2-2-5. Organic Photovoltaics

Overview

Organic photovoltaics (OPVs) are next-generation solar cells featuring a photoactive layer of electron-accepting and electron-donating π-conjugated organic molecules, sandwiched between buffer layers and electrodes. With their lightweight, flexible nature, and compatibility with scalable printing techniques, OPVs enable cost-effective fabrication and versatile applications. Recent advances in photoactive materials, particularly non-fullerene acceptors, have enhanced light-harvesting and reduced voltage losses, achieving power conversion efficiencies above 20%.

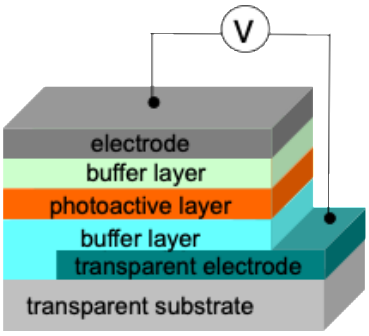

Figure 1. Structure of OPVs.

Current Status and Frontiers

Research on OPVs has advanced across both efficiency and durability improvements, as well as fundamental studies on device physics. In Japan, pioneering work, such as the introduction of the p-i-n bulk heterojunction structure by Hiramoto et al. in 1991, laid the foundation for the field, with broader research activity expanding in the 21st century. For an overview up to the mid-2000s, refer section "2-2-4. Organic Solid-State Solar Cells" in the Photochemistry Div Report described in Japanese. URL: https://division.csj.jp/div-report/02/0220204.pdf Over the past two decades, material innovations have markedly boosted efficiency, with key examples of electron acceptors and donors introduced below.

1. Fullerene-based electron acceptor materials

In the OPV development, fullerene electron acceptors with low reorganization energy have played a crucial role. [6,6]-Phenyl-C_{71}-butyric acid methyl ester ([70]PCBM), with high electron mobility and good miscibility, has been widely used since the 2000s. Advances such as SIMEF with superior thermal crystallization properties (Matsuo) and studies on [70]PCBM isomer effects (Umeyama) have enhanced efficiency and deepened device physics. Although non-fullerene

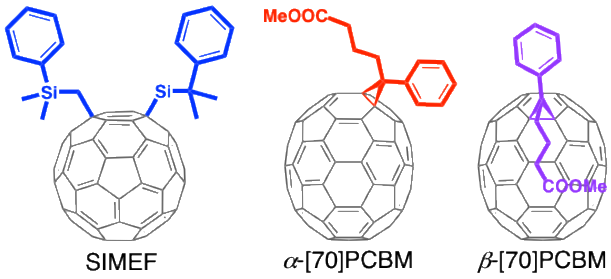

Figure 2. Structures of fullerene acceptors.

strong acceptors now dominate, fullerene derivatives remain important for ternary photoactive layers.

2. Non-fullerene electron acceptor materials

To address the narrow absorption range and limited energy-level tunability of fullerenes, non-fullerene acceptors (NFAs) have been actively developed. Molecular designs such as the A–D–A framework exemplified by ITIC and the A–DA'D–A framework exemplified by Y6 enable visible-to-near-infrared absorption, suitable energy-level alignment, and high electron mobility, achieving power conversion efficiencies above 20%. Increasing attention is also directed toward NFAs with simpler, non-fused structures for easier synthesis (for example, TT-TF-DCI by Ie et al.).

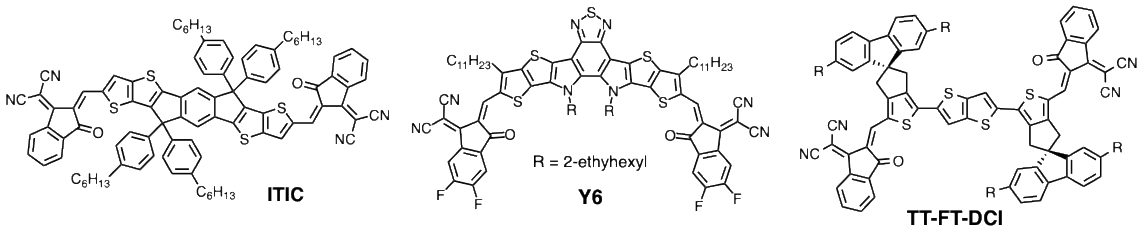

Figure 3. Structures of NFAs.

3. Electron donor materials

In the early stages, poly(3-hexylthiophene) was widely used as an electron donor, but its narrow absorption range and limited energy-level tunability were persistent limitations. To address these, low-bandgap D–A copolymers combining electron-donating and electron-accepting units were developed, enabling red-shifted absorption and precise energy-level control. In addition, optimizing solubility, orientation, and crystallinity through fused-ring backbones and tailored alkyl side chains has also been shown to be critical (Osaka).

References

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3. S. Jinnai, et al., *J. Mater. Chem. A*, **10**, 20035–20047 (2022).
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Future Perspectives and Directions

Challenges to be addressed within 10 years: achieving 20% efficiency and long-term stability in modules via green manufacturing; advancing large-area, low-cost fabrication; enhancing performance and applications of semitransparent and flexible devices.

(Author: Tomokazu Umeyama)