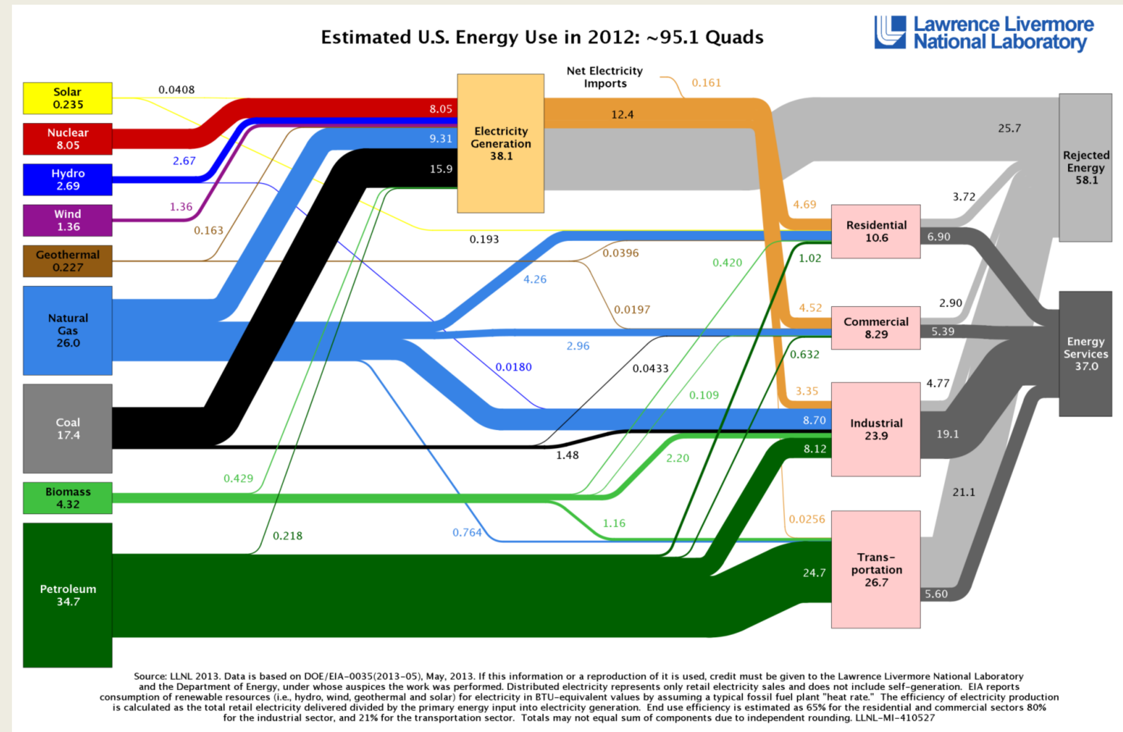
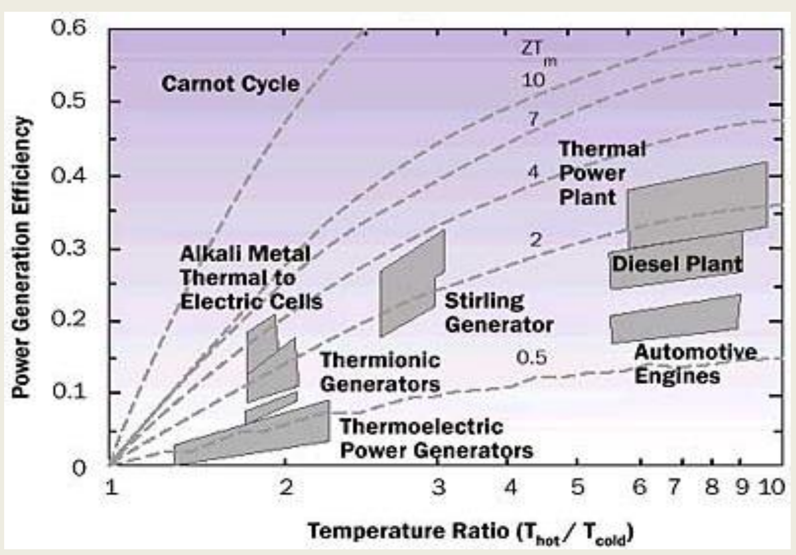
Electronic Materials for Energy Applications

