

# First-Principles Calculation of Lattice Thermal Conductivity of NaCl and MgO at High Pressures

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Physics Department, Auburn University, Alabama



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# Outline

## ➤ Motivations

Earth Science & Solid State Theory

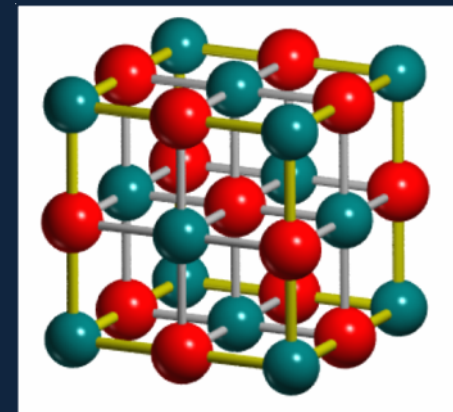
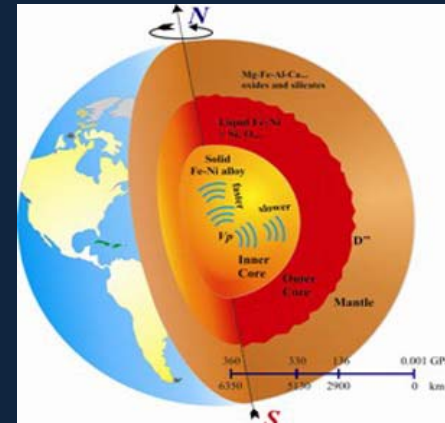
## ➤ Methodologies

First-principles calculations & Transport theory

## ➤ Results and Discussion

MgO v.s. NaCl

## ➤ Summary and Future Work



# Motivations

## ➤ Heat budget of Earth's Interior

### ➤ Conduction

$$\vec{j}_Q = -\kappa \vec{\nabla} T$$

### ➤ Convection

$$R_a = \frac{\rho_0 g \alpha \Delta T d^3}{\kappa \nu}$$

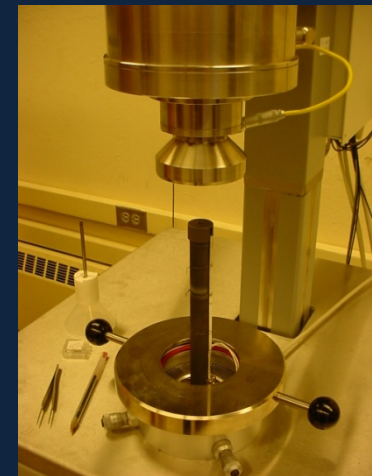
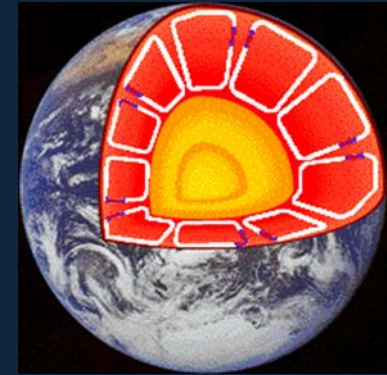
## ➤ Challenges in High Pressure Measurements

### ➤ $T > 2300\text{K}$ & $P > 100\text{ GPa}$

## ➤ Case Study: NaCl vs MgO

### ➤ MgO : $B \approx 180\text{ GPa}$ , $d\ln(\kappa)/dP \approx 4-5\ \% \text{GPa}^{-1}$

### ➤ NaCl : $B \approx 30\text{ GPa}$ , $d\ln(\kappa)/dP \approx 17 - 30\ \% \text{GPa}^{-1}$



# METHODOLOGY

**Lattice Thermal Conductivity: Anharmonic Lattice Dynamics + Fermi-Golden Rule + Peierls-Boltzmann Kinetic Transport Equation**

Peierls-Boltzmann Kinetic Transport Equation

$$\kappa = \frac{1}{3} \sum_{i, \vec{q}} C_V(i, \vec{q}) v_g^2(i, \vec{q}) \tau(i, \vec{q})$$

Fermi-Golden Rule:

$$P_i^f = \frac{2\pi}{\hbar} |\langle f | \Delta H | i \rangle|^2 \delta(\epsilon_f - \epsilon_i)$$

$$\Delta H = \frac{1}{6} \sum_{i, j, k=1}^{3N} A_{ijk} \Delta x_i \Delta x_j \Delta x_k$$

