First-principles High-throughput Design and Discovery of Novel Materials, and its Application to Thermoelectrics

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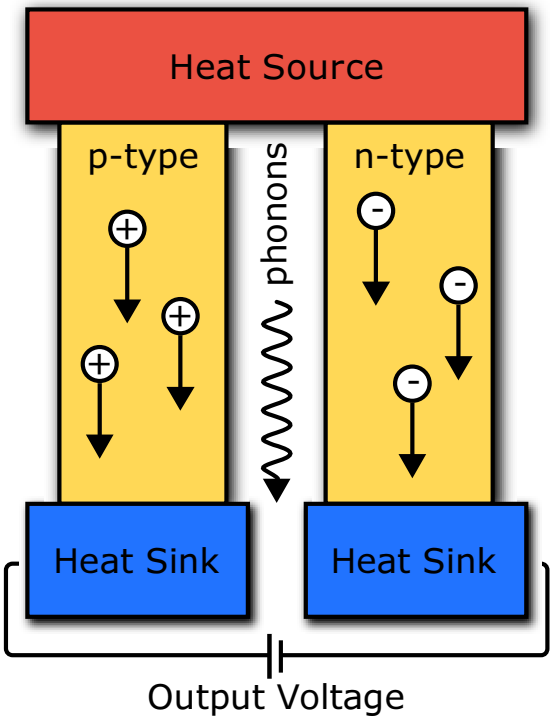

The development of a green, sustainable and affordable energy economy is one of the preeminent scientific challenges of our time. Thermoelectric materials, i.e. materials that allow a direct conversion of a temperature gradient into an electric voltage, have the potential to recover significant amounts of otherwise wasted heat, e.g., in power plants, in car exhausts, or even in mobile electronics [1]. Current low efficiencies of thermoelectric materials have confined their use only to high-tech and expensive applications, such as astronautical engineering, and limited a wide commercial adoption. [1]. Experimentally, the optimization –for instance by introducing compositional and structural disorder at various length scales [2]– is a complex, tedious and costly task, since the efficiency depends on a variety of material properties that are extremely difficult to optimize concurrently, and that subtly depend on each other: the electrical conductivity σ, the Seebeck coefficient S, and the electronic k_{el} and phononic k_{ph} thermal conductivities. This project aims at developing the fundamental theories and tools to compute the thermoelectric transport coefficients σ, S, k_{el}, and k_{ph} from *first principles* and to apply the developed framework to complex materials. By this means, we are able to shed light on the largely unknown mechanisms of thermal [3,4] and electronic transport [5] that determine thermoelectric efficiency and to guide and accelerate the optimization of thermoelectric devices.

[1] J. Snyder and E. Toberer, Nature Materials 7, 105 (2008).
[2] K. Biswas *et al.*, Nature 489, 414-418 (2012).
[3] C. Carbogno *et al.*, Phys. Rev. B 90, 144109 (2014).
[4] G. Fugallo *et al.*, Nano Lett. 14, 6109 (2014)
[5] C. H. Park *et al.*, Nano Lett. 14, 1113 (2014)