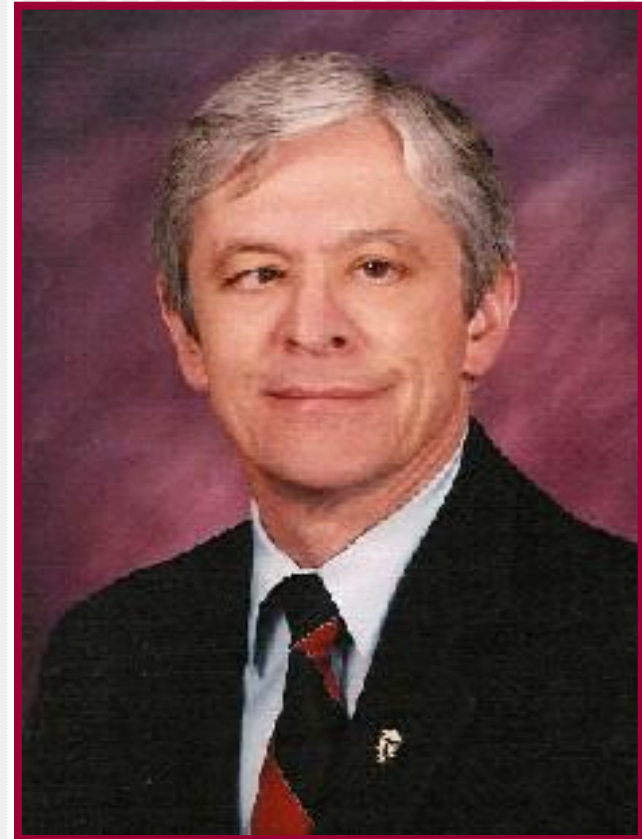


Dr. Charles W. Myles

Professor of Physics

**Theoretical & Computational
Materials Physics**

- **Semiconductor Materials**
- **Thermoelectric Materials**
- **First-Principles Calculations**
- **Structural & Electronic Properties**
- **Vibrational & Thermal Properties**
- **Transport Properties**



Physics Research

Theoretical/Computational Materials Physics
Professor Charles W. Myles

Properties of Semiconductors

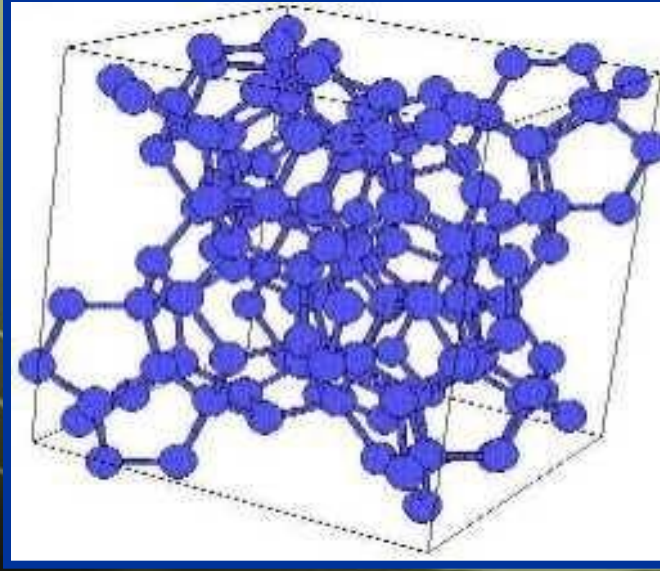
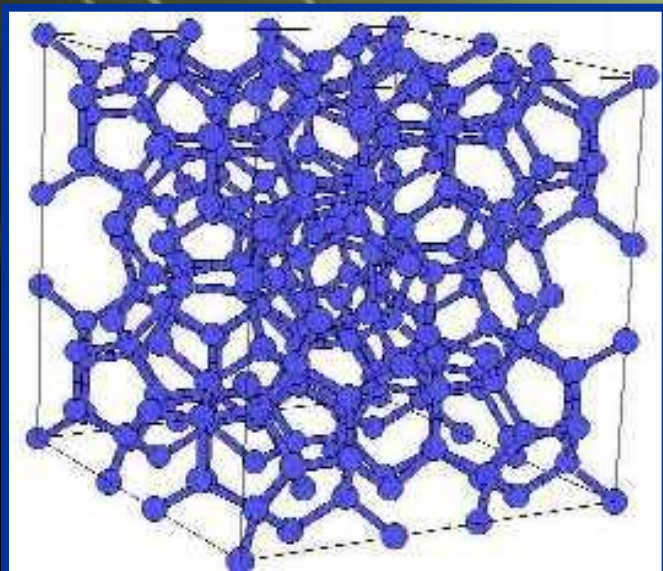
- First-Principles Calculations
- Clathrate Semiconductors & Thermoelectrics
- Structural, Electronic, & Vibrational Properties
- Electronic & Thermal Transport

