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Thermoelectric Properties of Ultra Narrow Silicon Nanowires from Atomistic Calculations NEOPHYTOU NEOPHYTOS, HANS KOSINA, Institute for Microelectronics, Technical University of Vienna — The progress in nanomaterials' synthesis allows the realization of thermoelectric devices based on 1D nanowires (NWs). In these confined systems the electrical and thermal conductivities, and the Seebeck coefficient can be designed to some degree independently, providing enhanced ZT values as compared to the bulk material's value. We calculate the electrical conductivity, the Seebeck coefficient, and the electronic part of the thermal conductivity of scaled Si NWs. We use the atomistic sp³d⁵s*-spin-orbit-coupled tight-binding model and linearized Boltzmann transport. Our calculations include up to 5500 atoms, a task still computationally affordable within this model. We examine n-type and p-type NWs of diameters between 3nm and 12nm for [100], [110] and [111] transport orientations, at different doping levels. Using experimentally measured values for the lattice thermal conductivity, the expected ZT values of the nanowires are estimated. We further provide directions for power factor optimization with structure confinement.

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