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Thermal Transport in Thermoelectric Materials with Chemical Bond Hierarchy

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Understanding thermal transport in complex materials is a critical issue in searching for high-performance thermoelectric materials. This talk will summarize our recent work on the diverse lattice dynamics and unusual thermal transport in compound materials with different level of structural complexity. Usually, the thermal transport is described by the traditional concept of phonon and phonon scattering anharmonicity. A concept of part-crystalline part-liquid state (or liquid-like), and even part-crystalline part-glass state (or glass-like), was demonstrated in some materials such as Cu_3SbSe_3 and $Cu_2(S,Se)$ with chemical-bond hierarchy, in which certain constituent species weakly bond to other part of the crystal. Those materials intrinsically manifest the coexistence of rigid crystalline sublattices and the other fluctuating noncrystalline sublattices with large atomic displacement amplitude and even flow of the subgroups of atoms. The large-amplitude vibrations and liquid-like flow of atoms generate unusual severe phonon scattering and thermal damping due to the collective low-frequency vibrations similar to the Boson peak in amorphous or liquid materials, leading to the phenomenon of phonon scattering beyond the traditional anharmonicity.