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# Buckyball Derivatives as Acceptors in Organic Photovoltaics: A Review

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**Abstract**

Organic materials are a focus of primary attention in the field of organic photovoltaics (OPV) due to low cost (in terms of fabrication, operation, and maintenance), high portability, quick production, and mechanical flexibility. Buckyball derivatives play a prominent role as acceptors in these devices. They are investigated in combination with various organic donor polymers to increase power conversion efficiency (PCE) of OPV devices. This review gives an extensive insight about buckyball derivatives in organic photovoltaics (OPV) under three sections. The first section gives a broad overview on types of organic solar cells and how PCE can be improved by finetuning nine factors. The second section explores classification of buckyball derivatives and their properties. In the final section, the roles of key buckyball derivatives such as C60, PC60BM, PC70BM, bisPCBM, [60]IPB, ICBA, [60]PCBH in the field of OPV are discussed.

***Keywords:*** bisPCBM; Fullerene; Fullerene Derivatives; Organic Acceptors; Organic Photovoltaics; Organic Solar Cells; PCBM; Power Conversion Efficiency.

## 1. What is Organic Photovoltaics (OPV)?

It all started with the discovery of photovoltaic effect in 1839 by French physicist, Edmund Becquerel, when he found out that certain materials, especially metals, conduct a minute amount of electricity when exposed to sunlight. Albert Einstein explained the photoelectric effect in 1905 for which he won the Nobel Prize for Physics in 1921. Encyclopedia Britannica defines photovoltaic effect as “the process in which two dissimilar materials in close contact produce an electrical voltage when struck by light or other radiant energy”. Hence, two different conducting materials which are placed in close contact with each other, when exposed to sunlight, would give rise to a potential junction which can be exploited to produce electricity. This is exactly what photovoltaic cells are designed to do. The early photovoltaic industry sought after popular semiconductors such as silicon, germanium, and indium arsenide.

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However, the attention diverted towards organic semiconducting thin films due to low energy-cost of fabrication[1], high economy, low operating and maintenance costs, easy processing[2], high portability, fast manufacturing, mechanical flexibility[3], compatibility with a wide range of substrates and no noise pollution compared to its inorganic counterpart [4,5]. This is what gave birth to the Organic Photo Voltaic (OPV) technology.

The OPV devices are made of electrically conducting organic materials which consists of electron donors and electron acceptors. Hence a strategic role is played by the donor-acceptor pair in organic conductors as charge transfer takes place between them[6].

Photovoltaic systems are based on four main processes[7] namely light absorption, exciton diffusion, charge separation and charge extraction. The separated charges move towards the respective electrodes in the charge extraction stage. If the separated charges recombine, it gives rise to the "dark current" which reduces the efficiency of OPV devices.

There are different types of OPV devices such as tandem cells[8], bulk- hetero junction (BHJ) solar cells[9], organic/inorganic nanostructures like dye-sensitized solar cells [9–11] and multilayers of small organic molecules[12].

The very first OPV solar cells comprised of a single organic layer sandwiched between two metal electrodes of different work functions [13,14]. This was followed by the "bilayer hetero junction" concept, where two organic layers with specific charge carrier (i.e. electron or hole) transporting properties were sandwiched between the electrodes[9].

Tandem solar cells followed as a solution to reap a broader spectrum of sunlight as they are a combination of two or more solar cells which absorb solar radiation in different wavelengths. The major challenge faced in development of tandem cells is the unavailability of suitable low band gap polymer.

The BHJ solar cells were born by blending two polymers having electron donor (D) and acceptor (A) properties, in solution. The binary solutions then resulted in a solid phase mixture of both polymers when they were spin casted.

A dye-sensitized solar cell (DSSC) also known as dye-sensitized cell (DSC) is based on a photo-electrochemical system where there is a semiconductor formed between a photo-sensitized anode and an electrolyte. This is theoretically similar to the BHJ fundamentals.

Improvement in the field of solar cells is highly pursued as a solution for the energy crisis. It is believed that OPV devices would yield the most substantial cost reduction among the alternatives to silicon based solar cells [12,15].

The popularity of this field is highly evident from the drastic increase on the number of publications on organic solar cells from 1953 in the year 2010 [4,16] to approximately 5000 in 2016[17]. Hence, a vast amount of

research is currently underway to increase the Power Conversion Efficiency (PCE) of organic photovoltaics. To increase PCE, it is crucial to reduce the energy loss during the initial electron transfer step.

PCE is defined as **Pmax/Pin** where Pmax is "maximum electrical power produced by the device" and Pin is "incident light power"[18]. Pmax is equal to the product of Fill Factor (FF), Short Circuit Current Density ($J_{sc}$) and Open Circuit Voltage ($V_{oc}$).

The following are some of the important requirements to be fulfilled to increase the PCE:

### *1.1. Broad range of solar spectrum*

Tandem solar cells are the main solution to this requirement as multiple photoactive layers with complementary absorption spectra can be stacked in series[8], [19]–[22]. The front cell is of a high-band gap material, then comes an interconnecting layer (ICL), followed by a rear cell comprising a low-band gap material in the case of a typical double-junction cell. This also helps to improve the $V_{oc}$ as it is usually limited by the bandgap of the active materials[8], [19]–[22].

### *1.2. The Open Circuit Voltage ($V_{oc}$)*

Scharber et.al.[12] define the $V_{oc}$ of the solar cell as the voltage which compensates the current flow through the external circuit. In Metal–Insulator–Metal (MIM) model of BHJs, $V_{oc}$ equals the work function difference of the two metal electrodes. This was highly controversial as $V_{oc}$ was also influenced by reduction potential of the fullerene due to Fermi-level pinning[23], morphology of the active layer[24] and the electrochemical potential of the cathode[25]. Even though, the MIM theory was extended, it failed to give a satisfactory explanation on $V_{oc}$ for BHJs.

