Contribution ID : **228** Type : **Oral Presentation**

Mixed Halide Effects on Structure and Electronic Properties in Perovskite-Inspired Materials

Lead halide perovskites have garnered significant attention for optoelectronic applications due to their outstanding properties, such as high absorption coefficients, tuneable bandgaps, long charge carrier lifetimes, and excellent defect tolerance. However, their widespread use is hindered by the toxicity of lead, prompting the search for environmentally benign alternatives. Bismuth-based perovskite-inspired materials have emerged as promising lead-free candidates, offering comparable electronic characteristics and enhanced stability [1].

In this study, we employ density functional theory (DFT) to systematically investigate the structural, electronic, and carrier transport properties of the mixed-halide system Cs3Bi2(I1-xBrx)9 exploring several compositions with x ranging from 0 to 1. We predict a composition-driven phase transition from the iodine-rich P63/mmc phase to the bromine-rich P-3m1 phase occurring near 42% Br content. The P63/mmc structure is found to be stable below ˜39% Br, while the P-3m1 phase becomes energetically favourable above ˜44% Br, in agreement with experimental trends [2].

The bandgap generally increases with higher Br concentrations, consistent with experimental observations. Effective mass calculations reveal that electrons consistently have lower effective masses than holes across all compositions, indicating higher electron mobility. Additionally, hole localization becomes more pronounced with increased Br content, likely due to self-trapping effects associated with Br atoms, which could impact overall charge transport [3].

These findings highlight the pivotal role of halide composition in tuning the phase stability, electronic structure, and charge transport properties of Bi-based perovskite-inspired materials. The insights provided here are instrumental for the rational design and optimization of lead-free materials for next-generation photovoltaic and photocatalytic applications.

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