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Ab-initio calculations of the lattice thermal conductivity from an exact solution of the Boltzmann-Peierls equation LAURENT CHAPUT, Institut Jean Lamour — In this work we present *ab-initio* calculations of the lattice thermal conductivity and related quantities for several semiconductors of interest in energy transport and thermoelectricity. Excellent agreements with experiments are found. A new method is proposed to obtain a numerically exact and fast solution to the Boltzmann-Peierls equation. This is made possible using the symmetry of the systems and open the way to the theoretical design of new materials. The collision kernel of the equation is constructed using an efficient parallelization of the code over the irreducible triplets of phonon wavevectors involved in the different possible collisions. These irreducible triplets are the equivalent of the irreducible part of the Brillouin zone for single particle quantities. Therefore a formulation of the self energy and collision kernel based on their use drastically reduce the computational time.

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