There is no such thing as a simple metal

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Thermoelectric (TE) materials have garnered very large amounts of interest in the past 10 years as alternative solutions for energy generation and waste heat harvesting, as well as for cooling applications, e.g. in cpus. Only very recently has it become possible to predict quantitatively the thermal and electrical conductivity of materials from a first principles basis. We will review a few recent advances in methodology, with applications to (simple and less simple) metals. The Seebeck coefficient is one of the most delicate quantities to determine and to optimize, and it is central to TE efficiency - we will detail the first ab initio calculations of S and contrast them with the very widely used constant relaxation time approximation.