

Review

Donor–Acceptor Interactions in Organic Solar Cells: Linking Molecular Design, Energy-Level Alignment, and Device Performance

Mirza Sanita Haque  and Simon Y. Foo 

Electrical and Computer Engineering, FAMU-FSU College of Engineering, Florida State University, Tallahassee, FL 32304, USA; mhaque@fsu.edu

* Correspondence: foo@eng.famu.fsu.edu

Abstract

Organic solar cells (OSCs) are a potential photovoltaic technology because they can be manufactured in scalable systems, are lightweight, and have mechanical flexibility. Power conversion efficiencies close to 20% have been achieved in recent years due to the quick development of donor–acceptor material systems. Better control over nanoscale shape and the creation of non-fullerene acceptors are major factors driving this advancement. Nevertheless, there are still complicated connections between morphology, interfacial energetics, and molecular structure. It is yet unclear how these elements interact to affect charge creation and transport. In this review, donor–acceptor interactions in organic solar cells are examined from a fundamental chemical and physical perspective. From conventional fullerene derivatives to contemporary non-fullerene acceptors, we first look at the development of acceptor materials. We demonstrate how molecular engineering has enhanced device efficiency, energy level adjustment, and light absorption. We then examine the energetic alignment at donor–acceptor interfaces, paying particular attention to charge-transfer state creation, border orbital offsets, and the factors influencing voltage losses. We also investigate how intermolecular interactions, including hydrogen bonding, π – π stacking, and noncovalent interactions involving heteroatoms, control electrical coupling and nanoscale shape in bulk heterojunction active layers. We also go over device engineering techniques including processor control, interface engineering, and bulk heterojunction architecture optimization. These tactics demonstrate how improved solar performance might result from molecular design. Lastly, we highlight new possibilities for next-generation OSCs, such as scalable production techniques, adaptive molecular design, and morphological stabilization. This work provides a strong framework for comprehending donor–acceptor interactions and for directing the careful design of high-performance organic photovoltaic systems by combining knowledge from molecular chemistry, morphological control, and device engineering.



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1. Introduction

Organic solar cells (OSCs) use a donor–acceptor (D–A) photoactive layer to transform sunlight into electrical power. Excitons are produced and separated at nanoscale heterojunctions in this layer. Fullerene acceptors, including phenyl-C61-butyric acid methyl

ester (PCBM), were used in early devices. Although these offered robust processing, they had disadvantages including substantial voltage losses and restricted spectrum tunability. Starting with ITIC (3,9-bis(2 methylene (3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4 hexylphenyl)-dithieno [2,3-d:2',3'-d'] s-indaceno [1,2-b:5,6-b']dithiophene) type A-D-A molecules, the field moved to non-fullerene acceptors (NFAs). The absorption, energy levels, and packing of these NFAs can all be chemically modified. This modification maintains effective charge generation while reducing voltage loss and increasing absorption [1,2]. By offering excellent visible–NIR absorption and appropriate energetics with medium-bandgap polymer donors, the ITIC family demonstrated the viability of A-D-A NFAs. This signaled the start of an era where optoelectronic properties could be cleverly improved by using end-group design, π -bridge extension, and backbone planarity. Y-series acceptors, such Y6/BTP-4F and its chlorinated variant Y7/BTP-4Cl, added halogenated end groups and bent fused backbones to build upon that foundation. This resulted in low nonradiative losses and great external quantum efficiency. In contrast to BTP-4F/Y6, chlorination in BTP-4Cl significantly increased absorption while reducing nonradiative energy loss. As a result, single-junction efficiencies of roughly 16.5% with improved open-circuit voltage (V_{oc}) were possible. Further structure–property analyses connected Y6's unique π - π packing to exciton/electron delocalization and small energy offsets [3,4]. Molecular design on the donor side concentrated on copolymers based on quinoxaline, BDT, and DPP. These polymers possessed side-chain polarity and regulated halogenation. This strategy sought to maximize the packing, miscibility, and depth of the highest occupied molecular orbital (HOMO) using Y-series NFAs. The idea of “low-offset, low-loss” was demonstrated in two case studies: (i) PTQ10:Y6, where efficient charge creation with small offsets was evaluated by time-resolved spectroscopy; and (ii) PM6:Y6, where charge generation looked to be practically barrierless despite modest driving force. This demonstrated that effective free-carrier generation may be separated from significant offsets by well-matched D–A chemistry [5,6]. In addition, D18-Cl and D18-class donors displayed excellent hole mobility, strong π - π stacking, and deep HOMOs. When combined with Y-series acceptors, such as D18:Y6, which reached approximately 18.22% with a certified efficiency of 17.6%, this combination helped attain single-junction efficiencies exceeding 18%. These results introduced useful design concepts like side-chain engineering, selective halogenation, and fused-unit backbones. Without sacrificing V_{oc} these techniques, increase fill factor and short-circuit current (J_{sc}) [7]. Additionally, process-aware chemistry has been highlighted in recent publications. It is essential for manufacturability that several D-A references pairs (PM6:Y6, PM6:L8-BO, D18:Y6) be synthesized from non-halogenated solvents (o-xylene or toluene) and scaled using blade or slot-die coating with minimal additive loading. The effects of solvent selection on the liquid-to-solid transition, fibrillation, and vertical stratification are explained in reviews of green-processed Y-series systems and bio-renewable solvent windows. This relationship enables effective and scalable processing by connecting chemistry, morphology, and device physics [8–10]. Figure 1 shows the evolution of donor–acceptor (D-A) chemistry in organic solar cells, highlighting four phases: the fullerene baseline (P3HT: PCBM), the rise of A-D-A non-fullerene acceptors (ITIC family), the Y-series breakthrough period, and the current focus on green and scalable processing. Theoretical and energetics, (ii) Y-series advancements like chlorinated Y7 (BTP-4Cl) and low-loss transport made possible by delocalization, (iii) proof of barrierless free-charge generation in PM6:Y6 blends, (iv) the appearance of donors of class D18 and an estimated efficiency of 18% for single junctions, and (v) a shift toward o-xylene or toluene processing and slot-die or blade coating for scaling. The timeline shows how decisions in process (solvent or additives, coating method) and molecular design (end-group halogenation, backbone planarity, side-chain engineering) evolved in tandem to reduce non-radiative losses and boost efficiency.

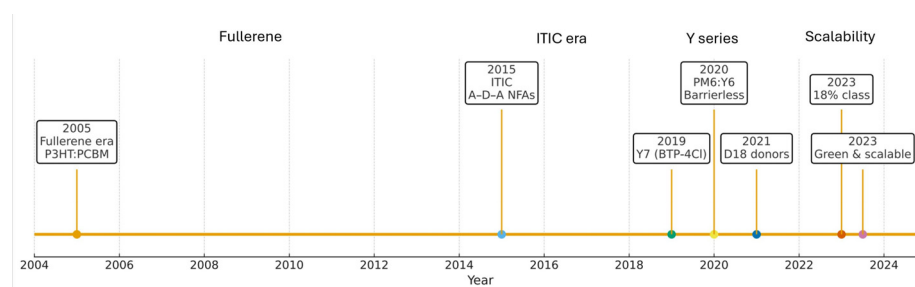


Figure 1. Evolution of donor–acceptor chemistry in organic solar cells, from fullerene baselines to ITIC-type NFAs, Y-series breakthroughs, PM6:Y6 mechanism, D18-class donors, and green, scalable processing.

Table 1 lists representative donor–acceptor systems and practical processing notes drawn from recent literature.

Table 1. Represents donor–acceptor systems and typical processing notes.

Donor	Acceptor	Solvent/Additives	Processing Notes
PM6 (PBDB–T–2F)	Y6 (BTP–4F)	o-XY or Tol; CN/DIO optional; also, CB/CF variants	Green-solvent blade/slot-die demonstrated; barrierless free-charge generation reported in PM6:Y6 [6,8]
PM6 (PBDB–T–2F)	L8–BO (BTP–eC9)	o-XY, Tol; typically, additive lean	High-speed doctor/slot-die coating; large-area and thick-film compatible; scalable coating trends reported [8,10]
PTQ10	Y6	CB/CF; light CN/DIO if needed	Low-offset (small driving force) yet efficient charge generation demonstrated through time-resolved spectroscopy [5]
D18/D18–Cl	Y6/N3	CB/CF; green processing routes also reported	High J_{SC} and FF; single-junction devices approaching 18%(certified 17.6%); donor design motifs summarized [7]
PBDB–T (PCE12)	IT–4F (ITIC–4F)	CB/CF + DIO (typical for morphology control)	Baseline non-fullerene A–D–A system; ITIC family established the viability of NFAs [1,2]
PM6 (PBDB–T–2F)	Y7 (BTP–4Cl)	CB/CF; CN	Chlorination broadens absorption and reduces nonradiative loss; efficiency class around 16.5% [3,4]

2. Fundamental of Donor–Acceptor Chemistry

In bulk heterojunction (BHJ) and bilayer devices, photoexcitation generates Frenkel excitons that, to form an interfacial charge-transfer (CT) state with the electron on the acceptor and the hole on the donor, must reach a D–A interface within their diffusion length. Conjugated semiconductors typically have diffusion lengths between 5 and 20 nm, and accurate measurements necessitate controlled bilayer photoluminescence (PL) quenching, sensitized stacks, or exciton–exciton annihilation investigations [11]. The CT state energy can be approximated as

$$E_{CT} = E_{LUMO}^A - E_{HOMO}^D - E_{coul}$$

where E_{coul} accounts for interfacial Coulomb binding and image-charge stabilization. Open-circuit voltage V_{OC} is then governed by E_{CT} and by radiative and nonradiative recombination from CT states; EL and FTPS are standard tools to locate E_{CT} and to track the CT emission tail that correlates with voltage losses [12]. The Figure 2 highlights direct excitations within D and A and the CT manifold at the D–A interface.

