

White-light emitting Ruddlesden-Popper perovskites

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Recently, owing to their excellent optoelectronic properties combined with an enhanced material stability, two-dimensional (2D) organic halide perovskites have emerged as an attractive alternative to 3D perovskites for photovoltaics^{1,2}. More, their ability to emit white-light at room temperature with a good color rendering projected this family of materials into the spotlight of potential future low-cost white LED components³. However, the underlying physical mechanisms behind these emissive properties are not fully understood. Herein we propose to investigate the origin of the broad-band emission observed at different temperatures in a series of $(\text{C}_6\text{H}_{11}\text{NH}_3)_2\text{PbX}_4$ 2D Ruddlesden Popper perovskites (X= Br or I)^{4,5} by coupling advanced structural measurements with an atomistic approach based on the density functional theory (DFT). Indeed, as the temperature is decreased, phase transitions between undistorted and distorted structures were observed for the two compounds of the series by means of temperature dependent X-ray diffraction. While this crystallographic phase transition goes along with a measured polarization-electric field hysteresis for the bromide compound, apparition of satellite incommensurate reflections was instead obtained for the Iodine one. We believe that these satellite reflections might also be connected to a low temperature ferroelectric ordering. In order to set a clear interplay between the structural distortions and the observed optoelectronic properties, theoretical studies intend to provide insights of the electronic band structures and polarization characteristics for these compounds.

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