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Thermoelectric properties of nanoporous Si JOO-HYOUNG LEE, JEFFREY C. GROSSMAN, University of California-Berkeley, JOHN REED, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California-Davis — Improvements in thermoelectric (TE) materials could lead to efficient solid-state energy-conversion for environmentally benign power generation and refrigeration. This realization would require a large increase to ~ 3 in the thermoelectric figure of merit ZT at room temperature. Recent experiments have shown promise for practical applications of TE materials such as Bi_2Te_3/Sb_2Te_3 superlattices and PbSeTe/PbTe quantum dot superlattices, yielding ZT of 2.4 and $1.3 - 1.6$, respectively. In addition, there have been recent attempts to use Si for TE pplications due to its structural simplicity and the possibility of utilizing existing Si-based manufacturing processes. In the present work, we report theoretical studies on thermoelectric properties of Si with periodically arranged nanometer-sized pores (*nanoporous Si*). Specifically, we calculate the electrical conductivity, Seebeck coefficient and figure of merit of nanoporous Si for a range of configurations using a combined *ab inito* electronic structure calculation and Boltzmann transport approach at room temperature. The results show a substantial increase in ZT compared with that of bulk Si, similar to recent findings for ZT in Si nanowires. Approaches for increasing ZT further in this porous material will also be discussed.

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