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ROLE OF CRYSTAL STRUCTURE AND CHEMICAL BONDING IN THERMAL TRANSPORT OF THERMOELECTRIC MATERIALS: THE CASE OF FILLED *β*-Mn-TYPE PHASES

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Finding the way to interlink heat transport with crystal structure and order/disorder phenomena is crucial for designing materials with ultralow lattice thermal conductivity. Here, we revisited the crystal structure and explored the thermoelectric properties of several compounds from the family of the filled *β*-Mn-type phases $M^{n+}_{2/n}Ga_6Te_{10}$ (*M* = Pb, Sn, Ca, Na, Na+Ag). The strongly disturbed thermal transport observed in the investigated materials originates from a three-dimensional Te-Ga network with lone-pair-like interactions, which results in large variations of the Ga-Te and *M*-Te interatomic distances and substantial anharmonic effects. In the particular case of $NaAgGa_6Te_{10}$, additional presence of different cations, leads to bonding inhomogeneity and strong structural disorder resulting in the dramatically low lattice thermal conductivity (~0.25 W m^{-1} K^{-1} at 298 K), being the lowest among reported *β*-Mn-type phases. This study offers a way to develop materials with ultralow lattice thermal conductivity by considering bonding inhomogeneity and lone-pair-like interactions.

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