ESRF	**Experiment title:** Study of perovskite based materials for solar cell applications	**Experiment number**: 20-02-738
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Report:

As an outcome of our experiment, the manuscript entitled "*Electronic Structure and Band Interface of Cesium Bismuth Iodide on Titania heterostructure using Hard X-Ray spectroscopy*" with the following author list: **D. Phuyal, S. M. Jain, B. Philippe, M. B. Johansson, M. Pazoki, J. Kullgren, K. O. Kvashnina, M. Klintenberg, E. M. J. Johansson, S. M. Butorin, O. Karis, and H. Rensmo**, has been submitted to J. Mater. Chem. A.

Abstract:

Bismuth halide compounds as a non-toxic alternative are increasingly investigated for their potential in optoelectronic devices and for their rich structural chemistry. Hard x-ray spectroscopy was applied to the ternary bismuth halide $Cs_3Bi_2I_9$ and its related precursor BiI_3 and CsI to understand its electronic structure at an atomic level. We specifically investigated the core-levels and valence band using x-ray photoemission spectroscopy (PES), high-resolution x-ray absorption (HERFD-XAS), and resonant inelastic x-ray scattering (RIXS) to get insight into the chemistry and the band edge properties of the two bismuth compounds. Using these element specific x-ray techniques, our experimental electronic structure show that the primary difference between the two bismuth samples are the position of the iodine states in the valence and conduction bands, and the degree of hybridization with bismuth lone pair ($6s^2$) states. The crystal structure of the two layered quasi-perovskite compounds play a minor role in modifying the overall electronic structure, with variations in bismuth lone pair states and of iodine band edge states. Density Functional Theory (DFT) calculations are used to compare with experimental data. The results demonstrate the effectiveness of hard x-ray spectroscopies to identify element specific bulk electronic structure and their use in optoelectronic devices.