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Experimental validation of high thermoelectric performance in $RECuZnP_2$ predicted by advanced DFT calculations

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Thermoelectric materials can convert waste energy back to useful electricity and hence, can significantly contribute to the generation of clean energy. However, thermoelectric materials are currently limited by high cost and low efficiencies. The search for high-efficient thermoelectric materials is hindered by the interrelated electrical and thermal transport properties. High-throughput screenings based on density functional theory (DFT) can accelerate the search and discover novel high-performance thermoelectric candidates. In a recent screening of 48,000 compounds, enhanced electronic properties were observed for various $RECuZnP_2$ compounds. The thermoelectric transport properties were measured for three different $RECuZnP_2$ compounds indicating high thermoelectric efficiencies. Advanced DFT calculations (i.e., AMSET and compressive sensing lattice dynamics) were performed confirming the high thermoelectric performance. These methods can compute the scattering rates of electrons and phonons (even with strong anharmonicity) and provide unique insights of the underlying physics in thermoelectric compounds.

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