SYNCHROTRON RADIATION PHOTOELECTRON SPECTROSCOPY STUDY OF THE ELECTRONIC STRUCTURE OF Ag-Bi-I RUDORFFITE NANOPARTICLES

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Abstract. Organic/inorganic lead halide perovskites are among the most studied materials for absorption layers in solar cells due to their optimal band gap, high charge carrier mobility, and valence band alignment with materials used for electron and hole transport (Milosavljević et al. 2018). However, there are several obstacles for large-scale production of these materials such as degradation in the presence of oxygen and moisture and lead toxicity. Silver-bismuth-iodide (Ag-Bi-I) rudorffites have garnered significant research interest as lead-free, chemically stable, and low-cost absorber materials. Fabricating Ag-Bi-I in nanocrystal form could facilitate their integration into solar cells and enhance the performance due to the quantum confinement effect. Here, we present the synthesis of ligand-free Ag-Bi-I rudorffite nanomaterials and a photoelectron spectroscopy study of the obtained systems. We fabricated Ag₃BiI₆ aerosol nanoparticles with an average size of

~ 100 nm (Danilovic et al. 2020) and colloidal nanoplatelets with lateral dimensions of approximately 110 nm and thickness ranging from 1 to 8 nm (Danilovic et al. 2022). The electronic structure of isolated nanoparticles was explored using synchrotron radiation X-ray aerosol photoelectron spectroscopy (XASP). By integrating XASP results with UV-Vis absorption spectroscopy and XPS data, the complete valence electronic structure of Ag-Bi-I nanosystems was reconstructed. Furthermore, an analysis that shows the relation between the positions of the bands in the Ag₃BiI₆ nanosheet absorption spectra and the thickness of the nanosheet will be discussed.

References

Milosavljević, A. R., Božanić, D. K., Sadhu, S. : 2018, *J. Phys. Chem. Lett.* 9, 3604. Danilović, D., Božanić, D. K., Dojčilović R. : 2020, *J. Phys. Chem. C* 124, 23930. Danilović, D., Milosavljević A. R., Sapkota, P. : 2022, *J. Phys. Chem. C* 126, 13739.