VIDEO ARTICLE

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Advanced Thermoelectric Materials with High Performance and Low Cost: *Ab Initio* Study

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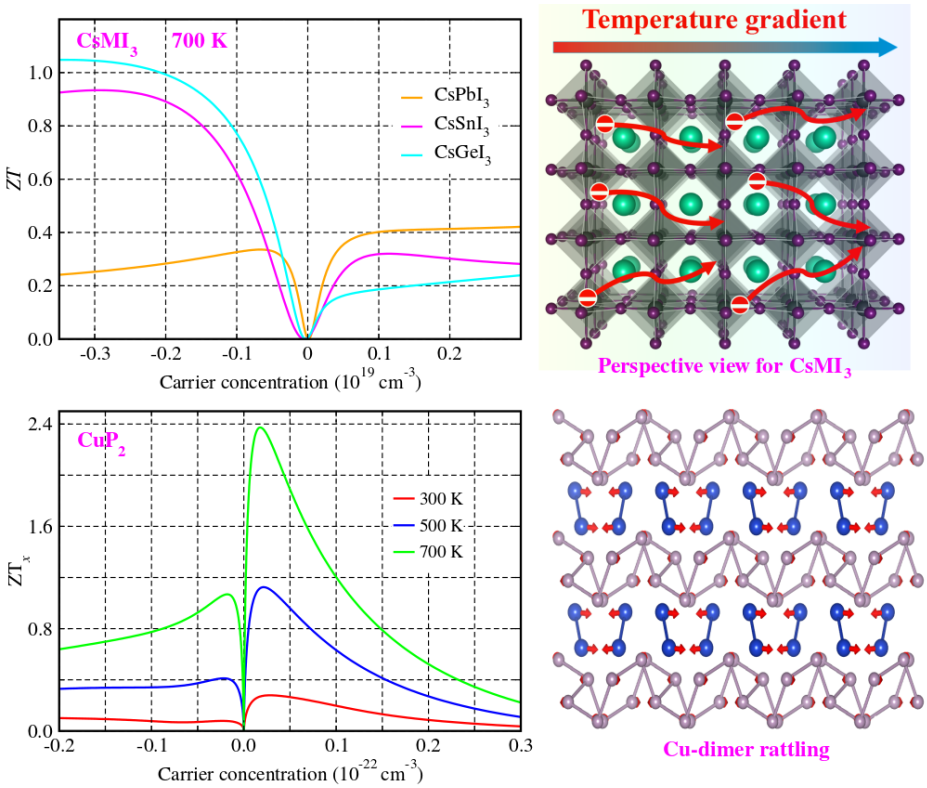
Graphical Abstract



Thermoelectric figure of merit ZT predicted by use of first-principles calculations for all-inorganic iodide perovskite $CsMI_3$ and metal phosphide CuP_2 with perspective view of $CsMI_3$ crystalline structure and Cu-dimer rattling in CuP_2.

Abstract

Conventional thermoelectric materials such as chalcogenides and Bi–Te alloying systems exhibit high thermoelectric conversion efficiency, but unfortunately, they include expensive rare-earth element Te thus hindering their application for large-scale power generation by using them. Searching novel thermoelectric materials with high performance and low cost is now receiving special attention and great challenges in the field of material design. To do this, we perform first-principles lattice dynamics combined with temperature-induced anharmonic phonon renormalization and connected to the Boltzmann transport equation in all-inorganic iodide perovskites $CsMI_3$ (M = Pb, Sn, and Ge) and metal phosphide CuP_2. First, we predict

thermoelectric performance in the cubic $CsMI_3$ at a high temperature of 700 K. Under stabilization of the cubic phase that exhibits strong anharmonic phonon modes at 0 K, our calculations show that at T = 700 K, these perovskites have ultralow lattice thermal conductivities below 0.6 W m^{-1} K^{-1} and high thermopower factors over 1.5 mW m^{-1} K^{-2}, being comparable or superior to those of GeTe. Moreover, we find that cubic $CsGeI_3$ and CsSnI3 have higher thermoelectric figure of merit ZT over 0.95 upon n-type doping, being attributed to the strong lattice anharmonicity and flat-dispersive electronic bands with high degeneracy. Next we study the thermoelectric properties of metal phosphide CuP_2 in the monoclinic phase. Our lattice dynamics calculations reveal that CuP_2 exhibits Cu-dimer rattling modes, which strongly scatter the heat-carrying acoustic and low-lying optical phonons, resulting in an unusually low lattice thermal conductivity below 3.6 W m^{-1} K^{-1}, being about a half of the conventional thermoelectrics GeTe. We predict Seebeck coefficients, the value of which at 300 K is in good accordance with the experiment, and power factors that are superior to the conventional thermoelectrics GeTe, possibly due to flat- and dispersive-band structures with high orbital degeneracy. Finally, we assess its thermoelectric performance by evaluating the figure of merit ZT, finding that upon p-type doping ZT can reach over 1.3 at a high temperature of 700 K by optimizing the hole concentration. To conclude, our results highlight the potential of using metal phosphide CuP_2 and inorganic iodide perovskites $CsMI_3$ as a promising material for thermoelectric applications with practical performance and low cost.

Keywords: Thermoelectric materials; inorganic halide perovskite; metal phosphide; lattice dynamics; transport properties

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References

1. U.G. Jong, Y.S. Kim, C.H. Ri, Y.H. Kye, C.J. Yu, *The Journal of Physical Chemistry C*, **2021**, 125, 6013.
2. U.G. Jong, C.J. Yu, Y.H. Kye, S.N. Hong, H.-G. Kim, *Physical Review Materials*, **2020**, 4, 075403.
3. U.G. Jong, C.H. Ri, C.J. Pak, C.H. Kim, S. Cottenier, C.J. Yu, *New Journal of Chemistry*, **2021**, 45, 21569.

Biography of Presenting Author

Un-Gi Jong is a senior researcher of Faculty of Materials Science, Kim Il Sung University. He has got his Ph.D. degree in materials science from Kim Il Sung University in 2019. His research interest includes a computational materials design of energy conversion materials such as light absorber of perovskite solar cells and thermoelectrics by applying first-principles method. In 2021, he was awarded the Complimentary Membership from the American Chemical Society and became a Guest Editor for the journals of Frontiers in Physics and Frontiers in Energy Research.

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