Anharmonic Lattice Dynamics

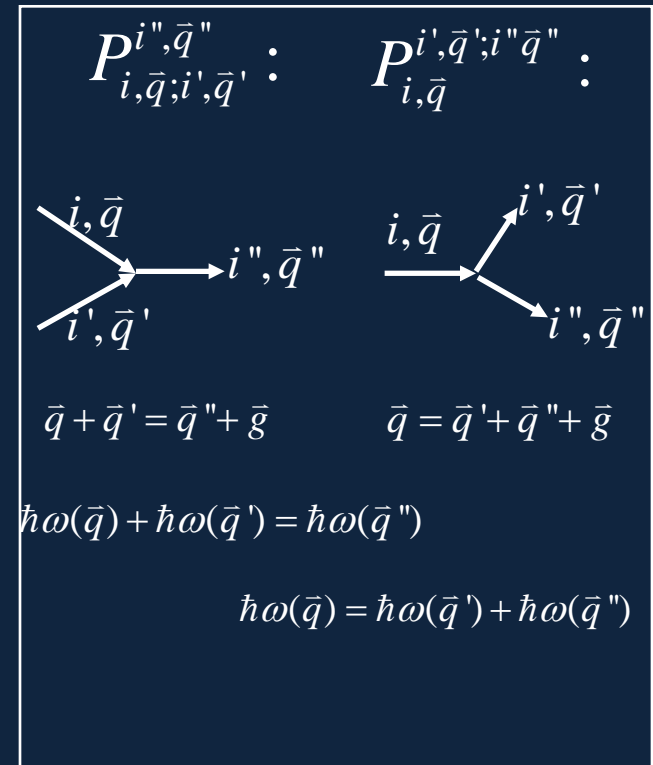
$$A_{ijk} = \frac{\partial^3 E}{\partial x_i \partial x_j \partial x_k}$$

Real-Space  
Finite-Displacement  
Algorithm

DFT

F-H Theorem

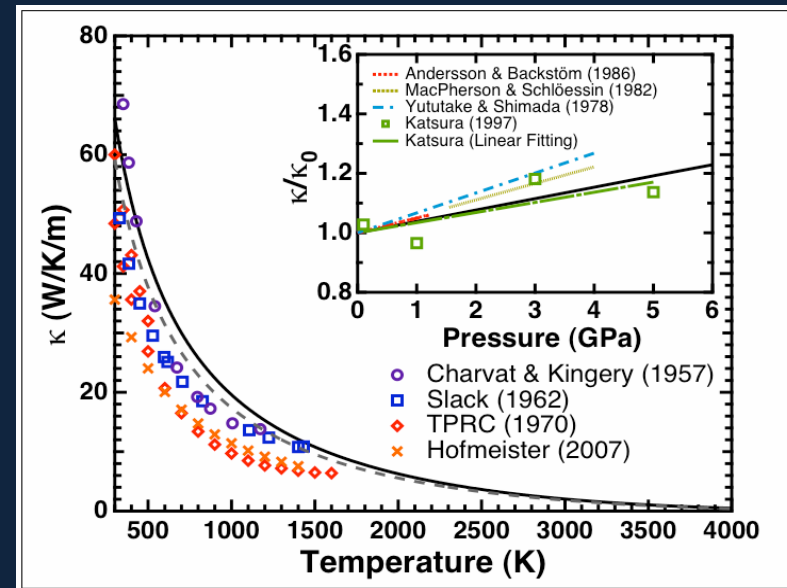
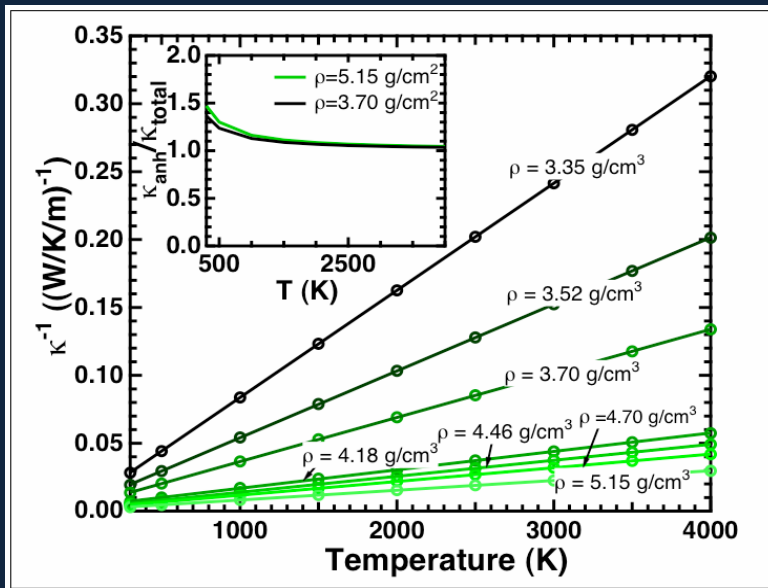
$$F_i = \frac{\partial E}{\partial x_i}$$



# Results & Discussion: MgO

- X. Tang and J. Dong, “Pressure dependence of harmonic and anharmonic lattice dynamics in MgO: A first-principles calculation and implications for lattice thermal conductivity”, PEPI, Vol 174, Pages 33-38, (2009).
- X. Tang and J. Dong, “Lattice thermal conductivity of MgO at conditions of Earth’s interior”, submitted , June 2009.

