



SPECIAL TOPIC: Photovoltaic Materials, Devices, and Applications

Editorial: special topic on photovoltaic materials, devices, and applicationsLifu Zhang¹, Bin Kan², Yiwang Chen^{1*}, Yongsheng Chen^{3*} and Yongfang Li^{4*}

To reduce society's dependence on fossil fuels, new photovoltaic technologies are driving a fundamental change in the way renewable energy is utilized. This issue of "Photovoltaic Materials, Devices, and Applications" focuses on the latest breakthroughs in this field, and systematically discusses the path of technological innovation, practical challenges, and future opportunities.

As the frontier of photovoltaic technology, third-generation thin-film photovoltaics (e.g., organic and perovskite photovoltaic (PVK)) have significantly improved photovoltaic conversion efficiency and stability through innovative design of photoactive materials and optimization of device structures. With their solution processability, lightweight, and flexibility, these technologies show unique competitive advantages and industrialization potential in cutting-edge applications including wearable electronic devices and integrated photovoltaic systems.

The selected research papers and reviews systematically present the latest breakthroughs in novel photovoltaic technologies, covering key research directions such as photovoltaic material design and synthesis, interfacial engineering modulation, active layer morphology optimization, and semi-transparent photovoltaic applications. These results not only reflect the outstanding progress in this field in recent years, but also point out the promising innovative paths for future technological development.

The active layer material is the most important component of organic photovoltaic (OPVs). Precise control of its structure through molecular design remains a long-term challenge in developing high-performance OPVs. For instance, Min *et al.* [1] found that the benzotriazole with a 2-ethylhexyl side chain enhanced molecular crystallinity and donor-acceptor interactions, achieving a high-power conversion efficiency (PCE) of 18.09% and 95% operational stability retention over 700 h. Similarly, Liu *et al.* [2] designed and synthesized an all-fused-ring acceptor FM4 with low trap density, integrated it into the PM6:Y6-based active layer, and developed a near-infrared organic photodetector with ultra-low noise currents. Fluorination strategies further enhance material properties. Zou *et al.* [3] synthesized a fluorinated acceptor with semi-perfluoroalkyl

chains, and the device achieved a PCE of 16.3% with a fill factor of 77.3% and retained 90% efficiency after 1240 h in air. Additionally, dimerized acceptors have gained attention for their morphological stability. Yi *et al.* [4] employed multiscale simulations to study end-group (EG) engineering in acceptors. The designed NB-V (combining naphthalene and benzene EGs) balanced intramolecular and intermolecular interactions, enabling enhanced light absorption and charge transport.

In OPVs, except development of the active layer materials, the interface layer materials are also important. At present, as a hole transport layer, poly(3,4-ethylenedioxythiophene):poly(4-styrenesulfonate) (PEDOT:PSS) has been widely used. However, the inherent acidic and hydrophilic nature of PEDOT:PSS can lead to electrode corrosion of the device and affect the device performance. Liu *et al.* [5] designed and synthesized a new material named bisphosphonate molecule (3BPIC-cF) using the central fluorination strategy. The 3BPIC-cF improved the light transmittivity of the device and its compatibility with the organic active layer interface. The device has a higher hole extraction rate, lower interface impedance and smaller non-radiative recombination loss. Liao *et al.* [6] reported a simple method to enhance the water resistance of PEDOT:PSS by adding tris[bis-(methoxymethyl)amino]-1,3,5-triazine (HM) as a cross-linking agent. The addition of HM neutralized the acidity of PEDOT:PSS and formed a stable hydrophobic network morphology, and the efficiency and stability of the device are significantly improved. Meanwhile, many cathode interface materials (CIMs) are not suitable for printing manufacturing due to their thickness sensitivity. Zhang *et al.* [7] designed and synthesized three self-doped polymer CIMs, in which PN-Pi significantly reduced the work function of the Ag electrode, reduced the interface defects, and obtained impressive PCEs.

