# Thermoelectric Materials


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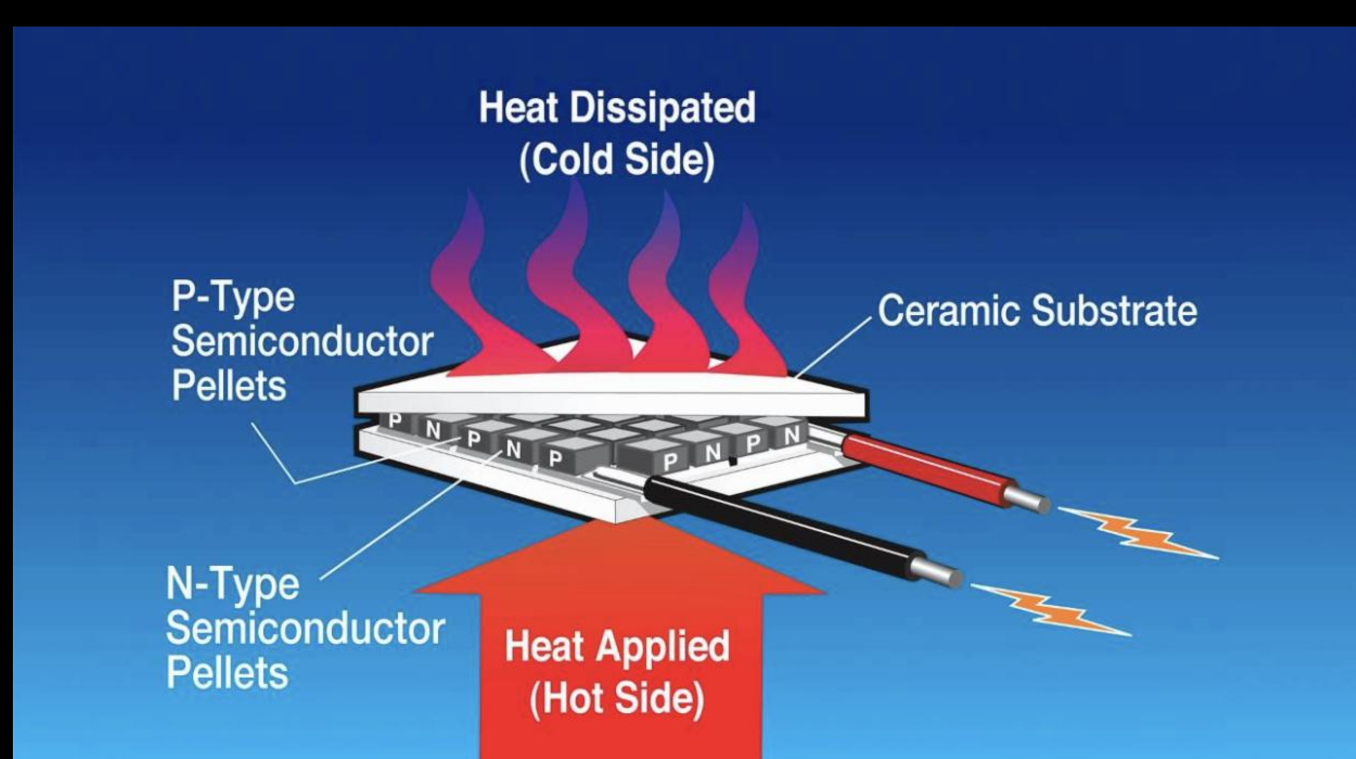
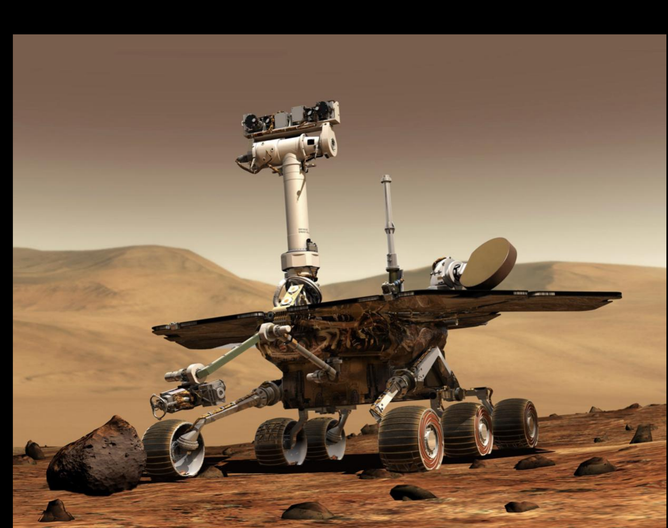
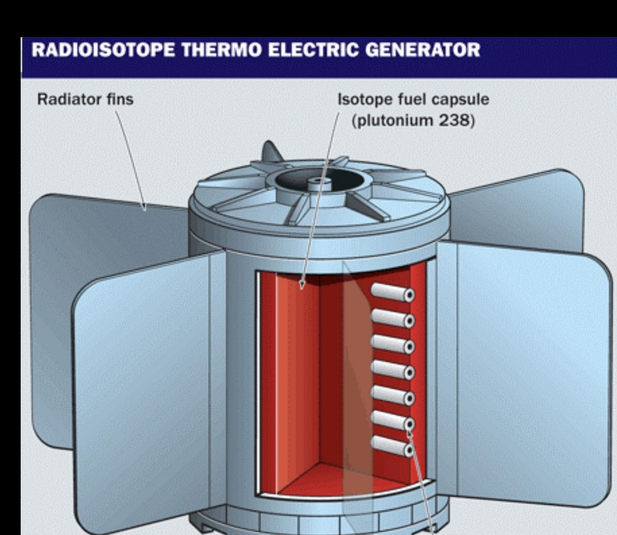
## Introduction

- 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- electric 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 its either going to be all hot or all cold.



