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Computational and experimental force multipliers for the discovery of new thermoelectric materials[1]

ERIC TOBERER, Colorado School of Mines

This talk will focus on the development of advanced thermoelectric materials within the Materials Genome Initiative paradigm and the prospects for widespread thermal-to-electric power conversion. These thermoelectric material discovery efforts are driven by a close coupling of theory, computation, and experimental validation. The implementation of a high through-put search of known and hypothetical compounds for thermoelectric performance (NSF-DMREF) has led to the identification of new classes of thermoelectric materials. High throughput experimental measurement of thermoelectric materials serves to complement these computational efforts. Further material development involves demonstrating materials with exceptionally strong phonon-point defect scattering cross-sections and strong lattice anharmonicity. In concert with computation, general design principles for next generation thermoelectric materials emerge.

[1]NSF DMREF 1333335