Group Leader: Professor Donald Morelli
Postdoctoral Scholar: Dr. Vijay Ponnambalam
Graduate Students: Xu Lu, Gloria Lehr, Winston Carr, Spencer Waldrop, and Jared Williams

- Thermoelectrics are solid state devices that **convert heat to electricity** with no moving parts.
- Nearly two thirds of all energy produced in the US is lost in the form of waste heat.
- Thermoelectrics allow us to recapture some of that heat and convert it back into electricity.
- Important applications for these devices include power plants and exhaust systems of cars.



Of all of the energy produced in the United States, **waste heat** accounts for nearly two-thirds. From *Lawrence Livermore National Lab* (2013).



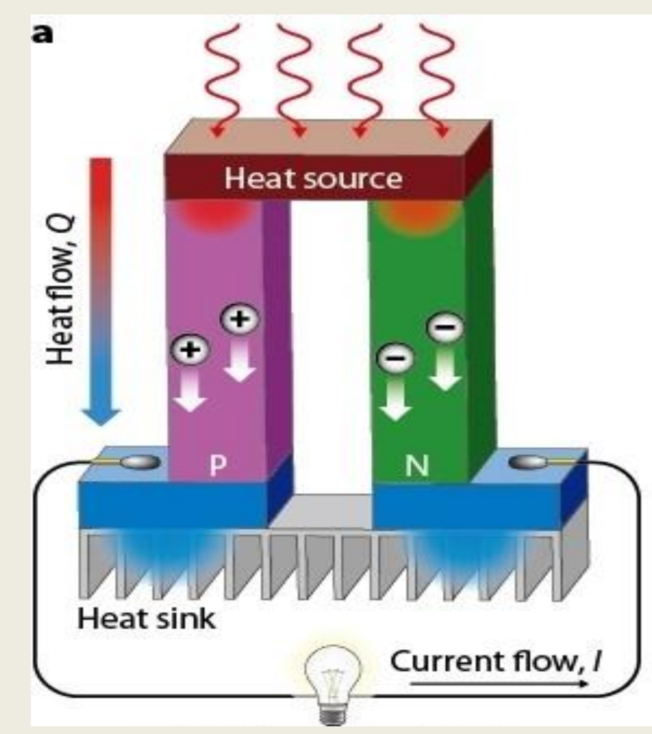
Power Generation Efficiency: A comparison of several popular power generators, including thermoelectric devices with varying zT. From *Electronics Cooling Magazine*, Nov 2005.

- Thermoelectric devices can also be used as **heating or cooling** units when a current is applied.
- This technology is important for niche applications, such as cooling of infrared sensors on satellites or maintaining lab equipment at precise temperatures, where size and reliability are more important than efficiency.

- The efficiency of thermoelectric devices is limited by the thermoelectric materials.
- By developing better materials, we can increase the efficiency of a multitude of processes.
- ***The goal of the Morelli group is to find new approaches to increasing the efficiency of thermoelectric materials for waste-heat recovery and climate control applications.***