The correlation between the photo-voltage and the oxidation potential of the conjugated polymer was reported by Gadisa and his colleagues [26]. The correlation was detected between the electrochemical properties of six similar polythiophene derivatives (donors) and the $V_{oc}$ of polymer–fullerene solar cells where PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) was used as the acceptor. However, from most literature, it can be concluded that the origin of the open-circuit voltage of the bulk-heterojunction solar cell still has no general consistent understanding.

According to published models and experimental results, most authors agree that $V_{oc}$ is directly linked to the HOMO (Highest Occupied Molecular Orbital) of the donor and the LUMO (Lowest Unoccupied Molecular Orbital) of the acceptor [6, 12, 23, 26–29].

Both the HOMO and the LUMO levels of the donor lie higher than the analogous levels of the acceptor in 'Type II' heterojunctions[30]. The heterojunction can aid charge separation which is used in photovoltaic cells[31–33]. This concept is schematically shown in Figure 1.

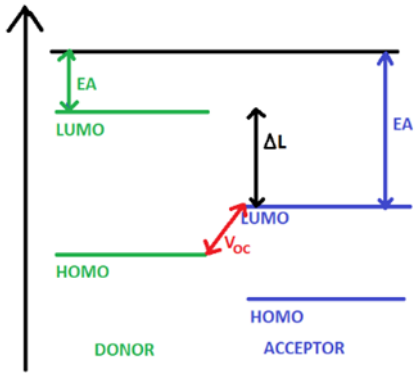



**Figure 1:** Simple HOMO-LUMO diagram for a donor-acceptor interface.

The following equation by Scharber[12] is used to evaluate $V_{oc}$ of conjugated polymer-PCBM system:

$$V_{oc} = (1/e)\,(|E^{Donor}HOMO| - |E^{PCBM}LUMO|) - 0.3\ V \qquad (1)$$

where e is the elementary charge and using –4.3 eV for the PCBM lowest occupied molecular orbital (LUMO) energy.

A key note in designing the HOMO-LUMO levels is to allow a minimum of 0.3 eV energy difference between the donor LUMO and acceptor LUMO for sufficient charge separation[12], [34] which is directly related to the $J_{sc}$ of solar cells.

Hence it's widely accepted that introducing donor polymers with lower lying donor HOMO levels leads to enhanced $V_{oc}$ [28]. Another popular method for increasing the $V_{oc}$ of fullerene-conjugated polymer devices is to increase the LUMO level of the acceptor (fullerene)[35], [36] or to use donors with improved energy levels[37].

It was also revealed that larger $V_{oc}$ can be obtained if polymers with bulky side chains are used as they have lower HOMO energy levels. The influence of the side groups and the side chain is not only applicable to $V_{oc}$ but also hole mobility, absorption and miscibility with fullerides[38].

Interestingly, lowering of $LUMO_{Donor}$ in polymer-fullerene BHJ solar cells could yield efficiencies around 6.5%[39]. As already known, promoting the $LUMO_{Acceptor}$ will increase the $V_{oc}$ with no effects on absorption of the solar spectrum by the cell. In the case of single layer solar cells, the latter is more favorable theoretically as the efficiency approached a value of around 8.4% when the LUMO offset was reduced to 0.5 eV[40]. Unfortunately, inefficient charge transport, insufficient charge-dissociation, morphology problems are some of the drawbacks encountered when acceptors with a higher LUMO than that of PCBM are used.

Although Vandewal and his colleagues observed a drop in photocurrent and efficiency with the lowering of the fullerene content, an increase in $V_{oc}$ was recorded[27].

The energy difference between the HOMO of the donor polymer and the LUMO of the acceptor fullerene determines the spectral position[41]. The spectral position is also affected by other factors such as binding energy of the charge- transfer exciton and its electrostatic environment.

Other individual studies also show that $V_{oc}$ too has a direct correlation with the spectral position of the charge-transfer band; either with the peak of charge-transfer emission[42,43] or the onset of the charge-transfer band[44]. Correspondences between the $V_{oc}$ and photoluminescence[43] or electroluminescence[42] were also observed.

The thermal excitations of ground-state charge transfer complexes (formed between the acceptor and the donor) gives rise to the dark current which has a direct impact on $V_{oc}$ [6,27,45,46]. Stronger the charge-transfer interactions, lower will be the $V_{oc}$ and hence lower the PCE [6,27,47]. Interfacial dipoles affect not only the driving force for charge separation but also the $V_{oc}$ [6,27]. $V_{oc}$ is also influenced by preparation conditions[48].

Given below is yet another formula [27] for $V_{oc}$; but this formula does not state any explicit relationship with band gap. Spectral band positions are present only implicitly through current density (J0) where k is the Boltzmann constant, T is the temperature in Kelvin and q is the Coulombic charge.

$$V_{oc} = \frac{kT}{q} ln\left(\frac{J_{sc}}{J_0} + 1\right) \qquad (2)$$

$V_{oc}$ is also decided by the recombination at the donor/acceptor interface [27,45,49]. Perez and colleagues[47] showed that $V_{oc}$ also depends on the coupling between donor and acceptor materials. Such coupling can suppress the charge transfer band oscillator strength, reduce J0, and thus increase $V_{oc}$. Hence $V_{oc}$ can also be improved if the origin of non-radiative recombination pathways could be explored [27].