The morphology of the active layer in OPVs is crucial for fabricating high-performance large-area devices. The utilization of two acceptor materials (M36, M13) with excellent miscibility enables the formation of a mixed phase [8], which significantly promotes the extension of exciton diffusion length. Simultaneously, the ternary active layer can generate an ideal phase-separated microstructure, effectively reducing the probability of

¹ Key Lab of Fluorine and Silicon for Energy Materials and Chemistry of Ministry of Education, Jiangxi Normal University, Nanchang 330022, China

² School of Materials Science and Engineering, National Institute for Advanced Materials, Nankai University, Tianjin 300350, China

³ State Key Laboratory and Institute of Elemento-Organic Chemistry, Frontiers Science Center for New Organic Matter, The Centre of Nanoscale Science and Technology and Key Laboratory of Functional Polymer Materials, Renewable Energy Conversion and Storage Center (RECAST), College of Chemistry, Nankai University, Tianjin 300071, China

⁴ Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

* Corresponding author (email: ywchen@ncu.edu.cn; yschen99@nankai.edu.cn; liyf@iccas.ac.cn)

charge recombination. The surface coordination between the bridging medium PBTO and CuSCN enhances the interfacial interaction [9], optimizes charge transport, and induces a vertical phase distribution, thereby reducing carrier recombination. Adjusting solute concentration controls ink viscosity to suppress flow stripes, while temperature regulation prevents material aggregation during gravure printing [10]. A 1 cm² flexible OPVs made by roll-to-roll gravure printing on a low-cost polythiophene system reaches 10.55% PCE. Despite challenges, controlling active layer morphology is essential for OPVs commercialization.

The use of additives serves as a key strategy for active layer morphology optimization, with its influence being multi-dimensional. Jen *et al.* [11] have comprehensively reviewed the functionality of solid additives in all-polymer systems, uncovering their mechanistic actions. Their findings demonstrate that solid additives predominantly govern active layer morphology by regulating the early-stage self-assembly dynamics of donor and acceptor components. Notably, the voids created by additive volatilization enable enhanced molecular mobility of photovoltaic materials, ultimately leading to optimized nanophase separation. Moreover, solid additives serve to strengthen the interfacial donor-acceptor coupling, which refines charge transport networks and consequently suppresses charge recombination. For instance, Han *et al.* [12] have introduced a solid additive into the active layer to reduce the intermolecular π - π stacking distance, thereby improving the molecular ordering and facilitating the movement of acceptors, ultimately leading to the formation of an optimal vertical phase-separated morphology. Besides, additives can reduce polymer chain entanglement, effectively mitigating undesirable polymer over-aggregation. Wang *et al.* [13] have demonstrated that incorporating dual additives into the polymer system not only promotes disentanglement of polymer chains but also enhances interchain interactions, facilitating well-ordered molecular stacking. This synergistic effect enables precise control of phase-separated structures, leading to concurrent improvements in both charge transport and exciton dissociation efficiency.

Moreover, the modulation of crystallization kinetics is decisive for enhancing the performance of PVK devices. Meng *et al.* [14] used a crystal growth modulation strategy to prepare high-quality CsPbI₃ films using a new precursor solution with CsI/DMAPI₃/PbI₂ in a dimethylamine acetate (DMAAc)/dimethylformamide (DMF) mixed solvent. The DMAAc/DMF mixed solvent can facilitate phase transformation and reduce the nucleation rate, achieving a high PCE of over 21% for small-size devices, and 19.9% with an active area of 11.40 cm². The modification of the buried bottom interface of perovskite can effectively optimize the performance of the devices. Li *et al.* [15] explored a buried interface modification strategy by introducing the functional molecule *N*-acetyl-L-glutamic acid (NALG) to address the above issues. The carboxyl and amide groups of NALG can help passivate interfacial defects and enhance perovskite crystallization. Xue *et al.* [16] designed a series of SAMs featuring gradually extended π -conjugation structures to improve device performance by enhancing hole extraction and transport, resulting in inverted PVKs with enhanced operational stability and a PCE of up to 25.2%. Regarding the problem of the heavy p-doping effect and inherent defects of tin-based perovskites, Chen *et al.* [17] proposed a novel n-type organic small molecule dopant, namely, NDI2HD-Br₂, to synergistically alle-

