Lone Pairs and Thermoelectric Properties

OLIVIA LONG
What is a thermoelectric

1821 – Thomas Seebeck

High electron mobility and low phonon mobility
What makes a good thermoelectric?

Figure of merit:

\[ zT = \frac{\sigma \times S^2}{\kappa_L + \kappa_e} T \]
Band gap engineering

Band gap arises from difference between HOMO and LUMO

Ways to alter:
- Electronegativities
- Bond strength
- Doping
Phonon scattering

Boundary scattering
Doping

Large molecular weight

Complex crystal structure
Charge density wave distortions
Lone pair effects

Typically comes from Group 13-15 cations

O$_h$, quenched s$^2$

C$_{3v}$, expressed stereo-active s$^2$

Band diagrams
Temperature dependence

Increasing band gap with increasing temperature
Anharmonicity

Large Grüneisen parameter ($\gamma$) = high phonon scattering

Arises from distortions, loss of inversion symmetry
Coordination geometry

Coordination geometry of metal center

Ligand dependent

O_h, quenched s^2

C_3v, expressed stereo-active s^2
Why do we want thermoelectrics?

Harness waste heat and recycle into energy
Summary

Many ways to alter band gap and optimize zT
Lone pairs distort lattice and disrupt high symmetry
Able to decouple electrical and thermal conductivity
Questions?