### *1.3. Short-circuit current density ($J_{sc}$) and Fill Factor (FF)*

As the name implies, the short circuit current is the current from the solar cell when it is 'short circuited'; in other words when the voltage across the solar cell is zero. Hence it is also the maximum current that can be drawn from the solar cell. Since it's highly dependent on the surface area of the solar cell, the term short circuit current density is used. $J_{sc}$ depends on the number of photons, the spectrum of the incident light, collection probability of the solar cell and optical properties such as absorption and reflection. The equation[50] given below can be used to numerically evaluate $J_{sc}$.

$$J_{sc} = e \int^{\frac{\lambda}{hc}} A(\lambda) I_{AM1.5}(\lambda)\, d\lambda \qquad (3)$$

where e is the elemental charge, h is the Plank's constant, c is the speed of light in vacuum and I is the spectrum of the incident light (the standardized spectrum is the AM1.5 spectrum; hence the symbol IAM1.5). There is also a direct linear correlation between $J_{sc}$ and incident light power[51].

The maximum power which can be derived from a solar cell is determined by Fill Factor (FF) which is defined

as the ratio of maximum power output to the product of $J_{sc}$ and $V_{oc}$ [52].

One study has shown that active layers based on P3HT donor - non-fullerene small molecular acceptor blend can lead to low $J_{sc}$ due to unfavorable phase separation morphologies[53]. In order to achieve high $J_{sc}$ and FF, high charge carrier mobility and fine phase separation with the acceptor are a must[8].

Another study[54] has proved that organic solar cells with thick active layers has significantly improved $J_{sc}$ (21.11 mA cm−2) while suppressing the tradeoff between $J_{sc}$ and $V_{oc}$ by a remarkable amount. Yet the fill factor was found in the 51-54% range due to low electron–hole mobility ratio.

Trukhanov et.al.[52] have demonstrated that the Shockley-Queisser limit (SQL) established for inorganic p–n junction solar cells can be exceeded by FF in OPVs through field-dependent recombination of free charges at the donor-acceptor interface, heterojunction and interface generation.

According to latest research, strengthening of intramolecular charge transfer in certain molecules have contributed to higher $J_{sc}$ [55].

Schilinsky and his colleagues recently reported a model from which correlation between charge mobility and FF could be deduced.[12], [56]. Kiermasch et.al.[57] in a recent study have theoretically explained fill factor with and without masking. Some factors which pose a limitation of FF are field dependent carrier generation, distributed series resistance effects and light intensity dependent shunts.

### *1.4. Efficient Exciton Formation and Dissociation*

The efficiency of OPV cells also depends on how efficiently exciton-dissociation and charge-separation occur. Many factors such as geometric arrangement, electronic structure and electric field at the donor-acceptor interface affect these processes[6]. The rate of charge dissociation or recombination is determined by the relative energies of the exciton states, charge-transfer states and charge-separated states[58]. Figure 2 demonstrates the schematic example of this concept.

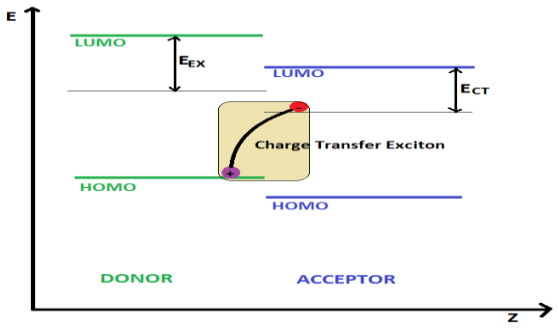



**Figure 2:** Dissociation of a singlet exciton which forms an exciplex across the interface.

### *1.5. Electron/Charge Transfer*

Charge-transfer states is the state where an electron has jumped from the excited donor to a neighboring acceptor (or vice versa in the case of a hole). The charge-separated state is where the electron and hole are far away from each other. Exciplexes are additional electronic excited states which possess both mixed molecular-exciton and/or charge-transfer characters and are formed during optical or electrical excitations[6].

Each charge-transfer state and/or exciplex can undergo separation to give rise to photocurrent or recombine radiatively to the ground state producing light or decay non-radiatively into the ground state or into non-emissive state.

The excitons which reach the donor: acceptor interfaces should be made to dissociate (forming a charge transfer, CT complex) by modifying the electronic structure of donors and acceptors, changing electric fields or using impurities[12].

### *1.6. Charge Mobility*

Once the exciton dissociates at the donor–acceptor interface, the released electron should be transported to the cathode and the hole to the anode. The interface-to-volume ratio and percolation ratio of donor: acceptor decides charge mobility[7]. Steric hindrance due to the branched side chains of the donor[38] and isolated domains[7] too can affect charge mobility.

### *1.7. Orientation*

The orientation between the donor and the acceptor has a great impact on charge transfer[4]. Hence, designing of donor – acceptor blend should be optimized to derive the full benefits of the interfacial interactions.

### *1.8. Morphology*

The domain size of the donor, interface-to-volume ratio of the blend, percolation between the donor and acceptor, collection at the electrodes, proper molecular alignment are all morphological factors which affect PCE[4]. Even device fabrication parameters such as thin-film deposition spinning speed[59]–[61], polymer molecular weight[62], temperature[63,64], solvent choice [65,66] and drying time of the thin films[67] affect the morphology.

### *1.9. Stacking Structure*

A strong correlation between stacking structure of molecules and electronic structure as well as subsequent hole effective mass was discovered[58]. Staggered geometry, zigzag structure, linear alignment[68] and tilted structure[69] are some among the investigated structures.

More attention is given to bulk-hetero junction solar cells due to their high potential of being a low cost OPV technology, efficient conversion of the absorbed photons to electrons and efficient collection of the separated

charges at the electrodes enhanced by the bi continuous interpenetrating network[12].

