CORE-CM SEMINAR
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Romancing the Rock: High Performance Thermoelectricity in Mineral-Based Materials

The thermoelectric effect was discovered in the early 1800's by Seebeck in studies on metals and minerals. Later, in the first half of the 20^{th} Century, further studies on minerals were undertaken by Haken and Telkes. With the advent of semiconductor physics and technology, effort turned in the latter half of the 20^{th} century to synthesizing compounds with controlled compositions from purified elements, a fabrication strategy that has largely continued to the present day.

Concerns over element toxicity and the low abundance of some elemental components such as tellurium, cobalt, and the rare earths, have compelled us to return to the study of earth-abundant materials for thermoelectricity. However, we return to this starting point armed with powerful tools that help us to predict the relevant properties of large families of compounds and natural minerals. Guided by density functional theory calculations of lattice dynamics and electronic structure, we have identified the tetrahedrite family of minerals as potential high performance thermoelectric materials. Importantly, the tetrahedrites comprise the most widespread sulfosalts on Earth. The general composition of tetrahedrite may be written as $Cu_{12-x}M_xSb_{4-y}As_yS_{13}$, where M is mainly iron or zinc. An unusual band structure gives rise to large Seebeck coefficient over a wide range of x, spanning the compositions of tetrahedrite that occur in nature. Meanwhile, large anharmonicity drives the lattice thermal conductivity down to near minimum values. As a result, tetrahedrites can possess dimensionless figures of merit exceeding unity at 400C, comparable or even exceeding that of some of the best synthetic thermoelectric materials in this temperature range. We also show that samples synthesized using natural mineral tetrahedrite directly as a source material possess similar values of figure of merit. The results suggest a new paradigm for thermoelectric material development. Rather than extracting and purifying elements at great effort and cost, and then recombining them into new compounds at more effort and cost, one can use natural minerals directly as sources for highly efficient thermoelectric materials.

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