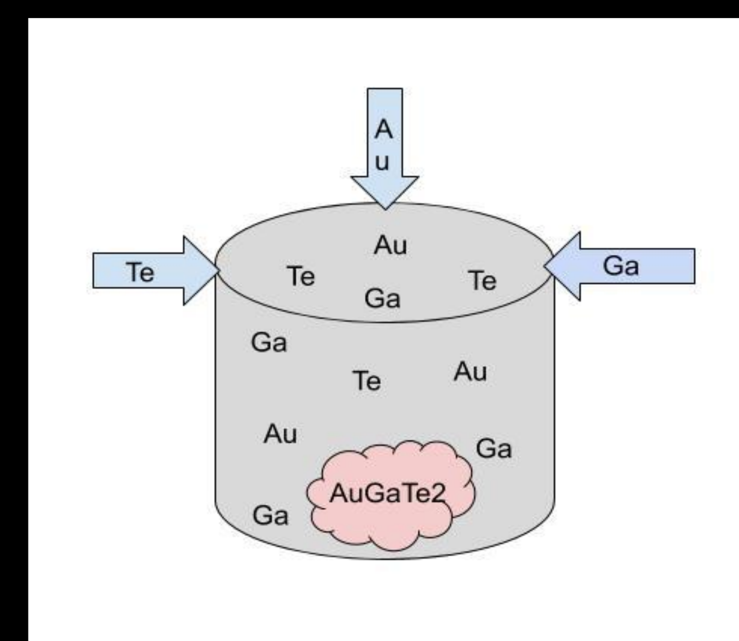



## Motivation

- 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.

## Method

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




**Competing compounds** are created if too much of an element gets into the mixture creating a different material.

**Rich environment** is an environment with an excessive amount of element.

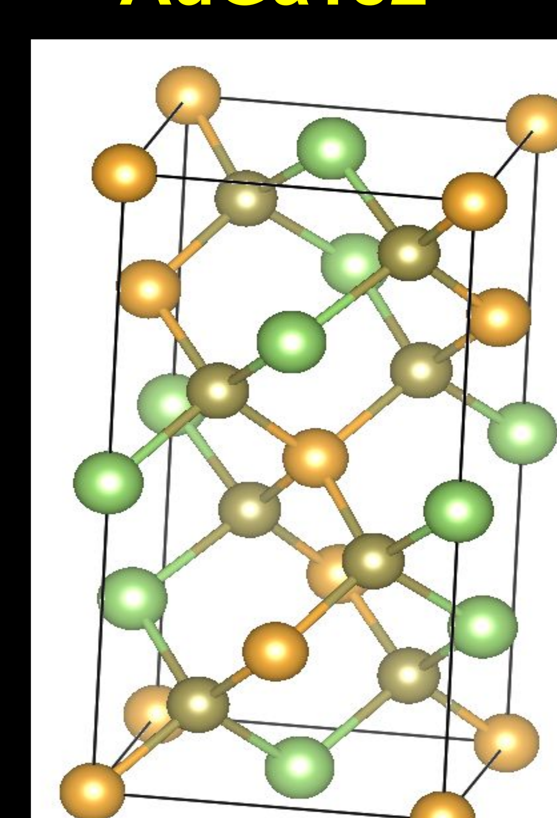
- With the right amount of each element the material can be formed.

