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Ab-initio modeling of thermoelectric materials: a new route towards higher efficiency (I)

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Today roughly 60% of the energy humans produce is lost as waste heat. Thermoelectrics (TE) can convert this heat source into useful electrical power, and thus have the potential to impact our energy future. The key challenge is to increase the TE conversion efficiency, which depends on the TE material properties. The past decade has seen remarkable progress in TE materials, but that have originated from experimental trial-and-error. This creates an opportunity for predictive materials modeling to theoretically explore and discover promising TE materials to help guide experimental efforts and accelerate innovation.

In this talk, I will give a brief introduction to TEs and present our recently developed formalism for first-principles modeling of TE transport properties. I will demonstrate how this cutting-edge technique, based on density functional theory and the Boltzmann transport equation, can accurately predict TE characteristics and provide new insights into the scattering and transport physics of these materials.

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