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Emerging Hybrid Halides for Optoelectronics beyond Perovskites

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High-performance hybrid metal halides, featuring exotic structures and unique functionalities, show great promises for optoelectronic applications. Rational chemical design strategies, leveraging diverse metal, halide, and organic components, can accelerate the discovery and the understanding of these materials. Our work focuses on designing new metal halide families with tailored properties, including highly emissive photoluminescence, circularly polarized luminescence, second harmonic generation and ferroelectrics. Key strategies involve (1) engineering emissive metal centers (Mn, Cu, Sb) with selective chiral/achiral organic cations/ligands for bright emission;[1-3] (2) inducing asymmetry through lone pair metal such as Ge,[4] controlling the symmetry through directional coordination of organic cationic ligands,[5] (3) incorporating hygroscopic rare earth metals into bimetallic 0D systems with group V metals using neutral solvent ligands;[6-7] (4) not only chemical pressure matters for the local coordination environments, but physical pressure[8] can also induce and help obtaining metastable non-centrosymmetric phases. We have demonstrated these design strategies in multiple systems with superior properties and outlined the structure-property relations within each family.