Type I Clathrates

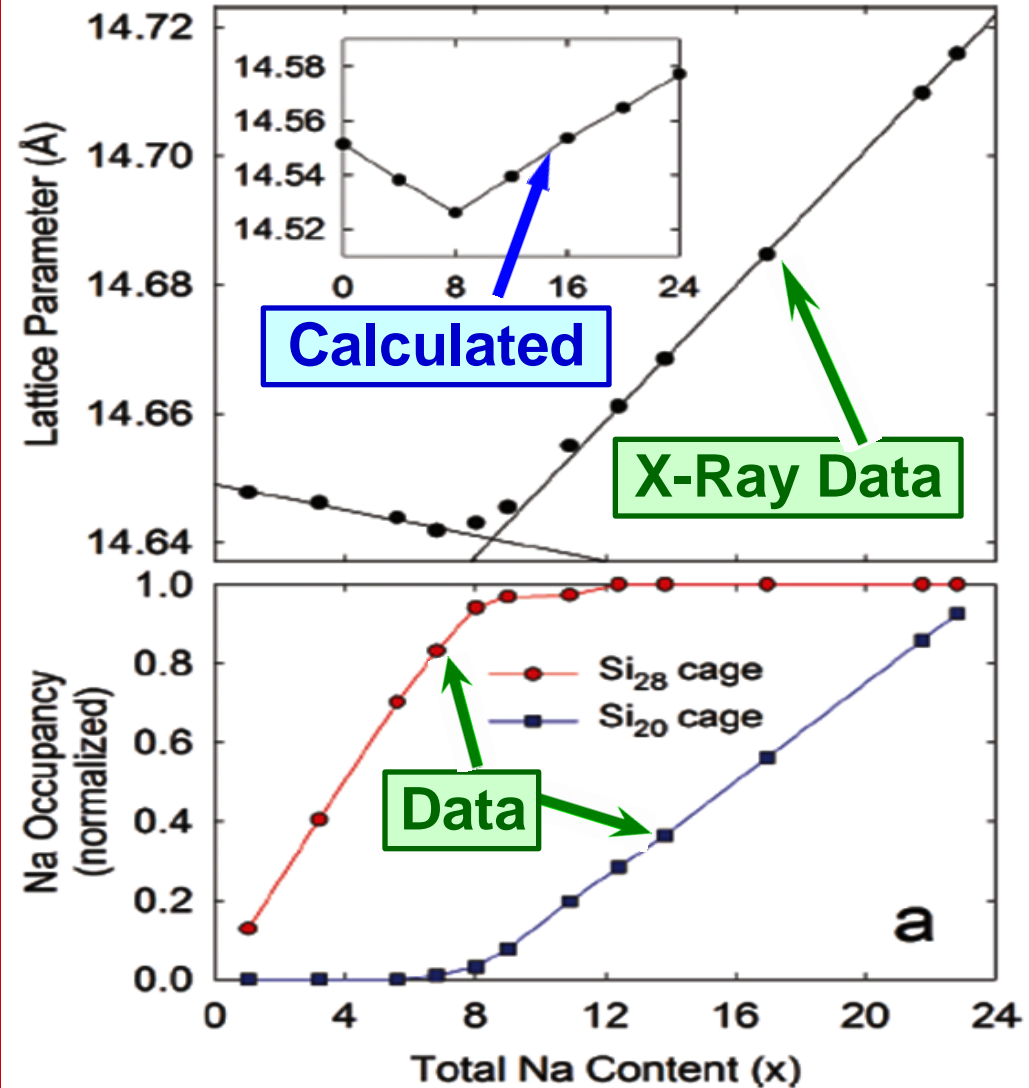
Si_{46} , Ge_{46} , Sn_{46}

Type II Clathrates

Si_{136} , Ge_{136} , Sn_{136}



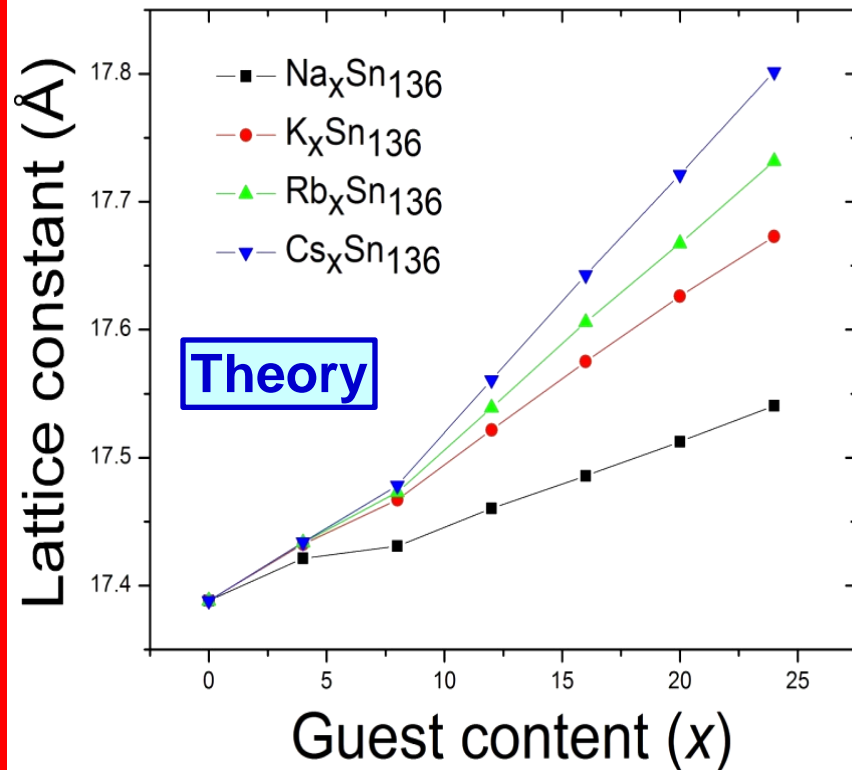
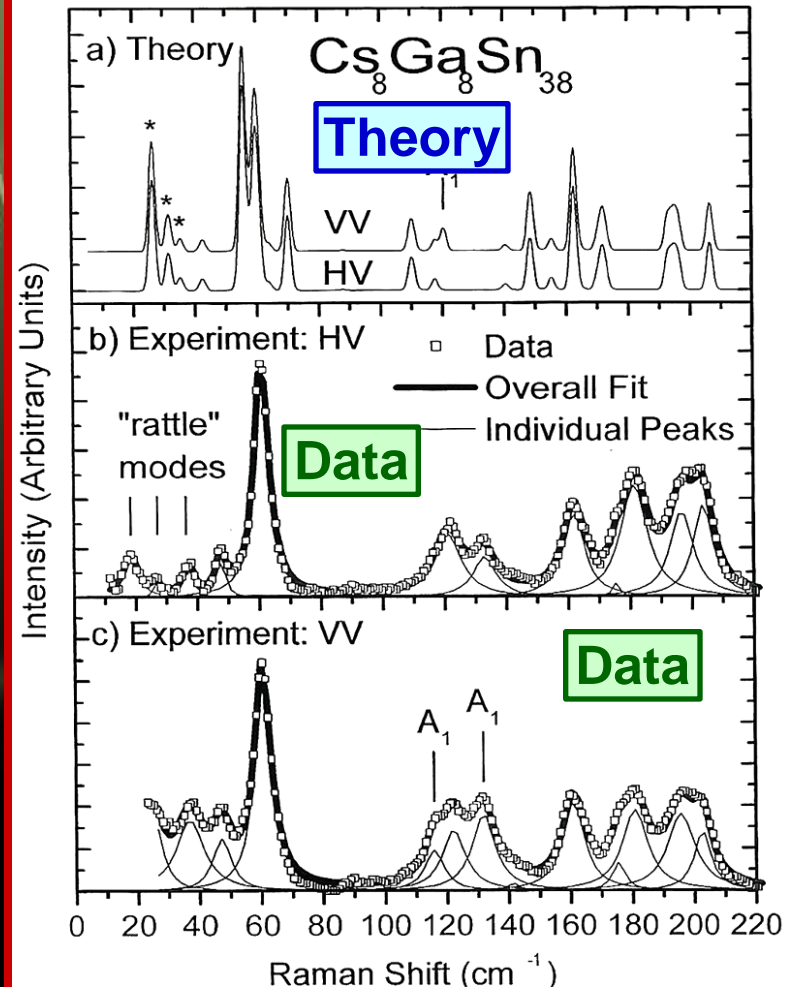
Lattice Constant vs. x in $\text{Na}_x\text{Si}_{136}$



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Calculated & Measured Raman Spectra: Nolas, Myles, et al.
J. Appl. Phys. 92, 7225 (2003).



Calculated Lattice Constant vs. x in $\text{Na}_x\text{Sn}_{136}$, $\text{K}_x\text{Sn}_{136}$, $\text{Rb}_x\text{Sn}_{136}$ & $\text{Cs}_x\text{Sn}_{136}$, Xue & Myles, unpublished (2015)

Calculated & Measured Heat Capacity vs. Temperature: Biswas, Myles, et al., *J. Appl. Phys.* 104, 033535 (2008).

