

# Conjugated Molecules for Advanced Organic and Perovskite Photovoltaics

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Perovskite solar cells (PSCs) and organic photovoltaics (OPVs) have emerged as leading candidates for next-generation energy solutions, owing to their high power conversion efficiencies and compatibility with solution-processed fabrication. These attributes make them particularly promising for addressing the energy demands of Internet of Things (IoT) applications. A key strategy for enhancing PSC and OPV performance is the mitigation of interfacial defects through the design of advanced charge transport layers, including electron transport layers (ETLs), hole transport layers (HTLs), and interfacial layers (IFLs). In this talk, I will present our recent progress in developing conjugated molecules for ETLs, HTLs, and IFLs, which has led to significant performance enhancements.<sup>[1]</sup> We developed strategies including efficient electron-selective layers, perovskite bulk passivation, and bilayer HTL architectures to boost indoor PSC efficiency. By integrating organic semiconductors, sol-gel NiO<sub>x</sub>, and self-assembled layers, we optimized interfacial energy alignment and carrier transport. Under 3000 K LED illumination at 1000 lux, our Cs<sub>0.18</sub>FA<sub>0.82</sub>Pb(I<sub>0.8</sub>Br<sub>0.2</sub>)<sub>3</sub> devices achieved over 43% indoor PCE.<sup>[2]</sup> Furthermore, we optimized bulk heterojunction (BHJ) blend layers — such as PM6:PY-IT, and PM6:Y6 and its derivatives — and their ternary counterparts to realize high-performance OPVs.<sup>[3]</sup> Our studies show that optimized ternary blend morphologies enhance exciton dissociation, carrier transport, and overall power conversion efficiency. We also demonstrate improved thermal and ambient stability in OPVs, advancing their robustness and reliability. These results highlight the pivotal role of molecular design in passivation, electron transport, and interfacial engineering — driving next-generation PSCs and OPVs toward energy-efficient IoT applications.

## References

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