

26th Congress of SCTM

Sept. 20-23, 2023, Metropol Lake Resort, Ohrid, N. Macedonia

Synthesis and Characterization of Hybrid Organic-Inorganic Perovskites with Morpholinium as an Organic Cation

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Hybrid organic-inorganic perovskites (HOIPs) have been an intensely studied class of materials since the synthesis of the seminal compound $(CH_3NH_3)PbI_{3}$, due to their promising optoelectronic properties and their potential application in the design of diodes, photosensors and photovoltaic cells. In this work, we describe the synthesis and characterization of a class of iodide organic-inorganic perovskite with morpholinium as an organic cation, while the second cations are varied (B = Bi³⁺, Sb³⁺, and Pb²⁺). The emphasis of the research is in the direction towards their application as semiconductors, estimated through the direct and indirect band gap energies.

The synthesis of the perovskites was conducted in acetonitrile as a solvent, to which corresponding iodide salts of the organic cations were added. The reaction mixtures were heated for 30 minutes to an hour. Crystallization of the lead perovskite was observed almost instantaneously. However, in the case of Bi and Sb perovskites, the solutions had to be evaporated almost completely, before lighter-colored crystals precipitated from the solution. The crystals were left overnight, that lead to the formation of a darker crystalline phase. Studies were conducted on these darker phases of each of the studied perovskite.

The obtained compounds were investigated by powder XRD and vibrational spectroscopy (IR and Raman) in a wide temperature range (liquid nitrogen temperature to 20 °C). Thin films of the HOIPs were obtained with the use of spin coating techniques, and they were investigated by UV-vis spectroscopy. These data were used to construct the Tauc plots, from which the direct and indirect band gaps were determined.

Keywords: hybrid organic-inorganic perovskites, morpholinium, thin films, PXRD, vibrational spectroscopy, UV-vis spectroscopy.