$$zT = \frac{S^2\sigma}{\kappa_e + \kappa_l}T$$

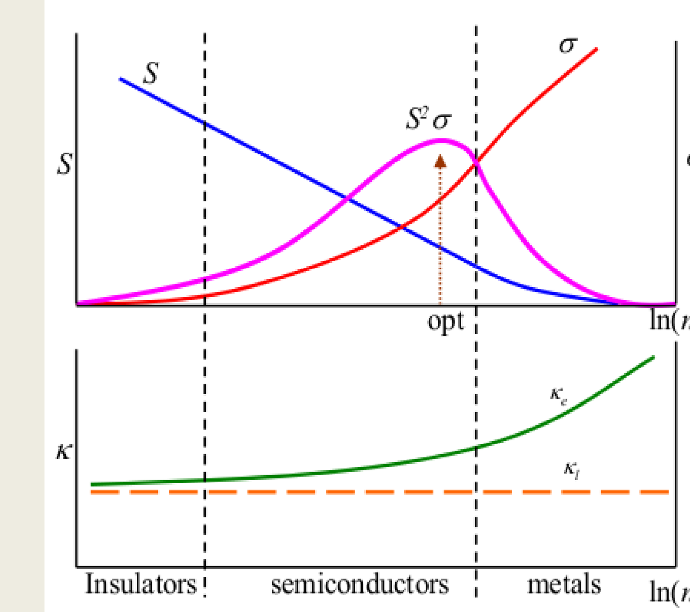
S: Seebeck Coefficient
σ: Electrical Conductivity
κ_e: Electronic Thermal Conductivity
κ_l: Lattice Thermal Conductivity
T: Temperature



Power Generation: A temperature gradient across two different materials arranged in a unicouple circuit creates a current. From http://www.risoe.dk/

Material Capabilities

- A material's capabilities are determined using the *thermoelectric figure of merit* or **zT**.
- The efficiency of a device composed of thermoelectric materials can be estimated using the zT value.
- The properties included in the zT are *contraindicated*, meaning that by enhancing one property, another is directly affected (in a negative way).
  - Optimizing the value of σ reduces S
  - Optimizing the value of κ reduces σ



Power Factor is optimized for highly doped semiconductors. From *Frontiers of Physics in China*, **3** 269 (2008).

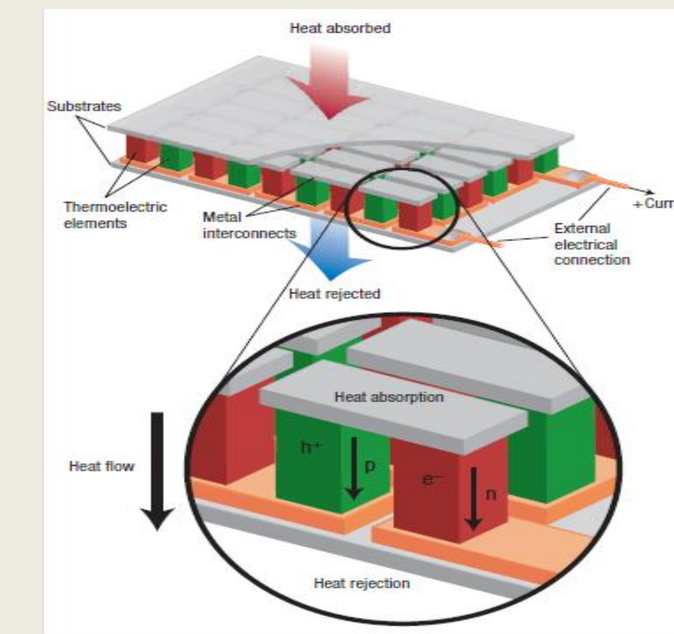
Enhancing Thermoelectric Properties

Optimizing Power Factor ($S^2\sigma$)

- **Doping** with elements near the base composition (in the periodic table) can be used to change the number of charge carriers, thus optimizing the power factor.

Reducing Thermal Conductivity

- **Solid solutions/alloying** can reduce κ_l by scattering phonons.
- **Reducing particle size** is known to decrease κ_l without affecting any other properties.
- **Doping** also introduces point defects, assisting in lowering of the κ_l.



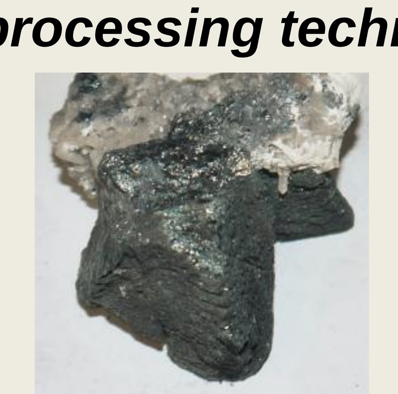
Thermoelectric Device: A device is composed of many unicouples arranged electrically in series and thermally in parallel. These devices can be fabricated in many shapes and sizes. From *Nature Materials* **7**, 105 (2008).

