**Computational Materials Modeling (Collaboration with Dr. Lan Li)**

**Density Functional Theory (DFT)**
- Calculates energy as a function of electron density
  - Thorough investigation of structure-properties relationship for materials screening and design
- Structural properties predict:
  - Bond length/angle, energetics, and phase stability
- Electrical properties predict:
  - Seebeck coefficient, bonding, electrical conductivity, and power factor
- Phonon properties predict:
  - Thermal conductivity and phonon drift velocity

**Experimental Approach**
- Electrical thermometry platform allows for probing the role of defects on thermal transport.
- Structure controlled through process parameters.
- Finite element modelling allows for extraction of thermal conductivity.
- FEA agrees with analytical models.

**Thermal Conductivity**
- Single-layer transition metal dichalcogenide (MX₂) materials investigated as potential transistors, optical emitters, and spintronic devices
- Exhibit hexagonal graphene-like structures
- We employ first-principles modeling techniques to investigate thermoelectric properties of MX₂ materials

**Computational Approach**
- Phonon scattering reduces thermal conductivity
- Phonon dispersion relations can be used to calculate lattice thermal conductivity, \( \kappa_l \)
  - Computationally expensive
- One can qualitatively estimate trends in lattice thermal conductivity based on the following factors:
  - Atomic weight
  - Bond stiffness
  - Phonon frequency band gap
  - Dispersion gradient, \( \frac{\partial \omega}{\partial k} \propto v_d \propto \kappa_l \)