**S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES**
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Condensed Matter and Materials Physics

06th August 2025 **4.00 PM** **FERMION**

SPEAKER

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TITLE OF THE TALK

Structure-Property Correlation and Cation Dynamics in $APbX_3$ Perovskite

ABSTRACT

Hybrid Organic-Inorganic Lead Halide Perovskites (HOIP) have emerged as efficient photovoltaic materials and are promising candidates for developing solar cells with high photo-conversion efficiencies. HOIPs are represented by $APbX_3$, where A is the organic cation e.g. MA ($(CH_3NH_3)^+$) or FA ($(CH(NH_2)_2)^+$), X is halide anion. We have investigated the structure and photoluminescence properties of the solid solution series, $MA_{1-y}FA_yPbI_3$ for various compositions with $0 \leq y \leq 1$. Through temperature dependent single-crystal and powder XRD, we could establish a structural phase diagram for these solid solutions. Most interesting finding in this system is that, structure and dielectric property are strongly correlated. It is known that the organic units in hybrid halide perovskites are free to rotate, but it is not clear if this freedom is of any relevance to the structure-property relationship of these compounds. We have employed quasi-elastic neutron scattering using two different spectrometers, thus providing a wide dynamic range to investigate the cation dynamics in methylammonium lead bromide ($MAPbBr_3$) and formamidinium lead bromide ($FAPbBr_3$) over a large temperature range covering all known crystallographic phases of these two compounds. Our results establish a plastic crystal-like phase forming above 30 K within the orthorhombic phase of $MAPbBr_3$ related to 3-fold rotations of MA units around the C−N axis with an activation energy, Ea, of ~27 meV, which has no counterpart in the FA compound. MA exhibits an additional 4-fold orientational motion of the whole molecule via rotation of the C− N axis itself with an Ea of ~68 meV common for the high-temperature tetragonal and cubic phases. In contrast, the FA compound exhibits only an isotropic orientational motion of the whole FA unit with Ea ≈ 106 meV within the orthorhombic phase and a substantially reduced common Ea of ~62 meV for the high-temperature tetragonal and cubic phases. Our results suggest that the rotational dynamics of the organic units, crystallographic phases, and physical properties of these compounds are intimately connected. Effect of halide variation specifically on the cation dynamics would also be discussed briefly.

HOST FACULTY

Prof. Priya Mahadevan, Senior Professor
Dept. of Condensed Matter & Materials Physics
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