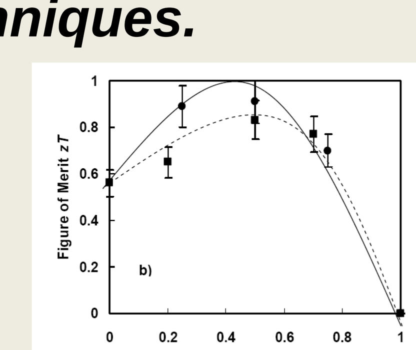
Energy Frontier Research Center

Revolutionary Materials for Solid State Energy Conversion

Earth-Abundant Materials

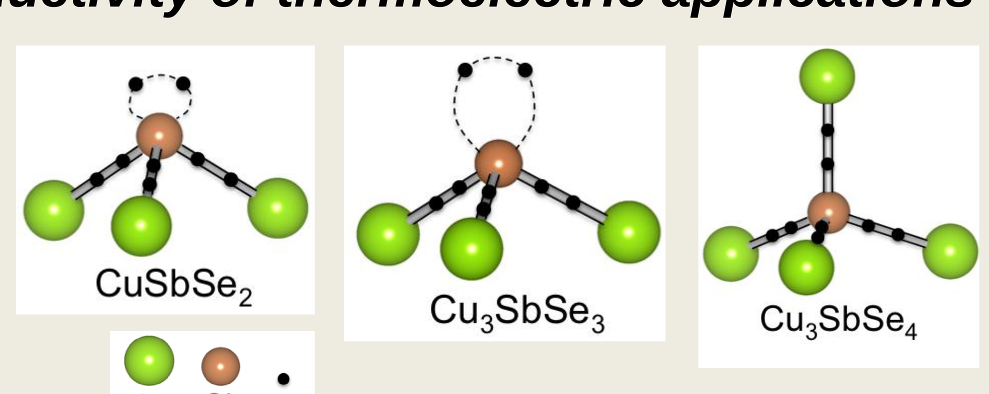
- Good thermoelectric materials often consist of elements that are in low abundance and require careful doping and complex synthesis procedures.
- Earth-abundant thermoelectrics can open the door to many new and inexpensive power generation opportunities.
- Tetrahedrites, earth's most abundant sulfosalt, can be used to achieve a zT of over 1.0 for a wide range of compositions with minimal processing requirements.
- ***The goal of this project is to maximize the thermoelectric efficiency of materials composed of earth-abundant elements using facile synthesis and processing techniques.***





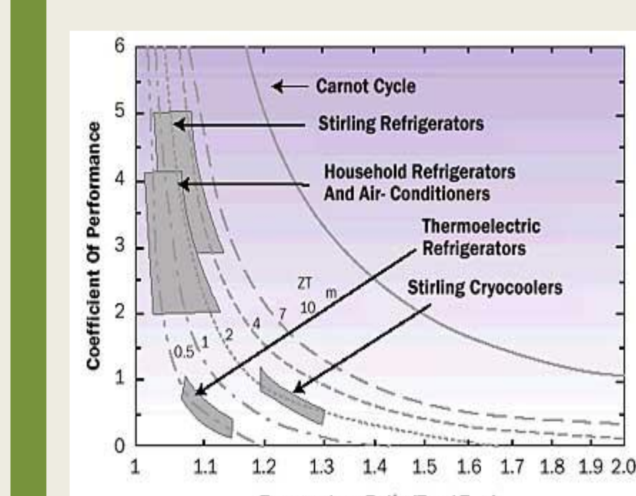
Highly Anharmonic Solids with Low Thermal Conductivity

