National Institute of Technology Rourkela

Progress Seminar

Seminar Title	: Synthesis, Structure, and Optoelectronic Properties of Lead-Free Metal Halides with Low Dimensional Structures
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Venue	: Chemistry Seminar Hall
Date and Time	: 06 Sep 2024 (04:00 PM)
Abstract	: Low-dimensional organic-inorganic metal halides (OIMHs) have garnered immense research attention in the field of solid-state lighting materials owing to their outstanding self-trapped exciton (STE)-induced luminescence properties. Though there has been significant research activity in the field of lead-based hybrid metal halides, these compounds suffer from environmental toxicity and atmospheric instability. Thus, it is significant to explore new and promising materials, containing non-toxic elements with excellent atmospheric stability and superior luminescence properties. This has led to the dawn of Bi/Sb-based OIMHs as potential substitutes for lead-based OIMHs with very good thermal and ambient stability and containing relatively less toxic and earth-abundant elements, which are crucial for large-scale commercial use. Further, it has been observed that reduction in the dimensionality of the Bi/Sb-based OIMHs enhances their photoluminescence (PL) properties for applications in solid-state lighting devices. Moreover, understanding the relationship between the structure and luminescence properties of these materials is of utmost importance for tuning the luminescence properties for various practical applications. Hence, we have developed lead-free Bi/Sb-based novel metal halides, $(3,5\text{-DMP})_2BiCl_5$ and $(3,5\text{-DMP})_2SbCl_5$ [(3,5-DMP) = 3,5-dimethylpiperidine], possessing zero-dimensional (0D) structures and crystallizing in triclinic (*P*&minus1 space group) and monoclinic ($P2_1/c$ space group) crystal systems, respectively. The structural phase transition from monoclinic to triclinic phase and its effect on optical properties like band gap and photoluminescence (PL) is further studied through the synthesis of solid solution, $(3,5\text{-DMP})_2Bi_{1\&minus x}Sb_xCl_5$, by the substitution of Sb in pristine Bi compound. Furthermore, by replacing the X site containing the Cl atom with Br atom, we have successfully synthesized a new 0D Sb-based OIMH compound with a general formula, $(3,5\text{-DMP})_3Sb_2Br_9$ crystallizing in the triclinic P&minus1 space group and possessing a typical 0D structure with isolated face sharing $[Sb_2Br_9]^{3\&minus}$ units. The synthesized compound is studied for its optical and luminescent properties. In the next objective, we tried to use a bulkier A-site organic cation and successfully synthesized two new 0D OIMH compounds with formula, $(2\text{-ABI})_3MCl_6.H_2O$ [(2-ABI) = 2-aminobenzimidazole, M = Bi, Sb] both of which crystallized in the monoclinic $P2_1/n$ space group. The pristine Sb compound exhibited bright yellow emission with broad PL band centering at 580 nm while its Bi analogue displayed no emission. The effect of Sb substitution on the structural, optical and PL properties will be further studied in detail to understand the underlying relationship between structural variation and the optoelectronic properties in these compounds. These compounds are further characterized by using different spectroscopic techniques.