



Tunable ferroelectric polarization and its interplaywith spin-orbit coupling in tin iodide perovskites

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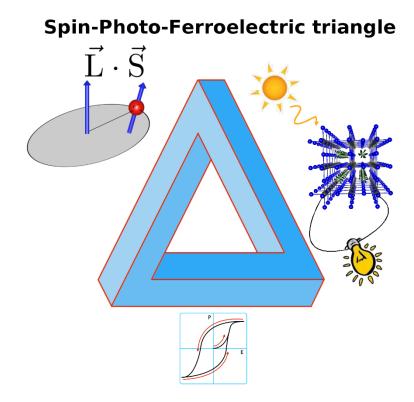
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Halide perovskites represent an emerging photovoltaic technology. Using density functional theory simulations and symmetry analysis, we discuss the properties in lead-free perovskite iodide (FA)SnI₃, containing the polar formamidinium cation FA, (NH₂CHNH₂)⁺. We have shown that the perpendicular arrangement of FA molecules , leading to a 'weak' ferroelectric polarization, is energetically more stable than parallel arrangements of FA planes, being either antiferroelectric or 'strong' ferroelectric. Moreover, we show that the 'weak' and 'strong' ferroelectric states with the polar axis along different crystallographic directions are competing in energy, thus suggesting that, at least at low temperatures, an electric field could stabilize different states with the polarization rotated by 45°, resulting in a highly tunable ferroelectricity appealing for multistate logic. Intriguingly, the relatively strong spin–orbt coupling in noncentrosymmetric (FA)SnI₃ gives rise to a co-existence of Rashba and Dresselhaus effects and to a spin texture that can be induced, tuned and switched by an electric field controlling the ferroelectric state.



A pictorial triangle representing the interplay of dipolar ordering, photovoltaic properties and spin-orbit related phenomena in lead-free solid-state organic-inorganic halide perovskite solar cells.