Performance of BHJs is mainly influenced[7] by three morphological factors namely electron donor phase's domain size, interface-to-volume ratio of the blend and percolation ratio. It's crucial for the electron donor phase's domain size to be small enough for exciton to diffuse to the donor–acceptor interface. The interface-to-volume ratio of the blend should be sufficiently large for efficient exciton dissociation. The percolation ratio is the volume fraction of electron donor and acceptor phases that penetrates through the blend. It must be large to ensure charge carrier transport. Hence it can be rightly said that the performance of BHJs is highly dependent on the nano-scale morphology of the photoactive layer.

**2. Introduction to Fullerenes**

The discovery of Buckminsterfullerene in September 1985 by Kroto et.al. at Rice University was the start of a new chapter in the nanotechnology world [70]. It was named after Buckminster Fuller, an American architect, whose geodesic dome it resembled. They shared a Nobel Prize in 1996 for their novel discovery. Famously known as "The Buckyball" or "C60", it is a spherical molecule comprising of 60 carbon atoms only arranged in to 12 pentagonal and 20 hexagonal rings. The diameter of a C60 molecule is approximately 7Å.

Fullerenes are the third allotrope of C following behind graphite and diamond. Fullerenes are made of C atoms only arranged in pentagonal and hexagonal rings. Its shapes can vary from sphere to ellipsoids to cylinders or more. These C atoms are sp2 and sp3 hybridized. The C atoms with sp2 configuration are responsible for the angle strain in the molecule [71] which leads to the curvature at each pentagon. This curvature gives rise to the distinctive hollow cage configuration of fullerene molecules. The Isolated Pentagon Rule (IPR) which states that "no two pentagons in a stable fullerene can be adjacent" is followed by the most stable configuration of rings.

C70, comprising of 70 C atoms, can be stated as the next most well-known fullerene after C60. The isolated pentagon rule is obeyed only by one configuration of each of C60 and C70 molecules. Fullerenes can range from 20 to thousands in the number of C atoms[72]. Those with less than 300 C atoms are limited to single-shell structures and are generally referred to as 'buckyballs'.

Giant fullerenes are those with the number of C atoms exceeding 300. They can be single or multi-shelled; the latter is referred to as 'onions' since the adjacent multiple layers resemble those of an onion. The multi-shelled form consists of concentric layers gifting them with remarkable properties which can be exploited in the field of photovoltaics, hydrogen energy storage, wear resistance and superconductivity[73].

In addition, fullerene nanotubes/buckytubes were first reported in 1991[74]. These are made up of hexagonal ringed cylindrical walls. These walls are capped at each end by six pentagonal rings and required hexagonal rings to close the structure. Popularly known as Carbon Nanotubes (CNT), they can range from (4A) to tens of nanometers [75] in diameter. They can be single-walled nanotubes (SWNT) or multi-walled nanotubes (MWNT) comprising of several concentric cylinders. The applications of CNTs span a wide spectrum due to their unique characteristics which is beyond the scope of this article.

Nanospheres[76], nanovesicles[77], nanorods[78], nanonetworks[79], nanowires[80], liquid crystals[81] are some of the fullerene nanostructures used in very recent, diverse applications. In this review the main focus will be on buckyballs and derivatives along with their roles in OPV applications.

### *2.1. Properties of Buckyballs*

Irreversible oxidation and reversible reduction properties are exhibited by C60 and C70 buckyballs. They can be reduced with up to 6 electrons resulting in high electron affinity. This is due to the presence of triply-degenerate low-lying LUMOs (lowest unoccupied molecular orbital). It also possesses fivefold-degenerate (π-derived) highest occupied molecular orbital (HOMO). The HOMO has hu symmetry while the LUMO has t1u symmetry (25 cited in [82]). C60 has a localized π-electron system. Hence it is not a super-aromatic structure but behaves only as an electron deficient molecule making it an ideal candidate to be an electron acceptor. It can accept electrons not only in solid state but also in solution form. C60 is highly insoluble in water due to their hydrophobic nature.

Closely packed solid structure of C60 molecules form face-centered cubic (f.c.c.) symmetry while C70 exhibits f.c.c. or hexagonal-close packed (h.c.p.) symmetry[82].

Their ultrafast electron transfer mechanisms (Glatthaar and his colleagues 2005 cited in [50]) with a much slower back transfer[71] had aided in solving the low yield restrictions faced in OPV devices.

High strength and high stability are among the key characteristics of Fullerenes which enable them to retain their shapes even after colliding with stainless steel at 15,000mph[71].

C60 and C70 can be considered as ‘energy reserves’ due to the vast amount of energy stored in the delocalized π-bond system. This is evident from the high heats of formation compared to other fullerenes[83]. They also possess higher ionization potentials compared to the other clusters[84]. C60 undergoes addition reactions[85], nucleophilic and electrophilic substitutions, radical reactions and polymerization[86].

Such characteristic features help to establish Buckminster fullerenes as an ideal candidate in many diverse applications such as superconductors[87], semiconductors[88], hydrogen storage[89], transport and delivery[90], extraction and purification[91], organic reaction catalysts[92], lubrication[93], cancer treatment[94], nanocrystalline diamond film growth[95] and rubber industry[96].

### *2.2. Types of Buckyball derivatives*

Derivatives of fullerenes are important to ‘customize’ their electronic, magnetic, mechanical, optical and catalytic properties so as to optimize their applications in the relevant field. Figure 3 exhibits the main classes of buckyball derivatives based on literature review.

