Heterostructural Alloying – A Design Tool to Improve Functionality

Scientific Achievement
Metastable (SnCa)Se with improved thermoelectric functionality was realized by combining theory-guided alloying with non-equilibrium growth.

Significance and Impact
Alloying to target desired structures is emerging as a powerful materials design tool for applications requiring multi-property optimization. In this case, a factor of 100 increase in the power factor, which depends on Seebeck coefficient and electrical resistivity, is achieved in going from orthorhombic SnSe to cubic Sn$_{0.84}$Ca$_{0.16}$Se (Fig. 2).

Research Details
**Theory:** DFT/RPA accurately calculates alloy phase diagrams (Fig. 1).

**Synthesis:** Sn$_{1-x}$Ca$_x$Se films by pulsed laser deposition (PLD).

**Characterization:** Crystal structure by X-ray diffraction, decomposition microstructures by scanning transmission electron microscopy / energy-dispersive X-ray spectroscopy, transport measurements by Hall effect, Seebeck effect, electrical resistivity. Optical absorption determines bandgap and thickness.


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**Fig. 1:** Predicted phase diagram. Isotropic rock-salt (RS) structure desired.

**Fig. 2:** Measured transport properties of PLD-grown (SnCa)Se thin films.