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A review from fullerene dominance to non-fullerene innovation: theoretical perspective on next-generation organic photovoltaics

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The mechanical flexibility, solution processability, and the capability for low-cost processing of organic photovoltaics (OPVs) make them a viable class of next-generation solar energy technology. The design of effective electron acceptors that promote exciton dissociation, charge transfer, and long-term device stability is a key feature in finding OPV performance. With a focus on their electronic structure, charge-transfer mechanisms, and structure–property connections, this analysis offers theoretical insights into the fabrication of electron acceptors from traditional fullerene derivatives to sophisticated non-fullerene acceptors (NFAs). The creation of NFAs has been fueled by the restricted tunability, weak visible absorption, and morphological instability of fullerene-based acceptors, which have previously dominated because of their suitable energy levels and isotropic charge transmission. Studies using density functional theory (DFT) and time-dependent DFT (TD-DFT) show how end-group engineering, frontier orbital distribution, and molecule geometry in NFAs improve charge mobility, exciton separation, and light absorption. Additionally, theoretical models demonstrate how important molecular planarity, π–π stacking, and dipole moments are in controlling donor–acceptor interfacial energetics and blend morphogenesis. When taken as a whole, these computational insights offer a basic framework for the logical development of next-generation acceptors targeted at increased photostability, lower energy losses, and higher power conversion efficiencies in OPVs.

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1. Introduction

Humanity has historically relied extensively on a range of conventional energy sources, such as coal, natural gas, fossil fuels, agricultural waste, and many more. Long-term use of these finite restricted energy reserves has resulted in a number of environmental risks, including but not inadequate to air pollution, water pollution, climate change, and a dangerous effect on biodiversity. Renewable energy sources, which are sustainable and ecologically benign, are therefore desired.[1] However, to lessen the usage of fossil fuels, interest in renewable energy resources has been rising due to their finite obtainability and growing awareness of the results of CO_2 and other greenhouse gas emissions. The world's energy use is likely to increase from about 17 TW in 2010 to about 27 TW by 2040, with developing countries making up the majority of this demand.[2] Renewable energy has numerous advantages, but there are drawbacks to its use. The initial expense of creating and implementing renewable energy technology is one of the biggest obstacles, as it may be more expensive than nonrenewable sources in the short run. However, because renewable energy sources don't need to constantly buy fuel, their long-term costs are frequently lower. Additionally, as technology improvements and economies of scale are realized, their costs are probably going to go down.[3]

Solar energy, which covers 0.1% of the planet's surface with 10% solar conversion equipment enough to power the entire world, is one of the most attractive options, though terribly underutilized, another energy sources. One of the main ways to collect and transform solar energy is sunlight conversion into electricity by photovoltaic (PV) cells, commonly known as solar cells. Despite recent growth of 35–40% annually, this type of solar electricity only made up less than 0.1% of the world's electricity.[4,5] Organic solar cells (OSCs), which incorporate the use of solar energy, electronics, and flexibility, have therefore piqued the interest of academics with expertise in chemistry, physics, materials science, and even engineering. Thanks to interdisciplinary cooperation, OSCs have advanced rapidly in recent years and now have a power conversion efficiency (PCE) of 18%.[6,7] Additionally, OPVs may be made on plastic substrates, have tandem architectures, are lightweight, and are flexible enough to fit the human body for possible use in consumer electronics. OPVs can be included into construction elements for a range of uses since they can also be transparent or color-tunable.[8]

Fig. 1 illustrates the rapid evolution of power conversion efficiency (%) for Polymer Solar Cells (PSCs) from 2000 to 2025. It specifically highlights how non-fullerene OSCs (NFA) have significantly outperformed fullerene-based PSCs (FA) since their emergence around 2014, reaching efficiencies of 20%.

Open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF) are the three key factors that define the PCE of OSCs. Many studies concentrated on finding optimum donors and acceptors with suitable energy level alignments to enhance the OSC performance. Fullerene derivatives like $PC_{61}BM$, $PC_{71}BM$, and ICBA are widely implemented as electron acceptors for their high electron mobility. But a more effective technique to improve OSC performance has been made possible by non-fullerene acceptors (NFAs) with customizable structures and broader, stronger absorption.[18] One of the key factors influencing the commercialization of OPV cells is power conversion efficiency. The PCE of OPV cells has improved in recent years as result of the introduction of novel materials. For example, fullerene acceptors' dominant position was altered by the introduction of non-fullerene acceptors (NFAs) like ITIC in 2015 because to their higher photovoltaic performance.[19,20] PCEs of about 15% have resulted from further optimization of this type of NFA.[21] However, according to a thorough investigation of the optimal PCE under a set of plausible assumptions, Brabec and colleagues' theoretical computation indicates that a PCE of 19% might be realized.[22] This suggests that OSCs have a lot of potential for the future, giving researchers a lot of space to work. A PCE of 15% was seen to be a fair goal for OSCs recently. The elements limiting the device efficiency in OSCs must be found in order to exceed this goal.[23]

It can be concluded that choosing high-performance acceptor materials is the key to resolving the OSC performance issue since it is essential to improving OSC performance.[24] The stability and PCE of OSCs can be greatly increased by high-performance acceptor materials, which enhances overall performance and makes it possible to develop OSCs over time. It is therefore crucial to do studies on high-performance acceptor materials for organic solar cells (OSCs).[25] Fullerenes are the favored acceptors in polymer-fullerene systems, which have attained high PCE in OPVs. Due to high costs, poor light absorption, narrow bandgaps, and restricted tunability, progress has stagnated. Additionally, fullerene nanoparticles move and agglomerate, reducing device lifetime and efficiency.[26] The creation of unique non-fullerene acceptors (NFAs) is a more dynamic and modular strategy to further improve OPV device

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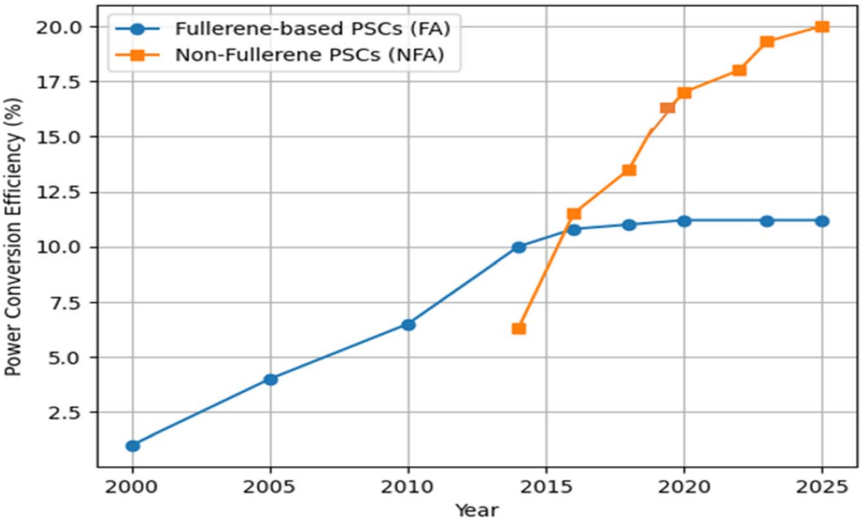


Fig. 1 Shows record PCEs of organic solar cells (OSCs) reported between 2000 and 2025 for fullerene acceptor (FA) and non-fullerene acceptor (NFA) systems. While FA-based devices show steady progress, NFAs exhibit a rapid efficiency surge, surpassing FA performance and approaching ~20% by 2025 [based on the work reported in ref. 8–17].

performance. Additionally, they should exhibit easier synthesis, better solubility, higher optical absorptivity, and a structural flexibility that permits donor and acceptor materials' frontier energy levels to match favorably.[27]

The comparatively reduced stability of the device is one of the primary obstacles to its eventual commercialization, despite the fact that OSCs showed significant potential from the PCE perspective.[28] OSCs experience degradations brought on by several circumstances, and their operational performance can rapidly decline.[29] It is still very difficult to achieve long-term stability in OSCs. As a result, stability in OSCs has attracted a lot of scientific interest recently.[30] The following functional layers can be used to categorize the several strategies that have been suggested in recent years to increase the stability of OSCs: (1) creating new photoactive materials, adding third components, employing solid additives, and implementing layer-by-layer (LBL) production techniques for the active layers. (2) Modifying the widely used HTL/ETL materials and creating more sophisticated ones for the interlayers. (3) For the electrodes: identifying more flexible and stable materials. (4) Creating hermetic and flexible encapsulation materials for full-stack devices.[31]

The potential of organic photovoltaic cells to be used in special applications such as wearable electronics,[32] portable energy sources in underdeveloped nations,[33] prosthetic retinas, and power-generating polarizing filters[34] is frequently mentioned. Rather than utility-scale power generation, many of these applications are explicitly geared toward the consumer market. It may be more crucial to reduce environmental impact than to enhance the lifespan or even performance of some devices for some applications, given the speed at which once-state-of-the-art consumer electronic devices are being replaced by new models.[35] Some of the different applications of OSCs illustrated in Fig. 2.

This review's main goal is to compile and evaluate the theoretical knowledge of fullerene and non-fullerene acceptors (NFAs) that has developed in the field of organic photovoltaics (OPVs) over the previous 20 years. Theoretical research has become crucial for revealing the principles governing device behavior as OPV efficiency and stability depend more and more on the delicate connections between molecule structure, electrical characteristics, and intermolecular interactions.

The target of this paper is to present a theoretical foundation that clarifies how acceptor materials affect important processes in bulk-heterojunction structures, including light absorption, exciton diffusion, charge transfer, charge separation, and charge transport. Comparing the unique electrical properties of fullerene acceptors with the quickly growing class of NFAs is one of the main goals of this investigation. Due to their advantageous electron mobility and isotropic charge transport, fullerenes have historically dominated OPV research; however, their limited absorption, high cost, and limited tunability have

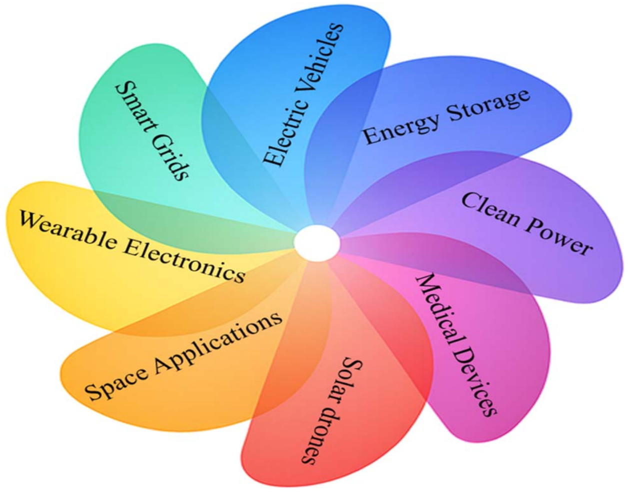


Fig. 2 Different applications of OSCs.

spurred the move toward non-fullerene systems. This review demonstrates how molecular design strategies in NFAs result in improved light harvesting, optimized energy level alignment, stronger intermolecular interactions, and lower voltage losses by compiling and interpreting theoretical studies.

This review's ultimate goal is to help researchers comprehend how theoretical tools can speed up the creation of next-generation acceptor materials. This paper seeks to help the logical development of highly efficient, stable, and economical OPV systems by connecting theoretical predictions with experimentally observed trends. This thorough theoretical approach will assist in identifying information gaps, elucidating the links between structure and property, and outlining viable directions for acceptor engineering in the future.

