	Experiment title:	Experiment number:
	Role of bismuth doping on the electronic bandgap of hybrid perovskites	MA-5455

Beamline:	Date of experiment:	Date of report:
BM8 + BM16	from: 27/9/22 to: 30/1/23	31/3/23
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Report:

$((CH_3)_3SO)_3Pb_{3x}Bi_{2(1-x)}I_9$ powders were prepared by precipitation from aqueous solutions as described in J. Phys. Chem. C (2021). Phase purity of all samples was checked with laboratory XRD before shipping.

BM16:

X-ray absorption (XAS) spectra at Pb L_2 (15200 eV) and Bi L_2 (15708 eV) edges were collected for $(TMSO)_3Pb_{3x}Bi_{2(1-x)}I_9$, $(TMSO)_3Pb_{3x}Bi_{2(1-x)}Br_9$ (x = 0, 0.15, 0.25, 0.5, 0.75, 1) and Bi_2Te_3. The spectra were collected with an energy range depending on the overlapping of the absorption edges of the elements composing the compounds. The storage ring operated at 6 GeV mode with a minimum current of 195.02 mA. The XAS spectra have been collected in fluorescence mode using ionization chambers filled with He gas. A Si (220) monochromator was used achieving an energy resolution ΔE of ~ 1.2 eV. The XAS data have been collected with an energy step of 5 eV in the pre-edge region and 0.4/0.5 eV in the XANES region. The spectra have been collected in vacuum at liquid N_2 temperature (80 K), using a cryostat available at the beamline, beacause the hybrid perovskites ($(TMSO)_3Pb_{3x}Bi_{2(1-x)}I_9/Br_9$) show photo-degradation under the X-ray beam. The samples suitable for XAS measurements in fluorescence mode were prepared by mixing the compound with boron nitride (BN) in different proportions and pressing the mixture into 5 mm diameter pellets, so that measurements could be made on pellets with different sample dilution. Data analysis is underway.

BM8:

X-ray absorption (XAS) spectra at Bi L_3 (13.4 keV) and kSn (20.2 keV) - edges have been collected for $(TMSO)_3Pb_{3x}Bi_{2(1-x)}I_9$, $(TMSO)_3Sn_{3x}Bi_{2(1-x)}I_9$, $(TMSO)_3Pb_{3x}Bi_{2(1-x)}Br_9$ (x = 0, 0.15, 0.25, 0.5, 0.75, 1), BiI_3, SnI_2 and $SnBr_2$. The spectra were collected with an energy range depending on the overlapping of the absorption edges of the elements composing the compounds. The XAS spectra have been collected in transmission mode. The XAS data have been collected with an energy step of 10 eV in the pre-edge region, 1 eV in the XANES

region and 2-3 eV in the EXAFS region. The spectra have been collected in vacuum at liquid N_2 temperature (100 K), using a cryostat available at the beamline, beacause the hybrid perovskites ($(TMSO)_3Pb_{3x}Bi_{2(1-x)}I_9/Br_9$) show photo-degradation under the X-ray beam. The samples suitable for XAS measurements in transmission mode were prepared by mixing the compound with polyethylene in an adequate ration for measurements in transmission mode and pressing the mixture into pellets of 13 mm of diameter. Data analysis is underway.