ENGINEERING

Interface Engineering to Kinetically Trap the Photovoltaic Crystal Phase of Formamidinium Lead Iodide Perovskite

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Renewable energy, especially solar energy, has gained increasing popularity in common households and industries. While silicon is the dominant material used in commercial solar panels, emerging photovoltaic materials called perovskites have demonstrated a fast increase in the power conversion efficiency from in-lab experiments. The record efficiency of perovskites has increased from 3.8% to the most recent 25.5% within only 12 years, which rivals the 26.1% of single-crystal silicon solar cells.

Formamidinium lead iodide (FAPbI₃) is used in the highest-performing perovskite solar cells for its near-ideal band gap, but its photovoltaic crystal phase is thermodynamically unstable at room temperature. An effective solution to this is to modify the interface and passivate crystal defects to kinetically trap the photovoltaic phase. Typically, long-chain alkylammonium ligands are used to bond to the perovskite surface and create a hydrophobic and strained interface. While this method is effective, it is limited by the insulating nature of alkyl chains, the rotations of carbon-carbon bonds, and the poor thermal stability of the methylammonium group. In this research, we extend the intentions of previous passivation studies by creating a strained interface with a more stable and semiconducting passivation layer. In-lab synthesized p-conjugated oligothiophene ligands with formamidinium anchoring groups are used to match the formamidinium vacancies in the FAPbI₃ perovskite lattice. In

Schematic showing 2D perovskite passivation of formamidinium lead iodide (FAPbI₃) using ligand post treatment.

addition, the bulky and rigid conjugated ligands can both tune the surface optoelectronic properties and stabilize the surface against moisture ingress and phase transformation. With these novel passivation agents, FAPbI₃ perovskite solar cells with power conversion efficiency over 20% and improved stability were achieved.

Research advisor Letian Dou writes: “Formamidinium lead iodide perovskite is a low-cost, high-performance solar material. Unfortunately, it is not stable due to an unwanted phase transition. Yiyuan (Melody) Zhang’s work provides a promising solution for increasing the transition barrier and stabilizing this exciting material. Her work paves the way to a photovoltaic device better than silicon.”