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Part-crystalline part-liquid state and electrical/thermal transport in materials with chemical-bond hierarchy

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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 Cu3SbSe3 with chemical-bond-hierarchy, in which certain constituent species weakly bond to other part of the crystal. Such a material could intrinsically manifest the coexistence of rigid crystalline sublattices and other fluctuating noncrystalline sublattices with thermally induced large amplitude vibrations and even flow of the group of species atoms. The large-amplitude vibrations and movement of atoms can 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. While different phase or state may have large energetic discrepancy, whether the thermally-induced part-crystalline state is undergoing phase transition becomes an interesting issue. In addition, our earlier work reported that second-order phase transition could induce extreme electron and phonon scattering in thermoelectrics. The above work clearly demonstrated that the unusual effect from structural fluctuations on thermal and electrical transport in thermoelectrics should be paid attention to. While materials with these structural changes can retain extremely low lattice thermal conductivity and unusual electron transport and become promising candidates for high-performance thermoelectrics, underlying mechanism is yet to be explored.