2. Background

OPVs had low PCE from the start because they were straightforward, single-layer devices (Fig. 3a) made up of a Schottky diode design, a pristine polymer, and two electrodes.[36] A double-layer structure composed of n-type perylene diimide derivative and p-type copper phthalocyanine served as its foundation (Fig. 3b).[37] Yu *et al.* presented bulk heterojunction (BHJ) OSCs in 1995 in which the donor and acceptor were stacked together to create the active layer. Device performance was greatly improved by the improved D/A interface and decreased the distance needed for exciton separation of the BHJ construction (Fig. 3c).[38] The PCE of BHJ OSCs has grown to 18% since the modification of the BHJ structure, thus counted as an OSC novel discovery. For this reason, BHJ OSCs are a feasible PV technology.[39]

In recent decades, major efforts have been undertaken to produce π-conjugated polymers for usage as p-type and n-type (*i.e.*, donor and acceptor) semiconducting materials to improve the performance of organic photovoltaics (OPVs).[41,42] PCEs greater than 18% have been observed in OPVs using π-conjugated polymers as the electron donor[43,44] due to the replacement of non-fullerene acceptors for fullerene acceptors.[45] One of the processes necessary for OSCs, organic light-emitting diodes, and organic thin-film transistors to function is the active layer's ability to transmit created or injected charges, either holes or electrons. This process often hinders their performance. The molecular and chemical makeup of the material's components,[46] defects and impurities in the active layer that may serve as charge-trapping sites and decrease carrier mobility,[47] and the molecular packing in solid states[48–50] are some of the factors that affect charge-carrier mobility, or the speed at which charges travel throughout a material.

2.1. Working principle of OPVs

Generally speaking, an OPV gadget operates in four main processes. Excitons are first created when photons are absorbed. After then, these excitons split and diffuse at the donor/acceptor (D/A) material interface. Following the exciton splitting, the charges are then moved throughout the apparatus. Ultimately, the charges are gathered and added to the solar cell's total output.[51] Energies of photon equivalent to or elevated than the bandgap of the blended materials are captured by an OPV when it is exposed to light. When an absorbed photon activates the electron D polymer in the energetic region of OPV devices, the excitation process starts.[52] To go from a material's occupied molecular orbital (HOMO) to its unoccupied molecular orbital (LUMO), an electron must cross the bandgap, an energy difference.[53] For the separation of excitons, where a significant potential energy difference exists, the carriers must go to the interface amongst the D and A materials. Nonetheless, the diffusion lengths of excitons in most conjugated polymers, which are typically between 5 and 20 nm, are shorter than the optical absorption route, which is roughly 200 nm. Therefore, in order to produce charges effectively, excitons must be made within their diffusion length.[54,55] Transferring these charges to the appropriate electrodes is a critical next step after creating free charge carriers, as presented in Fig. 4.[56]

Electrons from the absorber layer are injected by the ETL. Electrons pass through the materials that conduct electrons throughout this process before being gathered by the electrode. Additionally, by lowering series resistances, the ETL can improve the device efficiency and charge collecting efficiency.[57,58] The loss of photogenerated current may potentially have an impact on the OPV's performance. The absorber layer's

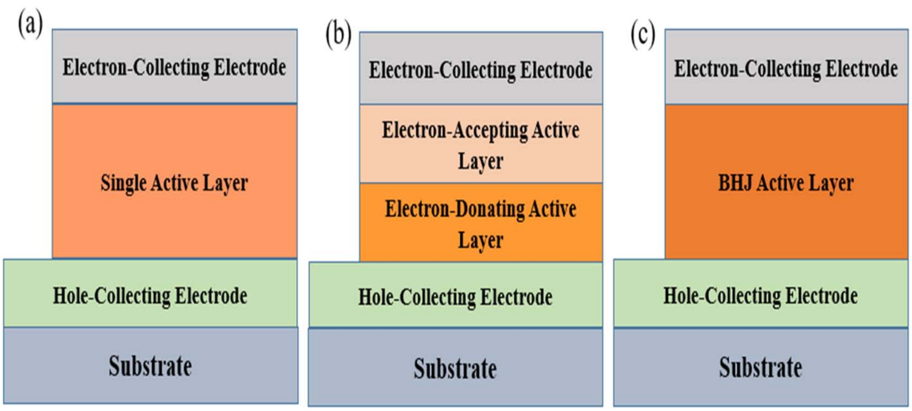


Fig. 3 Schematic representations of OSCs with (a) single active layer, (b) bilayer heterojunction, and (c) bulk heterojunction structures are displayed. Redrawn and modified from ref. 40.

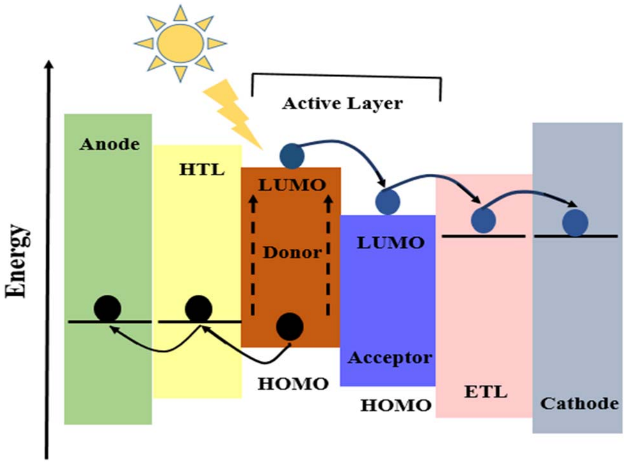


Fig. 4 Diagrammatic depiction of the energy levels in OPV that involve photon conversion to photocurrent. Redrawn and modified from ref. 56 with permission from Wiley-VCH GmbH, © 2024.

thickness affects the channel available for photogenerated electrons and holes, which is linked to this loss. Increasing the thickness rises the possibility of charge carrier recombination, which significantly lessens the device's total performance. Therefore, it may be inferred that device performance can be enhanced by improving parameters associated to light absorption, exciton dissociation, charge transit, and charge collecting.[59] OPV performance is also greatly influenced by interface layers (HTL and ETL) and photoactive organic semiconductor materials. This is due to the fact that light-induced charge injection in the cells mainly depend on the physical and chemical characteristics of interface, which influence the energy level among metal contacts and organic semiconductors in line with the purported ripple effect created by means of molecular orbital energy levels.[60]

OPV devices are made up of multiple layers (Fig. 5). A translucent conductor that works as an anode is placed over a clear substrate, like a glass or plastic plate, in standard configuration (Fig. 5a). In a similar vein, an electron passage buffer layer by the back of the active medium serves the cooperative role, proceeded by the (light reflected) cathode. Because the electron-transport layer metals in this design are frequently extremely reactive, which can cause the device to deteriorate, inverted designs (Fig. 5b) with reversed electrodes and other buffer layers have been employed. It is also possible to make even greater OPV efficiencies by making tandem solar cells using several active layers with various bandgaps, to broaden light absorption across the solar spectrum (Fig. 5c).[61]

Due to their increased stability even in the absence of encapsulation, inverted OPV cells (i-OPV) typically do not disintegrate for several days, they have drawn particular interest. Additionally, because of their superior chemical and physical characteristics over the organic interface layer, metal oxides are the materials of choice for the interface layer in i-OPV[62] (Table 1).

Theoretically, depending on the assumptions, the efficacy of only heterojunction OSC is expected to be between 10% and 11%, or nearly the values believed to be needed for large uses. To address the drawbacks of single heterojunction solar cells, which may have an efficiency of about 15%, tandem techniques are required.[70,71]

2.2. Electron acceptors

Fullerenes are spherical molecules with a conjugated π-system consisting of fused pentagons and hexagons; the smallest and most prevalent example of an I_h-symmetric molecule is C_{60}. Despite having over 12 500 potential Kekulé structures, indicating an aromatic nature, C_{60}'s sp^2 network is devoid of hydrogen-saturated barriers. As a result, normal aromatic

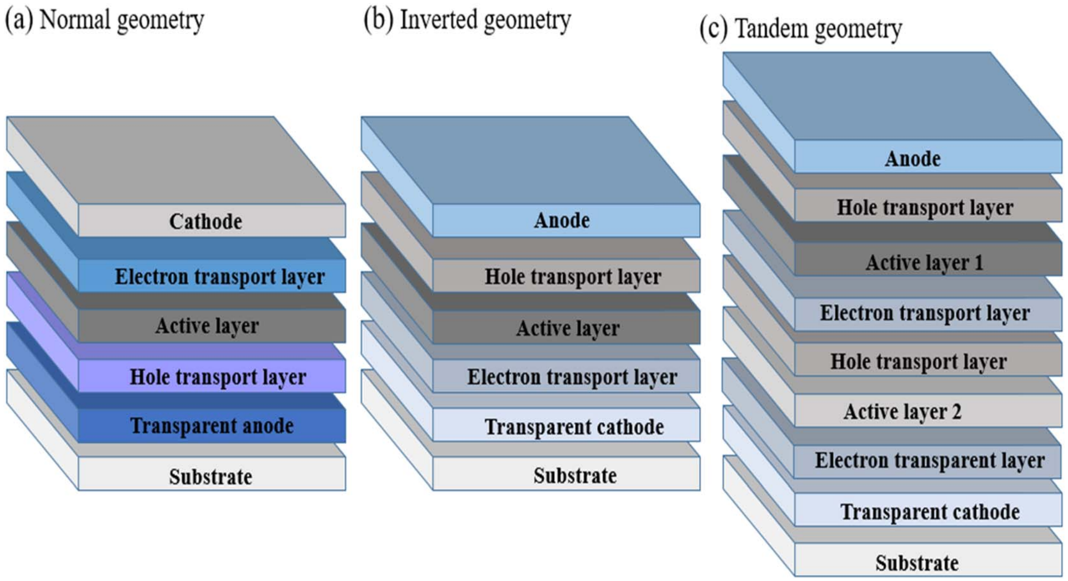


Fig. 5 OPV device common layer structure schematics in (a) normal, (b) inverted, and (c) tandem geometries. Redrawn and modified from ref. 61 with the permission of the author, Darling SB.

