Density functional theory in the search for new thermoelectric materials

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Thermoelectric materials have applications in both Peltier-cooling and in converting waste heat to electrical energy. Due to the discovery of new materials the area has received much attention the past decade.

The search for new thermoelectric materials is a quest to maximize the dimensionless figure of merit $zT = (\sigma T/\kappa)S^2$, where S is the Seebeck coefficient and σ and κ are the electronic and thermal conductivities respectively. zT quantifies the performance of a thermoelectric and one must therefore maximize the power factor $S^2\sigma$ and minimize κ. S, σ and κ are coupled and all depend strongly on the detailed electronic structure, carrier concentration and crystal structure, which makes the task of finding new compounds with large values of zT extremely difficult.

Based on a case study of $CsBi_4Te_6$ I will show how electronic structure calculations can be used to rationalize the behavior of known materials. In this process some fingerprints, which characterize good performance, are identifies. These observations are used to construct a screening of the inorganic crystal structure database for potential thermoelectric materials. I will show how this resulted in the discovery of two new materials: $FeSb_2$ and LiZnSb.

Finally, I will discuss how density functional theory can aid the development of modern nano-structured materials.