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

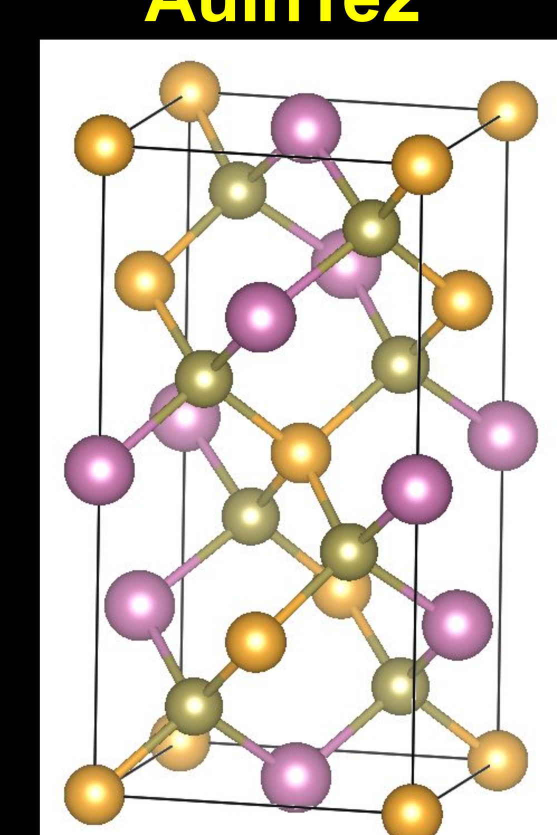
## Equation

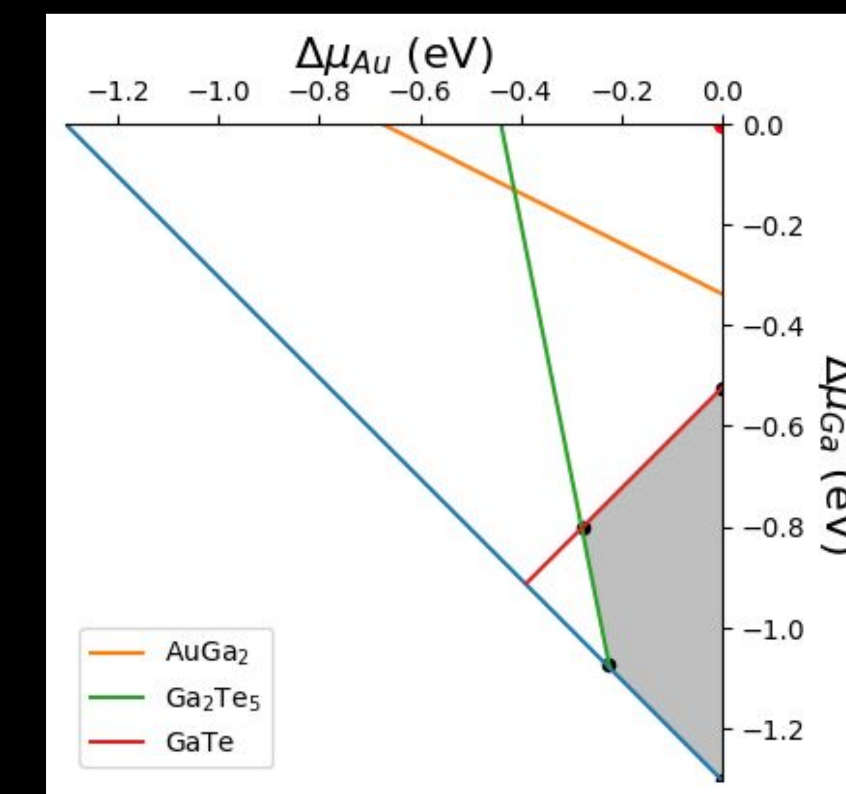
- You want ΔH to be the most negative for the material you want to form.
- The result tells us how much of an element exist in the environment of the lab.

**AuGaTe2**



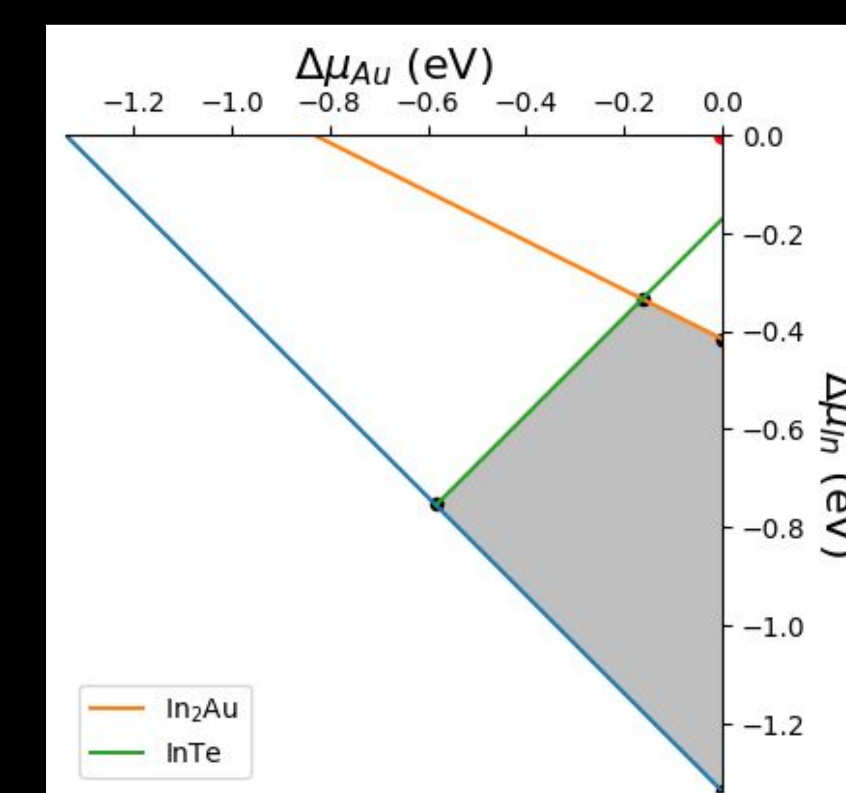
**AuInTe2**






## 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 a 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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