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Role of A-site molecular ions dynamics in the polar functionality of perovskite metal-organic frameworks

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Recent studies on organic-inorganic hybrid perovskites (OIHPs) and ferroelectric metal-organic framework perovskites (MOFPs) reveal their superb performance as highly efficient photovoltaics and promising ferroelectrics. This has enabled a new generation of optic-electronic-mechanical devices based on green chemistry. However, the ultimate strategies to optimize these polarization-related functionalities are not yet clear, leading to confused reports in the literature. In this work, we investigate a rationally selected series of molecular ions within Mg(HCOO)3− frameworks to form [CH3NH3]Mg(HCOO)3 (MAMOF), [(CH3)2NH2]Mg(HCOO)3 (DMAMOF), and [C(NH2)3]Mg(HCOO)3 (GUAMOF). Single-crystal X-ray diffraction, inelastic neutron spectroscopy and ab initio molecular dynamics are used to achieve detailed structural pictures of three MOFPs. Intriguingly, our study reveals that the alignments of protonated amines are highly dependent on the directional hydrogen bonds that link N-H units to the surrounding MgO6 octahedra. The alignments of different amines and their dynamics are therefore determined by the acceptor O provided by the distortive frameworks. We successfully assigned the alignments of the A-site ions associated with different polar behavior to the dielectric properties for three MOFPs and propose that the configuration of the A-site molecular ions and potential hydrogen bonds are critical to enable the design of polarization-related functionalities in both MOFPs and OIHPs.

Speakers Gender

Male

Level of Expertise

Early Career <5 Years

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