

# How the Energetic Landscape of Non-Fullerene Acceptor Organic Solar Cells Controls Device Performance

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Organic solar cells (OSCs) use blends of electron-donating and electron-accepting organic semiconductors, providing the necessary driving force for charge separation and photovoltaic energy conversion. Using non-fullerene acceptors (NFAs), power conversion efficiencies of more than 20% have recently been achieved.

In this talk, I will establish a link between the chemical structure of NFAs and their efficiency in state-of-the-art bulk heterojunction organic solar cells. In fact, the structural motif of NFAs is the origin of peculiar properties: strong light absorption is combined with exceptionally long exciton diffusion lengths;<sup>[1]</sup> their molecular quadrupole moments facilitate exciton-to-charge transfer state conversion and reduce the field dependence of charge separation.<sup>[2-3]</sup> In blends, fast energy transfer from the donor to the acceptor occurs and causes the device efficiency to depend primarily on the ionization energy (IE) difference: for offsets <0.3 eV, the charge generation efficiency is reduced,<sup>[4]</sup> for offsets >1.0 eV, fast charge recombination competes efficiently with charge extraction, limiting device performance.<sup>[5]</sup> Interestingly, our very recent experiments on blends using Y-series acceptors indicate that high charge separation yields can be maintained for offsets as low as ~0.2 eV.<sup>[6]</sup> Understanding the relation between the molecular structure, interfacial energetic landscape, photophysics, and device performance is crucial for a guided design of new organic semiconductor materials using, for instance, computational material chemistry approaches to predicting more efficient molecular target structures.

[1] W. Yang et al., *Adv. Energy Mater.* **2025**, 2405322;

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[3] A. Markina et al., *Adv. Energy Mater.* **2021**, 11, 2102363;

[4] J. Gorenflot et al., *Adv. Mater. Interfac.* **2023**, 22202515;

[5] Althobaiti et al., *Energy Env. Sci.* **2025**, accepted.

[6] Karuthedath et al., in preparation.