processing, and thermal stability. Hence, the design of the fullerene derivative plays a vital role in the efficiency of the OSCs. Numerous papers were published on the $PC_{61/71}BM$ and various functionally modified fullerene acceptors in the past several years with higher efficiency, higher LUMO level, and improved solubility. The symmetrical structure of $PC_{61}BM$ showed high aggregation properties, insufficient absorption in the visible region, but unsymmetrical $PC_{71}BM$ had a good optical absorption in the visible region, hence it was the most desirable choice for best performing solar cells. From the comparison, it was clear that the modification in the $PC_{61/71}BM$ core with aryl group, alkyl chain length, and end group modification didn't show any significant difference in the PCE with the P3HT polymer donor in BHJ-OSCs device structure. Fullerenes multi-adducts performed better than the $PC_{61/71}BM$ due to the development in the V_{oc}. In multi-functionalization, mainly bis-functionalization showed better performance than mono-adduct. C_{60} and C_{70} based hetro bis-adducts namely, $C_{60}(CH_2)$(Ind), and OQMF70 showed the highest PCE of 5.90%, and 6.61% respectively, which was comparable with the indene based bis-adducts. Commonly, tris-adduct fullerenes showed the lowest PCE due to the isomer effect and electron trapping, but OQBMF was a hetro tris-adduct of C_{60}-methanofullerenes, which showed a excellent PCE of 6.43% due to improved V_{oc}. Similarly, indene substituted C_{60} and C_{70} fullerenes based bis-adducts showed supreme PCE, of 6.5% ($IC_{60}BA$) and ~6.7% ($IC_{70}BA$) respectively, peak PCE was attributed to the high electron donating indene group, which enhanced the LUMO level due to the shrinkage in the π-system. The dihydronapthyl based fullerene bis-adduct derivatives such as, $NC_{60}BA$, and $NC_{70}BA$ showed the best performance of 5.37%, and 5.95% respectively, than the mono-adduct. Even though abundant fulleropyrrolidines were reported, the performance of the fulleropyrrolidines based device was very deprived than the $PC_{61/71}BM$ based devices. Though the OSCs are comparatively efficient for commercial application due the insufficient efficiency and lower environmental stability factors controls the early arrival to the market. Therefore, it is essential to go through the recent fullerene derivatives based literatures, including mono-, bis-, tris- and multi-adducts of various methanofullerene derivative, indene based fullerene derivatives, dihydronaptyl substituted fullerenes, fulleropyrolidines, 1,2 and 1,4-adducts and fullerene

Abbreviations: BHJ, bulk heterojunction; OSCs, organic solar cells; SMOSCs, small molecular organic solar cells; D:A, donor:acceptor; HTL, hole transporting layer; ETL, electron transporting layer; PCE, power conversion efficiency; EQE, external quantum efficiency; IPCE, incident photon to current conversion efficiency; UV, Vis-ultraviolet-visible; NIR, near-infrared; PL, photoluminescence; V_{oc}, open circuit voltage; J_{sc}, short circuit current; FF, fill factor; μ_e, electron mobility; μ_h, hole mobility; μ_e/μ_h, hole to electron mobility ratio; AFM, atomic force microscopy; ITO, indium tin oxide; PEDOT:PSS, poly(3,4-ethylene-diox- ythiophene):poly(styrene sulfonate); CN-1, chloro naphthalene; wt%, weight percentage; THF, tetrahydrofuran; CF, chloroform; P3HS, poly(3-hexylselenophene); CB, chlorobenzene; TCB, 1,2,4-trichlorobenzene; ODCB, orthodichlorobenzene; DIO, 1,8-diiodooctane; OT, 1,8-octanedithiol; SA, solvent annealing; PTA, post-thermal annealing; TA, thermal annealing; rms, root means square; ICBA, indene-C_{60} bisadduct; $IC_{60}MA$, indene-C_{60} monoadduct; $IC_{70}BA$, indene-C_{70} bisadduct; $IC_{70}MA$, indene-C_{70} monoadduct; MEH-PPV, poly(2-methoxy-5-(2'-ethylhexyloxy)-1,4- phenylene vinylene); MDMO-PPV, poly(2-methoxy-5-(3,7-dimethyloctyloxy)- 1,4-phenylenevinylene); $PC_{61}BM$, [6,6]-phenyl-C_{61}-butyric acid methyl ester; $PC_{71}BM$, [6,6]-phenyl-C_{71}-butyric acid methyl ester; $PC_{84}BM$, [6,6]-phenyl-C_{84}-butyric acid methyl ester; P3HT, poly(3-hexylthiophene)

* Corresponding author.
E-mail addresses: sakthivel.p@vit.ac.in, polysathi@gmail.com (P. Sakthivel).

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derivatives for OSCs applications. In this regard, we discussed the present development in fullerene derivative and summarized the efficient fullerene derivatives for the BHJ-OSCs application and suggest a possible scenario for the future development in the fullerene cage.

