A New Class of Low Dimensional Organic-Inorganic Hybrid Halides for Optoelectronic Applications

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Abstract: In the world of perovskite halides, the lower dimensionality is showing high structural tunability and more stability with the introduction of hydrophobic organic cations by blocking the moisture penetration in comparison to 3D structure. This result in attractive optoelectronic properties for different field of applications such as solar cells, lasers, photodetectors, memory devices and LEDs[1],[2],[3]. The progress and field of applications of perovskite halides in the last decade is tremendous, however they contain toxic lead which is restricting the applications due to stability, health and ecological concerns. So, there is an urgent need to include the non-toxic elements[4].
Here, we are reporting a new photoluminescent lead-free class of materials, BZA_3BiX_6 [BZA is benzylamine, Bi is bismuth and X is bromine and iodine]. They have been synthesized by a solution-based approach with a monoclinic structure that has isolated MX_6 octahedra surrounded by the organic cations. The powder morphology of the grown crystals is analysed by HR-SEM which concluded the layered growth. BZA_3BiBr_6 and BZA_3BiI_6 exhibits semiconducting behaviour with a bandgap of 2.7eV and 2.2eV respectively. Upon 350 nm excitation, BZA_3BiBr_6 exhibits broad emission centered at 415 nm and 450 nm with a long tail. On the other hand, BZA_3BiI_6 is not an emitter. We consider them as 0D perovskite halides as the octahedral cations are completely surrounded by the organic cations[5]. In this work we are doing a systematic study of the crystal structure, degree of distortion and its purity using the single crystal X-ray diffraction, powder X-ray diffraction and Fourier-transform infrared spectroscopy. The thermal stability of the sample has been examined by TGA/DTA analysis. The optical studies have been thoroughly studied on UV-spectrophotometer and spectrofluorometer. This study will open the doors for a new type of materials by exploring the individual sites in the structure.

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Figure 1: Powder samples of BZA_3BiBr_6 (left) and BZA_3BiI_6 (right).