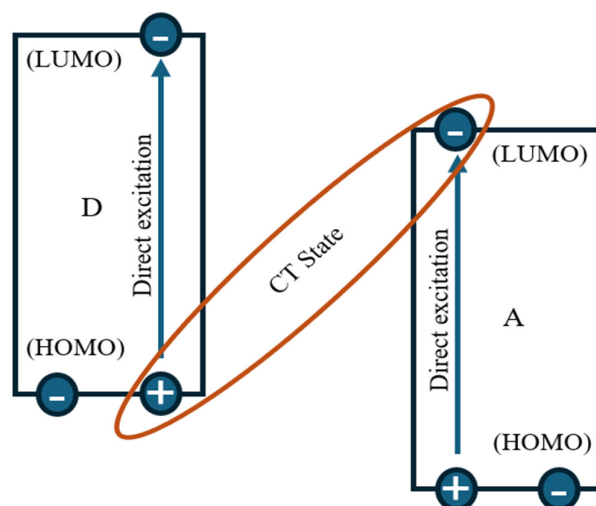


Figure 2. Donor–acceptor HOMO–LUMO alignment and interfacial CT state. The red highlighted region denotes the donor–acceptor interfacial CT state.

Classical screening rules linked frontier levels to achievable PCE and encouraged sizable driving-force offsets between donor HOMO and acceptor LUMO [13,14]. Modern analyses separate the radiative and nonradiative contributions to voltage loss: in the reciprocity (radiative limit) framework, the nonradiative voltage loss is

$$\Delta E_{\text{nonrad}} = -kT \ln(EQE_{\text{EL}})$$

Therefore, increasing device electroluminescence quantum efficiency directly raises V_{oc} [15]. To avoid biased peak placements and miscalculated losses, thin-film optical microcavity effects must be modeled when extracting E_{CT} from EL or FTPS. Effective charge separation can happen at modest energy offsets (0.1–0.3 eV) if interfacial order, electronic coupling, and CT exciton hybridization encourage quick dissociation. This is a significant result of the NFA era. Temperature-dependent photocurrent, ultrafast spectroscopy, and theory have all supported this small-offset paradigm, demonstrating that delocalization-assisted separation reconciles high V_{oc} with high J_{sc} [16]. These observations are framed in the larger BHJ framework by historical and fundamental viewpoints on plastic solar cells and CT/free-carrier equilibria [17,18]. A consistent map is used to translate orbitals to device metrics. While acceptor LUMO determines electron affinity and the transport landscape, donor HOMO depth limits the achievable V_{oc} . The blend optical gap E_g^{opt} restricts spectral coverage, and the ceiling of J_{sc} . Material families provide useful tuning knobs: donor backbones like BDT, quinoxaline, and DPP provide HOMO control, planarity, and miscibility through halogenation, π bridge selection, and side-chain engineering [19]; all-polymer systems (polymer donors with polymer acceptors) prioritize mechanical robustness and processing latitude [20–22]. Recent stability studies include lessons for NFA materials and interfaces [23,24], and stability and morphology baselines in fullerene-free systems (e.g., o-IDTBR) offer helpful references for non-fullerene comparisons [25].

Performance–Sustainability Trade-Offs in Molecular Design

The performance of contemporary organic solar cells has been greatly enhanced by molecular engineering techniques such side-chain optimization, backbone rigidification, fluorination, and chlorination. To adjust frontier energy levels, improve molecular packing, strengthen intermolecular contacts, and lower nonradiative voltage losses, fluorination and chlorination have been widely used. The success of Y-series non-fullerene acceptors

and donor polymers like PM6 and D18-Cl has been greatly aided by these adjustments. Despite these benefits, sustainability and manufacturability must be taken into consideration while making molecular design decisions. Halogenated materials may need less ecologically friendly processing methods and frequently need more intricate synthetic pathways. The effects of highly halogenated organic semiconductors on the environment, end-of-life management, and regulatory issues are also receiving more attention. As a result, more recent research has concentrated on developing non-halogenated materials, environmentally safe solvent systems, and scalable manufacturing techniques to balance photovoltaic performance with green chemistry principles. Instead of concentrating only on record power conversion efficiency, future material development will probably need to simultaneously optimize efficiency, stability, scalability, and sustainability as organic photovoltaic technologies advance toward commercialization.

3. Donor Landscape: Architectures and Use Cases

Building on the three primary platforms (DTQ10, D18, and PBDB-T variants) [26], a range of more recent and older donors remain crucial for scalable processing, stability base-lines, and pairing rules. We arrange them by backbone class below, emphasizing the usual contributions of each family to V_{oc} , J_{sc} , and FF, as well as comprehensive studies in [27]. With a face-on texture and extended coherence length, P3HT created the semicrystalline donor model, which is now the industry standard for morphology and endurance. It has modest HOMO and thick film tolerance. To stabilize V_{oc} and spectrum coverage, PCDTBT offered a deep HOMO and amorphous packing. These donors are crucial for evaluating domain length scales under green solvents and for device-physics controls [28].

3.1. PTB7/PTB7-Th and BDT-TPD Families

One significant class of low-bandgap copolymers is represented by the PTB7 and PTB7-Th donor polymers. Prior to the widespread use of PBDB-T derivatives, they advanced our understanding of the relationship between structure, characteristics, and processing in polymer solar cells. Their importance stems not from record efficiency but rather from the important insights they provide regarding stability, scalable processing, energy offsets, and nanoscale morphological control. According to research on thermal aging, PTB7-Th is more thermally stable than PTB7 in both ambient and inert environments. Stronger intermolecular interactions from thiophene substitution and enhanced backbone planarity are associated with this development [29]. Additionally, in both blends, the PCBM and PC₇₁BM fullerene acceptors had comparable thermal behavior. This implies that the thermal breakdown routes in these systems are mostly influenced by the chemistry of the donor backbone rather than the acceptor selection. The nanoscale phase separation in PTB7:PC₇₁BM and PTB7-Th: PC₇₁BM blends is affected by donor-acceptor miscibility in the casting solvent and drying rates during film production, according to first principles and multiscale simulations and experimental morphology analysis [30]. These findings explain why, in comparison to PTB7, PTB7-Th usually forms more stable, delicately interpenetrating networks. Higher fill factors and reduced bimolecular recombination are the results of this stability. Future non-fullerene acceptor systems, where lower energy offsets necessitate highly regulated interfaces, will benefit from these discoveries. PTB7 and PTB7-Th have been recognized by numerous investigations as model systems for testing nonaromatic and non-chlorinated solvents. Low-toxicity solvents and solvent mixtures were used to create high-efficiency devices without sacrificing charge transfer or morphological control [31]. Notably, chlorobenzene was successfully substituted by terpinolene and other Hansen-solubility-guided solvents. This demonstrated that environmentally friendly processing settings can preserve positive donor-acceptor interactions [32]. These results indicated that

green solvents are now being used in PBDB-T and Y-series systems. When paired with low-boiling-point solvent additives, PTB7-Th blends also made it possible to process very thick active layers (up to around 230 nm) without vacuum drying [33]. This behavior highlighted how important additive volatility and solvent evaporation rates are to obtaining ideal morphology. These ideas are now crucial for roll-to-roll and slot-die coating techniques. In donors PTB7, PTB7-Th, and later PBDB-T, detailed external quantum efficiency and scanning tunneling microscopy studies linked the interfacial electronic structure with charge generation efficiency [34]. These investigations supported the notion that efficient photocurrent extraction depended on the density and energetic dispersion of interfacial charge-transfer states in addition to absorption. This gave subsequent charge transfer state investigations in NFA blends an experimental foundation. PTB7/PTB7-Th donors were employed in ternary and all-polymer designs in addition to binary fullerene systems. In these instances, morphology and recombination routes were greatly affected by donor compatibility and pendant group substitution [35]. These investigations demonstrated the strategic use of donor chemistry to balance energetics, morphology, and absorption. For contemporary multi-component organic solar cells, these ideas are still applicable. All things considered, the PTB7/PTB7-Th and BDT-TPD families laid the groundwork for comprehending the joint effects of backbone design, side-chain engineering, solvent selection, and drying kinetics on morphology, stability, and performance. Donor selection and processing methods for existing non-fullerene acceptor systems are still influenced by these discoveries. Figure 3 presents molecular structures of PTB7 and BDT-TPD families.

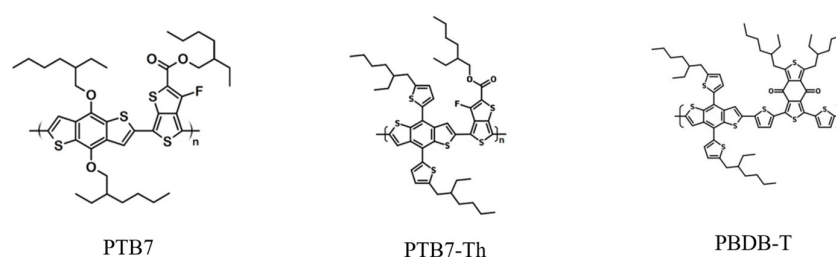


Figure 3. Molecular Structures of PTB7 and BDT-TPD families.

3.2. PffBT4T Donors

One class of BDT-benzothiadiazole copolymers is the PffBT4T family. Charge transfer, shape, and processing strength in these materials are all influenced by side-chain engineering and temperature-dependent aggregation. PffBT4T-2OD has high preaggregation in solutions, according to early research. When films are created, this produces tiny, cohesive crystalline domains. Even in thick active layers, this microstructure enables great hole mobility and good fill factors [36]. Subsequent investigation revealed that backbone planarity and intermolecular interactions are enhanced by regulated fluorination of the donor portion. This maintains advantageous domain sizes while increasing carrier mobility and photovoltaic performance [37]. Preaggregation in solutions is a crucial element influencing solid-state morphology, according to both theoretical and experimental investigations. It affects how fibrillar networks and percolation pathways evolve in bulk heterojunctions [38]. Phase separation length scales in non-fullerene blends are determined by the connection between donor aggregation and donor-acceptor liquid immiscibility. If aggregation grows too high, PffBT4T-2OD systems may switch from ideal bi-continuous networks to three-phase architectures [39]. Aggregation alters both electronic coupling and vibronic structure, according to spectroscopic studies. Recombination dynamics and charge-generation efficiency at donor-acceptor interfaces are impacted by this [40]. One important chemical element that regulates backbone form and aggregation strength is the location of side-chain branching. This enables morphology to be chemically adjusted without changing

the conjugated core [41]. These results make PffBT4T-type donor's important models for comprehending how high mobility, thickness tolerance, and processing robustness are caused by aggregation-driven microstructure. The design of contemporary wide-bandgap donors for scalable organic solar cells is still influenced by these ideas. The molecular structures of the PffBT4T family are shown in Figure 4.

