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Beyond the constant Lorenz number for separating thermal conductivities of electrons and phonons: A DFT study[1] MINGXING CHEN, Department of Physics, University of Wisconsin-Milwaukee, RAIMUND PODLOUCKY, Department of Physical Chemistry, University of Vienna, Austria — Lorenz number is an important quantity for separating thermal conductivities of electrons and phonons in the field of thermoelectrics, which is material- and temperature-dependent. Combing DFT calculations with Boltzmann transport equations, we have derived the Lorenz number for realistic compound $BaAu_6Ge_{40}$, a good thermoelectric material. It is demonstrated that using the constant Lorenz number of the Wiedemann-Franz law for simple metals leads to strong discrepancies, in particular at higher temperatures. The results suggest that one has to rethink the way of extracting both κ_{el} and κ_{ph} as usually done based on the measured electrical conductivity. We propose a strategy of correcting the Wiedemann-Franz Lorenz number that subtracts the metallic limiting value by S^2 as obtained from Seebeck measurements.

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