Table 1 Summary comparison of OPV cell device structures

Structure	Benefits	Weaknesses	Major property	References
Single layer	• The structure of the device might be made simpler • Lower production costs	• Inadequate mobility of charge carriers • Reduced effectiveness	Most basic OPVs are composed of a single organic layer with an active light-capturing and power-generating system	63 and 64
Bi-layer	• More light absorption than a single layer • Higher efficiency when compared to OPV with a single layer	• Low carrier mobility in comparison • More intricate device architecture than single layer OPV	Two organic semiconductor layers are positioned between two electrodes to form bilayer OPVs, a kind of thin-film solar cell. Usually, there are two layers: an electron-accepting (n-type) layer and an electron-donating (p-type) layer	65
Bulk hetero-junction	• Exciton dissociation is efficient because of the large contact area • Increased charge mobility over bilayer • Outstanding flexibility and efficiency	• Possibility of bi-molecular recombination losses • The comparatively low device efficiencies that have been shown thus far	Spin coating is typically used to apply a network of materials that are both electron donors and acceptors	66 and 67
Tandem	• Increase the solar cell's absorption in various sun spectrum regions • By stacking sub-cells with complimentary absorption spectra, efficiency is increased	• More intricate fabrication-related device architecture • Possible problems with sub-cell current matching	A set of two or more sub-cells with altered bandgaps are used to absorb different bands of the light spectrum	68 and 69

substitution processes cannot take place while the conjugated π-system of the fullerene is retained.[72] Fullerenes are carbon molecules and their bond structures are exactly the planar cubic graphs that have only pentagon and hexagon faces (Fig. 6).[73]

The icosahedral symmetry sealed cage structure of fullerenes is based on twenty hexagonal and twelve pentagonal rings. Through sp^2 hybridization, each carbon atom is joined to three further atoms. Two bond lengths are present in the C_{60} molecule. The 6 : 6 ring bonds are referred to as "double bonds" since they are reduced compared to the 6 : 5 bonds. Since it has susceptibility to prevent double bonds in the pentagonal rings, C_{60} exhibits weak electron delocalization and is not "Highly aromatic". Therefore, C_{60} functions as an electron-lacking alkene and interacts with electron-abundant species. The structure's geodesic and electronic bonding features account for the molecule's stability. Theoretically, there might be an endless number of fullerenes with structures based on hexagonal and pentagonal rings that are built in accordance with icosahedra laws.[74] The most prevalent fullerene in the fullerene family, C_{60}, was described by Krätschmer *et al.* utilizing electron and X-ray diffraction, mass spectroscopy, and infrared (IR) spectroscopy. The most prevalent fullerene in the fullerene family, C_{60} was described where structures and properties of fullerenes, carbon nanotubes, and graphene were discussed in detail to uderstand much about fullerenes particularly.[75] Fullerenes have garnered significant emphasis as fundamental constituents to create supramolecular architectures and purposeful micro/nanostructures at various scales beneath controlled production due to their distinctive architectures, strong electron-transporting properties, and superior electron-accepting capacity. Moreover, a unique approach that combines other moieties, such as metal-porphyrins and carbon nanotubes (CNTs) with fullerene, has produced several beneficial hybrids or composites.[76] Table 2 describes the various forms of fullerene.

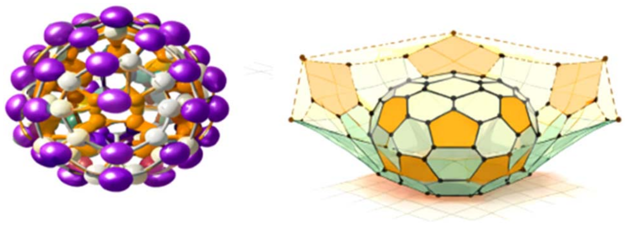


Fig. 6 C_{60} fullerene's structural illustration displaying its delocalized π-electron cloud and curvature created by fusing hexagons and pentagons. Redrawn and modified from ref. 73 with the permission of the author Schwerdtfeger P whose article is available under CC BY-NC-ND for non-commercial use and has properly cited © 2014 The Authors. *WIREs Computational Molecular Science* published by John Wiley & Sons, Ltd.

The conservative reasons for the benefits of fullerene derivatives as electron acceptors are strong, but they fail to take into consideration the lack of practical substitutes. The simplicity of electron acceptance may certainly be equaled by other

Table 2 Types of fullerene

Types	Description	Application	References
Buckyball clusters	Although C_{20} is the smallest member of buckyball clusters, C_{60} is the most prevalent buckyball. Other atoms may become trapped inside this hollow structure	Their spherical form makes them excellent lubricants Their hollow nature is helpful for administering medication	73
Nanotubes	Nanotubes are quite tiny. These have one or more borders and are hollow from the inside like a tube	Electronic industries are the primary users of nanotubes	75
Megatubes	The diameter of megatubes is greater than that of nanotubes. They have different-sized walls	The primary purpose of megatubes is to move molecules of various sizes	77
Polymers	High temperatures and high pressures cause the formation of polymers. These can have a variety of shapes, including two-dimensional, three-dimensional, and one-dimensional chains	Uses a variety of industries, including toys, construction, aerospace, plastics, textiles, packaging, stationery, and rope	78
Nano-onions	The shape of nano-onions is spherical. They are composed of several layers of carbon with a buckyball core in between	Nano-onions are used as effective lubricants	79

compounds with similar more electron affinity,[80] and good electron mobility[81] is not unparalleled.[82] With the correct processing additives, fullerene derivatives can also produce a good nanoscale architecture with donor and acceptor regions that are comparable in dimension to the exciton diffusion length.[83] The features of fullerene derivatives may also benefit from their capacity to enable electron transport in three dimensions, as opposed to two or one like most compounds or polymers. In an attempt to increase the group of acceptors, numerous synthetic groups are developing another electron acceptor materials (both polymeric and molecular) under these guidelines.[80,84] Some of the shortcomings of fullerene derivatives, for instance very little light absorption[85] and the very high cost of the most effective derivatives,[86] can be resolved by exploring further fullerene derivatives, which will instantly increase the variety of mixtures that can be considered. However, the limitations of fullerenes, such as their rigid energy levels, limited optical captivation (producing efficiencies of around 11–12%), and difficulty in altering the chemical structure, have prompted the research community to develop alternative non-fullerene electron acceptors (NFAs) recently.[87]

In the area of organic OPVs, non-fullerene acceptor molecules (NFAs) are a new family of materials that garnered a considerable attention.[88,89] These compounds are intended to get around some of the drawbacks of fullerene acceptors, which have major OSC investigation for many years. The ability of NFAs to captivate a extensive range of the sunlight spectrum and their customizable chemical architectures are what define them. In order to enable effective electron acceptance and transport, these compounds usually made of conjugated systems with sturdy electron-withdrawing groups.[90,91] OSC performance has markedly improved due to the creation of NFAs, including increased power conversion efficiency, stability, and scalability. Device efficiency and operational longevity are further improved by these materials' capacity to produce advantageous structure and phase separation with donor polymers. Numerous problems, including as the interface, scanty molecular packing, interlayer's strong reactivity with the active layers, and the reaction amongst photoactive materials and oxygen (*via* photooxidation), adversely affect the constancy of NFA-created OSCs. Due to these concerns, new techniques have been devised to expand the stability of the interlayer, optimize the symmetry, planarity, crystallinity, and side chain structure of NFAs, and produce more photochemically stable materials.[92,93] NFA-based OSCs are less affected by moisture-induced chemical breakdown processes than Perovskite Solar Cells (PSCs). Because perovskites include hygroscopic ammonium and Pb(II) salts, they become unstable when exposed to moisture. Therefore, in order to prolong the device's life and boost its economic viability, higher encapsulation process costs are implied.[94] A–D–A type acceptors, such as ITIC, Y6, and their derivatives or analogues, are the most effective NFAs in terms of chemical structures; "D" and "A" denote the electron-donating (D) and electron-receiving (A) moieties in an identical compound. PCEs of 15–19% for Y6 and its derivatives[99–101] and 9–16% for ITIC and its equivalent[95–98] have now been achieved. The predominant portion of polycyclic acceptors have difficult processes of synthesis, low reaction yields, and expensive making costs despite their exceptional characteristics and device performances, which will severely restrict the use of OSCs in the future.[102] To solve this issue, formation of non-fused ring electron acceptors (NFREAs) generated considerable attention. For their straightforward synthesis procedure and typically high yields, NFREAs can be significantly less expensive than fused-ring NFAs.[103,104] Nevertheless, the conjugated backbones of NFREAs are united by C–C single bonds, which are detrimental to the formation of planar and competent conjugated structures, in contrast to fused-ring acceptors with stiff and planar configurations. Consequently, the twisted conformation between neighboring units will prevent π-electrons from delocalizing, which is undesirable to intramolecular charge transfer (ICT). The fragile molecular conformations of NFREAs will also have an impact on effective molecular packing. As a result, NFREA-based devices have significantly lower PCEs, particularly at first. Researchers have established a variety of molecular design schemes to report the unstable conformation problem of NFREAs.[105–107] Because of the steric effect, bulky side chains like alkylbenzene, diarylamine, 2,4,6-triisopropyl benzene, *etc.*, can be added to provide a constant conformation.[108] Recently, OSCs based on NFREA have shown notable advances due to careful molecular design.[108,109]

2.3. Importance of theoretical studies in OSC acceptor design

While bulk heterojunction (BHJ)-type organic solar cells (OSCs) and dye-sensitized solar cells (DSSCs) are two new solar systems with unique design and operating processes, both rely significantly on accurate optoelectronic property characterization to attain maximum performance. For instance, the energy level alignment at the donor–acceptor interface enables effectual exciton dissociation and charge separation in BHJ-based OSCs.[110,111] Theoretical approaches offer a molecular-level framework for investigating the intrinsic properties of organic materials as well as their intermolecular interactions.[112] Density functional theory (DFT), one of these methods, has become a potent and economical tool for directing the formation of OPVs by allowing the methodical assessment of important parameters that are frequently challenging to obtain experimentally.[113–116] The energy conversion efficiency of photovoltaic systems is directly impacted by frontier molecule orbital energies, band gaps, and light absorption characteristics, all of which may be accurately predicted using DFT calculations.[111,117] DFT offers important understandings into the structure–property connections that control device performance by linking molecular arrangement with electronic characteristics including HOMO and LUMO energy levels.[118,119] Excitation energies, oscillator strengths, and absorption spectra are examples of excited-state parameters that can be analyzed in conjunction with time-dependent DFT (TDDFT), offering atomistic insight into the optical behavior of organic semiconductors.[120,121] The innovation cycle in organic photovoltaic research is accelerated by these theoretical insights, which allow the logical screening and selection of prospective donor and acceptor materials.[122] Conventional DFT and TDDFT techniques have intrinsic limitations despite their extensive success, especially when it comes to describing charge-transfer excited states that are frequent in OSCs. Advanced exchange–correlation functionals have been developed as a result.[123,124]

Since not all functionals include necessary effects, such extended ones, choosing the right functional is crucial for precisely capturing particular system attributes. For example, despite their popularity, hybrid functionals frequently fail to appropriately characterize extended impacts, which are important for precisely modeling the usual charge-transfer excited states of OSCs.[125–127] The so-called hybrid exchange–correlation functionals, such as B3LYP, B3PW91, and PBE0, which combine DFT exchange–correlation with Hartree–Fock exchange, have generally been demonstrated to provide qualitative accuracy in electronic structure modeling. Nevertheless, because these functionals lack corrected extended changes, that are crucial for examining the charge transfer excited states, they are still unsuitable for modeling the physical features of the system.[117,128] For a more realistic representation of excited-state characteristics in organic photovoltaic materials, extended corrected functionals like CAM-B3LYP have proven crucial.[129] Appropriate basis-set selection also contributes to the balance between accuracy and processing cost. For the investigation of the ground- and excited-state characteristics of organic semiconductors, polarized basis sets in particular, 6-31G (d) have been extensively used and verified.[117] All things considered, molecular modeling techniques, particularly DFT-based approaches, are an essential supplement to experimental research because they offer precise, predictive insights that direct material design. Theoretical research helps reduce development costs, shorten material optimization cycles, and make it easier to build high-performance donor–acceptor systems for next-generation organic photovoltaic devices by minimizing reliance on trial-and-error synthesis.[130–132]

