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**Band Degeneracy, Low Thermal Conductivity, and High Thermoelectric Figure of Merit in SnTe-CaTe Alloys** R. AL RAHAL AL ORABI, Department of Environmental Science and Engineering, Ewha Womans University, N. MECHOLSKY, Department of Physics and Vitreous State Laboratory, The Catholic University of America, J. P. HWANG, W. KIM, School of Mechanical Engineering, Yonsei University, J. S. RHYEE, Department of Applied Physics, College of Applied Science, Kyung Hee University, D. WEE, Department of Environmental Science and Engineering, Ewha Womans University, M. FORNARI, 5Department of Physics, Central Michigan University and Science of Advanced Materials Program — Pure lead-free SnTe has limited thermoelectric potentials because of the low Seebeck coeffcients and the relatively large thermal conductivity. In this study, we provide experimental evidence and theoretical understanding that alloying SnTe with Ca greatly improves the transport properties leading to ZT of 1.35 at 873 K, the highest ZT value so far reported for singly doped SnTe materials. The introduction of Ca (0-9%) in SnTe induces multiple effects: (1) Ca replaces Sn and reduces the hole concentration due to Sn vacancies, (2) the energy gap increases limiting the bipolar transport, (3) several bands with larger effective masses become active in transport, and (4) the lattice thermal conductivity is reduced of about 70% due to the contribution of concomitant scattering terms associated with the alloy disorder and the presence of nanoscale precipitates. An effciency of 10% (for $\Delta T$ = 400 K) was predicted for high temperature thermoelectric power generation using SnTe-based n- and p-type materials.

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