Poster

Structure-property behaviour of $(N(C_2H_5)_3CH_3)FeBr_4$ powder under high pressure

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Hybrid organic-inorganic ferroelectrics (HOIFs) exhibit outstanding structural diversity due to their high degree of freedom, and their versatile properties change in response to changes in external stimuli. Although chemical engineering methods have been used to modify the structures, morphologies and properties of these materials, there are still a number of issues related to stability, long-term functionality and environmental compatibility (e.g. the use of non-toxic or less toxic elements compared to lead). Given these challenges, it is important to fully explore the structural properties of *lead-free ferroelectrics* at high pressure. Post-synthesis *high-pressure treatment* is a clean tool for elegantly reshaping HOIFs to precisely regulate their crystal lattice and electronic behaviour with atomic-level knowledge, resulting in tuned bandgap narrowing, carrier lifetime extension, photoluminescence intensity enhancement, metallization, amorphization and phase transitions – properties that expand the application possibilities of HOIFs, but have so far been mainly reserved for the well-studied lead-containing hybrid molecular ferroelectrics, which are toxic and suffer from stability problems [1-3].

Given the limited data available due to the influence of pressure on the resolution limits of experiments on powder samples, with a high-pressure diamond anvil cell, there is a wide range of tunable photophysical properties of $(N(C_2H_5)_3CH_3)FeBr_4$ that can be controlled by high-pressure synchrotron X-ray diffraction and Raman experiments, absorption and emission spectroscopy, and electrical transport measurements in compression and decompression [3]. Reversible *pressure-induced narrowing of the band gap* by 1.22 eV at 20.3 GPa and an irreversible *pressure-induced emission enhancement* (PIEE) observed above 8 GPa revealed subtle changes in the electronic scene, with a fully reversible piezochromism phenomenon. The mechanism underlying these photophysical properties has been shown to be related to the *pressure-induced amorphization* triggered by the *phase transition* from hexagonal ($P6_3mc$) to monoclinic ($P2_1$) symmetry. It involves frustrations in the inorganic framework, driven by strong interactions with disordered organic cations and the recovery track of the $(N(C_2H_5)_3CH_3)FeBr_4$ lattice.

The soft nature of the environmentally friendly (compared to hybrid organic-inorganic perovskites containing lead) $(N(C_2H_5)_3CH_3)FeBr_4$ studied by pressure-induced amorphization and recrystallization could be advantageous for *bandgap tuning* and especially for the realization of HOIF, where excellent piezoelectric performance and mechanical softness can coexist.

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