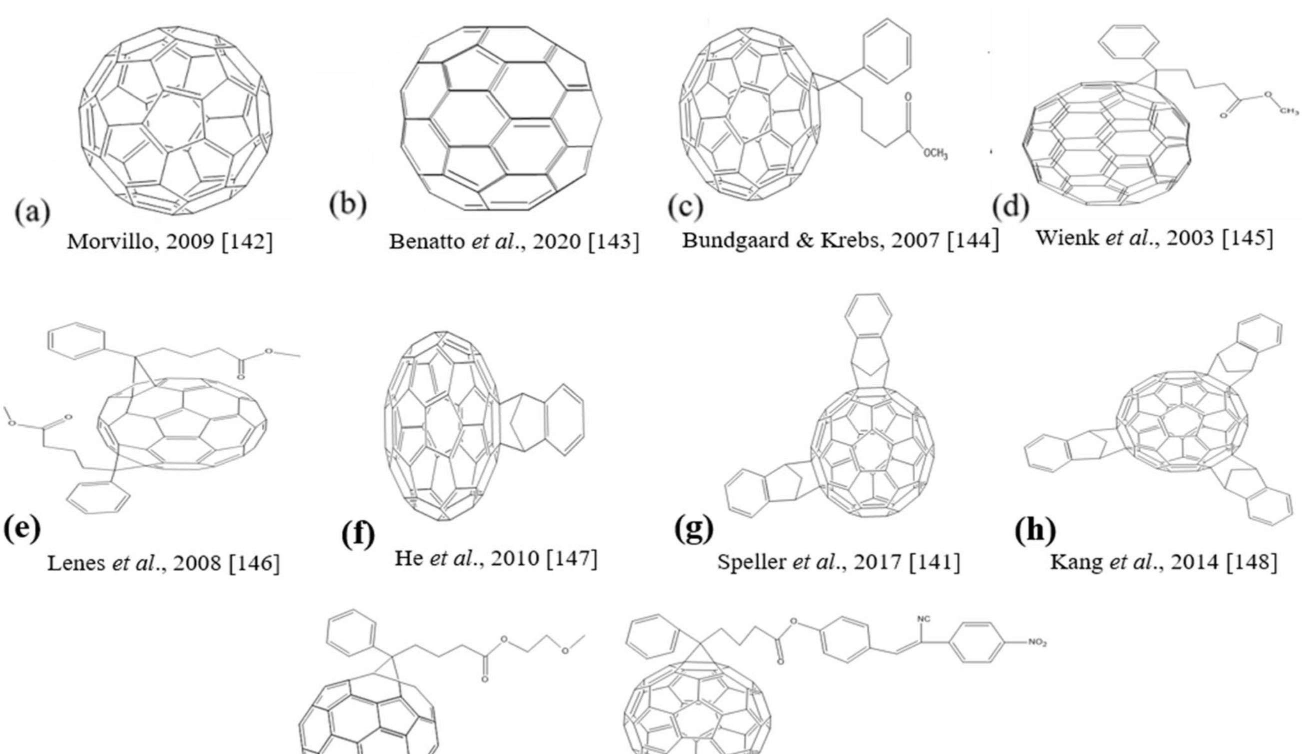
3. Fullerene acceptors

3.1. Structure and properties

In 1995, fullerenes and their derivatives were formally introduced into OPV applications. In fewer than ten years, fullerene derivatives with novel features were developed for molecular electronics and perovskite solar cells, which are currently in dire need of them. Therefore, novel device production of fullerene derivatives and organization methodologies must be investigated.[133] Carbon nanotubes (CNTs) and organic semiconducting molecules can be added to lithium-ion inner surface fullerenes to improve stability and PCE.[134] Two unique solvable bis(pyrrolidino)[60]fullerenes with lower electron affinities than regular fullerenes were created by Mumyatov *et al.* As a result, they can suppress the photooxidation of conjugated polymers and raise the open-circuit voltage by around 200 mV. Research on long-lasting and highly effective organic photovoltaic systems may benefit from these characteristics.[135] Additionally, the researchers learned that pyrrolidino[2,1-*a*]phthalazino[60]fullerenes are favorable organic electronic engineering and photovoltaics due to their tunable optoelectronic features and ease of preparation. They have a PCE of over 14% when utilized as electron-transport materials, and the processes engaged offer an entirely fresh concept for the successive synthesis of greater range of fullerene derivatives.[136] Fullerenes and their derivatives are important for ternary OSCs in addition to being used to increase the effectiveness of optical devices. Because they offer the best light-absorbing and electron-accepting qualities, ternary OSCs are frequently utilized as materials for PVs and photo detectors. They are created by blending donor polymers with various fullerene acceptor combinations.[137] The photostability of NFAs and conjugated polymers can be improved by fullerene-derived acceptors in ternary mixes with specifically created topologies.[138] Because they can increase PCE and change the blend geometry as the third component of OSCs, fullerene derivatives are perfect matter for effective OSCs which can be made through accurately changing the structural features. $IC_{60}BA$, a type of fullerene substitute, can be introduced to the PTZ1:IDIC hybrid system to enhance its photovoltaic performance and active layer shape.[139]

Early on, OSCs had very low power conversion efficiency (PCE). For example, in 1993, the PCE of OSCs dependent on fullerene was approximately 0.04%.[129] After C_{60}, C_{70}, which has 70C atoms, is the next most well-known fullerene. Only one configuration of each of the C_{60} and C_{70} molecules complies with the isolated pentagon rule. The number of C atoms in fullerenes can vary from 20 to thousands. Generally referred to as "buckyballs," those with fewer than 300C atoms are restricted to single-shell structures.[140] C_{60} fullerene[141,142] and C_{70} fullerene[143] derivatives are commonly used electron acceptors in organic solar cells. Phenyl-C_{61}-butyric acid methyl ester ($PC_{61}BM$)[144] is the most widely utilized acceptor, while $PC_{71}BM$[145] contains a C_{70} fullerene. It demonstrated that the bisadduct isomer mixture, which is devoid of monoadducts and higher adducts, can be utilized without the need for additional isomer separation leading to a better cell performance than PCBM.[146] Indene-C_{60} bisadduct (ICBA), a novel soluble C_{60} derivative, has a LUMO energy level that is 0.17 eV greater than PCBM.[147] Changes in charge mobility, optical characteristics, and miscibility with electron donating polymers were brought about by the fullerene multiadducts in the mixture, which altered the blend's morphology. At the same time, because of the high LUMO level, they usually raised the V_{oc} value.[148] Zhao and colleagues examined the impact of $PC_{61}BM$'s alkyl chain length on OSC performance; in their study, the alkyl chain length was altered by changing the carbon atoms from 3 to 7, which corresponded to F1 to F5. With a PCE of 3.7%, the OSC based on the P3HT:F1 system outperformed the P3HT:$PC_{61}BM$ system (3.5%).[149] When compared to $PC_{61}BM$, the LUMO energy level of modified fullerene F increased by 0.2 eV and demonstrated greater absorption.[150] Fig. 7 shows commonly used fullerene acceptors in OSCs.

In OSCs, materials that donate electrons include polymers, oligomers, and small molecules. These materials span distinct length scales and belong to different classes, but their basic properties are the same. The ideal electron donating material would have strong, broad absorption across the solar spectrum, high hole mobility for efficient and rapid charge transport, energy levels that correspond most closely to and combine with the energy levels of the electron acceptor for fast charge transfer, and appropriate miscibility with the electron acceptor in order to produce the expected nanoscale patterns. Numerous



(a) Morvillo, 2009 [142]
(b) Benatto *et al.*, 2020 [143]
(c) Bundgaard & Krebs, 2007 [144]
(d) Wienk *et al.*, 2003 [145]
(e) Lenes *et al.*, 2008 [146]
(f) He *et al.*, 2010 [147]
(g) Speller *et al.*, 2017 [141]
(h) Kang *et al.*, 2014 [148]
(i) Zhao *et al.*, 2010 [149]
(j) Li *et al.*, 2022 [150]

Fig. 7 Fullerene and typical fullerene electron acceptor chemical structures. (a) C_{60} fullerene; (b) C_{70} fullerene; (c) $PC_{61}BM$; (d) $PC_{71}BM$; (e) BisPCBM; (f) ICMA; (g) ICBA; (h) ICTA; (i) F1; (j) F. Redrawn and adapted conceptually from reference of each FAs.[141–150] design techniques have been created to give OSC devices good performance for new donors, such as alternating electron-rich and electron-poor groups and modifying the energy levels chemically (*e.g.*, by substituting fluorine).[151,152] A post-production treatment for plastic solar cell devices has been devised to significantly increase the power conversion efficiency of polymer solar cells. The properties of plastic solar cells based on poly(3-hexyl thiophene) (P3HT) as an electron donor material and [6,6]-phenyl C_{41}-butyric acid methyl ester (PCBM), a soluble C_{41} derivative, as an electron acceptor material can be enhanced by annealing the devices and concurrently applying an external voltage.[153]

Small molecules have a number of potential benefits over polymers that make them desirable materials, including a more adaptable molecular structure, simpler techniques for regulating energy levels and more repeatable synthetic processes that produce materials with greater purity.[154] Chen *et al.* created the D–A copolymer donor PTB7-Th[155] in 2013 using the 2D-BDT unit. PTB7-Th performed better than PTB7. PTB7-Th is the most extensively researched low-bandgap donor to date in OSCs, providing a 9.35% PCE.[156] For this, researchers have focused on creating organic compounds with specific geometries and electrical molecular properties in order to attain the necessary nonlinear optical qualities. Additionally, it has been noted from previously reported data that the necessary ground-state charge asymmetry is provided by D (donor) and A (acceptor) moieties.[157] One of the most effective polymer donors in BHJ solar cells containing fullerene acceptors, like phenyl-C_{61}-butyric acid methyl ester or its C_{71} analog (PCBM), is poly(benzo[1,2-*b*:4,5-*b*′] dithiophene-alt-thieno[3,4-*c*]-pyrrole-4,6-dione) (PBDTTPD). High open-circuit voltages >0.9 V, high fill-factors of around 70%, and power conversion efficiencies >8% are produced by conventional BHJ devices built of PBDTTPD and PCBM. It demonstrate how small modifications to the side-chain layout of PBDTTPD polymers influence the π-conjugated system's tendency to crystallize in the π-stacking direction and control the ordered crystallites' preferred orientation in thin films.[158] DRCN7T exhibits good film-forming qualities for solution processing, outstanding thermal stability, and high solubility in common solvents. OPVs with different donor/acceptor ratios, film thicknesses, annealing temperatures, and ETLs were created employing fullerene derivatives as the electron acceptor.