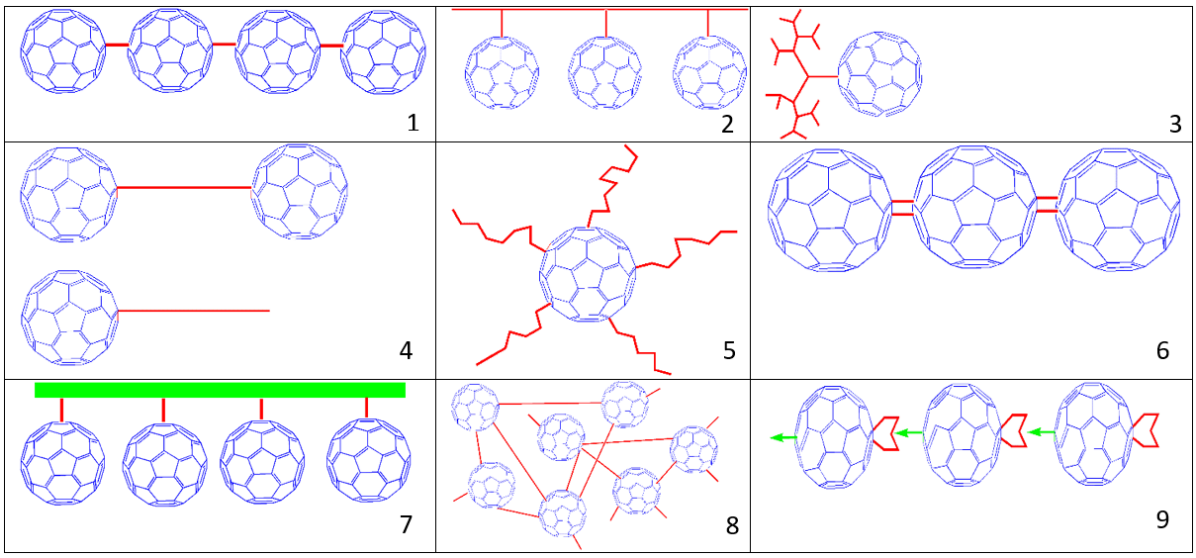



**Figure 3:** Main classes of Buckyball derivatives.

### *2.2.1. Main-chain fullerene polymers*

Electrochemical polymerization was used by Benincori and his colleagues [97] to produce main chain fullerene polymers in 1996. Taki and his colleagues [98] is credited for having produced the first true main chain fullerene polymers by attaching fullerene to diamine linkers via methanocarbonyl connectors.

Raissi and his colleagues [99] recently reported organic photovoltaic devices based on a multi-block copolymer incorporating main-chain fullerene polymers for the first time. They have employed atom transfer radical additional polymerization (ATRAP) method to prepare the fullerene moiety. Poly[poly(3-hexylthiophene)-block-poly{([1,4]-fullerene)-alt-[1,4-dimethylene-2,5-bis(cyclohexylmethyl ether) phenylene]}] (P3HT-b-PFDP) is the novel candidate used which has recorded a 50 fold performance improvement in inverted structures.

### *2.2.2. Side-chain fullerene polymers*

Wudl and his colleagues made the first attempt to produce side-chain fullerene polymers by obtaining a C60 containing polyester by poly-condensation; Geckeler and Hirsch succeeded in producing the very first side-chain fullerene polymer by first preparing an amino-polymer and then reacting it with fullerene to produce the side-chain fullerene polymer (Wudl and his colleagues 1992 and Geckeler & Hirsch, 1993 cited in [75]). Side-chain fullerene polymers can also be prepared using Diels-Alder cyclo-addition reactions[100] and Friedel–Crafts reactions[101]. How nearest neighbor interactions affect device performance[102] and how soft hydrocarbon chains can be used to enhance heat transfer from fullerene molecule to liquid[103] among many others are current research topics for this class of buckyball derivatives.

### *2.2.3. Fullerodendrimers*

Fullerene-functionalized dendrimers or fullerodendrimers comprises of controlled number of 'dendrons' attached on a C60 core. Depending on the type of polymers that make up these 'dendrons', the properties of the fullerodendrimers can be fine-tuned to suit various applications such as OPV devices, artificial photosynthetic systems, solubility of compounds among many others. In addition, amphiphilic 'fullerodendrons' with characteristic properties can be produced by incorporation of C60 moiety at each branching units[104].

### *2.2.4. Fullerene end capped polymers*

Single C60-end-capped oligophenylenevinylene prepared by Gu and his colleagues [105] was a great solution to overcoming barriers faced at the acceptor-donor junction in OPV devices using fullerene-polymer 'blends'. The reason is that this approach directly 'links' the acceptor and the donor in a bicontinuous network. Martineau and his colleagues [106] demonstrated that mono-, bi- and tri-, C60-end- capped oligothienylenevinylenes possessed small band gaps for light harvesting in organic photovoltaic devices.

### *2.2.5. Star-shaped fullerene polymers*

In this type of polymerization, C60 acts as a radical absorber which can multiply absorb primary and propagating polymer radicles. Due to this radicle absorbing property of C60, chain polymerization is restricted. Yet with time, the number of polymers attached to C60 may increase. Two types of hexa-arm star copolymers were prepared by Mignard and his colleagues [107] which showed some beneficial properties such as the number of arm being limited to 6, better solubility in common organic solvents and good photoconductivity which can be exploited in OPV devices. Efficient three-dimensional intermolecular electron transport and hopping behavior among doped oligoanilino-arms were also reported in poly(oligoanilinated) fullerenes[108].

### *2.2.6. 'All-fullerene' polymers*

This is where two fullerene molecules will be directly connected via covalent bonds. Electron beam-induced polymerization[109], plasma-induced polymerization[110], photopolymerization[111] and pressure-induced photopolymerization[112] are some methods of preparation. The formed polymer structures can range from one to three dimensions. Photochemical [2+2] cycloaddition reaction is supposed to be the main cause of crosslinking among fullerene molecules when they are in the excited triplet states.

