



## **Advanced Progress of Organic Photovoltaics**

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Modern civilization and economic development of humankind have been largely based on the exploitation and utilization of fossil energy. It is worth noting that the consumption and over-exploitation of fossil fuels have led to serious environmental pollution and energy shortage. Nowadays, the vigorous development of renewable energy (biomass, geothermal energy, wind energy, solar energy, etc.) to replace fossil fuels has been recognized as a key way to solve these global environmental pollution and energy shortage problems. As a new generation of green energy technology, organic photovoltaics (OPVs) have attracted wide attention due to the unique advantages of light weight, low cost, flexibility, and translucency. In addition to being normal power-generation devices, OPVs also have great application potential in the integration of energy-saving buildings, wearable devices, etc. OPVs have been developed for more than 30 years since 1986, and over 19% of power conversion efficiency (PCE) has been achieved due to the innovation of materials synthesis and the evolution of device engineering. In this Special Issue titled "Advanced progress of organic photovoltaics", we provide a comprehensive overview of OPVs from different perspectives, including contributions from nine different research groups.

This Special Issue on "Advanced progress of organic photovoltaics" includes nine papers from different groups, which refer to the theoretical research for excitons generation, charge separation and recombination of OPVs [1], the innovation of active layer materials [2–4] and interfacial layer materials [5], the optimization of photoelectric conversion process based on a ternary strategy [6], the investigation of encapsulation technology [7], the reviews related to film-forming kinetic process of OPVs [8], and high efficiency OPVs with PCE over 17% [9].

A brief summary of the content associated with each of the selected papers belonging to this Special Issue is included below.

The theoretical analysis is helpful for the in-depth understanding and construction of OPVs. The accuracy of the analytical results is largely determined by the way of treating exciton generation, exciton dissociation, and the charge recombination process. In Md. Shofifiqul Islam, [1] the optical transfer matrix method (OTMM) was employed by the author to calculate photogenerated excitons inside OPVs. It is also found that spherically averaged Gaussian distribution (SAGD) is the most logical and appropriate way to analyze dissociation probability. The performance of OPVs can be evaluated by the improved analytical solution of electrical transport equations, including (i) exciton generation obtained from OTMM, (ii) dissociation probability incorporating Gaussian distribution, and (iii) recombination of charge carriers.

Throughout the history of OPVs' development, the innovation and investigation of active layer materials should be the cornerstone of realizing efficient OPVs. In Haiyan Chen et al. [2], a simple terminal alkyl chain engineering was employed to adjust the active layer morphology towards highly efficient all-small-molecule OPVs. Two isomeric small-molecule donors (BT-RO-Cl and BT-REH-Cl) were synthesized, in which linear n-octyl (O) and branched 2-ethylhexyl (EH) were employed as the terminal alkyl chain. The BT-REH-Cl: Y6-based OPVs show higher PCE as compared to BT-RO-Cl: Y6-based



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**Copyright:** © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). OPVs due to improved phase separation and molecular arrangement for efficient charge transport in active layers. This work demonstrates that alkyl chain engineering should be an effective method for designing efficient small molecule donors. In Alexander N. Solodukhin et al. [3] the authors comprehensively investigated six star-shaped donor-acceptor molecules with electron-withdrawing terminal hexyldicyanovinyl fragments linked through the 2,20-bithiophene  $\pi$ -spacer to the different branching cores: TPA, m-TPA, f-TPA, s-CBZ, t-CBZ, and BTI. The effects of donor branch core type on the optical and electrochemical properties of films, the phase separation of active layers, and the performance of single-component and bulk heterojunction OPVs can be revealed. In Zahoor UI Islam et al. [4] the potential applications of zinc phthalocyanine (ZnPc) as active layers was explored, in which ZnPc was sandwiched between ITO/PEDOT:PSS and the Ag electrode. The ZnPc thin films show broad absorption spectra in the visible range and uniform surface morphology with a small roughness value of 15.48 nm, which should support efficient photon harvesting, exciton dissociation, and charge transport process. This work demonstrates that ZnPc is one of the candidates for the construction of OPVs.

