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Phonon-Glass Electron-Crystal like High Performance Thermoelectrics

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With about 2/3 of all utilized energy is being lost as heat. Thermoelectric materials can convert waste heat to electrical energy, and it will have significant role in future energy management. Achieving glass-like ultra-low thermal conductivity in crystalline solids with high electrical conductivity, a crucial requirement for high-performance thermoelectrics, continues to be a grand fundamental challenge. Despite this inherent trade-off, the experimental realization of an ideal thermoelectric material with a phonon-glass electron-crystal (PGEC) nature has rarely been achieved. We demonstrated high thermoelectric performance with a near room-temperature figure of merit, zT ~1.5 and a maximum zT ~2.6 at 573 K by optimizing atomic disorder in Cd doped $AgSbTe_2$.[1-3] Cd doping in $AgSbTe_2$ enhances cationic ordering, which simultaneously improves electronic properties by tuning disorder-induced localization of electronic states and reduces lattice thermal conductivity via spontaneous formation of nanoscale (~2-4 nm) superstructures. Further, we showed that isovalent Yb-doping induced enhanced atomic ordering decreases the overlap between the hole and phonon mean free paths and consequently leads to a PGEC-like transport in $AgSbTe_2$. A twofold increase in electrical mobility is observed while keeping the position of the Fermi level nearly unchanged, which leads to zT ~2.4 at 573 K.[4] Recently, we discovered PGEC-like thermoelectric transport in entropy stabilized new telluride single crystal, $AgGeSnSbTe_4$. Local distortion caused by the off-centering of Ge atoms, driven by a stereochemically active $4s^2$ lone pair in a globally symmetric rock-salt structure, plays a key role in suppressing thermal conductivity to its glass limit while maintaining good electrical transport.[5]

References:

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