

# New photoactive lead free perovskite absorber: process and preliminary characterization

Alexandre Py<sup>1</sup>, Yifeng Zhong<sup>1</sup>, Pallavi Singh<sup>2</sup>, David Cahen<sup>2</sup>, Davide Ceratti<sup>1</sup>, Paul Alexis Pavard<sup>1</sup>, Shan-Ting Zhang<sup>1</sup>, Nathanaelle Schneider<sup>1</sup>, Jean-François Guillemoles<sup>1</sup> and Philip Schulz<sup>1</sup>

<sup>1</sup> CNRS, Ecole Polytechnique, Institut Photovoltaïque d'Ile-de-France UMR 9006, 30 RD 128, 91120 PALAISEAU, France

<sup>2</sup> Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot 76100, Israel

Lead-free halide perovskites (HaPs) are gaining traction in the photovoltaic community as candidates to solve some of the issues inherent to lead HaPs<sup>1</sup>. Among these candidates, the gold HaPs family (AAuX<sub>3</sub>, with monovalent cation A<sup>+</sup> and halide anion X<sup>-</sup>) has been getting increasing attention, both from the theoretical<sup>2,3</sup> and the experimental point of view<sup>4,5</sup>. Compared to conventional Pb-based perovskite used in the state-of-the-art perovskite solar cell technology, this sub-class of HaP materials relies on the B-site substitution of Pb by Au that we expect to affect the optoelectronic properties most prominently via the BX<sub>6</sub> octahedral sub-unit in the crystal structure. More precisely, we aim to explore the effect of potential symmetry breaking in the B-site, i.e. via a double valence element (I+III) on the unusual defect science in HaPs. In this study, we report the first inorganic gold HaPs thin films (CsAuX<sub>3</sub>, with X = I, Br, Cl) and compare their structural and optoelectronic properties with data from the literature on corresponding single crystals.

We describe the process we designed to obtain these thin films, and discuss the most important deposition parameters. We present the Raman spectra of the obtained thin film which are in excellent agreement with the data obtained from powder/crystalline samples, experimentally and from the literature. The X-Ray diffraction pattern measured on the samples prove that the samples are crystalline enough for detection, with no secondary phase identifiable in the pattern. Scanning Electron Microscopy images confirm that the sample is a continuous thin film, with grain sizes for the crystallites ranging from 200 nm to 500 nm. Finally, we report the first photoluminescence spectrum obtained to our knowledge from this family of materials. This demonstrates the photoactivity of the obtained thin films, and opens the door to more advanced characterization and potential integration in devices in the future.

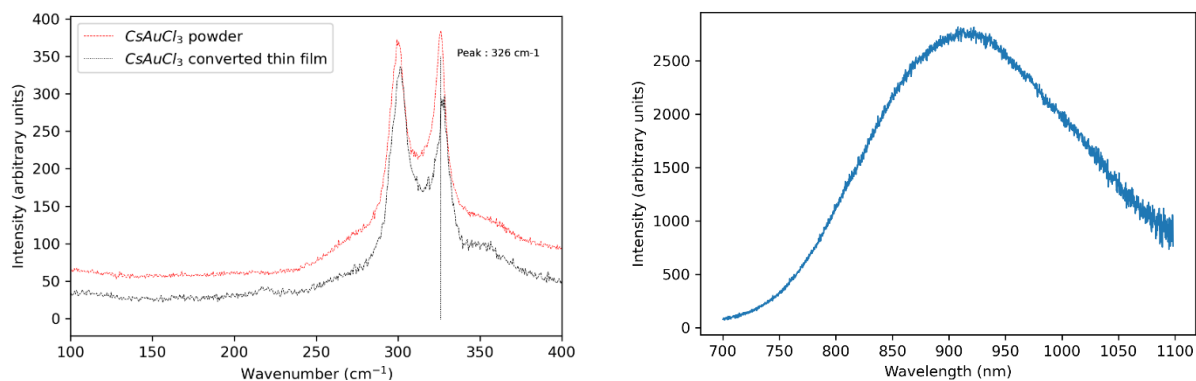


Figure 1: Raman spectrum of a converted CsAuCl<sub>3</sub> thin film versus powder samples (left) and photoluminescence spectrum (right) obtained from the same CsAuCl<sub>3</sub> thin film at room temperature

<sup>1</sup> V. Pecunia, L.G. Occhipinti, A. Chakraborty, Y. Pan, and Y. Peng, APL Mater. **8**, 100901 (2020).

<sup>2</sup> L. Debbichi, S. Lee, H. Cho, A.M. Rappe, K.-H. Hong, M.S. Jang, and H. Kim, Adv. Mater. **30**, 1707001 (2018).

<sup>3</sup> J. Kangsabanik, S. Ghorui, M. Aslam, and A. Alam, **6**, 1 (2019).

<sup>4</sup> H. Murasugi, S. Kumagai, H. Iguchi, M. Yamashita, and S. Takaishi, Chem. – A Eur. J. **25**, 9885 (2019).

<sup>5</sup> B. Ghosh, B. Febriansyah, P.C. Harikesh, T.M. Koh, S.S. Hadke, L.H. Wong, J. England, S.G. Mhaisalkar, and N. Mathews, Chem. Mater. (2020).