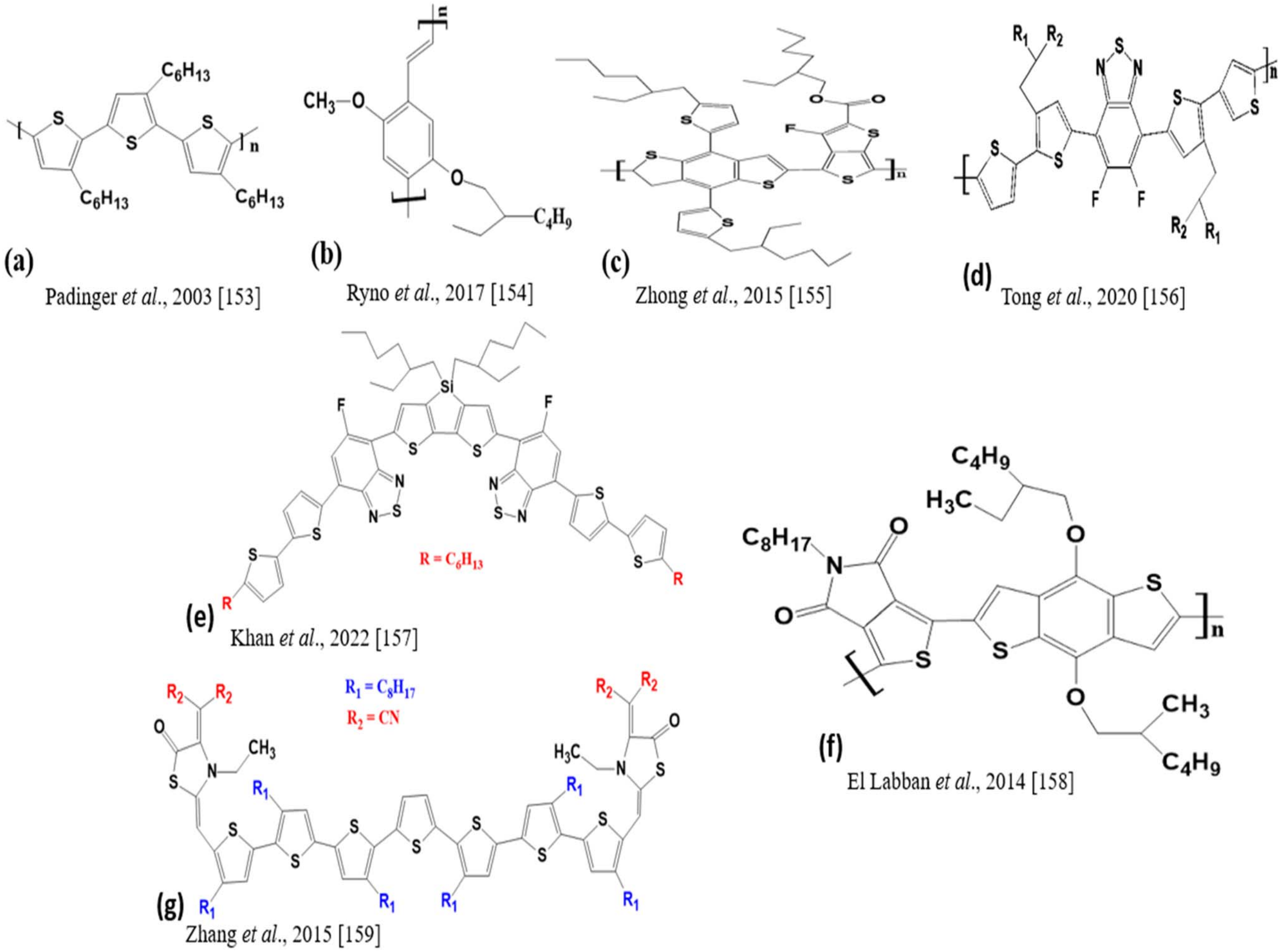


Fig. 8 Chemical architectures of small molecules and typical polymers that donate electrons. Structures: (a) P3HT; (b) MEH-PPV; (c) PTB7-Th; (d) PffBT4T-C_9C_{13}; (e) DTS($FBTTh_2$)$_2$; (f) PBDTTPD; (g) DRCN7T. Redrawn and adapted conceptually from reference from the reference of each electron donor.[153–159]

Table 3 Typical fullerene acceptor features and the associated performance of device[a]

Acceptor	HOMO/LUMO (eV)	Donor	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)	References
$PC_{71}BM$	—/—	MDMO-PPV	7.6	0.77	51	3.0	145
bis$PC_{61}BM$	−6.1/−3.7	P3HT	9.14	0.724	68	4.5	146
ICBA	—/−3.74	P3HT	9.67	0.84	67	5.44	147
F1	—/−3.91	P3HT	10.8	0.564	60.3	3.7	149
$PC_{61}BM$	—/—	P3HT	8.5	0.55	60	3.5	153
$PC_{61}BM$	—/—	MDMO-PPV	5.25	0.82	61	2.5	160
$PC_{61}BM$	—/—	P3HT	10.6	0.61	67.4	4.37	161
F	−5.90/−3.75	P3HT	10.3	0.81	63	5.25	162
$PC_{71}BM$	—/—	P3HT	12.2	0.61	55	4.1	163
$PC_{71}BM$	—/—	PTB7	14.5	0.74	68.97	7.40	164
$PC_{71}BM$	—/—	PffBT4T-2OD	18.2	0.77	74	10.4	165
ICBA	—/−3.74	P3HT	10.61	0.84	72.7	6.48	166
$IC_{70}BA$	−5.61/−3.72	P3HT	11.34	0.81	63	5.79	167
$IC_{70}BA$	—/−3.83	PTB7	15.4	0.79	55	6.67	168

[a] J_{sc} stands for short circuit current density, V_{oc} for open circuit voltage, FF for fill factor, PCE at 80 mW cm^{-2} under AM 1.5 lighting, CB for chlorobenzene, and DCB for 1,2-dichlorobenzene.

With $V_{oc} = 0.91$ V, $J_{sc} = 14.87$ mA cm^{-2}, and FF = 68.7%, a PCE of 9.30% (certified at 8.995%) was attained.[159] Fig. 8 illustrates various commonly used donor in OSCs.

Typical fullerene acceptors are matched with various donor materials in Table 3, which highlight their salient characteristics and associated device performance.

DFT and TD-DFT has been used to study the electrical and optical features of fullerene-acceptors utilized in organic photovoltaic devices. Roy *et al.* optimized the molecular geometries of C_{60} and C_{70} and evaluated frontier molecular orbital energies, including HOMO and LUMO levels, using DFT simulations. Bulk-heterojunction (BHJ) systems, where FD is the electron acceptor and poly(3-hexylthiophene) (P3HT), an ordinary photovoltaic polymer, as the donor material, are used to collect data from experiments for all solar cells.[169] GaussView 6.0 was used to sketch the molecular structures of FDs,[170] and Gaussian 16 software was used to optimize them using the semi-empirical PM6 method[171] (Fig. 9).

The trustworthiness of the PCE values was demonstrated by all ten FDs passing the Euclidean distance-based AD inquiry.

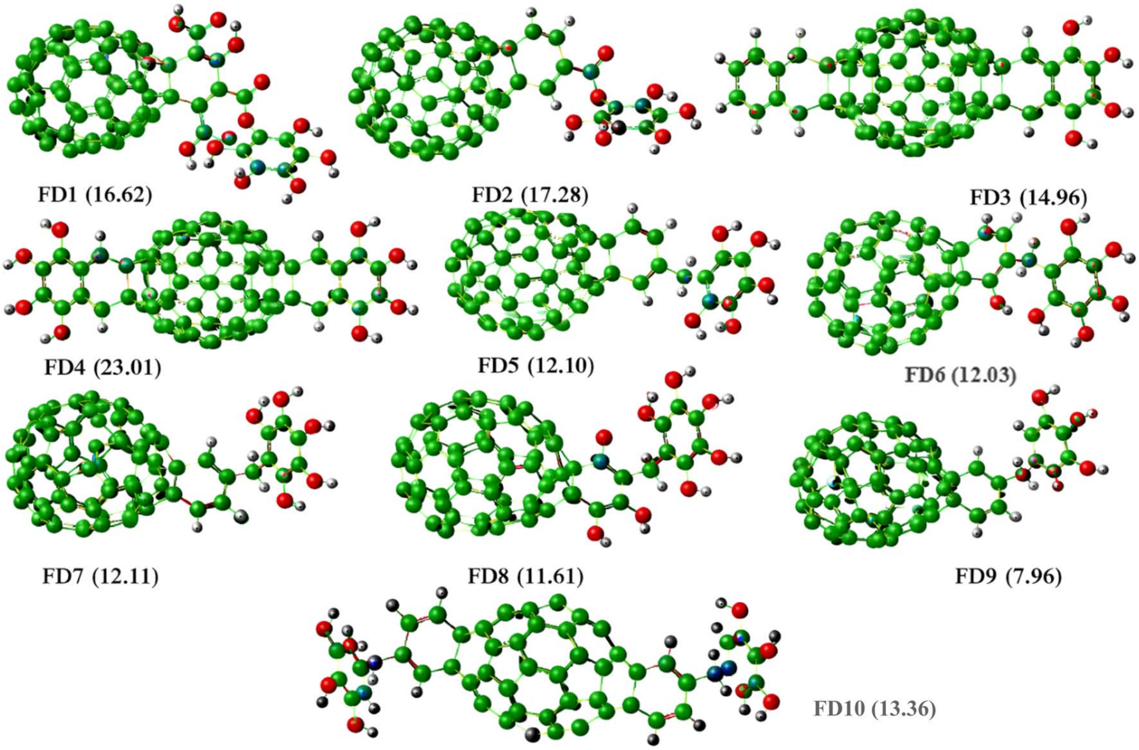


Fig. 9 Design of fullerene derivatives (FDs) as the primary acceptor molecule for polymer solar cells, values given in parentheses are %PCE. Modified from the ref. 169.

This qualifies them for further analysis to show their potential as efficient acceptors for PSCs based on fullerene in future. The forecasted PCE of FDs ranges from 7.96 to 23.01 when taking in account both C_{60} and C_{70} FDs. FD7, FD8, and FD9 are C_{70} FDs with PCE of between 7.96 and 12.11, whereas the other FDs are C_{60} FDs with PCE values between 12.03 and 23.01. Without a doubt, all results are positive and greater than any FD acceptor now in use for PSCs.[169]

3.2. Drawbacks of fullerene acceptors

Due to the obstacle of modification of their optical/electronic features, interest in fullerene-based acceptors has decreased. Although PCBM derivatives are commonly utilized, higher open-circuit voltages and efficiency frequently require lower electron-affinity acceptors[138] (Fig. 10).

Therefore, the hypothesis predicted that the performance of OSCs utilizing poly(3-hexylthiophene) (P3HT) would nearly double when fullerene derivatives with lower electron affinity were utilized as electron acceptor material.[172] Fullerene acceptors have been applied to create the most effective OSCs to date, but they have some disadvantages. First, very little sunlight is absorbed by fullerenes.[169,173] Second, fullerenes' overly strong electron affinity limits the OSC's open circuit voltage. Third, they are easily photo-oxidized, which substantially shortens the life of a solar cell. Furthermore, the synthesis of fullerene derivatives necessitates considerable energy consumption and costly solvents.[174] Pristine fullerenes did badly in OSCs because of their symmetrical shape, less solubility, absorption, and low lying LUMO levels. A decreased PCE results from pure fullerene's aggregation tendency, which is determined by its solubility and miscibility.[175,176] Under extreme photo-oxidation conditions, such as an oxygen-containing environment with UV radiation in ambient settings or argon laser light that resembles a section of the solar spectrum and resonates the polymer band gap, FTIR has shown that PCBM degrades.[177] This oxidation has been shown to degrade the photoconductivity of the mix film containing the fullerene cage.[178] The energy shift of a neutral atom upon obtaining an electron to form a negative ion affects the degree of light-induced oxidation of a polymer:fullerene hybrid, in addition to the electron affinity of the fullerene acceptor.[179] Since prior research has examined PCBM and other fullerene acceptors with greater LUMO levels but none with lower LUMO levels, it is expected that creating a fullerene acceptor with a lower LUMO level will improve the photochemical durability of the polymer.[141] Fig. 11 Comparison of the optical density loss per hour (%) for various polymer donors (PBDTTPD, P3HT, PBTTT, and MDMO-PPV) across a series of fullerene acceptors.

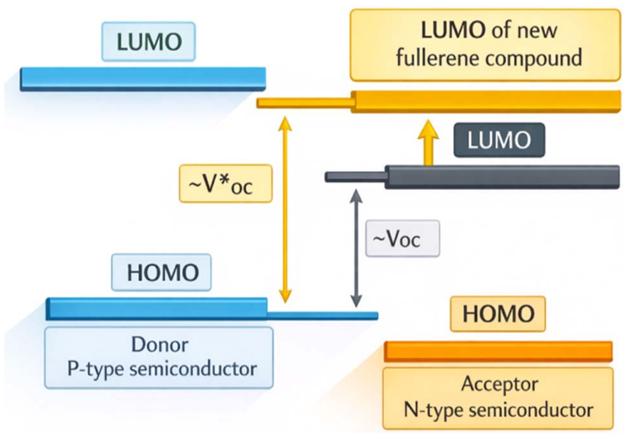


Fig. 10 Diagram illustrating the border orbitals of p-type and n-type semiconductor materials in a bulk heterojunction solar cell. It is demonstrated that V_{oc} increases as the fullerene derivative's LUMO energy increases. Redrawn and modified from ref. 138.

