

ABSTRACT:

Facet Engineering for High-Efficiency and Stable Perovskite Solar Cells

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Metal halide perovskites have emerged as star materials for next-generation photovoltaic technology due to their outstanding optoelectronic properties, with laboratory device efficiencies exceeding 27%. However, their intrinsic stability remains a core challenge for industrialization. Research indicates that different crystal facets in perovskite polycrystalline films exhibit significantly varying environmental stability—the (111) facet demonstrates excellent moisture resistance, while the (100) facet is prone to water and oxygen erosion, serving as a weak point for phase transitions and degradation. Therefore, achieving precise control over crystal orientation, suppressing unstable facets, and promoting the preferential growth of stable facets is a key pathway to simultaneously enhance device efficiency and stability.

This talk systematically presents our team's synergistic strategies for controlling perovskite crystal orientation. First, in inverted structures, the introduction of NaCl into the PEDOT:PSS hole transport layer induced preferential orientation of perovskites along the (100) direction, revealing the role of lattice matching in heterogeneous nucleation. Subsequently, for conventional structures, the multifunctional molecule biguanide hydrochloride (BGCI) was introduced at the SnO₂/perovskite interface. Through Lewis coordination and electrostatic coupling, this optimized interfacial energy level alignment, passivated defects, and promoted high-quality perovskite crystallization, achieving a high efficiency of 24.4% and excellent environmental stability. Furthermore, we utilized the natural compound tea saponin (TS) to modify the SnO₂ surface. Through synergistic hydrogen bonding and Lewis coordination, this successfully guided the dominant growth of the perovskite (111) facet, resulting in a photoelectric conversion efficiency of 24.2% and significantly enhanced humidity tolerance.

To fundamentally address the instability of the (100) facet, we innovatively designed a functional additive containing triformyl (TFPA). Combined with advanced characterization techniques such as in-situ GIWAXS, terahertz spectroscopy, and scanning electron diffraction navigation imaging, we confirmed that TFPA selectively anchors to the (100) facet, suppressing its growth while guiding preferential orientation toward the (111) facet. This strategy not only significantly increased the energy barrier for the α -to- δ phase transition, enhancing intrinsic stability, but also optimized charge transport properties, ultimately achieving a balance between high efficiency and long-term stability.

In summary, through a synergistic three-pronged strategy of “interface engineering—molecular design—facet regulation”, this work achieves precise control over perovskite crystal orientation. It

provides a universal technical pathway for developing perovskite solar cells with both high efficiency and high stability, strongly advancing their practical application.

Keywords: perovskite solar cells; facet engineering; crystal orientation.

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