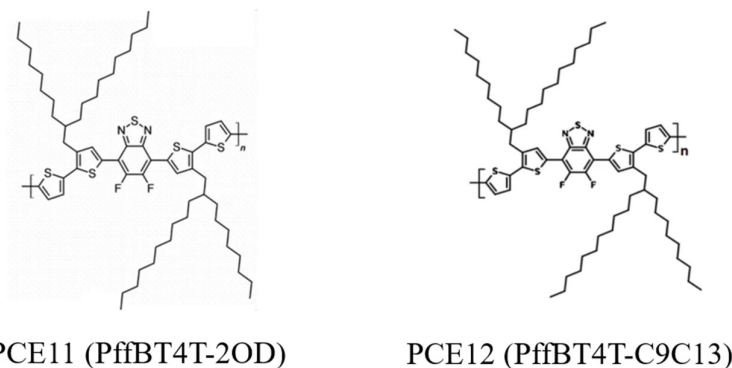


Figure 4. Molecular Structures of PffBT4T family.

3.3. DPP and Isoindigo Donor Families

A well-known class of low-bandgap donor materials includes isoindigo-based polymers and diketopyrrolopyrrole (DPP). They have substantial intermolecular interactions, widespread conjugation, and powerful electron-withdrawing cores. Their excellent charge-carrier mobility, chemical stability, and capacity to absorb light from red to near-infrared make them appealing. Strong aggregation tendencies accompany these advantages, necessitating careful management at the molecular and processing levels. Bandgaps of 1.3 to 1.5 eV can be attained while maintaining long conjugation lengths and effective transport within the chains, according to early research on semi-crystalline random copolymers with various DPP-to-isoindigo ratios [41]. According to these investigations, increasing the DPP content increases hole mobility and crystallinity, but if the miscibility between donor and acceptor is not carefully regulated, it can also result in excessive phase separation and trap-assisted recombination. Deeper HOMO levels and improved thermal stability were introduced by donors containing isoindigo, such as PII2T [42]. For ternary and all-polymer solar cells, where spectral match and stability during operation are crucial, this made them attractive. The structural flexibility of isoindigo derivatives was emphasized in reviews. For a variety of organic electrical applications, this enables exact control over backbone planarity, substitution symmetry, and intermolecular packing. The position and asymmetry of alkyl-chain branching significantly affect backbone form and aggregation strength in systems connected to PffBT4T and DPP, according to studies that incorporate spectroscopy, theory, and in-depth simulations. This offers a way to modify crystallinity while maintaining absorption efficiency. It was later demonstrated that techniques employing asymmetric and random copolymers could lessen excessive aggregation while preserving wide absorption and efficient charge generation [43,44]. The remarkable mobility of DPP and isoindigo polymers in organic field-effect transistors provided significant insights into the connection between structure and transport outside of solar cells [45]. This demonstrated how balanced transport is supported by intermolecular contact and backbone rigidity. The design of organic solar cells has been directly impacted by these discoveries, and DPP and isoindigo donors continue to be important models for comprehending the trade-offs between low bandgap, morphological control, and nonradiative losses [46]. A few molecular structures from these families are shown in Figure 5.

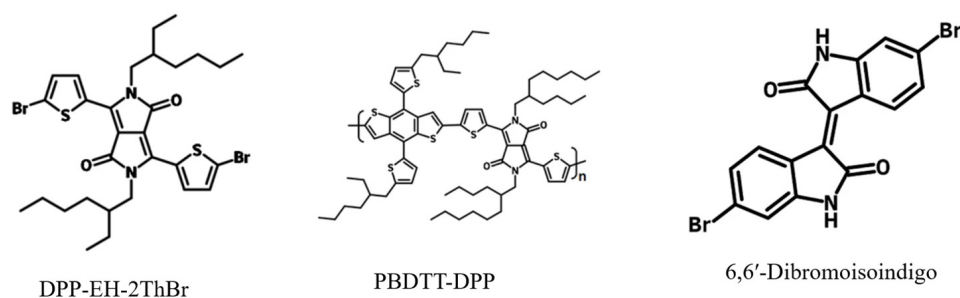


Figure 5. Molecular Structures of DPP and Isoindigo Families.

3.4. PBDB-T and Derivatives

In contemporary organic solar cells, one of the most significant wide-bandgap donor platforms is the PBDB-T family of polymer donors. It has helped NFA-based devices that are more efficient than 15–18% grow quickly. Electron-deficient thiophene-based units and a benzodithiophene (BDT) core are structural properties of PBDB-T. Strong intramolecular charge transfer, excellent energy alignment with low-bandgap acceptors, and high absorption coefficients in the visible range are all made possible by this combination [47]. The electrical structure and solid-state packing of the PBDB-T backbone can be effectively modified by systematic halogenation and modification. PM6 (PBDB-T-2F) and PM7 (PBDB-T-2Cl) are examples of fluorinated and chlorinated variations that lower the donor HOMO level and strengthen noncovalent conformational locking (e.g., S...F, S...Cl interactions). As a result, intermolecular coherence and backbone planarity are enhanced [48]. These adjustments enable regulated trade-offs between aggregation strength and open-circuit voltage. For compatibility with Y-series acceptors, these elements are essential. The interactions between transport, morphology, and device performance in PBDB-T-based blends have been elucidated by thorough experimental and theoretical investigations in addition to molecular energetics. Polarons in PBDB-T backbones are moderately delocalized, according to charge-transport analysis and electron paramagnetic resonance experiments. This minimizes excessive recombination and promotes effective hole transport [49]. PBDB-T derivatives produce finely intermixed yet percolated donor domains with both fullerene and non-fullerene acceptors, according to morphology studies, which result in strong fill factors throughout a broad processing range [50]. The investigation of scalable synthesis and processing techniques has also been made possible by the PBDB-T scaffold's chemical stability. High-performance PBDB-T materials with reduced synthetic complexity can be produced via direct C-H arylation polymerization methods, which makes them appropriate for large-scale production [51]. Furthermore, research employing green processing conditions and nonhalogenated solvents shows that PBDB-T derivatives may withstand eco-friendly manufacturing methods without sacrificing stability or efficiency [52]. A contemporary design strategy in donor chemistry is exemplified by the PBDB-T donor family. These wide-bandgap polymers have good compatibility with NFA systems, modest aggregation strength, and designed noncovalent interactions. As a result, PBDB-T derivatives remain important benchmark donors for studying the links between structure, property, and performance as well as for transforming laboratory-scale efficiencies into scalable organic photovoltaic solutions. Figure 6 represents few molecular structures from these families.

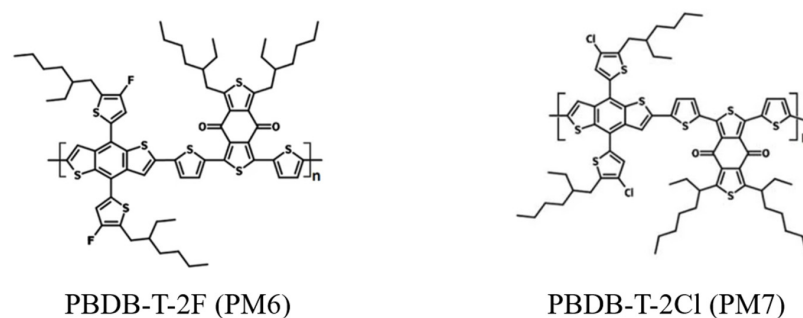


Figure 6. Molecular Structures of PBDB-T and Derivatives.

3.5. PTQ10 and Related Low-Cost Polymer

PTQ10 is now a crucial inexpensive polymer donor. It has a straightforward chemical composition and offers competitive photovoltaic performance for a range of device types. Early tests demonstrated PTQ10's thickness tolerance. Its ability to sustain high power conversion efficiency in thicker active layers underscores its promise for roll-to-roll processing and scalable production [53,54]. According to additional research, devices that use PTQ10 in conjunction with well-designed non-fullerene acceptors can achieve efficiency levels above 18%. This efficiency results from balanced transport, efficient charge creation, and complementary absorption [55]. The ability of PTQ10 to crystallize in a regulated manner is a crucial feature. According to thorough spectroscopic and structural investigations, PTQ10 produces extremely crystalline domains with coherence lengths of several nanometers. These domains facilitate effective hole transport and permit sufficient donor–acceptor mixing for exciton dissociation [56,57]. According to morphological analyses of PTQ10: IDIC, PTQ10: ITIC, and PTQ10: Y-series blends, PTQ10 forms stable, percolated networks with a moderate degree of phase separation. This form reduces vulnerability to differences in processing and aids in achieving robust fill factors. Research on charge photogeneration and recombination reveals that PTQ10 devices minimize bimolecular recombination while producing free carriers effectively, particularly when paired with Y-series acceptors. Despite minor energetic offsets, time-resolved and steady-state investigations show that PTQ10's long exciton lifespan and advantageous interfacial energetics contribute to effective charge separation [58]. Because of these features, PTQ10 is a valuable model for researching recombination loss pathways and low-offset donor–acceptor interfaces. PTQ10 has been effectively employed in ternary and quaternary active layers in addition to binary blends. It serves as both a selective hole-transport component and a morphological regulator in these multi-component systems. PTQ10 contributes to the development of hierarchical “rivers-and-streams” topologies that enhance charge extraction without sacrificing stability or voltage [59]. All these results point to PTQ10 as a crucial donor for investigating the connections between crystallinity, morphological control, molecular simplicity, and scalable device production in contemporary organic solar cells. Figure 7 represents molecular structures of PTQ10 and its derivatives.

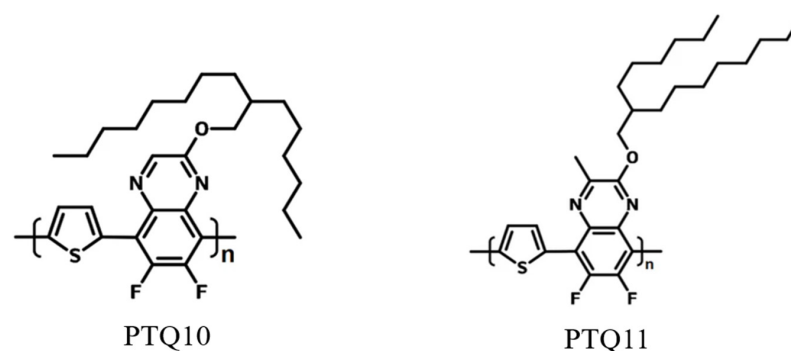


Figure 7. Molecular Structures of PTQ10 and derivatives.

