X-ray excited optical luminescence of metal halide hybrid perovskites: Effect of the halide composition, illumination spectrum and moisture conditions

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Metal halide hybrid perovskites are of great interest in applications in optoelectronic devices. It has been observed that $Cs_xFA_{1-x}Pb(I_yBr_{1-y})_3$ perovskites show an improvement in the structural and optical stability, features highly aimed in solar cells and optical devices, after the addition of Cs. Yet, they still suffer under operation conditions. Despite this, the damage by the environment, such as moisture, and radiation, on the optoelectronic properties of these perovskites are still to be studied. We have implemented a setup at the XRD2-LNLS beamline that allows for structural characterization by X-ray diffraction (XRD) while measuring X-ray excited photoluminescence (XEOL) with the sample at a fixed angle. Both XEOL and XRD evolution were monitored simultaneously while other parameters (moisture and illumination wavelength) were modified. The study of the compounds x:y = (10:38, 40:38), indicates that they present different responses under the flux of hard x-ray photons (7keV) due to the excitation beam. It has been observed that the XEOL signals of both samples increased in the humid-ambient atmosphere (photobrightening). Simultaneously to the photobrightening, the structural variations in sample 40:38 indicate the segregation of a Cs-rich phase, which does not happen to 10:38. These changes are proven to be due to the continuous 7keV X-ray beam excitation, and we propose that the different structural responses are due to the different Cs-contents. In the dry atmosphere both samples remained stable. Photoluminescence (PL) measurements show that, despite the different decay mechanisms, XEOL and PL have comparable behaviour. We have shown that coupling XRD and XEOL is a powerful tool to investigate perovskite material under different environmental conditions.

References: [1]Knight, A. J., et al. ACS energy letters 6.2 (2021): 799-808.

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