4. Non-fullerene acceptors

4.1. Structure and properties

The power conversion efficiency (PCE) of OSCs has increased to over 18% thanks to recent developments in nonfullerene acceptors paired with suitable polymer donors and utilized as the photoactive layer. This is comparable to commercial silicon-based solar cells, suggesting a promising future for OSCs' practical applications.[180] Both electron-rich and electron-deficient units often make up NFAs. The interaction between these units can change the shape of films, increase the light absorption, and vary the energy levels of acceptor materials. In the meanwhile, OSCs based on NFAs are consistently performing better.[181] NFAs have been extensively investigated for use by the general population due to their capacity to increase the absorption range, stability, and PCE of OSCs.[182] Among these, Y6, a NFA molecule, has progressively come to the attention and has previously made a significant contribution to many OSC sectors, allowing single-junction OSCs to reach efficacies of over 15%.[183] The two main approaches to obtaining successful NFAs are A–D–A type NFAs and imide-based NFAs. NFAs of the A–D–A type, which have a conjugated donor–acceptor structure, are the subject of this section. In the A–D–A type, "A" and "D" denote the electron-donating and electron-withdrawing functional groups. It is possible to lower bandgap and extend conjugation by linking electron-rich and electron-deficient moieties.[184] ITIC-Th is a member of a family of organic non-fullerene fused-ring electron acceptors that have recently greatly increased the efficiency of organic solar cells. Additionally, because of the well-matched energy levels, the passivation of defects, and the complementary absorption spectra, the presence of ITIC-Th in the perovskite thin film results in increased photocurrent and improved fill factor. This suggests a new path toward future high-efficiency solar cells integrating halide perovskite materials and organic non-fullerene acceptors into the same active layer.[185] The ideal polymer solar cell (PSC) of PBDB-T:IT-M under AM 1.5G, 100 mW cm^{-2} lighting produced a high PCE of 12.05%, a V_{oc} of 0.94 V, a short-circuit current (J_{sc}) of 17.40 mA cm^{-2}, and a fill factor (FF) of 0.735. A PBDB-T:IT-M-based PSC was forwarded to the National Institute of Metrology, China (NIM) for certification since PCE above 12% is the highest value for single-junction PSCs (certified cell area of 3.729 mm^2). To the best of our knowledge, this type of single-junction PSC has the highest certified PCE of 11.6% with a V_{oc}

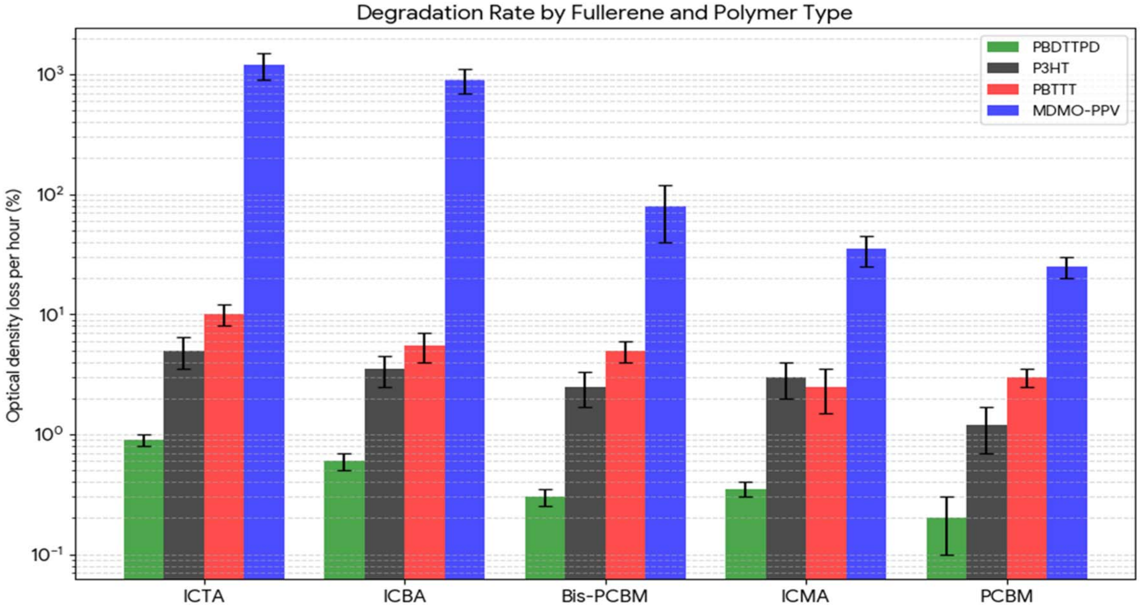


Fig. 11 The bar chart shows the degradation rates (optical density loss per hour) for four different polymers when mixed with various fullerene acceptors. PBDTTPD (green) consistently shows the highest stability, while MDMO-PPV (blue) exhibits the highest rate of degradation across all tested combinations. Adapted conceptually based on the work reported in ref. 179. With the permission of WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim Copyright © 2012.

of 0.92 V, a J_{sc} of 17.15 mA cm^{-2}, and an FF of 0.735.[186] For fullerene-free organic solar cells (OSCs), a novel polymer donor (PBDB-T-SF) and a novel small molecule acceptor (IT-4F) were created. The effects of fluorination on the donor and acceptor's charge mobilities, molecular energy levels, and absorption spectra were methodically investigated. The PBDB-T-SF:IT-4F-based OSC device demonstrated a record high efficiency of 13.1%, and a thickness of 100–200 nm can achieve an efficiency of over 12%, indicating the potential of fullerene-free OSCs in real-world applications.[187]

The optimization of the central core units, the electron-withdrawing terminal units, and the bridges between the core and terminal units increased the PCEs of the fused-ring core-based NFAs based on binary OSCs to more than 13%.[188] Based on indacenodithiophene, a planar fused-ring electron acceptor (IC-C6IDT-IC) is created. With an extinction coefficient of up to 2.4 × 105 M^{-1} cm^{-1} and a high electron mobility of 1.1 × 10^{-3} cm^{2} V^{-1} s^{-1}, IC-C6IDT-IC exhibits considerable absorption in the 500–800 nm range. Power conversion efficiencies of up to 8.71% are demonstrated using as-cast polymer solar cells based on IC-C6IDT-IC without further modifications.[189] We create a fused-ring electron acceptor (IOIC3) based on an alkoxy side-chain naphtho[1,2-*b*:5,6-*b*′]dithiophene core and contrast it with its alkyl side-chain equivalent (IOIC2). The analogues' morphological, electrical, optical, and charge transport characteristics are all impacted by side-chain changes. Power conversion efficiency (PCE) of PTB7-Th:IOIC3-based organic solar cells (OSCs) can reach 13.1%, which is much higher than that of PTB7-Th:IOIC2 (9.33%). Compared to PTB7-Th:IOIC2 (PCE = 7.32%, AVT = 13.1%), the semitransparent OSCs based on PTB7-Th:IOIC3 provide PCEs of up to 10.8% with an average visible transmittance (AVT) of 16.4%.[190]

Cui *et al.* recently replaced the halogen atoms in the fluorinated Y6 to create a novel "Y-series" NFA called BTP-4Cl. When compared to Y6,[191] BTP-4Cl acceptor showed a decrease in the LUMO energy level and a redshift in optical absorption. When employing PBDB-TF, devices used BTP-4Cl[192] showed a decreased non-radiative energy loss (0.206 eV), which contributed to an increase in V_{oc}. The enhanced absorption and V_{oc} were found to benefit a PCE of 16.5%.[194] Compared to BTP-eC11, BTP-eC9 has better electron transport properties and high solubility. Notably, the BTP-eC9-based single-junction OPV cells record a maximum PCE of 17.8% and receive a certified value of 17.3% because of the concurrently improved short-circuit current density and fill factor. These findings show that reducing the alkyl chains to achieve appropriate solubility and improved intermolecular packing has a significant potential to further improve its photovoltaic performance.[193] *o*-BTP-PhC6, *m*-BTP-PhC6, and *p*-BTP-PhC6 are three isomeric NFAs that were created and produced. The substitution positions (*ortho*, *meta*, and *para*) of the hexyl chains on the phenyl rings connected to the β-positions of the thienothiophene units are the primary structural differences between these isomers, allowing for the methodical study of side-chain orientation effects. Variations in side-chain geometry have a major impact on molecular aggregation, which in turn affects physicochemical characteristics and electron mobility, according to morphological studies and theoretical simulations. The NFAs showed varying photovoltaic capabilities when combined with the wide-bandgap donor polymer PTQ10. Notably, *m*-BTP-PhC6 attained a PCE of 17.7% with improved fill factor (FF) and short-circuit current density (J_{sc}), which is among the greatest efficiencies documented for PTQ10-based OSCs and emphasizes the significance of side-chain engineering in Y-series NFAs.[195] By improving the active layer's shape, the solid additive strategy is a successful method for raising the efficiency of organic solar cells (OSCs). 2,4,6-Trichloro-1,3,5-triazine (TCT), a highly volatile solid additive, was employed to control the morphology *via* potent intermolecular interactions with the polymer donor and acceptor. TCT improves device stability by stabilizing the bicontinuous fibrous morphology of the active layer and increasing crystallinity, molecular ordering, and carrier mobility. In contrast to the D18:L8-BO device (18.13%), the D18:L8-BO:TCT device attained a greater power conversion efficiency (PCE) of 19.50%.[196] A sampling of small molecule NFAs are shown in Fig. 12.