viate the intrinsic severe p-type self-doping and passivate the Sn-related defects of tin-based perovskites. The carbonyl groups (C=O) with high electron density in the NDI2HD-Br₂ can donate additional electrons to the perovskite band edge, resulting in the conversion of the tin-based perovskite from a p-type to a weak n-type semiconductor. Moreover, Ding *et al.* [18] demonstrated chiral organic phosphors towards efficient circularly polarized electroluminescence signals by incorporating central chiral (*S/R*)-2-methylbutane into the D-O-A organic phosphor. External quantum efficiencies of 14.9% and 13.0% were obtained with dissymmetry factors $|g_{\text{EL}}|$ of 7.00×10^{-4} and 9.87×10^{-4} , respectively.

Additionally, semi-transparent photovoltaic technology has attracted a lot of attention from researchers in recent years due to the excellent spectral tunability of photovoltaic materials. Zhu *et al.* [19] provide a systematic review of the latest research progress in the field of semi-transparent OPVs, covering the key directions of theoretical modeling, transparent top electrode design, optical modulation strategy, and optimization of active layer materials. Looking forward, the research in this field should focus on improving the stability of the devices, and promote the industrialization of the technology through the collaborative innovation between industry, academia, and research.

In summary, this issue of “Photovoltaic Materials, Devices, and Applications” summarizes the latest research progress in the field of synthetic chemistry and device physics of photovoltaic materials. It not only summarizes the important breakthroughs in this field in recent years, but also discusses the challenges and opportunities for future development. We expect that these research results will contribute to the innovative development of photovoltaic technology and provide scientific support for the development of efficient and sustainable energy solutions.

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Lifu Zhang is currently an associate professor at the School of Chemical Engineering, Jiangxi Normal University. He received his PhD degree from Nanchang University in 2022 under the supervision of Professor Yiwang Chen. His current scientific interests mainly focus on the structure design of the active layer and device optimization for polymer solar cells and modules.



Bin Kan is currently a professor at the School of Materials Science and Engineering, Nankai University. He completed his BS degree at Lanzhou University in 2012 and received PhD degree from Nankai University in 2018 under the supervision of Prof. Yongsheng Chen. From 2018–2021, he worked as postdoc at the University of Washington and University of Houston, respectively. His primary research focuses on the molecular design, synthesis, and applications of organic functional materials, with particular emphasis on developing advanced materials for organic photovoltaics and flexible electronic devices.



Yiwang Chen is a full professor of chemistry at Nanchang University and Jiangxi Normal University. He has served as the president of Gannan Normal University since 2022. He is also the director of the Institute of Polymers and Energy Chemistry, Nanchang University and the director of the Key Lab of Fluorine and Silicon for Energy Materials and Chemistry of Ministry of Education, Jiangxi Normal University. His research interests include polymer/perovskite solar cells, hybrid supercapacitors, sodium ion batteries, intelligent elastomers, zinc-air batteries and electrocatalysis.



Yongsheng Chen received his PhD degree in chemistry from the University of Victoria in 1997. From 2003, he has been a chair professor at Nankai University. His main research interests focus on carbon-based nanomaterials and organic functional materials for green energy applications.



Yongfang Li is a professor at the Institute of Chemistry, Chinese Academy of Sciences (ICCAS) and Soochow University. He received his PhD degree at Fudan University in 1986, and then did his postdoctoral research at ICCAS from 1986 to 1988. He became a staff in 1988 and was promoted to professor in 1993 at ICCAS. He was elected as a member of the Chinese Academy of Sciences in 2013. His present research field is photovoltaic materials and devices for polymer solar cells.