

From Chalcogen Bonding to S– π Interactions in Hybrid Perovskite Photovoltaics

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Streszczenie

The stability of hybrid organic–inorganic halide perovskite semiconductors remains a significant obstacle to their application in photovoltaics. To this end, the use of low-dimensional (LD) perovskites, which incorporate hydrophobic organic moieties, provides an effective strategy to improve their stability, yet often at the expense of their performance. To address this limitation, supramolecular engineering of noncovalent interactions between organic and inorganic components has shown potential by relying on hydrogen bonding and conventional van der Waals interactions. Here, the capacity to access novel LD perovskite structures that uniquely assemble through unorthodox S-mediated interactions is explored by incorporating benzothiadiazole-based moieties. The formation of S-mediated LD structures is demonstrated, including one-dimensional (1D) and layered two-dimensional (2D) perovskite phases assembled via chalcogen bonding and S– π interactions, through a combination of techniques, such as single crystal and thin film X-ray diffraction, as well as solid-state NMR spectroscopy, complemented by molecular dynamics simulations, density functional theory calculations, and optoelectronic characterization, revealing superior conductivities of S-mediated LD perovskites. The resulting materials are applied in n-i-p and p-i-n perovskite solar cells, demonstrating enhancements in performance and operational stability that reveal a versatile supramolecular strategy in photovoltaics.

Słowa kluczowe

chalcogen bonding, layered perovskites, low-dimensional perovskites, photovoltaics, supramolecular engineering

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