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Ab initio thermal transport properties of nanostructures from density functional perturbation theory. THUSHARI JAYASEKERA, Southern Illinois University, Carbondale, IL, ARRIGO CALZOLARI, Istituto Nanoscienze, CNR-NANO S3 Center I-41125, Modena Italy, KI WOOK KIM, North Carolina State University, Raleigh, NC, MARCO BUONGIORNO NARDELLI, University of North Texas, Denton, TX — We present a comprehensive first principles study of the thermal transport properties of low-dimensional nanostructures such as polymers and nanowires. An approach is introduced where the phonon quantum conductance is computed from the combination of accurate plane-wave density functional theory electronic structure calculations, the evaluation of interatomic force constants through density functional perturbation theory for lattice dynamics and the calculation of phonon transport properties by a real space Green's function method based on the Landauer formalism. This approach is computationally very efficient, can be straight-forwardly implemented as a post-processing step in a standard electronic-structure calculation (Quantum ESPRESSO and WanT in the present implementation), and allows us to directly link the thermal transport properties of a device to the coupling, dimensionality, and atomistic structure of the system. It provides invaluable insight into the mechanisms that govern the heat flow at the nanoscale and pave the way to the fundamental understanding of phonon engineering in nanostructures.

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