A Global Search for the Optimal Bandstructure for Thermoelectric Applications

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The best thermoelectric (TE) materials over the last 30 years has been Bi2Te3 and it's alloys. However recent discoveries have renewed the interest in finding a better TE material. We've decided to use a global search genetic algorithm to try and determine the optimal bandstructure for materials with TE applications. This project involves bandstructure analysis and transport property calculations of known materials with interesting TE properties. We want to employ a genetic algorithm to try and locate general features in a bandstructure which have importance for the TE effect of the material.

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