To meet the requirements of several efficient devices, including tandem and semitransparent devices, chemists have logically developed and prepared a series of materials.[197,198] A new era of OSCs was also ushered in 2015 when Zhan and colleagues disclosed a ITIC acceptor with an early PCE of 6.80%.[20] The small-molecule NFA ITIC's acceptor–donor–acceptor (A–D–A) backbone enables the D and A units to be changed to change the level of energy, absorptions, molecular structure, and other characteristics. More importantly,

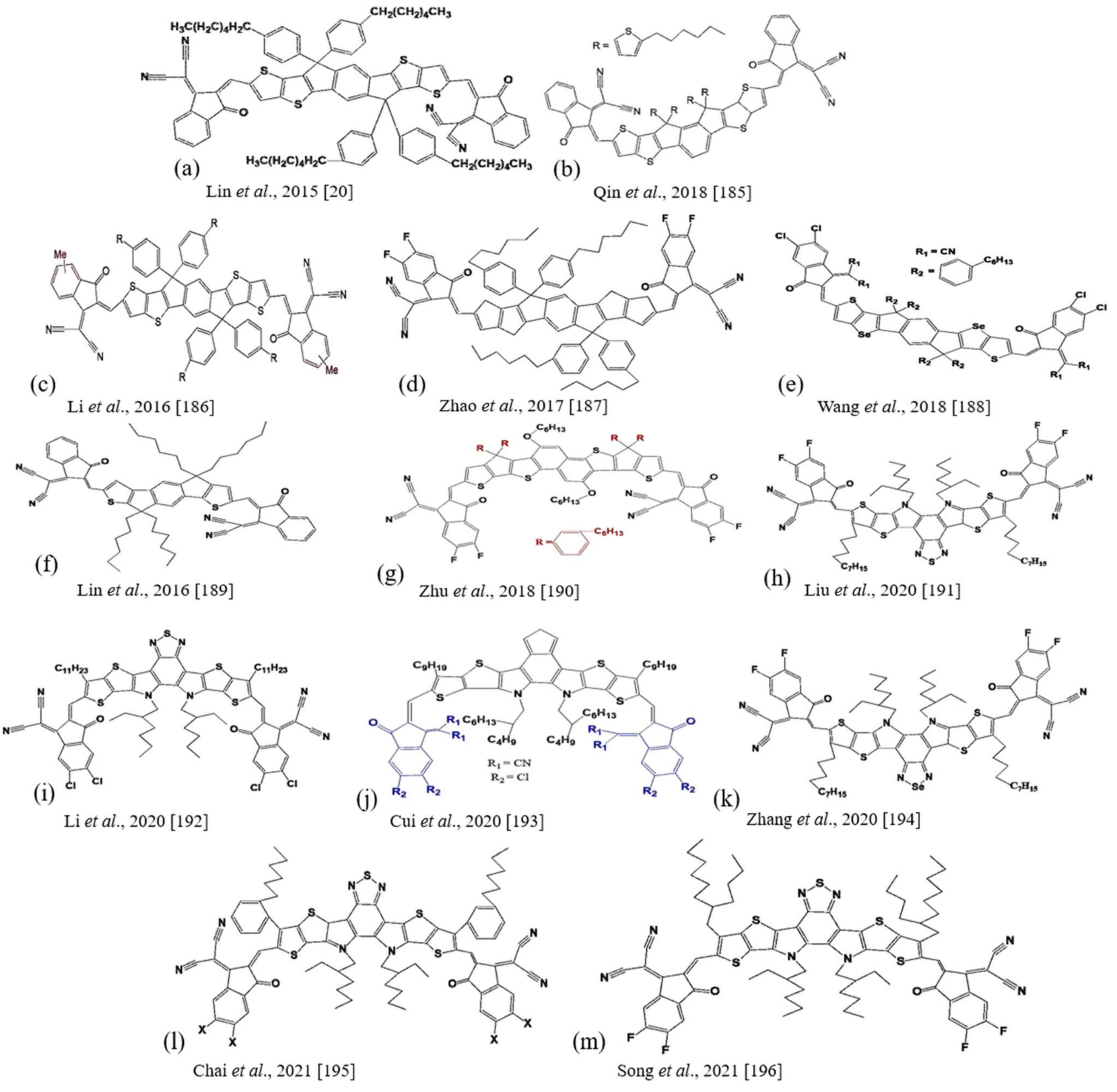

(a) Lin *et al.*, 2015 [20]
(b) Qin *et al.*, 2018 [185]
(c) Li *et al.*, 2016 [186]
(d) Zhao *et al.*, 2017 [187]
(e) Wang *et al.*, 2018 [188]
(f) Lin *et al.*, 2016 [189]
(g) Zhu *et al.*, 2018 [190]
(h) Liu *et al.*, 2020 [191]
(i) Li *et al.*, 2020 [192]
(j) Cui *et al.*, 2020 [193]
(k) Zhang *et al.*, 2020 [194]
(l) Chai *et al.*, 2021 [195]
(m) Song *et al.*, 2021 [196]

Fig. 12 Chemical structures of representative small molecular NFAs; (a) ITIC; (b) ITIC-Th; (c) IT-M; (d) IT-4F; (e) SeTI4Cl; (f) IDIC; (g) IOIC3; (h) Y6; (i) BTP-4CL; (j) BTP-eC9; (k) Y6Se; (l) *m*-BTP-PhC6; (m) L8-BO. Reproduced from reference of each NFAs.

Table 4 Typical tiny molecular NFA characteristics and related device performance

Acceptor	HOMO/LUMO (eV)	Donor	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)	References
ITIC	−5.48/−3.83	PTB7-Th	14.21	0.81	59	6.80	20
Y6	−5.65/−4.10	PM6	24.3	0.86	73.2	15.3	99
IT-M	−5.58/−3.98	PBDB-T	17.44	0.94	73.5	12.05	186
ITIC	−5.51/−3.78	PBDB-T	16.81	0.90	74	11.21	187
IT-4F	−5.66/−4.14	PBDBT-SF	20.5	0.88	71.9	12.97	187
IOIC3	−5.38/−3.84	PTB7-Th	22.9	0.762	74.9	13.1	190
Y6Se	−5.70/−4.15	D18	27.98	0.839	75.3	17.7	194
BTP-4Cl	−5.65/−4.02	PBDB-TF	25.4	0.867	75.0	16.5	204
ITIC-Th	−5.66/−3.93	PDBT-T1	16.24	0.88	67	9.60	205
SeTIC4Cl	−5.65/−4.08	PM6	22.92	0.78	75	13.31	206
IDIC	−5.69/−3.92	PTFBDT-BZS	14.51	0.891	62.2	8.04	207
FOIC	−5.36/−3.92	PTB7-Th	25.1	0.734	70.9	13.1	208
BTP-eC9	−5.64/−4.05	PM6	26.34	0.869	79.51	19.01	209
m-BTP-PhC6	−5.51/−3.46	PM6	26.71	0.871	80.04	18.60	210
L8-BO	−5.67/−3.90	PM6	25.06	0.874	78.57	17.74	211

intramolecular charge transfer (ICT) from the powerful electron-withdrawing end groups (A) to the large fused-ring electron-donating core unit (D) expands the absorption range to the near infrared (NIR) region. Through careful manipulation of the structures of A and/or D units, numerous NFAs with PCEs of 12% to 15% have been reported in the last five years.[199–202]

Zhang and associates introduced Y6Se, a high-performance acceptor made using a straightforward selenium change technique. PCE is reached up to 17.7% when composition of OSCs is ITO/PEDOT:PSS/D18:Y6Se/PNDIT-F3N-Br/Ag. An efficient hole transporting layer (HTL) made from cobalt(II) acetate with a framework of ITO/Co-based HTL/PM6:L8-BO/PNDIT-F3N/Ag was used by Meng *et al.* to build the OSCs. The V_{oc}, J_{sc}, and FF all upgraded along with HTL's work function and conductivity, resulting in a champion PCE of 18.77%.[180] Zou *et al.* reported Y18 in 2020 by substituting a benzotriazole fragment for the core benzothiadiazole fragment.[203] A reduced bandgap and better light-harvesting capacity resulted from this alteration, which also increased the core unit's capacity to donate electrons. Ternary cells based on Y18 produced a PCE of 17.11%. The interior and outer alkyl chains of chlorine-terminated Y-series acceptors were refined in 2020 by Yao *et al.*[193](Table 4).

Although fused NFAs have showed a lot of promise, their economic potential is limited by a few issues. Complex synthesis, frequently involving five to fifteen stages, is needed to create the fused backbone structure.[99,212] Low yield and higher costs are the outcomes of this challenging synthesis procedure. Due to its propensity to experience photo-oxidation when subjected to light and air, recent research has also revealed that fused ring NFA devices are not very stable.[213]

4.2. Non-fused ring electron acceptors

Because their molecular backbone is composed of single bonds, non-fused ring electron acceptors (NFREAs) have the potential to replace fused-ring acceptors. This makes it possible to adopt modular synthesis mainly through Stille and/or Suzuki coupling or C–H activation (without prefunctionalization) and eludes low-yield ring-closing reactions.[214] Zhang *et al.* developed an NFREA termed Ph-IC with a fully non-fused backbone using two thiophene units and alkoxyl benzene as the central core.[215] Ph-IC has a coplanar conjugated backbone and a very simple chemical structure due to within the molecular framework O⋯H and S⋯H noncovalent interactions. Consequently, material has an optic bandgap of 1.62 eV and an absorption edge about 800 nm. The Ph-IC-based device produced a PCE of 5.68%, V_{oc} of 0.89 V, J_{sc} of 12.37 mA cm^{-2}, and FF of 51.5% using the broadband gap polymer PBFTZ as a donor. Additionally, the same fundamental unfused acceptor, ICTP, was described by Chen *et al.*[216] Chen *et al.* later discovered three NFREAs having the matching skeletons as Ph-IC on the other hand altered fluoride-substituted IC groups and alkyl-substituted thiophene π bridges.[217] PTICH, PTIC, and PTICO are these NFREAs. Three NFREAs PhO4T-1, PhO4T-2, and PhO4T-3 were recently described. PhO4T-1 and PhO4T-2 demonstrated PCEs of 9.69% and 11.91%, individually, by the use of PBDB-T as a donor. PhO4T-3 attained a more PCE of 13.76% with the π-extension and chlorine replacement end group.[218] Li *et al.* ensured the planarity and stiffness of two straightforward average bandgap NFREAs, TPT4F and TPT4Cl, using a variety of intramolecular noncovalent conformational locking approaches. Ultimately, compared to the TPT4F-based device (7.67%), the device constructed by using TPT4Cl produced a PCE of 10.16%.[219]

In order to create a completely NFREA A4T-16 with 4T back that have a planar configuration and excellent conformational stability, Hou *et al.* recently added functional groups that have a considerable steric hindrance.[108] The DFT calculations show that the torsion angle in the middle of two thiophenes in TT-Pi is 0°, but dihedral angle amid the phenyl and thiophene units is 89.9° because of steric hindrance from the methyl groups. The energy difference among the two states (ΔE_{s-ms}) is 24 kJ mol^{-1}, but the rotational barrier between the stable and *meta*-stable phases ($E_{s\rightarrow ms}$) is 48 kJ mol^{-1}. These values show that TT-Pi has a very stable planar bithiophene structure because they are much higher than those of the other six 4T derivatives. The PBDB-TF:A4T-16 based device achieved an outstanding PCE of 15.2% together with a J_{sc} of 21.8 mA cm^{-2}, a V_{oc} of 0.876 V, and an overall FF of 0.798 (ref. 102) compared to A4T-21 (1.57%) and A4T-23 (10.4%) based devices. In reaction to their work on A4T-16, Hou *et al.* produced two NFREAs, A4T-25 and A4T-26, by describing large steric hindrance groups, triisopropyl phenyl, into different parts of the core thiophene units.[220] TPT4F was synthesized *via* Knoevenagel condensation for efficient OSCs. The molecule features an unfused TPT core with strong non-covalent interactions (NCIs), forming a rigid planar A–D–A structure with 2-(5,6-difluoro-3-oxo-indan-1-ylidene)-malonitrile acceptor units and showing a maximum absorption at 621 nm in chlorobenzene. When blended with PM6, the device exhibited a V_{oc} of 1.00 V and a fill factor of 0.57 (ref. 221) (Fig. 13).

