

**Experiment title:**

High pressure behaviour of Sn-based hybrid perovskites

Experiment number:

HC-3646

Beamline:	Date of experiment: from: 27 June 2018 to: 30 June 2018	Date of report:
Shifts:	Local contact(s): Federico Cova	<i>Received at ESRF:</i>

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Report:

Here we report on the first structural and optical high-pressure investigation of MASnBr_3 ($\text{MA} = [\text{CH}_3\text{NH}_3]^+$) and CsSnBr_3 halide perovskites. A massive red shift of 0.4 eV for MASnBr_3 and 0.2 eV for CsSnBr_3 is observed within 1.3 to 1.5 GPa from absorption spectroscopy, followed by a huge blue shift of 0.3 and 0.5 eV, respectively. Synchrotron powder diffraction allowed us to correlate the upturn in the optical properties trend (onset of blue shift) with structural phase transitions from cubic to orthorhombic in MASnBr_3 and from tetragonal to monoclinic for CsSnBr_3 . Density functional theory calculations indicate a different underlying mechanism affecting the band gap evolution with pressure, a key role of metal-halide bond lengths for CsSnBr_3 and cation orientation for MASnBr_3 , thus showing the impact of a different A-cation on the pressure response. Finally, the investigated phases, differently from the analogous Pb-based counterparts, are robust against amorphization showing defined diffraction up to the maximum pressure used in the experiments.

Publication resulting from the Experiment:

M. Coduri, T. A. Strobel, M. Szafranski, A. Katrusiak, A. Mahata, F. Héctor Cova, S. Bonomi, E. Mosconi, F. De Angelis, L. Malavasi*, *Band Gap Engineering in MASnBr_3 and CsSnBr_3 Perovskites: Mechanistic Insights through the Application of Pressure*, *J. Phys. Chem. Lett.* 2019, 10, 7398-7405.

