Thermoelectric Materials

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Introduction
- Thermoelectrics produce energy by a temperature difference. It uses waste heat and converts it into electricity.
- Thermoelectric materials convert energy based on the Seebeck and Peltier effect.
  - Peltier effect: electrical power to generate a temperature difference.
  - Seebeck effect: use temperature difference to generate electric power.
- We want high electrical conductivity. Low thermal conductivity.
  - If you have a high thermal conductivity it's either going to be all hot or all cold.

Method
- We ran simulations on Mirage to predict how much atoms move. They are run in HSE and PBE.
- The simulations give us the total energy.
  - Low energy means it's stable, high energy is unstable. We want it to be stable.

Motivation
- We want thermoelectric materials to be semiconductors; some electrons are bound and some are free to move.
- Metals, semiconductors, and insulators have different size atoms, which slows down the heat but allows electrons to move freely.

Equation
- You want $\Delta H$ to be the most negative for the material you want to form.
- The result tells us how much of an element exists in the environment of the lab.

$\Delta H = H_{\text{products}} - H_{\text{reactants}}$

Results for AuGaTe₂
- Simulated competing compounds like
  - AuGa₂
  - Ga₂Te₅
  - GaTe
- AuGaTe₂ can be created in a rich environment of gold and poor environment of gallium.

Results for AuInTe₂
- Competing compounds
  - In₂Au
  - InTe
- AuInTe₂ can be created in a gold rich environment and an indium poor environment.

Conclusion
- We discovered the new material AuGaTe₂.
- Now we know how to make these materials theoretically.
- Potentially good thermoelectrics because CuGaTe₂, AgGaTe₂, AgInTe₂ and CuInTe₂, which have similar structures, are good thermoelectrics.

Reference
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