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Chemical design rules for non-fullerene acceptors in organic solar cells

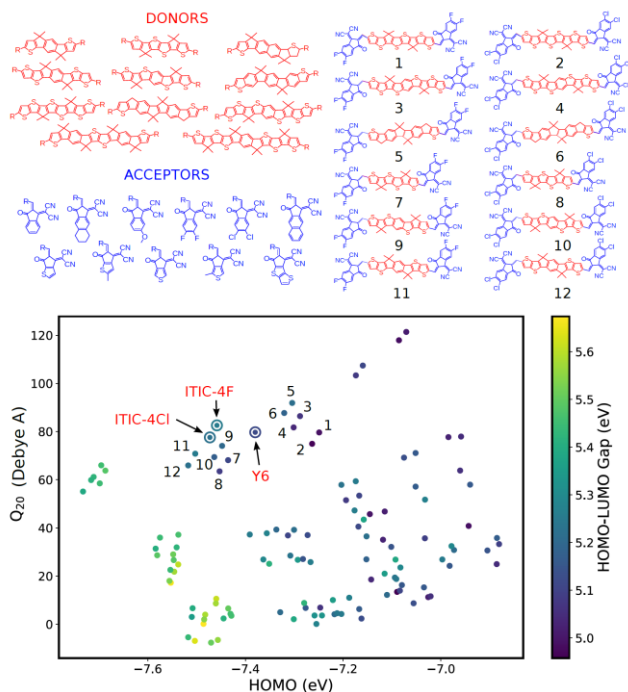
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Abstract:

Efficiencies of organic solar cells have practically doubled since the development of non-fullerene acceptors (NFAs). However, generic chemical design rules for donor-NFA combinations are still needed. We propose such rules by analyzing inhomogeneous electrostatic fields at the donor-acceptor interface. We show that an acceptor-donor-acceptor molecular architecture, and molecular alignment parallel to the interface, result in energy level bending that destabilizes the charge transfer state, thus promoting its dissociation into free charges. By analyzing a series of PCE10:NFA solar cells, with NFAs including Y6, IEICO, and ITIC, as well as their halogenated derivatives, we suggest that the molecular quadrupole moment of ca 75 Debye Angstrom balances the losses in the open circuit voltage and gains in charge generation efficiency.



Left: Chemical structures of acceptors and donors with R depicting the donor-acceptor bonds. Right: Molecular structures of 12 selected compounds. Bottom: Q₂₀-HOMO plot for 121 A-D-A compounds as well as high-performance NFAs ITIC-4F, ITIC-4Cl, and Y6. Each point is colored according to its corresponding HOMO-LUMO gap value. Reprinted with permission from *Advanced Energy Materials*, 2021

References:

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