

Department of Physics, National Central University



## Colloquium

## Highly resistive phonon transport in halide perovskites

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Abstract :

This presentation focuses on the inherent complexity of phonon dynamics in organicinorganic hybrid perovskites, arising from the intricate interplay between rotational organic cations and dynamically disordered inorganic octahedra mediated by hydrogen bonding. To elucidate these effects, this study investigates representative materials from the hybrid perovskite family, including three-dimensional (3D) MAPbCl<sub>3</sub> and MAPbBr<sub>3</sub>, as well as two-dimensional (2D)  $EA_2PbI_4$ , with an emphasis on their phonon scattering and thermal transport behaviors. We show that the thermal conductivity of these perovskites approaches the theoretical amorphous limit across a broad temperature range. Notably, during the phase transition from the orthorhombic to cubic phase in 3D perovskites, thermal transport shifts from crystalline-like to liquidlike behavior. This transition arises because, in the low-temperature orthorhombic phase, the restricted rotational freedom of organic molecules leads to Umklapp scattering dominating phonon resistance. In contrast, dynamic lattice distortions induced by the rotational hopping of methylammonium (MA<sup>+</sup>) cations become the primary factor influencing thermal transport in the high-temperature cubic phase. Additionally, we demonstrate that in EA<sub>2</sub>PbI<sub>4</sub>, the average phonon mean free path approaches the covalent bond length of the PbI<sub>6</sub> octahedron, contributing to the highly resistive thermal transport observed in this two-dimensional organic-inorganic hybrid structure.