In addition to the synthesis and exploration of newly active layer materials, the evolution of interfacial layer materials is also crucial for the preparation of high-efficiency OPVs. In Roberto Sorrentino et al. [5] the authors focused on increasing the performance of OPVs by designing and synthesizing a naphthalene diimide-based cathode interlayer (NDI-OH) with a facile three-step reaction. The NDI-OH possesses good solubility in alcohol solvents, good film-forming ability, and film thickness insensitivity, as well as self-doping properties, which makes NDI-OH suitable as a cathode interlayer. Both the PCEs of PTB7-Th:PC<sub>71</sub>BM and PTB7-Th: ITIC-based OPVs are increased by incorporating NDI-OH as cathode interlayer as compared to that of OPVs without cathode interlayer and with PFN or evaporated Ca as cathode interlayer.

From the device engineering perspective, ternary OPVs have been established to improve photon harvesting of active layers as much as possible by integrating two acceptors/one donor or two donors/one acceptor with complementary absorption spectra into one active layer. In Miron Krassas et al. [6] a conjugated and ladder-type multi-fused ring 4,7-dithienbenzothiadiazole:thiophene derivative (compound 'T') was synthesized and incorporated into PTB7:PC<sub>71</sub>BM host system to construct ternary OPVs. The incorporation of the compound T led to a favorable energy cascade between PTB7 and PC<sub>71</sub>BM, which should be beneficial to charge transfer. The PCE of ternary OPVs can be increased from 7.51% to 8.25% by incorporating 5 vol% compound "T", resulting from simultaneously improved short circuit current density, open circuit voltage, and fill factor. This work further demonstrates that a ternary strategy should be an effective and simple method to realize performance improvement in OPVs.

Benefiting from the synthesis of state-of-the-art active layer/interfacial layer materials and advanced device engineering, remarkable progress has been made in OPVs. It is worth noting that the intrinsically unstable nature of the organic materials involved is still delaying the OPVs' commercialization. It is essential to significantly improve the lifetime of OPVs. In Jarhoon Kim et al. [7] the authors investigated the effect of hydrophobic cyclized transparent optical polymer (CYTOP) encapsulation on the performance of OPVs. The CYTOP-encapsulated and bare OPVs can maintain 96% and 82% initial efficiency after 35 days of shelf storage, which suggests that the introduction of a CYTOP encapsulation layer can effectively block moisture and oxygen and improve the stability of OPVs.

Finally, two reviews are summarized from different perspectives, which are related to film-forming kinetic process [8] and the progress of OPVs with PCE over 17% [9], respectively. In Qiuju Liang et al. [8] the authors focused on the relationship between the film-forming dynamic process and the active layer morphology of OPVs. It is concluded that the film-forming dynamic process influences the degree of molecular crystallinity, molecular orientation, molecular domain sizes, and phase-separation structure of active layers. The authors also summarized the different methods employed by researchers to adjust the film-forming dynamic process, including thermal annealing, solvent vapor

annealing, adding solvent additives, and changing the solvent. Some typical examples were given and discussed in detail to reveal the relationship between the morphology and the device performance. Furthermore, the authors outlined the future development of the film morphology control, which may provide some guidance for further optimizing the device performance of OPVs. In Xuelin Wang et al. [9] the authors summarized the recent progress of OPVs with an efficiency over 17%. From the material synthesis perspective, typical donor/acceptor materials and newly interfacial materials for preparing highly efficient OPVs, as well as materials' evolution process, were introduced in detail. From the device-engineering perspective, multicomponent-based OPVs, and tandem OPVs, as well as their underlying wording mechanism, were summarized in detail. In the final part of the paper, the authors proposed that the next step of research should focus on how to make the fabrication technology of OPVs more suitable for scaling up and commercialization.

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