3.6. D18 and Derivatives

Strong crystallinity, high intrinsic hole mobility, and outstanding compatibility with Y-series non-fullerene acceptors make D18 one of the most effective wide-bandgap polymer donors for cutting-edge organic solar cells. Early research has shown that D18 is an exceptionally resilient donor that can maintain effective charge transport even in thick active layers, allowing for large fill factors and decreased sensitivity to processing changes [60]. D18 became a benchmark donor for near-record photovoltaic performance after subsequent device development and morphological control quickly drove D18-influenced single-junction efficiencies above 19% [61,62]. From the standpoint of molecular design, sidechain and backbone engineering are crucial for adjusting D18 derivatives performance. While retaining deep HOMO levels that enable large open-circuit voltages, chlorinated and side-chain-modified versions enhance solubility and film-forming characteristics [63]. Devices with concurrently high V_{OC} , J_{SC} , and FF can be achieved by synergistic side-chain engineering, which has been demonstrated to speed up charge extraction and reduce recombination losses [64]. These effects are intimately associated with the development of double-fibril or refined fibrillar morphologies that improve hole transport percolation channels [65]. In ternary systems, where the addition of guest non-fullerene acceptors allows for precise control over phase separation and crystallization kinetics, D18 has demonstrated exceptional efficacy beyond binary blends. These ternary approaches have produced efficiencies that are close to 19.3%, highlighting the D18 donor platform's adaptability in intricate active-layer formulations [66]. Simultaneously, new spectroscopic and computational research has started to clarify the photodegradation pathways of D18, offering crucial information about its long-term stability and degrading chemistry under light [67]. The D18 donor family represents an advanced stage of donor-acceptor polymer design, where record-level efficiencies are supported by the convergence of high mobility, controlled aggregation, and morphological accuracy. Because of this, D18 and its derivatives are still used as reference donors to investigate stability issues and upper performance limits of single-junction organic solar cells. The molecular structures of D18 and its derivatives are shown in Figure 8.

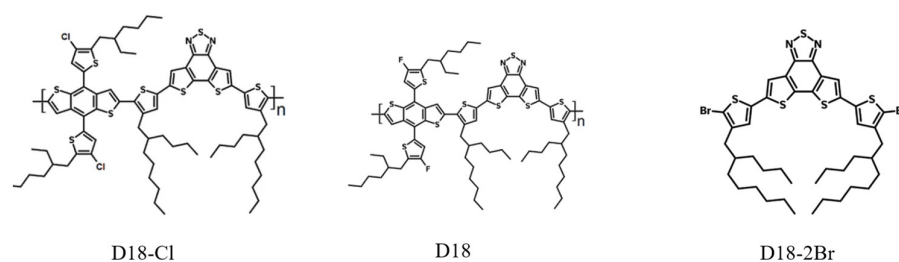


Figure 8. Molecular Structures of D18 and Derivatives.

3.7. Ternary Blend Strategies: Performance Enhancement Beyond Binary Donor–Acceptor Systems

Ternary OSCs, in which a third photoactive component is intentionally introduced into a conventional binary donor-acceptor blend, have emerged as a versatile strategy to overcome intrinsic trade-offs between voltage, current, morphology, and scalability. Depending on its energetic alignment and miscibility with the host materials, the third component can act as a morphological regulator, an energy cascade mediator, or a recombination suppressor, according to thorough reviews [68,69]. Ternary blends, as contrast to binary systems, provide more flexibility to maximize light harvesting, charge transport, and nonradiative voltage losses all at once. Early experiments demonstrated that by preserving advantageous nanoscale morphologies during film generation, ternary methods enable thicker active layers and enhanced large-area device performance [70]. Ternary blend design has moved toward carefully choosing secondary acceptors or donors that add

complementing absorption while preserving coherent charge-transport pathways since the introduction of non-fullerene acceptors [71]. In small-molecule and polymer: NFA systems in particular, these methods have been demonstrated to attenuate energy disorder and reduce voltage losses without compromising fill factor [72,73]. High efficiencies in both rigid and flexible devices can be achieved by engineering ternary blends to inhibit nonradiative recombination by optimal molecule packing and electrostatic potential tuning, according to recent studies [74]. The role of the third component as an active participant in charge separation and transport rather than a passive additive has been highlighted in advanced implementations where molecular electrostatics and ternary composition have been jointly optimized to achieve efficiencies approaching or exceeding 20% [75]. All these results point to ternary blend techniques as a potent and broadly applicable design paradigm for advancing organic solar cells beyond the constraints of binary donor–acceptor architectures. Donor polymer families utilized in high-performance organic solar cells are shown in Figure 9, which shows the structural progression from early BDT-based donors (like PTB7) to contemporary high-crystallinity systems like PBDB-T derivatives, PTQ10, and D18. Structure–property correlations are emphasized by highlighting key design motifs such as bandgap tuning, aggregation strength, and backbone planarity.



Figure 9. Representative donor polymer families used in high-performance organic solar cells.

Table 2 compared donor polymer families used in OSCs performance, scalability, and manufacturing considerations. PTQ10 has major advantages in terms of synthetic ease, cost, and scalability, even if D18-based donors currently provide the highest efficiency. While extremely crystalline donor systems like PffBT4T and DPP-based polymers would need more stringent morphology control during processing, PBDB-T derivatives offer a balance between performance and manufacturability. These trade-offs show that scalability, repeatability, and operational stability should all be considered when choosing a donor in addition to efficiency.

Table 2. Comparison of representative donor polymer families used in OSCs performance, scalability, and manufacturing considerations.

Donor Family	Strengths	Limitations	Synthetic Complexity	Scalability	Stability
PTB7/PTB7-Th	Good efficiency	Requires additives, stability concerns	Moderate	Moderate	Moderate
PffBT4T	High mobility	Strong aggregation	High	Moderate	Good
DPP/Isoindigo	Excellent transport	Excessive crystallization	High	Moderate	Good
PBDB-T/ PM6	Balanced performance	Halogenation dependence	Moderate	High	Good
PTQ10	Low cost, simple synthesis	Slightly lower efficiency ceiling	Low	High	Good
D18/D18-Cl	Record efficiencies	Higher synthetic complexity	High	Moderate	Good

It should be noted that direct comparisons of reported OSC efficiencies across different studies should be made cautiously. Variations in active-layer thickness, device architecture, processing conditions, solvent systems, post-treatment protocols, and measurement

procedures can significantly influence reported photovoltaic performance. In addition, batch-to-batch variations in polymer molecular weight, dispersity, and purity may affect morphology development and charge transport characteristics. Consequently, differences in reported efficiencies do not necessarily reflect intrinsic material superiority but may also arise from variations in device fabrication and testing conditions.

4. Fullerene-Based Electron Acceptors

The substance that takes electrons from the photoexcited donor after exciton dissociation at the donor–acceptor contact is referred to as an acceptor in organic solar cells. For more than 20 years, fullerene derivatives, particularly PC₆₁BM and PC₇₁BM—were the primary electron acceptors in bulk heterojunction solar cells. The fundamental donor–acceptor architecture of early organic photovoltaics was formed by combining these materials with conjugated polymer donors like P3HT, PTB7, and related systems [76,77]. Because of their spherical molecular structure, methano fullerene acceptors have deep LUMO energy levels, strong electron affinity, and almost isotropic charge-transport channels. These features allow for strong electron percolation networks, minimal energy disorder, and effective electron transfer from the donor, all of which helped early polymer–fullerene solar cells achieve relatively high fill factors and repeatable device performance [78]. Crucially, even though fullerene derivatives are tiny molecules, they only serve as electron acceptors and do not take part in hole transport or light harvesting in conventional device topologies. However, fullerene acceptors have inherent drawbacks that eventually prevent additional efficiency improvements. The donor material bears nearly all the burden of light absorption due to their weak and narrow optical absorption, which barely contributes to photocurrent production [79,80]. Furthermore, fullerene derivatives' deep LUMO levels impose significant energy offsets at the donor–acceptor interface, resulting in significant voltage losses linked to nonradiative recombination and charge-transfer state creation [81,82]. As donor bandgaps decrease, these losses get worse. Fullerene chemistry provides little structural tunability from the standpoint of materials design. Although side-chain functionalization enhanced solubility and processability, energy levels, absorption, and interfacial electrostatics were only slightly controlled. Additionally, under heat or protracted illumination stress, fullerene-based blends frequently show morphological instability, which can eventually result in phase segregation and performance loss [83,84]. A distinct performance ceiling for fullerene acceptors was established by the combination of weak absorption, restricted tunability, and voltage losses. The creation of non-fullerene acceptors with stronger and tunable absorption, adjustable frontier energy levels, and lower nonradiative losses was directly driven by these constraints. Fullerene acceptors are still a crucial reference system even though they are mostly supplanted in cutting-edge devices. They offer important design lessons in charge transport, morphological control, and interfacial energetics that continue to guide the development of contemporary acceptors. The chemical structures of NFAs with a fullerene acceptor are shown in Figure 10.

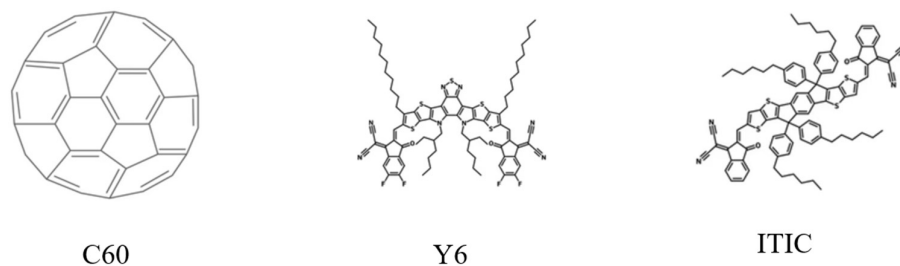


Figure 10. Chemical structure of fullerene C60, ITIC and Y6.

