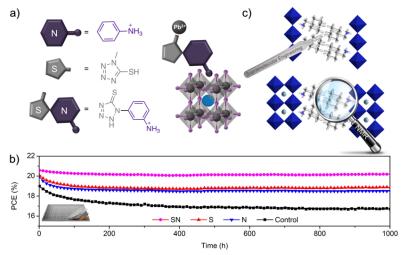


Supramolecular Engineering of Hybrid Perovskite Solar Cells: From Molecular Modulation to Layered Perovskite Architectures

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Hybrid perovskite solar cells exhibit remarkable solar-to-electric power conversion efficiencies, whereas their limited stability and molecular-level engineering remain challenging.^[1-3] In contrast to three-dimensional (3D) perovskites, their layered two-dimensional (2D) analogs show promising stabilities, though at the expense of the corresponding efficiencies.^[1,4-5] We demonstrate a strategy to provide stabilization without compromising the efficiency by employing multifunctional molecular modulators designed through fine-tuning noncovalent interactions complemented by structural adaptability.^[1,3] These systems are devised to interact with the 3D perovskite surface in a manner uniquely assessed by solid-state NMR spectroscopy.^[1-3,5] As a result, we obtain perovskite solar cells with superior properties and efficiencies exceeding 20%, accompanied by enhanced stabilities.^[2-3] Moreover, extending the design into layered 2D architectures leads to further stability enhancements.^[4-5] This approach has been investigated using a combination of techniques complemented by solid-state NMR spectroscopy to unravel the design principles and exemplify the role of supramolecular engineering in advancing hybrid perovskite solar cell research.



Schematic representation of a (a) molecularly modulated perovskite structure with the (b) evolution of the performance of the corresponding solar cells over time and the (c) illustration of the layered perovskite prototype

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