MONDAY

COLLOQUIUM

Pauling's Century-Old Rule Guided Unusual Heat Transport in Crystalline Materials

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13 Jul 2026 (Monday) | 14:30 Hrs (Tea / Coffee 14:15 Hrs) | Venue: TIFRH Auditorium

Controlling heat transport in crystalline solids requires fundamental understanding of how local bonding environments influence lattice dynamics. In this presentation I am going to show that a long-standing principle of crystal chemistry, Pauling's third empirical rule, offers a powerful and general route to engineering intrinsically low lattice thermal conductivity (κ_{lat}). When polyhedral units share edges or faces, close cation proximity generates electrostatic repulsion that destabilizes the lattice, producing dynamic distortion and enhanced anharmonicity. Using a combination of synchrotron X-ray pair distribution function (PDF), vibrational probes, and first-principles calculations, we demonstrate that such lattice instabilities are a recurring feature in several crystalline metal chalcogenides and halides. In TlAgSe, edge-linked coordination units promote Ag-Ag interactions that trigger correlated motion of Ag and Tl atoms. These dynamics introduce low-energy optical phonon excitations that interact strongly with acoustic phonons, leading to a pronounced reduction of κ_{lat} to approximately 0.17 W/m.K at 573 K. A broader survey of nearly 65 ternary metal chalcogenides reveals a systematic decrease in κ_{lat} as structural connectivity evolves from corner-sharing to edge- and face-sharing motifs, highlighting a chemistry-controlled trend rather than a material-specific anomaly. In structurally confined, zero-dimensional halides like Tl_2AgI_3, face-sharing-induced repulsion drives phonon localization and invalidates the conventional phonon-gas picture, resulting in a temperature-dependent crossover from particle-like to wave-like coherence-dominated phonon transport, described within the linearized Wigner transport framework. Together, these results show that polyhedral connectivity and chemical bonding in the crystal structure dictates phonon scattering, coherence, and localization in ordered crystals.

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