4.1. A-D-A Non-Fullerene Acceptors: ITIC and the First Paradigm Shift

A significant paradigm shift in cell design was brought about by the development of A-D-A structured NFAs, which addressed the basic drawbacks of fullerene-based electron acceptors. ITIC and its derivatives were important early NFAs because they showed that well-defined molecular designs could provide advantageous donor–acceptor interfacial energetics, tunable energy levels, and high optical absorption all at once [85–87]. Unlike fullerenes, ITIC-type acceptors actively contribute to the production of photocurrent by absorbing light intensely and widely into the near-infrared spectrum. ITIC’s A-D-A molecular motif is made up of strong electron-withdrawing end groups on either side of a planar fused-ring electron-donating core. Through chemical modification of the core and terminal units, this architecture allows for fine control of the LUMO level and intermolecular packing [88,89]. Consequently, ITIC-based blends showed better voltage and less energy disorder than polymer fullerene systems, proving that non-fullerene acceptors are practical substitutes rather than incremental alternatives [90]. ITIC-based devices allowed for new understanding of morphology control in bulk heterojunctions in addition to efficiency gains. ITIC derivatives form well-defined nanoscale phase-separated morphologies with common polymer donors, promoting balanced charge transport while inhibiting excessive recombination, according to extensive experimental studies [91]. Under ideal processing conditions, consistent device operation and repeatable high fill factors were made possible by these morphological benefits. Notwithstanding these developments, the ITIC family also revealed important issues that influenced later acceptor design. Long-term stability and final current production were limited by photochemical instability of the terminal electron-withdrawing groups and limited absorption beyond 850 nm [92,93]. Additionally, nonradiative recombination related to charge-transfer states remained non-negligible even though ITIC-based devices greatly reduced voltage losses in comparison to fullerene systems [94,95]. This prompted the search for acceptors with improved delocalization and electrostatic control. By defining important design principles—strong and controllable absorption, regulated molecule packing, and decreased energy disorder—ITIC and similar A-D-A acceptors ushered in the non-fullerene era of organic photovoltaics. These ideas directly influenced the creation of subsequent Y-series acceptors. As a result, ITIC serves as both an alternate acceptor class and the fundamental first step toward the development of contemporary high-efficiency non-fullerene solar cells.

4.2. Y-Series Acceptors: Delocalization, Quadrupole Moments, and Barrierless Charge Separation

The second and more revolutionary paradigm change in organic photovoltaics is represented by Y-series non-fullerene acceptors, which overcome the inherent drawbacks of previous A-D-A acceptors like ITIC. Y-series materials (e.g., Y6 and its derivatives) introduced fundamentally different electronic and morphological characteristics, such as extended intramolecular delocalization, large quadrupole moments, and near-barrierless charge separation, which together enabled power conversion efficiencies exceeding 18–20% [96], while ITIC established the viability of non-fullerene systems. Strong π stacking and three-dimensional charge delocalization are facilitated by the highly fused, ladder-type cores of Y-series acceptors. Even with slight donor–acceptor energy offsets, this delocalization lowers exciton binding energies and energetic disorder, allowing for effective charge separation [96]. Y-series materials have strong quadrupole moments that produce long-range electrostatic fields at donor–acceptor interfaces, in contrast to ITIC-type acceptors. By reducing interfacial energy barriers and facilitating spontaneous charge dissociation without the need for significant LUMO offsets, these fields successfully bend local energy landscapes [97]. A novel regime of bulk heterojunction organization is introduced morphologically by Y-series acceptors. Y-series blends frequently form delicately interpenetrating

networks with eutectic-like acceptor fibrils, balancing phase purity with percolation channels for both electrons and holes, according to advanced characterization investigations [98]. Even in thick active layers crucial to large-area processing, this architecture maintains minimal recombination losses while supporting high current densities [99]. Subtle differences in halogenation, side-chain engineering, and backbone curvature have a significant impact on nanoscale packing and vertical phase distribution, which directly affects fill factor and operational stability, as further shown by molecular-level investigations [100]. Crucially, Y-series acceptors significantly lower voltage losses in comparison to early non-fullerene and fullerene systems. Y-series blends routinely exhibit lower reorganization energies and suppress nonradiative recombination, which results in record-low energy losses (E_{loss}) in BHJ solar cells [101]. Studies on thermal annealing and processing also show that Y-series systems have a good balance between morphological stability and crystallization kinetics, which enhances device lifetimes under operating conditions [102]. By separating charge separation from significant energy offsets and reorienting performance optimization toward electrostatics, delocalization, and morphological control, Y-series acceptors reinvent the design space of organic photovoltaics. In addition to establishing Y-series materials as the most advanced acceptors available today, these discoveries offer a foundation for the logical design of next-generation non-fullerene systems. The history of electron acceptor design in organic solar cells is depicted in Figure 11, which shows the paradigm shifts from fullerene derivatives to A–D–A non-fullerene acceptors and then to Y-series acceptors. Optical absorption, energy disorder, and charge-separation barriers are among the major constraints addressed at each stage that are emphasized to highlight the structure–property linkages controlling device performance.

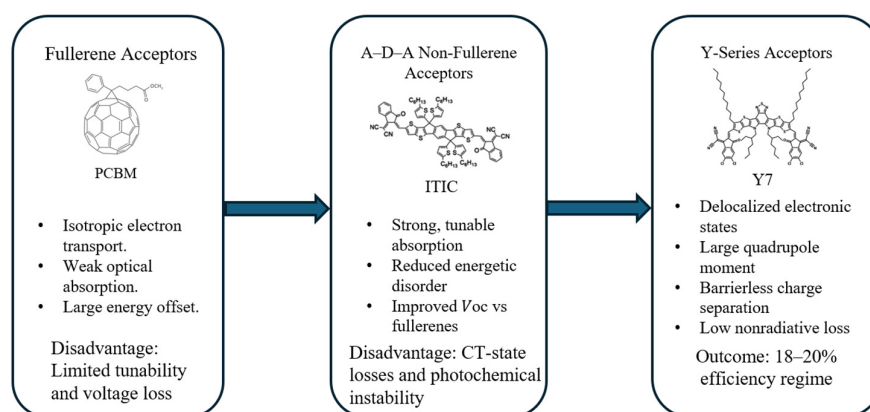


Figure 11. Representation of the evolution of electron acceptor design in organic solar cells. The arrows denote the progression from fullerene acceptors to A–D–A non-fullerene acceptors and finally to Y-series acceptors.

The transition from fullerene acceptors to ITIC-type A–D–A non-fullerene acceptors demonstrated that the optical and energy constraints of fullerene-based systems may be overcome by molecularly designed acceptors. Strong absorption and adjustable energy levels, however, were not enough to completely eradicate voltage losses and interfacial recombination, as seen by the performance ceiling and stability issues seen in ITIC variants. These restrictions prompted a more thorough investigation of charge-separation techniques that go beyond straightforward energy offsets. Y-series acceptors, which emphasize electronic delocalization, electrostatic phenomena, and morphology-controlled interfaces, established a radically different design philosophy in this setting. This shift decoupled efficient charge separation from large donor–acceptor energy offsets and enabled a new regime of low nonradiative loss and high photocurrent generation. The following

section discusses how these concepts are embodied in Y-series acceptors and why they define the current state of the art in organic solar cell performance.

5. Energy Level Alignment at Donor–Acceptor Interfaces

After discussing donor and acceptor materials, how these materials interact energetically when coupled inside a bulk heterojunction architecture is crucial to the functioning of organic solar cells. Because organic semiconductors have a relatively low dielectric constant, photoexcitation in organic photovoltaic systems produces tightly bound excitons rather than free carriers. Therefore, a carefully designed energetic interface between the donor and acceptor that promotes exciton dissociation and charge transfer is necessary for effective device operation [103,104]. The thermodynamic driving force for charge separation, the creation of interfacial CT states, and eventually the device's achievable open-circuit voltage is all determined by the alignment of the energy-level at the donor–acceptor interface. Excessive energy loss during charge transfer or ineffective exciton dissociation can result from improper alignment. Consequently, a key design element in contemporary organic photovoltaic research is the optimization of border orbital offsets between donor and acceptor materials [105,106]. The main energetic factors influencing donor–acceptor interfaces are covered in this part. These factors include charge-transfer state energetics, frontier orbital alignment, and methods for reducing voltage losses in high-efficiency organic solar cells. An energy-level diagram of a donor–acceptor interface is shown in Figure 12, which shows photoexcitation in the donor, electron transfer to the acceptor LUMO, and subsequent charge separation and transport away from the interface.

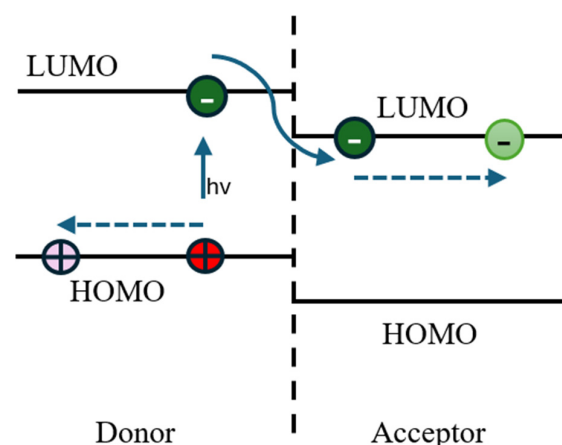


Figure 12. Schematic energy-level diagram of a donor–acceptor interface showing exciton generation, electron transfer to the acceptor, and charge separation.

5.1. Frontier Orbital Alignment and Exciton Dissociation

The efficiency of exciton dissociation in organic solar cells depends on the relative alignment of the HOMO and LUMO levels between donor and acceptor materials. An exciton is produced when the donor material is photoexcited, and it must diffuse to the donor–acceptor interface before recombining. If the energetic offset between these levels is greater than the exciton binding energy at the interface, electron transfer from the donor LUMO to the acceptor LUMO may take place [107]. In the past, to guarantee effective charge separation, early polymer-fullerene solar cells needed comparatively large LUMO offsets (usually 0.3–0.5 eV). Interfacial charge-transfer states were created because of the quick electron transfer from the excited donor to the fullerene acceptor made possible by this powerful driving force [108]. Large energetic offsets, however, also result in significant energy losses during the charge-transfer process, which lowers the maximum open-circuit voltage that may be achieved. It is now evident that effective charge separation can take

place even with much smaller energy offsets thanks to the development of contemporary non-fullerene acceptors. Charge transfer occurs efficiently with offsets less than 0.2 eV in many high-efficiency donor–acceptor systems, especially those based on Y-series acceptors. This result implies that beyond straightforward energy considerations, elements like molecule delocalization, electronic coupling, and dielectric screening play significant roles in promoting charge separation [109,110].

