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# Thermoelectric Properties from Ab Initio Calculations

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## ABSTRACT

As nanoscales become accessible to experimentalists, atomistic simulations of materials are becoming increasingly important for the prediction and design of materials properties. Recently, the search for energy efficient materials has driven the development of new theoretical methods, such as the Landauer-Datta-Lundstrom (LDL) generalized transport model, to explore thermoelectric properties of materials based on their electronic structure and lattice dynamics. The Landauer Transport Properties (LanTraP) tool, currently available in nanoHUB, allows the computation of thermoelectric transport coefficients from a full-band electron dispersion; however, generating such electron band structures from *ab initio* methods is a convoluted process. The aim of this project is to automate the generation of electron band dispersions using density functional theory (DFT) as implemented in the DFT materials properties simulator (DFTMatProp) nanoHUB tool. The new feature will produce the full-band electron dispersion of any material in a format suitable for use with LanTraP.

## KEYWORDS

Electronic structure, thermoelectric, transport coefficients, electronic conductivity, thermal conductivity, ZT figure of merit