- Thermal resistance in solids arises due to anharmonic processes – deviations from simple harmonic oscillator vibrations of lattice ions
- One class of solids exhibiting large anharmonicity are Cu-Sb-Se ternary semiconductors.
- Sb lone-pair electrons cause overlap of neighboring atom wave functions, causing large anharmonicity
- ***The goal of this project is to understand the origin of anharmonicity in crystals and design new materials with intrinsically low thermal conductivity of thermoelectric applications***



Multi-University Research Initiative

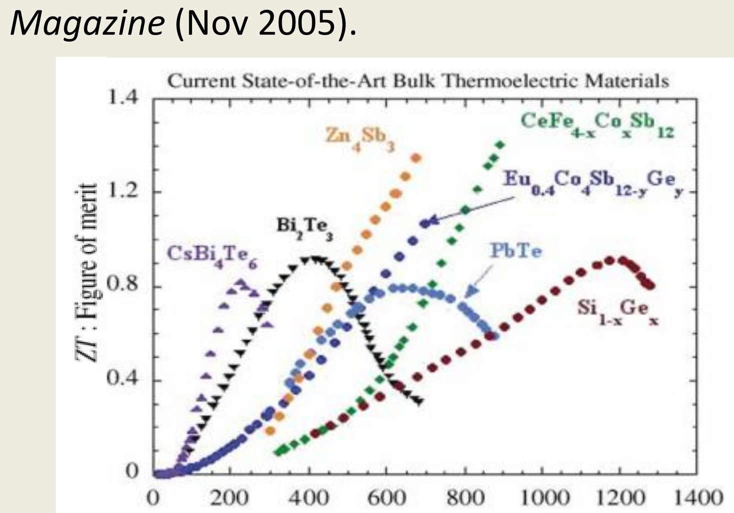
Cryogenic Peltier Cooling



Coefficient of Preformance: A comparison of several refrigeration methods, including thermoelectric devices with varying zT. From *Electronics Cooling Magazine* (Nov 2005).

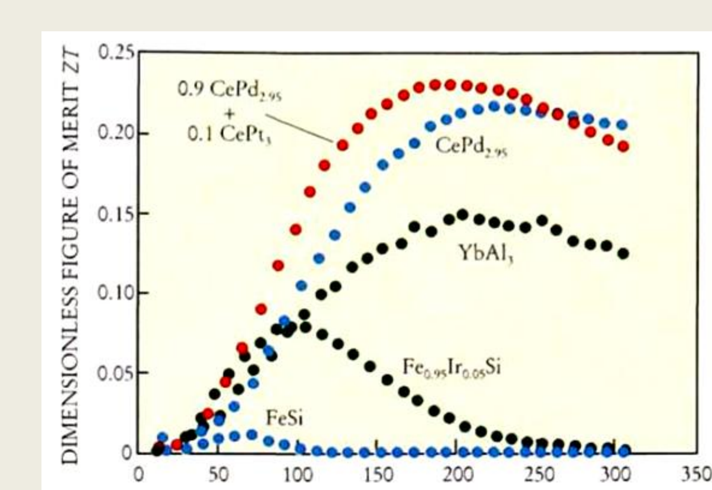
Low-Temperature Thermoelectrics

- To date, most good thermoelectric materials operate optimally at or above room temperature.
- Below room temperature the Seebeck coefficient tends toward zero, also sending the zT to zero.
- Some rare-earth compounds demonstrate unique properties in which the Seebeck coefficient peaks at cryogenic temperatures.
- ***The goal of this project is to understand and harness the unique properties of rare-earth compounds in order to create more efficient thermoelectric materials at cryogenic temperatures.***



ZT versus Temperature for several state-of-the-art bulk materials, of which Bi_2Te_3 is the most commonly used material for refrigeration applications.

From *Encyclopedia of Materials: Science and Technology* (2002).



ZT versus (Low) Temperature for several correlated metals including rare-earth compounds $YbAl_3$ and $CePd_3$.

From *Physics Today*, 42 (March 1997).