### *2.2.7. Immobilization of fullerene on solid surfaces*

This class of fullerene derivatives is mainly used to surface coat and transfer characteristic fullerene properties to bulk materials. It is crucial for C60 to strongly adhere to the substrate for successful coating without altering its cage structure. For this purpose C60 molecules are immobilized using self-assembled monolayers (SAM)[113] where strong covalent bonds are formed between C60 fullerene and terminal functional groups of SAM. This preserves fullerene's symmetric cage structure. Yang and his colleagues [114] present C60-DLC (diamond like carbon) nanostructure hybrid coatings with improved elasticity, damping capacity and ductility and reduced material loss.

### *2.2.8. Crosslinked fullerene polymers*

Initial morphology of the donor-acceptor blend being 'locked' or 'frozen' is the major benefit of crosslinking technique. It can be initiated through exposure to UV light or heat. Donskyi and his colleagues [115] present partially and fully crosslinked nanoclusters composed of self-assembled fullerene-polyglycerol amphiphiles (FPAs) which can involve in controlled transport of hydrophobic and hydrophilic agents. Photo-crosslinking of fullerene segments can tune the size and transport properties of the amphiphiles.

### *2.2.9. Doped Fullerene*

Doping is an important method of altering the electronic properties of fullerenes. The three main modes of doping are (i) intercalation (gives fullerene salts); (ii) on-ball (gives heterofullerenes); (iii) from inside (gives non-metal doped endohedral / metallofullerenes). Two different doping methods can be used leading to combinational doping[82].

Doping can be mainly classified as effective doping and ineffective doping. Significant changes in absorption spectra along with photoluminescence quenching and slight improvement in conductivity are the features of effective doping. On the other hand, small changes in the absorption spectra and conductivity along with enhanced photoluminescence and photoconductivity marks the characteristics of ineffective doping (Morita and his colleagues 1992 cited in [75]).

Many studies both experimental and theoretical had been undertaken to investigate various types of intercalating molecules ranging from single atoms like Mg to organic molecules on fullerene. Pontiroli and his colleagues [116] presented a new intercalated fullerene polymer Mg2C60 where four-membered carbon rings or single C–C bonds connect fullerenes to form a two-dimensional network which could be utilized in new types of Mg ion batteries. According to a study by Zhu and his colleagues [117], aromatic molecules can bond to C20 clusters via C-C or C-H-C bonds to form polymers which can preserve long term periodicity upon compression.

In heterofullerenes[118], a foreign atom replaces one or more C atoms in the fullerene cage. Trivalent heteroatoms like B or N are the most famous since they are closer to C in size and structure. Doping fullerenes with B and N lead to borafullerenes[119] and azafullerenes[120] respectively. If one such atom (odd number) is replaced, an open shell system is resulted. If even number of atoms is replaced, it leads to a closed shell system.

In endohedral fullerenes (EFs), an atom/ion/cluster other than C, is enclosed within the fullerene cage. If the enclosed element is a metal, it is referred to as endohedral metallofullerenes[121]. EFs are mainly classified into two: (i) which obey the IPR rule; (ii) non IPR EF: possess fused pentagons. Ceron and his colleagues [122] have elaborated about the 15 types of possible C-C bonds and 5 different types of EF junctions. The first cluster EF, Sc3N@Ih-C80 was discovered by Dorn and his colleagues in 1999 which is accepted to be the most abundant EF and the third most abundant fullerene as of today[122].

### *2.2.10. Supramolecular Fullerene*

Fullerene molecules can aggregate to give rise to supramolecular fullerene and other nanostructures depending on experimental conditions and donor medium without compensating their optoelectronic properties[123], [124]. Fullerene aggregation in supramolecular π gels[125], [126] is a reputed field of study in photoelectronic devices.

### *2.2.11. Molecular interlocked fullerene systems*

In a very recent study by Megiatto and his colleagues [127], molecular interlocked systems in relation to artificial photosynthetic machines were studied. These systems comprised of photo-redox components which were NOT covalently linked but rather mechanically. A mechanical bond cannot be separated without altering or breaking the chemical bonds between atoms. Two such fine examples of interlocked molecules are rotaxanes and catenanes. A molecular ring is confined in rotaxanes while two or more interlocked rings are present in catenanes. C60 fullerene (acceptor) and zinc(II)porphyrinate (donor) were used in designing rotaxanes and catenanes. Figure 4 is a schematic example of how a molecular interlocked fullerene system would look like.

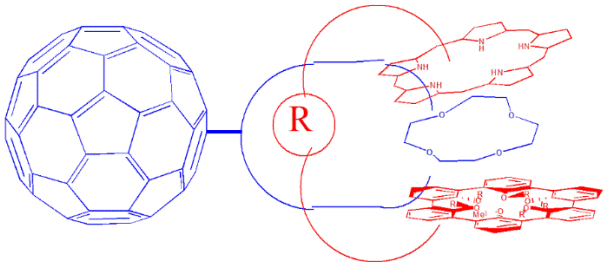



**Figure 4:** Schematic example of how a molecular interlocked fullerene system.

### *2.2.12. Other C60 Hybrids*

The characteristic features of Buckminster fullerene render high capacity to be associated with a wide range of molecules and polymers to yield a variety of C60 hybrids. C60 polymer hybrids for DNA attachment[128], C60-graphene hybrids[129], C60-nanotube hybrids[130], C60-gold hybrids[131] are some examples for recent studies in C60 hybrid fields.

## 3. Buckyball derivatives in the field of OPV

### *3.1. C60 and PC60BM/ PC61BM ([6,6]-phenyl C61 butyric acid methyl ester) as acceptor*

Most literature survey points to how much emphasis had been given to solar cells based on thiophene-based polymers as electron donors and PCBM (and derivatives) as acceptors during the early 2000's. Among the dominant individual systems studied, P3HT [poly(3-hexylthiophene)]- PCBM combination takes a prominent place achieving PCE of 4-5% [4, 12, 36, 38, 132, 133].

