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Harnessing Intervalley Scattering for High zT Thermoelectrics[1]
ROBERT MCKINNEY, Colorado School of Mines, PRASHUN GORAI, VLADAN STEVANOVIC, ERIC TOBERER, Colorado School of Mines, National Renewable Energy Lab (NREL) — Convergence of multiple valleys in the band edges improves the charge transport properties necessary for enhancing thermoelectric performance. Typically, these valleys are considered equivalent and intervalley scattering is neglected. Using the Boltzmann approach, we calculate the transport coefficients within the transport distribution function (TDF) formalism[2] for a multivalley band structure. We consider scattering between two valleys with very different effective masses that are offset in the reciprocal space. The resultant TDF is highly assymmetric about the Fermi level, which enhances thermoelectric performance. Guided by this model, we have performed a high-throughput computational search to identify band structures of known materials (calculated with density functional theory) that show similar characteristics - sharp increase in the density of states within a few k_BT of the band edge. More detailed and higher accuracy calculations have been performed on the identified candidates. We therefore demonstrate that intervalley scattering, which is usually ignored in thermoelectrics, can be harnessed as an energy-filtering method to enhance thermoelectric performance.

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[2]G.D. Mahan and J.O. Sofo, PNAS 93, 7436 (1996)

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