5.2. Charge-Transfer States and Voltage Loss

An essential intermediate stage in the functioning of organic solar cells is the creation of interfacial charge-transfer states. The electron and hole remain Coulombically coupled across the donor–acceptor interface during electron transfer, creating a CT state. The energy of this CT state has a significant impact on the device’s open-circuit voltage and charge-separation efficiency [111]. The energetic difference between the energy of the CT state and the optical bandgap of the donor–acceptor system is the source of voltage losses in many organic solar cells. The maximum attainable voltage is lowered if the CT state is substantially below the optical gap due to the resulting energy loss. Likewise, the device voltage can be further reduced by nonradiative recombination processes connected to CT states [112]. According to recent research, obtaining high open-circuit voltages requires decreasing the energy difference between the optical gap and the CT state. Modern organic solar cells may now reduce voltage losses to values close to 0.5 eV thanks to developments in molecular design, especially the creation of NFAs with adjustable energy levels [113]. To control CT states and reduce open-circuit voltage losses, several molecular design techniques have been developed. For instance, because of Y6’s delocalized electronic structure, which lowers CT-state binding energy and encourages charge separation, the PM6:Y6 system exhibits effective charge production despite a very tiny donor–acceptor energy offset. In a similar vein, chlorinated Y-series acceptors, such Y7, lessen voltage losses by reducing nonradiative recombination through better molecular packing and increased electroluminescence efficiency. The energy gap between the optical bandgap and the CT-state energy can also be reduced by optimizing interfacial energetics and reducing energetic disorder by donor polymer side-chain engineering and fluorination. These examples show that contemporary OSCs suppress V_{oc} losses by controlling CT-state energetics and lowering nonradiative recombination routes rather than by raising energetic driving force.

5.3. Energy-Level Engineering in Modern Organic Solar Cells

The possibilities for adjusting donor–acceptor energy alignment have greatly increased with the advent of non-fullerene acceptors. Modern acceptor molecules can be chemically tailored to obtain precise energy alignment with donor materials, in contrast to fullerene derivatives, which provide limited control over frontier orbital energies. HOMO and LUMO levels can be systematically tuned while also altering intermolecular interactions by structural changes including conjugation extension, side-chain engineering, and fluorination [114]. Specifically, Y-series acceptors have shown that when strong electronic coupling and delocalized charge-transfer states are present, effective charge separation can take place with little energetic driving force. Power conversion efficiencies surpassing 19% in single-junction organic solar cells are made possible by these materials’ high absorption coefficients, advantageous energy-level alignment with polymer donors, and decreased nonradiative recombination losses [115,116]. Overall, one of the most important factors influencing the performance of organic solar cells is still energy-level alignment. It is anticipated that further advancements in interface engineering and molecular design would minimize voltage losses while preserving effective charge generation. Thus, the

development of next-generation organic photovoltaic systems will continue to depend on an understanding of the connection between energy offsets, CT state creation, and molecular interactions. Successful donor–acceptor pairing necessitates a balance between energetic compatibility and morphological compatibility in addition to energy-level alignment. Excessive energetic offsets increase voltage losses, yet adequate HOMO–LUMO offsets are required to facilitate charge transfer. To create nanoscale phase-separated domains like the exciton diffusion length, donor and acceptor materials must simultaneously show considerable miscibility. To enable effective charge generation, charge transport, and decreased recombination losses, the most crucial compatibility concept in contemporary OSC design is to achieve advantageous energy-level alignment while preserving excellent donor–acceptor miscibility.

Table 3 summarizes representative energy-level engineering strategies that have been employed to regulate CT-state energetics, reduce voltage losses, and improve photovoltaic performance.

Table 3. Representative strategies for donor–acceptor energy-level engineering and their impact on OSC performance.

Strategy	System	Mechanism	Outcome
Reduced D–A offset	PM6: Y6	Delocalization assisted charge separation	High V_{oc} , low voltage loss
Chlorination	PM6: Y7	Reduced nonradiative recombination	Improved V_{oc} and PCE
Fluorination	PBDB-T-2F systems	HOMO tuning and reduced disorder	Higher V_{oc}
CT-state engineering	PTQ10: Y6	Reduced CT-state energy loss	Improved charge generation
Energy cascade design	Ternary OSCs	Facilitated charge transfer	Increased J_{sc} and PCE

6. Chemical Interactions and Morphological Organization in Donor–Acceptor Systems

In addition to the electrical structure of the donor and acceptor materials, the performance of OSCs is also influenced by the molecular interactions and nanoscale morphology that result from blending these materials. Exciton dissociation, charge transfer, and recombination take place in an interpenetrating network formed by the donor and acceptor in bulk heterojunction structures. As a result, the final morphology and device efficiency are significantly influenced by the chemical interactions between donor and acceptor molecules. As a result, current OSC research has advanced beyond straightforward material selection to a more profound comprehension of how molecular design controls phase separation, nanoscale ordering, and intermolecular interactions. The way donor and acceptor molecules self-assemble during film formation is largely determined by these interactions, which include π – π stacking, dipole–dipole interactions, hydrogen bonding, and noncovalent conformational locking. The effectiveness of exciton diffusion, charge transfer, and carrier transport in the device is ultimately determined by the resultant morphology [117,118]. Research on donor–acceptor blends has shown that controlled phase separation and molecular ordering must be carefully balanced for the best photovoltaic performance. While excessive phase separation might reduce exciton dissociation by decreasing the interfacial area, excessive mixing may decrease charge transport channels. Thus, one of the most significant hurdles in the design of next-generation OSC materials is still comprehending the molecular origin of morphology development [119]. The conceptual representation in Figure 13 illustrates how charge transport and photovoltaic performance are determined by intermolecular interactions in conjugated D–A systems, which regulate molecular packing, phase separation, and nanomorphology.

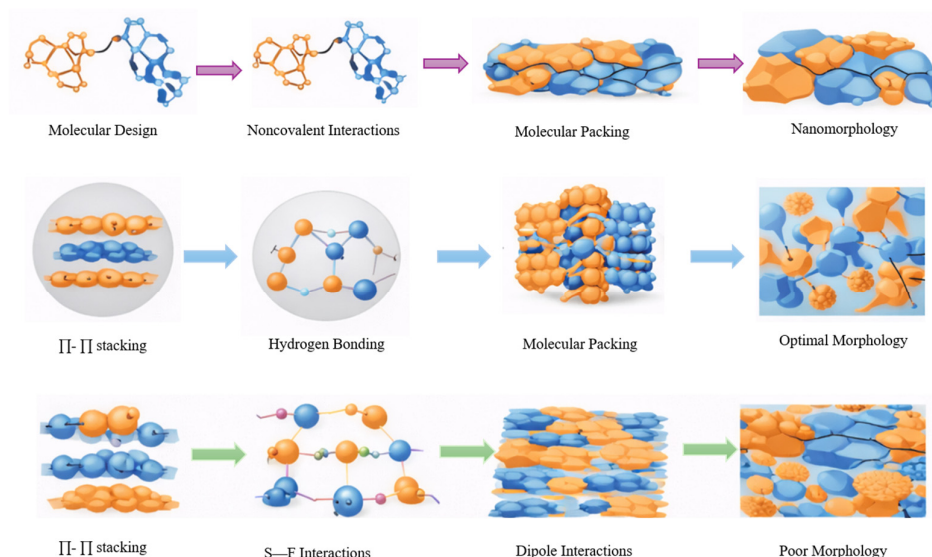


Figure 13. Relationship between molecular design, intermolecular interactions, nanomorphology, and device performance in donor–acceptor organic solar cells.

6.1. Intermolecular Noncovalent Interactions in Donor–Acceptor Blends

In conjugated organic semiconductors, noncovalent interactions are essential for regulating molecule packing and electrical coupling. π - π stacking, hydrogen bonding, dipole–dipole interactions, and heteroatom-based interactions like S $\cdots$ O, S $\cdots$ F, and N $\cdots$ H bonds are some examples of these interactions. Because they promote orbital overlaps and permit effective carrier mobility inside the active layer, π - π stacking interactions between conjugated backbones are especially crucial for charge transfer. Strong π - π interactions encourage orderly molecule packing, which enhances electronic delocalization and lowers the material’s energy disorder [120]. Modern donor polymer design has made extensive use of noncovalent conformational locking, such as sulfur–oxygen or sulfur–fluorine interactions, in addition to π - π stacking, to improve backbone planarity. Stronger intermolecular coupling and better molecular ordering are the outcomes of these interactions, which limit torsional motion along the conjugated backbone [121]. Controlling donor–acceptor assembly can also be significantly influenced by hydrogen bonds. In some donor–acceptor systems, cooperative hydrogen bonding interactions have been demonstrated to produce orientated nanostructures and enhanced phase organization. Favorable packing patterns that improve charge transport and exciton dissociation can be stabilized by such interactions [122]. The importance of quadrupole moments and electrostatic interactions NFAs, especially in Y-series materials, has been further emphasized by recent research. These electrostatic interactions affect the development of charge-transfer states at the donor–acceptor interface and aid in the construction of organized molecular aggregates [123].

6.2. Molecular Planarity and Stacking in Conjugated Systems

The electrical characteristics and packing behavior of organic semiconductors are significantly influenced by the planarity of conjugated molecules. Stronger π - π stacking interactions are encouraged by planar molecule backbones, which facilitate effective charge transport channels in the active layer. To improve backbone planarity and intermolecular interactions, several donor polymer families, such as DPP, isoindigo, BDT, and thiophene-based polymers, have been developed. These materials are appealing options for high-performance OSCs due to their strong intermolecular packing and high charge-carrier mobilities [124]. For instance, extremely planar aromatic units seen in DPP-based polymers encourage strong π - π stacking and long-range electronic delocalization. In a similar vein,

isoindigo-based polymers have stiff conjugated backbones that facilitate favorable molecular ordering and effective charge transfer in thin films [125]. The shape of D-A blends can be significantly influenced by the degree of π - π stacking. Ordered crystalline domains that enhance charge mobility can be formed by strong stacking interactions, but they must stay small enough to sustain effective exciton dissociation. Therefore, to balance crystallinity and miscibility within the active layer, careful molecular design is needed [126].