The P3HT/PCBM mixture enjoys an exceptional property of its PCE having a wide range. Changes in fabrication conditions contribute to alterations in hole mobility of the polymer[39], crystallinity[134], domain size[60] and absorbance in the visible range[135] which in turn can give rise to varying PCE. Lee and group[7] revealed that the optimum weight ratio for P3HT:PCBM blends is 1:1 in order to have the optimum interface-to-volume ratio and balanced charge carrier transport (in both phases). When PCBM was blended with P3HT, a significant increase in $V_{oc}$ was seen due to the increase of the LUMO level; a high $J_{sc}$ as well as FF were maintained.

Stephen and his colleagues [136] experimentally demonstrated the plausibility of producing a polymer with alternating fullerene and dye units (in the main chain) as acceptors for the first time. C60 or phenyl-C61-butyric acid methyl ester (PCBM) were the selected fullerenes while diketopyrrolopyrrole (DPP) was the selected dye. They were manufactured via the sterically controlled azomethine ylide cycloaddition polymerization (SACAP) method. It exhibits a promising field for future research since the $V_{oc}$ recorded was significant. This is a class of main chain fullerene molecules and hence possesses two main advantages over its side-chain counterparts: it has higher fullerene content and highly variant electronic properties. DPP has many favorable properties such as high stability, increase $V_{oc}$ of solar cells and good charge mobility. The authors encourage the incorporation of C60 and dye into repeating macromolecule to obtain highly variant LUMO levels of C60.

A novel azido cross-linkable group for PC60BM system had been introduced[137] which can effectively stabilize the BHJ morphology by improving the stability of P3HT:[60]PCBM system. This is a class of crosslinked fullerene polymers.

Supramolecular C60 fullerenes in the form of long crystalline fibers have shown increased photo-detection[138] while enhanced photoconductivity was reported in supramolecular rods composed of crystallized C60 fullerene[139].

Recent study[140] comprised of CuO nanoparticle doped PCBM:P3HT blend has proven to increase PCE by 3-4% compared to the non-doped ones.

Insertion of a PCBM layer in between P3HT:PCBM blend and the cathode[141] has greatly improved the device performance which is credited to enhanced light absorption and increased PCBM amount at the interface which in turn leads to facilitation of electron extraction and carrier recombination suppression.

### *3.2. PC70BM/ PC71BM ([6,6]-phenyl C71 butyric acid methyl ester) as acceptor*

It's quite accepted that C70 fullerene surpasses the C61 fullerene in absorption in the visible region and hence giving rise to a better overlap[142, 143]. Thus, the $J_{sc}$ of the PC71BM device is higher than that of the PC61 BM[28].

Dou and his colleagues [8] had fabricated around 300 single-layer devices using poly{2,6′-4,8-di(5-ethylhexylthienyl)benzo[1,2- b;3,4-b]dithiophene-alt-5-dibutyloctyl-3,6-bis(5-bromothiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4-dione} (PBDTT-DPP) as donor and PC71BM as acceptor. The highest they have achieved for $V_{oc}$,

$J_{sc}$ and FF are approximately 0.74 V, 13.5 mA cm-2 and 65% respectively. PCE value >6% was recorded for 90% of the devices. They reason that deeper HOMO level attributed to the increase in $V_{oc}$ while higher hole mobility attributed to increase in $J_{sc}$ and FF. They suggest a weight ratio (polymer: PC71BM) 1:2 for high performance.

The highest certified efficiency in the OPV field as of 2011 was recorded by them[8] where the tandem cell they've developed records a PCE of 8.62% with a $J_{sc}$ of 8.26 mA cm-2, a $V_{oc}$ of 1.56 V and an FF of 66.8%. The combination of PBDTT-DPP and PC71BM was used for the rear cell while the combination of P3HT and IC60BA (indene-C60 bisadduct) was used for the front cell.

Dai and his colleagues [144] demonstrated how incorporation of two binary additives namely 1,8-diiodooctane (DIO) and polyethylene glycol (PEG) contribute to improved $J_{sc}$ and PCE in BHJs comprising of PC71BM as acceptors. Donor/acceptor phase separation was facilitated by DIO additives leading to efficient exciton dissociation and charge transport. PEG additives improve the crystallinity of the studied donor system and thus optimizing charge transport pathway.

PC70BM was used as the acceptor in a research conducted by Chen & peers [145] where the average obtained efficiency was 7.38%. The main donor polymer used was poly[4,8-bis-substituted-benzo[1,2-b:4,5-b']dithiophene-2,6-diyl-alt-4-substituted-thieno[3, 4b]thiophene-2,6-diyl] (PBDTTT-E) with two main modifications giving rise to donor polymers PBDTTT-C and PBDTTT-CF. The optimized weight ratios of donors PBDTTT-E, PBDTTT-C and PBDTTT-CF to the acceptor (PC70BM) were 1:1, 1:1.5 and 1:1.5, respectively.

Latest research on PC71BM acceptor BHJs, shows that ternary composition with a non-fullerene small molecule improves efficiency over the traditional binary composition of donor polymer-PC71BM and can yield a PCE of 12.9%[146].

