

# Tunable Structural and Optoelectronic Properties of Methylammonium Lead Bromide Perovskite under Pressure

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The organic-inorganic lead halide perovskites MAPbX<sub>3</sub> (MA = CH<sub>3</sub>NH<sub>3</sub>, X = Cl, Br and I) have shown superior properties for applications in photovoltaic technology. These materials can be synthesized at a low cost, and have strong solar absorption and excellent power conversion efficiency that currently reaches ~22%. MAPbBr<sub>3</sub> is one of these materials, it displays orange colour and with band gap of ~2.3 eV at ambient conditions. The room-temperature structure of MAPbBr<sub>3</sub> is cubic with space group *Pm-3m* and shows a diversity of structures during cooling.<sup>1-2</sup> The framework of all the structures of MAPbBr<sub>3</sub> consist of vertex-sharing PbBr<sub>6</sub> octahedra, in which the disordered/ordered MA cations occupy the three-dimensional channels and hydrogen-bond to the host framework of the PbBr<sub>6</sub> octahedra. The high pressure response of structural and electronic changes of MAPbBr<sub>3</sub> have been reported recently.<sup>3-6</sup> We found considerable inconsistencies in these reports and lots of the unsolved issues need to be clarified and explained.

In this work,<sup>7</sup> we investigated the structural and optoelectronic properties of MAPbBr<sub>3</sub> using synchrotron single crystal and powder X-ray diffraction and photoluminescence measurements under various stress conditions. We found the properties of MAPbBr<sub>3</sub> can be tuned by employing different pressure-transmitting medium (PTM). While non-hydrostatic compression of MAPbBr<sub>3</sub> leads to amorphization above 2.4 GPa, under quasi-hydrostatic (Ar) and hydrostatic (He) pressure, the sample remains in crystalline phases. A sequence of phase transitions between two cubic phases and orthorhombic *Pnma* phase is observed when using Ar, or no PTM. In helium, only transitions between the two cubic structures and a new isostructural phase transition with a large volume collapse to a third cubic phase at 2.7 GPa was observed. The photoluminescence measurements indicate a pressure-induced band gap-narrowing in the cubic phase I, and a blue-shift in the orthorhombic structure.

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