1. Introduction

Electronic revolutions in the last fifty years yielded modern agriculture and irrigation system. Revolutions in the agriculture system leads to more energy demand which was accomplished by the non-renewable energy resources [1–4]. Utilization of non-renewable energy sources for the mass energy production which leads to the depletion of fossil energy resources at a faster rate and resulted the maximum greenhouse gas emission [5]. The emission of these gasses induced global warming and paves the way for sudden natural calamities [6]. To avoid this only option behind us is consuming the clean and green renewable energy. The solar cell will play the key role to contain the environmental pollution. A polymer solar cell is the one, which attracted remarkable attention due to the cheap production cost, flimsy, and elastic nature than the conventional silicon based inorganic solar cell. It directly converts the endless sunlight into current [7]. Polymer solar cells are classified on the basis of the active layer preparation into mono layer, bilayer, BHJ, tandem, and inverted solar cells. In each of the above solar cell donor and acceptor units are necessary, except mono layer solar cells. Conjugated polymer or small molecule is most widely used a donor, similarly polymer, small molecule, perylene diimide, and fullerene derivatives are used as an acceptor material [8]. The ultrafast photo-induced electron transfer from polymer to fullerene, resulted the flourish of OSCs [9]. The limited solubility of pristine C_{60} showed the lower performance in OSCs, hence, it is compulsory to find soluble fullerene derivative for efficient OSCs. This paves the way for the synthesis of new fullerene derivatives, such as $PC_{61}BM$, which is highly soluble in aromatic solvents, and efficient electron acceptor than the pristine C_{60}. In OSCs, P3HT polymer and $PC_{61}BM$ are most widely used donor and acceptor respectively [10].

To commercialize the low cost OSCs, the PCE should be improved; numerous research groups are trying to achieve the above objective by tailoring the donor and acceptor material with the wide and strong absorption in UV–vis to NIR region, appropriate energy levels, material miscibility and improved charge transporting properties. Particularly numerous functionalized fullerene derivatives have been reported with improved efficiency [11,12].

Recently, Chen et al. [13] reported a record high PCE of ~10% for a single junction BHJ-OSCs, which was obtained for the PTB7-Th polymer with $PC_{71}BM$ ([6,6]-phenyl-C_{71}-butyric acid methyl ester) acceptor. Recently, small molecule based single-junction BHJ-OSCs with $PC_{71}BM$ reached a record high PCE of ~10% [14]. In the case of tandem solar with $PC_{61}BM$ and $PC_{71}BM$ as acceptor layers reached PCE of ~15% [15]. Similarly, fullerene free bilayer and BHJ solar cell based on small molecule and PCDTBT polymer acceptors showed an improved efficiency of ~8.4% and ~10% respectively [16,17]. Heliatek achieved the highest certified efficiency of ~12% in December 2013, for a multi-junction solar cell [18]. Though, some highly conjugated n-type polymers, and small molecules performed better than the fullerene derivatives, but $PC_{61/71}BM$ acceptors still the cornerstone of all fullerene derivatives [19,20]. In polymer solar cells, BHJ device structure showed peak performance than the bilayer one due to the interpenetrating D-A interface. Hence, it is essential to review the applications of recent modified fullerene derivatives in BHJ-OSCs for higher performance. To improve the PCE of OSCs, which containing tailored fullerene as an acceptor must have the following important features, broad and strong absorption, better solubility than pristine fullerene (over solubility will give negative results), better miscibility with donor polymer (lower miscibility will reduce the bicontinuous interpenetrating network), higher lying LUMO level for maximum V_{oc}, smooth morphology for good electron mobilities, FF and J_{sc} [5,7,8]. Tailored fullerenes play a key role in the PCE of OSCs.

In recent years, extensive studies have been aimed to design optimal electron donors which resulted the dramatic improvement in the PCE of BHJ-OSCs [7–9]. On the other hand, less attention has been devoted in the fullerene based acceptors derivatives. Although fullerene derivatives have been widely used, the structural optimization still to be needed to increase the compatibility with the P3HT donors. Especially, efficient and novel chemical methods are needed to modify the fullerene cage with particular functional group to solve the device based concerns either in BHJ or conventional device structure. In the past fullerene derivatives based review papers which are published before 2013, they summarized the best results of the fullerene derivatives based solar cells [12,19,20]. During the recent past, it is not surprising to see that the chemistry of fullerene derivatives has budded significantly and many new fullerene derivatives have been introduced in the BHJ-OSC field. Some of the fullerene derivatives achieved the best efficiency. Considering the importance of the fullerene acceptors, in this review we are intended here to give a rationalized review regarding the developments in the fullerene derivatives for high performance BHJ-OSCs. In this review, we explained in brief about the classification of solar cell, working principle and history of fullerenes in first part and in the second part we summarized the best performing fullerene derivatives with elaborate explanation. In addition to that we highlight the recent development in fullerenes and the reason for the peak performance.

The authors express regret for any lapses of fullerene derivatives based scientific publications which are related to BHJ-OSCs applications. We hope that this review offers a clear summary of the present best performing fullerene derivatives in BHJ-OSCs and will give new thoughts for tailoring novel fullerene derivatives with suitable properties for better OSC application. In this regard, we reviewed the recent research development on tailored fullerene acceptors derivative for high performance BHJ-OSCs.

2. Classification of solar cells

The device which converts the solar radiation into current is called as a solar cell. The classification of solar cell is given in the following Fig. 1. It is mainly classified into three type first one non-organic or inorganic based solar cells, second one is the organic based solar cells; the final one is a hybrid solar cell which is made by the mixture of organic and inorganic materials.

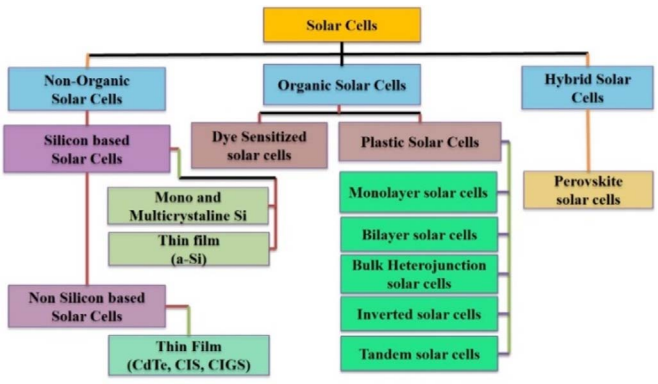

Fig. 1. Classification of solar cells.