6.3. Donor–Acceptor Miscibility and Phase Separation

To enable exciton dissociation and charge transmission, bulk heterojunction OSCs depend on nanoscale phase separation between donor and acceptor materials. Domain sizes in the active layer should ideally be on the order of the exciton diffusion length, or roughly 10–20 nm. Excitons produced within the donor material may recombine before they reach the D-A contact if domains are too big. On the other hand, excessive mixing between donor and acceptor molecules could interfere with charge transport pathways, which would lower the performance of the device [127]. The Flory–Huggin’s interaction parameter, which represents the thermodynamic compatibility of the two components, is frequently used to characterize the miscibility between donor and acceptor materials. The miscibility between donor and acceptor molecules can be drastically changed by minor structural modifications such side-chain engineering or fluorination, which can result in large morphological alterations [128]. The final active layer shape is also greatly influenced by processing conditions. Phase separation and molecular ordering in OSC films are frequently controlled by methods such solvent engineering, thermal annealing, and solvent vapor annealing. By using these techniques, researchers can increase device efficiency by optimizing the nanoscale morphology [129].

6.4. Impact of Morphology on Device Performance

Exciton diffusion, charge separation, charge transport, and recombination dynamics in organic solar cells are all significantly influenced by the nanoscale shape of D-A blends. To guarantee effective exciton harvesting at donor–acceptor interfaces, donor and acceptor domains must have characteristic dimensions like this length scale since exciton diffusion lengths in organic semiconductors are usually restricted to about 10–20 nm [130]. Moreover, to enable effective charge extraction, the shape must concurrently offer continuous percolation channels for electrons and holes [131,132]. Device performance can be severely impacted by undesirable shape. Excitons recombine before they reach a donor–acceptor interface due to excessive phase separation, which reduces photocurrent generation by creating donor or acceptor domains bigger than the exciton diffusion length. On the other hand, excessive donor–acceptor mixing can diminish charge-carrier mobility and FF by disrupting charge-transport routes, increasing energetic disorder, and promoting carrier entrapment [133]. Furthermore, whereas inadequate molecular ordering frequently restricts charge transport and raises transport losses, highly crystalline domains may promote bimolecular recombination and cause charge accumulation [134]. Additionally, morphology has a significant impact on OSCs’ operating stability. Phase segregation, crystallization, or changes in the vertical composition distribution might result from morphological evolution under extended illumination or heat stress, which can modify charge-transport pathways and raise recombination losses [135]. Therefore, one of the most crucial conditions for concurrently achieving high efficiency and long-term stability in organic solar cells is striking an ideal balance between molecular ordering, donor–acceptor miscibility, and nanoscale phase separation [136].

The relationship between intermolecular interactions, morphology development, and photovoltaic performance is summarized in Table 4.

Table 4. Molecular interactions in donor–acceptor systems and their influence on morphology and device performance.

Interaction Type	Representative Materials	Morphological Effect	Device Effect
π - π stacking	D18, PTQ10, Y6	Enhanced molecular ordering	Improved mobility and FF
Hydrogen bonding	Functionalized D-A systems	Directed self-assembly	Improved phase organization
S...F interaction	PM6, PBDB-T derivatives	Backbone planarization	Reduced energetic disorder
S...O interaction	BDT based donors	Increased crystallinity	Enhanced charge transport
Quadrupole interactions	Y6 NFAs	Controlled aggregation	Reduced non radiative losses
D-A miscibility	PTQ10: Y6, PM6: Y6	Optimal nanoscale phase separation	Higher PCE

7. Device Engineering and Process Strategies

The basic electrical characteristics of OSCs are determined by the molecular design of donors and acceptor materials, but the efficiency of these materials in real-world photovoltaic devices is ultimately determined by the device architecture and processing circumstances. If the active layer morphology, interface energetics, or electrode contacts are improperly constructed, even highly optimized donor–acceptor systems may show poor device performance. According to recent publications [137,138], device engineering has become a crucial part of current OSC development, enabling efficiency exceeding 19%. The active layer of bulk heterojunction solar cells is created by combining donor and acceptor materials to produce an interpenetrating network that promotes charge transfer and exciton dissociation. However, the conditions of film deposition, the choice of solvent, and post-processing procedures all have a significant impact on the creation of this morphology. Thus, during the past ten years, OSC efficiency has advanced rapidly due in large part to advancements in device engineering, including interface design, processing control, and device architectural optimization [139,140].

7.1. Bulk Heterojunction Architecture

The active layer of bulk heterojunction solar cells is created by combining donor and acceptor materials to produce an interpenetrating network that promotes charge transfer and exciton dissociation. However, the conditions of film deposition, the choice of solvent, and post-processing procedures all have a significant impact on the creation of this morphology. Thus, during the past ten years, OSC efficiency has rapidly increased due in large part to advancements in device engineering, including interface design, processor control, and device architecture. Because organic semiconductors have a low dielectric constant, tightly bound excitons are produced when photons are absorbed in the donor material [141]. Before they recombine, these excitons must diffuse to the D-A contact. Excitons produced within the donor can effectively reach the interface and undergo charge separation thanks to the BHJ architecture's significant increase in the accessible interfacial area [142]. After exciton breakup, holes travel through the donor phase toward their respective electrodes, whereas electrons travel through the acceptor network. Therefore, an ideal nanoscale morphology that strikes a compromise between phase separation and interfacial contact and continuous charge transport channels inside both donor and acceptor domains are necessary for efficient device functioning [143,144]. The various BHJ device architectures are shown in Figure 14.

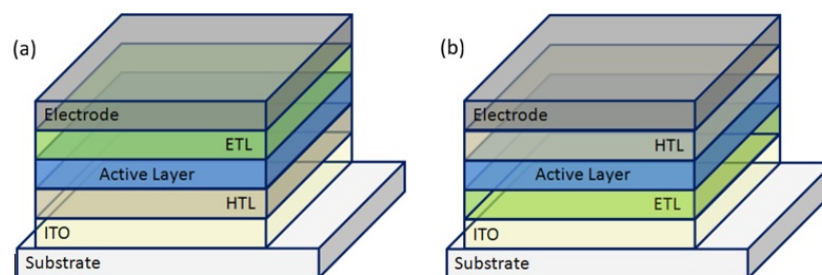


Figure 14. Different device architectures of bulk heterojunction solar cells. (a) Standard device design with the cathode on top of the device stack and (b) inverted device architecture with the cathode located on the transparent substrate.

7.2. Interface Engineering

Device efficiency is mostly determined by the interfaces between the organic semiconductor and the electrodes, in addition to the active layer. Recombination losses and decreased device performance might result from poorly aligned energy levels or ineffective charge extraction at these interfaces [138]. Interfacial layers are frequently added between the electrodes and the active layer to improve charge extraction and lower recombination to overcome these issues. Usually, these layers are categorized as either HTLs or ETLs. PEDOT: PSS, MoO_3 , and NiO_x are examples of common HTL. These substances prevent electron transport toward the anode while promoting effective hole extraction. Similarly, to encourage electron extraction and prevent holes at the cathode interface, ETL materials such as ZnO , TiO_x , and PFN-Br are employed [145]. Interfacial layers can modify the active layer's shape and molecular ordering during film creation, which can further impact device performance in addition to enhancing charge extraction. As a result, careful interface designing has emerged as a key tactic for maximizing OSC stability and efficiency [146].

7.3. Processing Techniques and Morphology Control

The processing parameters utilized during film deposition have a significant impact on the morphology of the donor–acceptor blend. The active layer's nanoscale morphology can be dramatically changed by small changes in the solvent selection, drying rate, or post-deposition treatment. Solvent engineering, which uses solvent mixtures or additives to adjust the crystallization behavior of donor and acceptor materials, is one popular method for controlling morphology. Chloronaphthalene (CN) and 1,8-diiodooctane (DIO) are examples of solvent additions that might improve molecular ordering in the film and slow the drying process [147]. Another popular method for improving phase separation and molecule packing in OSC films is thermal annealing. Improved charge transport and device performance can result from controlled heating that increases crystallinity in the donor and acceptor phases [148]. To fine-tune nanoscale morphology, solvent vapor annealing has been used in addition to thermal annealing. By using this method, the active layer can reorganize when exposed to solvent vapor, improving phase separation and molecular ordering without compromising the film structure [149]. These processing techniques are frequently required to produce high-efficiency OSC devices and are critical in shaping the final morphology of the active layer. The notable performance gains made possible via morphological optimization are demonstrated by representative experiments. For instance, Ma et al. found that thermal annealing of P3HT bulk heterojunction solar cells improved the morphology of the nanoscale interpenetrating network, leading to increased charge transport and an improvement in power conversion efficiency from about 2.5% to over 5% [150]. Like this, PTB7-based devices have made extensive use of solvent additives like DIO to maximize phase separation and molecular ordering, which has resulted in significant gains in fill factor and short-circuit current density when compared to additive-

free devices [151]. More recently, it has been demonstrated that morphological tuning can enhance molecular packing, lower recombination losses, and permit power conversion efficiencies of 18% in non-fullerene acceptor systems, such as PM6 and related Y-series blends [152]. These examples demonstrate that processing-induced morphology control is often as important as molecular design in determining OSC performance.

As shown in Table 5, processing strategies such as thermal annealing, solvent-additive engineering, and morphology optimization can significantly improve charge transport, reduce recombination losses, and enhance overall device efficiency. These results demonstrate that morphology control is a critical complement to molecular design in high-performance organic solar cells.

Table 5. Representative examples of performance enhancement in OSCs achieved through morphology optimization and processing engineering.

System	Optimization	PCE Before	PCE After
P3HT: PCBM	Thermal annealing	~2.5%	>5%
PTB7: PCBM	DIO additive	~6–7%	~8–9%
PM6: Y6	Morphology optimization	~15–16%	>18%

As OSC technologies advance to large-scale manufacturing, the connection between molecular design and manufacturability has grown in significance. Solubility, aggregation behavior, drying kinetics, and film-forming properties are all directly influenced by molecular characteristics such side-chain length, branching position, backbone planarity, and halogenation. Optimized side-chain engineering, for instance, can enhance compatibility with non-halogenated solvents like toluene and o-xylene, allowing for environmentally friendly processing. Similarly, in high-speed coating processes like roll-to-roll production and slot-die coating, controlled aggregation behavior is crucial for preserving morphological tolerance. As a result, current donor and acceptor design increasingly takes manufacturing compatibility and processing resilience into account in addition to photovoltaic performance.

