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Thermoelectric performance of Si-Ge heterostructured nanowires from first-principles ARASH MOSTOFI, MATTHEW SHELLEY, Imperial College London — We present calculations of the thermoelectric figure of merit ZT of both pristine and axially heterostructured Si/Ge nanowires as a function of their compositional disorder, growth direction and diameter. Our method is based on density-functional theory (DFT). Both charge and transport properties are calculated within the Landauer-Buttiker formalism. We compute ZT for realistic nanowires (ca. 10,000 atoms and 100 nm in length) by using maximally-localized Wannier functions to map large-scale DFT calculations onto short-ranged model Hamiltonians with negligible loss of accuracy. The approach is fully automated and robust, such that large numbers of configurations of the system can be explored with high throughput and efficiency. While we focus here on their application to thermoelectric nanowires, the algorithms we have developed are generally applicable to other classes of disordered quasi-one-dimensional nanostructures such as DNA, carbon nanotubes and graphene nanoribbons.

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