# INTERFACIAL ENGINEERING FOR EFFICIENT AND STABLE PEROVSKITE PHOTOVOLTACIS

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## ABSTRACT

Perovskite solar cells (PSCs) have reached power conversion efficiencies (PCEs) comparable to crystalline silicon, yet interfacial charge losses and operational instability continue to hinder commercialization. These challenges are addressed through molecular engineering of hole-transport layers and surface passivating ligands to regulate energy alignment, defect chemistry, and excited-state dynamics. A pyrrole-functionalized ProDOT-based polymer hole transport layer (PPr) was developed to achieve favorable energy-level alignment, enhanced interfacial contact, and improved film robustness without sacrificing solution processability. Devices employing PPr retain 94% of their initial efficiencies after 4,000 h of aging under ambient conditions. Beyond charge transport layer modification, an overlooked loss pathway in aromatic surface passivators is identified, in which low-lying ligand triplet states serve as non-radiative recombination centers. By rationally increasing the ligand triplet energy using triphenylene-based passivators, triplet-mediated charge trapping is effectively suppressed, leading to simultaneous improvements in device efficiency and photostability. In parallel, thiophene-based bidentate ligands enable selective reconstruction and spatially uniform passivation of residual $PbI_2$, reducing trap densities and enhancing operational stability, yielding PCE up to 26.19%. Complementary efforts extend these interfacial design principles to fluorinated ligands, ITO-free electrodes, stable bidentate ligands, and scalable large-area perovskite light-emitting diodes. Collectively, interfacial and excited-state engineering emerge as a unified framework for advancing the efficiency, stability, and scalability of perovskite optoelectronic devices.