7.4. Device Stability Challenge

OSC degradation can generally be classified into photochemical instability, thermal instability, morphological instability, and interfacial/electrode degradation. Photochemical degradation arises from prolonged exposure to light and oxygen, leading to molecular bond breaking and the formation of trap states. Thermal instability can induce phase segregation and crystallization within the active layer, while morphological instability alters nanoscale donor–acceptor organization and charge-transport pathways. In addition, diffusion of electrode materials and degradation of interfacial layers may increase series resistance and recombination loss over time [144]. The burn-in effect, in which the device effectiveness rapidly drops over the first few hours of operation before stabilizing, is a common degradation phenomenon seen in OSC devices. This impact is frequently linked to the creation of trap states within the material or structural alterations in the active layer morphology [153]. Also, donor and acceptor materials may undergo chemical degradation because of extended illumination, especially in the presence of oxygen. These degradation processes have the potential to change energy levels, decrease charge mobility, and eventually impair device performance. Molecular design, better encapsulation methods, and the creation of more stable device designs, especially inverted structures, have all been the focus of recent research efforts to increase OSC stability [154]. A comprehensive design framework that incorporates molecular design, energy-level engineering, intermolecular interactions, morphological control, and processing optimization is increasingly needed

to solve long-term OSC stability, according to recent studies. Structural disorder can be decreased and photochemical degradation suppressed by molecular design techniques such side-chain engineering, backbone rigidification, and the creation of intrinsically stable donor and acceptor materials. Recombination-induced breakdown pathways and charge accumulation are reduced by optimal donor–acceptor energy alignment. During operation, intermolecular interactions such as noncovalent conformational locking and π – π stacking decrease morphological evolution and encourage stable molecular packing. Like this, regulating phase separation and donor–acceptor miscibility aids in preserving advantageous nanoscale morphologies under heat and light stress. Lastly, processing methods including thermal annealing, solvent engineering, and scalable coating processes can enhance device repeatability and further stabilize active-layer morphology. When combined, these tactics show that the synergistic optimization of molecular, energy, morphological, and processing parameters across the device architecture determines operational stability rather than a single material parameter.

7.5. Ternary Blend Strategies

Ternary OSCs have become a successful device-engineering approach for concurrently enhancing light harvesting, charge transport, morphology, and voltage-loss management, going beyond traditional binary donor–acceptor systems. A third photoactive component is purposefully added to a binary donor–acceptor blend in ternary OSCs. The third component can serve as a complimentary absorber, morphological regulator, energy-cascade mediator, or recombination suppressor, depending on its energetic alignment and miscibility with the host materials [155,156]. The capacity of ternary blends to expand the absorption spectrum and boost photocurrent generation is one of their main benefits. Ternary systems can capture a greater portion of the solar spectrum while preserving effective charge transport channels by adding a donor or acceptor with comparable absorption properties [157,158]. Furthermore, the third component can enhance molecular packing and control nanoscale phase separation, resulting in more balanced electron and hole transport and less bimolecular recombination [159]. Ternary techniques can successfully minimize nonradiative voltage losses while maintaining high short-circuit current density and fill factor, according to recent studies. According to Jiang et al., the addition of a properly chosen third component allowed all-small-molecule OSCs to simultaneously optimize their morphology and reduce voltage loss by improving molecular ordering and lowering energy disorder [160]. Similarly, Duan et al. showed that high-efficiency rigid and flexible OSCs with improved operational stability were made possible by ternary blend engineering, which decreased nonradiative recombination [161]. In contemporary NFA systems, the efficiency of ternary methods has become especially clear. Ternary OSCs have attained efficiencies close to and even higher than 20% by carefully adjusting mix composition, energy-level alignment, and molecule electrostatics. For instance, Yang et al. demonstrated the capacity of ternary architectures to concurrently enhance charge generation, charge transport, and long-term stability by reporting over 20% power conversion efficiency through the cooperative optimization of ternary composition and molecular electrostatics [162]. Ternary blends not only improve efficiency but also offer increased scalability and processing tolerance. For large-area production and roll-to-roll fabrication, the addition of a third component can stabilize advantageous morphologies, lessen sensitivity to processing conditions, and enhance thick-film device performance [163,164]. To overcome the inherent trade-offs between current generation, voltage losses, morphology control, and device stability in high-performance organic solar cells, ternary blend engineering has emerged as a flexible and widely applicable approach. Future tandem organic solar cells must concurrently meet several material and production requirements. To optimize solar spectrum, use

while reducing optical losses, the photoactive materials utilized in the front and back sub cells should first have complimentary absorption spectra. Second, to guarantee effective carrier extraction and long-term operation, donor and acceptor materials must demonstrate appropriate energy-level alignment, balanced charge transport, and strong photostability. Third, to minimize electrical and optical losses and promote charge recombination between sub cells, extremely transparent and low-resistance connectivity layers are needed. Tandem architecture should work with scalable solution-processing methods like roll-to-roll fabrication, slot-die coating, and blade coating from a manufacturing standpoint. Finally, converting high laboratory efficiencies into commercially viable tandem OSC systems would require enhanced thermal, morphological, and environmental stability.

7.6. Emerging Device Architecture

The traditional OSC structure typically consists of the following configuration:

ITO/PEDOT: PSS/Active Layer/Metal Electrode

However, many modern high-performance OSCs now employ inverted device architectures, which reverse the order of the charge transport layers. In inverted devices, the structure typically follows:

ITO/ZnO/Active Layer/MoO₃/Ag

Improved stability and better compatibility with large-scale fabrication techniques are two benefits of this architecture [165]. Tandem organic solar cells have also surfaced as a viable strategy for boosting power conversion efficiency beyond traditional single-junction devices. To capture a larger range of the solar spectrum, tandem devices stack several active layers with complementary absorption spectra [166]. Furthermore, applications needing flexible and lightweight solar systems find OSC technology especially appealing. OSCs are interesting options for wearable technology, portable electronics, and building-integrated photovoltaics since they can be made on flexible substrates utilizing solution processing techniques. The device architecture of an inverted organic solar cell is depicted in Figure 15.

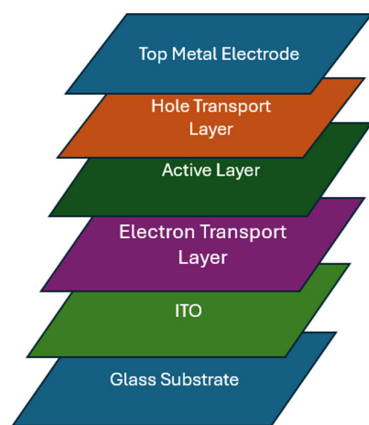


Figure 15. Device architectures of inverted solar cells.

8. Conclusion and Future Perspectives for Donor–Acceptor Chemistry in OSC

Over the past 20 years, organic solar cells have advanced remarkably thanks to developments in device engineering, donor–acceptor chemistry, and molecular design. With the advent of non-fullerene acceptors and the creation of highly optimized donor polymers, power conversion efficiencies have significantly increased, allowing devices that currently surpass 19% efficiency in lab settings. Despite these developments, there are still several scientific and technological obstacles to overcome before organic photovoltaics may be widely used in the commercial sector. Reducing energy losses during charge creation is one

of the most crucial areas of research. Device performance is still constrained by nonradiative recombination and voltage losses, even though contemporary donor–acceptor systems have greatly improved energy-level alignment. Future studies will probably concentrate on creating materials that maximize open-circuit voltage while preserving effective exciton dissociation by enabling effective charge separation with low energy offsets. The stability of organic solar cells over the long term is another important issue. Phase segregation and decreased device efficiency can result from the nanoscale morphology of donor–acceptor mixes changing during heat stress, extended illumination, or environmental exposure. Therefore, enhancing the intrinsic stability of donor and acceptor materials and creating more durable device topologies will be crucial for real world implementation. It is anticipated that advancements in encapsulation technologies and the creation of intrinsically stable materials would be crucial in resolving these problems. Another important area of research is comprehending and managing the emergence of morphology during film processing. Predicting the ultimate morphology of donor–acceptor mixes based on molecular structure is still difficult, despite the development of numerous processing strategies to maximize nanoscale phase separation. The intricate link between chemistry, processing conditions, and morphology development in organic photovoltaic systems may be better understood by combining sophisticated characterization techniques, computational modeling, and machine learning methodologies. The creation of tandem organic solar cells offers an interesting prospect for additional efficiency gains in addition to enhancing single-junction devices. Tandem designs can collect a larger fraction of the solar spectrum and possibly surpass the efficiency constraints of single-junction devices by stacking several active layers with complementary absorption spectra. Realizing the full potential of tandem OSC technologies will require ongoing advancements in interlayer materials and device integration. Lastly, the production of lightweight, flexible, and large-area solar systems benefits greatly from the solution-processable characteristics of organic semiconductors. These features make OSCs especially appealing for new applications, including building-integrated photovoltaics, wearable electronics, and portable energy systems. Transforming laboratory-scale efficiency into scalable production technologies would require ongoing advancements in materials design, processing methods, and device stability.

All things considered, the future of organic solar cells will rely on the ongoing fusion of device engineering, chemical interactions, morphological control, and molecular design. Researchers can create next-generation donor–acceptor systems that combine high efficiency, long-term stability, and scalable fabrication by gaining a better knowledge of the connections between these variables. These developments will be essential to making organic photovoltaics a practical technology for producing sustainable energy.

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Abbreviations

The following abbreviations are used in this manuscript:

A-D-A	Acceptor donor acceptor
BHJ	Bulk heterojunction
BDT	Benzodithiophene
CB	Chlorobenzene
CF	Chloroform
CT	Charge transfer
D-A	Donor acceptor
DIO	1,8-Diiodooctane
DPP	Diketopyrrolopyrrole
EL	Electroluminescence
EQE	External quantum efficiency
FF	Fill factor
FTPS	Fourier transform photocurrent spectroscopy
HOMO	Highest Occupied Molecular Orbital
ITC	3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexyl phenyl)-dithieno [2,3-d:2',3'-d']s-indaceno [1,2-b:5,6-b']dithiophene
JSC	Short circuit current
LUMO	Lowest unoccupied molecular orbital
NFA	Non-fullerene acceptor
NIR	Near-infrared
o-XY	o-Xylene
OFET	Organic field effect transistor
OPV	Organic photovoltaic
OSC	Organic solar cell
PC61BM	[6,6]-Phenyl-C61-butyric acid methyl ester
PC71BM	[6,6]-Phenyl-C71-butyric acid methyl ester
PCE	Power conversion efficiency
PL	Photoluminescence
V _{oc}	Open-circuit voltage

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