NFAs have clear favorable properties over fullerene-based acceptors, such as an outstanding absorption coefficient, a wide absorption range, variable energy levels, and orderly packing architectures. In general, altering the center D and terminal A units can control the optoelectronic characteristics and packing topologies of NFAs. Because of this, NFAs have been at the forefront of OSC development in over the past few years, and the PCEs of OSCs created on A–D–A type NFAs have exceeded 16%.[104] Ahmed *et al.*[222] used dynamic dynamic theory (TD-DFT) and indigo-dithiophenepyrrole, mainly D–A oligomers. According to Mehboob *et al.*,[223] the electron-acceptor groups prevent malononitrile or dinitromethane, and the host molecules obtain contain a benzodithiophene compound. By means of a split valence 6-31G (d,p) base set, such integrated molecules showed low bandgap values and positive charge mobility in B3LYP theory. The optical and electric characteristics were computed for newly produced dithieno[3,2*b*:2′,3′-*d*] silole 2,6-diyl molecular donors at the CAM-B3LYP/6-31G (d) using DFT and TD-DFT. In analyzing the energy molecules of FMOs, V_{oc}, regenerate energy, and excitation energy, improved molecules perform superior than reference molecules.[224] It was discovered in 2020 that the maximal regeneration power, FMOs, and V_{oc} of subphthalocyanine present in chromophores affected DFT consumption in the B3LYP/6-311G (d,p) base set. In solar systems, these recently created donor molecules are far additionally effective than dependable computers. DFT at the B3LYP theory level has therefore yielded promising results for solar data.[225]

One of the main barriers preventing NFA-OSCs from being used in commercial settings has been their volatility. Their stability is impacted by multiple variables, for instance both internal and external elements. The constancy of OSCs is significantly impacted by external elements such light, heat, water, and stress. To rise the solidity of NFA-based OSCs, particular molecular design guidelines are still lacking. Therefore, it is still crucial to learn more about the intrinsic deterioration processes of NFA-OSCs and to develop effective approaches for suppressing these processes.[226]

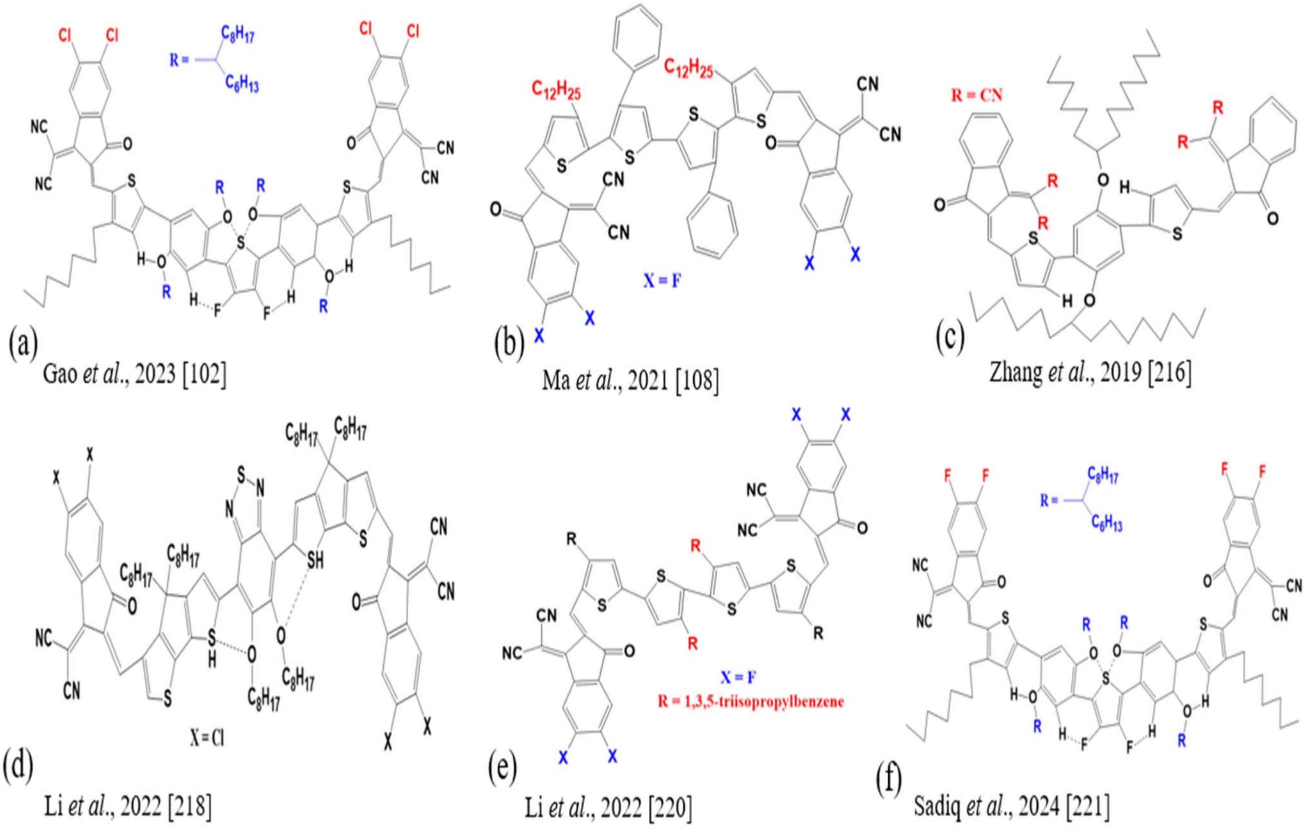


Fig. 13 The complete NFREAs' chemical structures; (a) TPT4Cl; (b) A4T-21; (c) ICTP; (d) BCDT-4Cl; (e) A4T-25; (f) TPT4F. Reproduced and modified from reference of each NFREA's.

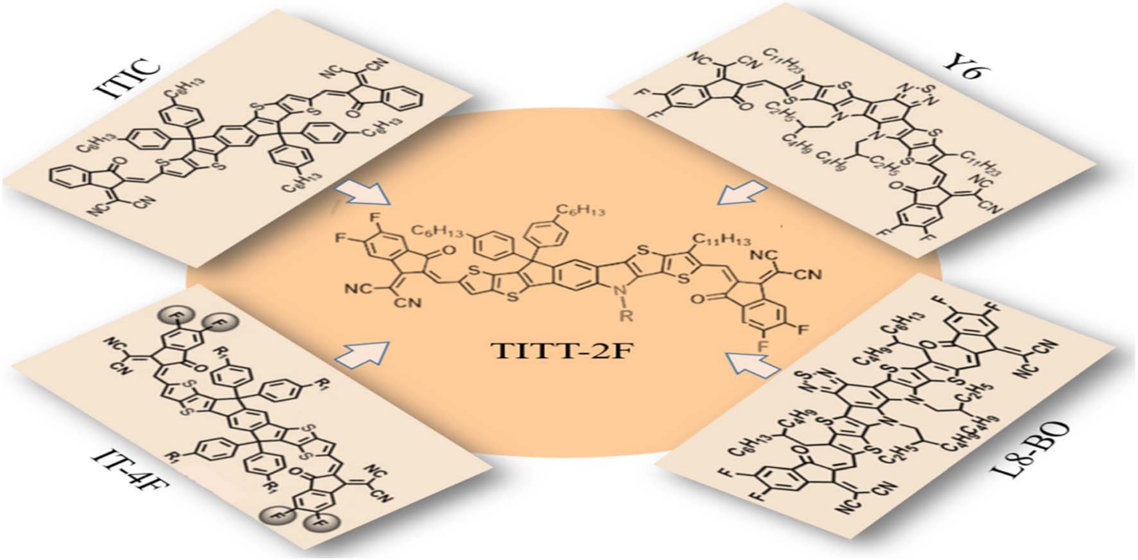


Fig. 14 Successful OSCs application of hybrid NFAs. Reproduced from ref. 237. With the permission of Elsevier Ltd © 2025.

5. Hybrid systems/fullerene + NFA

The ternary method, which integrates a reduced bandgap NFA into a fullerene-free binary host BHJ system, has drawn a lot of attention because it improves the absorption of the photo-active layer and, subsequently, the device J_{sc}.[227,228] While maintaining desirable film morphology and guaranteeing that the FF of the corresponding OSCs stays unharmed, the addition of two NFAs with comparable chemical assemblies may encourage advantageous material merging that results in homogenous acceptor phases.[229,230] Still, a typical weakness of employing a NFA of less bandgap as a third factor is the drop in V_{oc}, which always results in a lower PCE.[231–233] In order to solve these problems, recent research has proposed a novel scheme to raise the V_{oc}. This method produces a bigger V_{oc} by using a guest NFA that has a high LUMO energy than the host NFA-based acceptor in the binary host BHJ system.[234,235] Improvements in both FF and J_{sc} are made possible by the positive contact amid the host and guest acceptors as well as the guest's capacity to adjust to the host NFA's clustering behavior.[234] Two fullerene-non-fullerene hybrid acceptors, IDTIC-$PC_{61}BM$ (IP) and $PC_{61}BM$-IDTIC-$PC_{61}BM$ (PIP), are produced by uniting a non-fullerene acceptor (IDTIC) with a fullerene derivative ($PC_{61}BM$). To assess the capability of these hybrid acceptors, organic solar cells built on four different acceptors (IP, PIP, IDTIC, and $PC_{61}BM$) and the similar polymer donor (PBDB-T) were developed. With PCEs of 8.81% (PBDB-T:PIP) and 8.17% (PBDB-T:IP), respectively, the hybrid acceptor-based OSCs surpass the PBDB-T:$PC_{61}BM$ (7.62%) and PBDB-T:IDTIC (5.98%) OSCs. The outcomes show how well the hybrid acceptor scheme expands photovoltaic performance while overcoming the shortcomings of acceptors.[236]

Zhao *et al.* created a hybrid NFA TITT-2F built on the thieno[2′,3′:4,5]thieno[3,2-*b*]indole-thieno[3,2-*b*]thiophene core with a spiro group by combining structural elements of IT-4F and Y6. With an OSC centered on PM6:TITT-2F, a satisfactory PCE of 12.16% was obtained. Additionally, a ternary PM6:5%TITT-2F:95% Y6 cell showed a J_{sc} of 26.74 mA cm^{-2}, a V_{oc} of 0.86 V, a fill factor (FF) of 71.56%, and a promising PCE of 16.37%. These results show hybrid NFAs' enormous potential for successful OSC applications[237] (Fig. 14).

Pan *et al.* attained the best performance of 16.7% of OPV device by incorporating a tiny quantity of PCBM into the PM6:Y6 structure. After blending with PCBM, the host binary structure's consistent fine-film form and π–π interactions are preserved, but phase purity, hole and electron conduction efficiency, and unimolecular recombination are all enhanced. These effects, along with the apparent absorption of PCBM, account for the concurrently enhanced short-circuit current density and better fill-factor. This method should be widely applicable and can be applied to many OPV systems.[238]

6. Conclusion

Overall, theoretical research has shed light on charge separation, energy alignment, and electron transport in OPVs while emphasizing the drawbacks of fullerene acceptors, including their limited tunability and weak absorption of visible light. Recent developments concentrate on nonfullerene acceptors (NFAs) that provide tunable orbitals, broad absorption, and decreased recombination through end-group engineering, donor acceptor design, and molecular planarity. Furthermore, current theoretical and computational work is increasingly driving predictive material discovery and optimization rather than being limited to retrospective mechanistic analyses. AI-assisted design has the potential to speed up material innovation. For instance, integrated machine learning and genetic algorithm frameworks have been built to screen and design donor-NFA couples with expected power conversion efficiencies approaching ∼17% and higher.[239] The systematic optimization of absorbance profiles, bandgaps, and charge transport properties is further shown by complementary computational insights into unique NFA cores, which provide useful design guidelines for next-generation photovoltaic materials. One of the main obstacles to commercialization is being addressed by hybrid and multicomponent approaches that mix NFAs with fullerene derivatives. These approaches are also showing promise as ways to balance charge transfer and enhance thermal and operational stability. With continuous work on stability and scalable processing to bridge lab and practical performance, state-of-the-art NFA OPVs currently surpass 20% efficiency.

Conflicts of interest

There are no conflicts to declare.

Data availability

No primary research results, software or code have been included and no new data were generated or analyzed as part of this review.

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