### *3.3. Both PC60BM and PC70BM*

Outstanding electron affinity and excellent charge mobility are two characteristic features of PCBM[1–3]. Single layered polymer cells developed by Liang and coworkers[38] used alternating thieno[3,4-b]thiophene and benzodithiophene units as the donor in combination with PC61BM and PC71BM as acceptors. PCE of 4.8% was recorded with PC61BM while a PCE of 5.6% was recorded with PC71BM. Even though these solar cells had generated $J_{sc}$ and FF among the highest reported during the time, the $V_{oc}$ was comparatively insignificant (only 0.56-0.58 V). In a study conducted by Vandewal et.al.[27] comprising of five different donor polymers in combination with PC61BM and PC71BM, the polymer/fullerene ratio in most of the efficient devices was between 1:2 and 1:3. The varying combination of the donor-polymer blend has yielded different efficiencies.

### *3.4. bisPCBM as acceptor*

Lenes and coworkers[36] announced a bisadduct analogue of PCBM called the bisPCBM, which is a byproduct during PCBM preparation[147]. It is a n-type semiconductor material with a large number of regioisomers and

has a higher LUMO than PCBM[148]. The HOMO of bisPCBM is 6.1eV which is significantly higher than the work function of the electrode used (PEDOT:PSS, 5.2 eV). Hence, hole injection into the fullerene can be ignored and it can be assumed that only electrons flow under forward bias. It was also demonstrated that bisPCBM is a better acceptor than PCBM as $V_{oc}$ of the P3HT:bisPCBM system has increased to 0.73V; a value higher by 0.15V than the P3HT:PCBM. It has recorded a fill factor of 68% and a short-circuit current of 91.4A/m2. It resulted in a PCE of 4.5%. It was concluded that the 0.7% increase compared to the previous P3HT:PCBM system was entirely due to the increase of $V_{oc}$. A recent computational research using DFT (Density Functional Theory) simulations studied a bisPCBM donor system coupled with eight variants of a modified thiophene donor with F and Se atoms incorporated[149].

Stephen et. al.[136] demonstrated for the very first time that repeating structures of fullerenes (C60 or PCBM) and dyes (diketopyrrolopyrrole - DPP) can be used as acceptors in BHJs. Oligomerization and dimerization among PCBMs both of which are photo-induced homo-reactions lead to enhanced device stability and creation of charged traps, respectively. PCBM leaching leads to efficiency loss due to excessive interfacial concentrations and large crystals[150].

### *3.5. Other Modified Fullerenes*

Use of [60]IPB instead of PC60BM as acceptor is reported to have increased $V_{oc}$ by 50mV and PCE by 10-15% by comparison in P3HT BHJ solar cells[151]. Studies on P3HT with PCBM and ICBA/Indene-C60 Bisadduct(1',1'',4',4''-tetrahydro-di[1,4]methanonaphthaleno[5,6]fullerene-C60) blends too are available[152].

Phenyl-C61-butyric acid hexyl ester ([60]PCBH) is found to have higher $J_{sc}$ than PCBM cells[153]. Modified PCBH such as Lu3N@C80-PCBH is reported to have higher $V_{oc}$ over their hollow counterparts[154].

Bregadiolli and coworkers[155] had introduced a novel fullerene polymerization technique via the [1 + 3] cycloaddition mechanism to produce Oligo(azafulleroid)s and poly(azafulleroid)s. They claim to have obtained an FF comparable to that of PCBM. It is notable that imino-chemistry is focused on for the first time in main chain fullerene oligomer synthesis.

In order to overcome the pitfalls of BHJs, a novel concept of using polymer nanoparticle super lattices was introduced which lead to the field of OPV devices to take a new turn[156].

## 4. Conclusion

Any photovoltaic technology has two primary goals: one is to absorb the maximum amount of incident photons and the other is to generate the maximum amount of free energy possible from each photon. The former yields a large photocurrent while the latter leads to a large voltage. Clearly, the goals contradict each other since materials with a small band gap and a large bandgap are needed respectively to satisfy the first and second goals. Small band gap materials yield small voltage while large band gap materials yield smaller photocurrents due to the absorption of fewer photons.

This is one of the main reasons why investigated organic materials are not able to exceed the PCE (power conversion efficiency) limit to be considered commercially viable and still linger in the 10%-15% range. Low band gap polymer based OPVs and tandem cells have reported a PCE of 10.5% and >13% respectively in recent times[50].

From the literature survey, deficit in PCE cannot be attributed to any one factor alone but as a whole/ combination of two or more factors such as insufficient carrier mobility, miscibility with appropriate donors/acceptors, low solar spectrum coverage, suitable HOMO-LUMO energy levels to enhance $V_{oc}$, the morphology design and electron transfer process.

How the positive and negative charges are freed from Coulomb attraction to produce separated charge carriers is still a mystery and should be subjected to investigation.

Modeling of interfaces between the organic conjugated materials comprising of their electronic and geometric structures is a key area that awaits much needed attention. The interfacial effects whether it may be of the electronic or the optical process that takes place has been pointed out many a time to play a crucial role.

The morphology design being one of the fundamental challenges in OPV research is clearly a multi-dimensional problem.

Using PC70BM instead of PC60BM shows that further improvements in PCE can be obtained. Further developments are yet to be reported as the performance of the composite prepared with PC70BM is poorer compared to that with PC60BM. Also, the phase separation behavior of the polymer-PC70BM is shown to be different from that of polymer-PC60BM. Many alternatives can be explored when more research is directed this way.

Due to depleting fossil fuel sources and concerns for mother nature, renewable energy sources are a must at the earliest possible time. Organic photovoltaic is a promising field to cater this need. Advances in both theoretical and practical research is vital to improve the efficiencies of OPV devices.

Description of ground and excited state potential energy surfaces in complicated environments accurately still need substantial improvement than what is currently available. For this reason, novel concepts built on DFT & TDDFT, multi reference quantum calculations, GW/Bethe-Salpeter and quantum Monte Carlo are being developed by theoretical chemists which could be a significant aid in exploring novel acceptors.

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