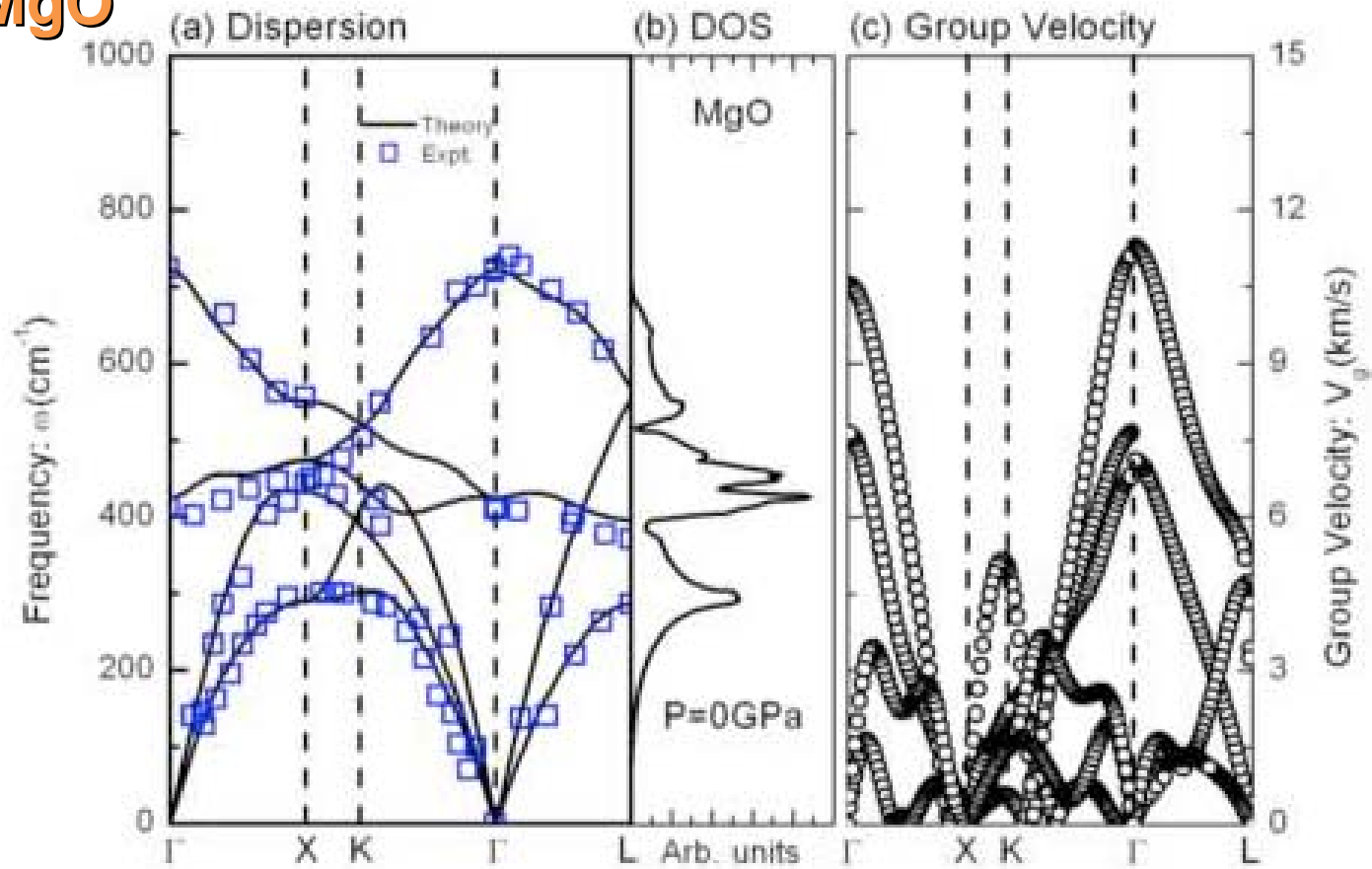
$$\kappa^{-1}(T, \rho) = A(\rho) + B(\rho)T = \exp\left[-17.5 + \frac{80.1}{\rho} + \frac{-132}{\rho^2}\right] + \exp\left[-9.31 + \frac{-35.9}{\rho} + \frac{119}{\rho^2}\right] \cdot T$$



$$\kappa^{-1}(T, \rho) = A(\rho) + B(\rho)T = \exp\left[a_1 + \frac{a_2}{\rho} + \frac{a_3}{\rho^2}\right] + \exp\left[b_1 + \frac{b_2}{\rho} + \frac{b_3}{\rho^2}\right] \cdot T$$

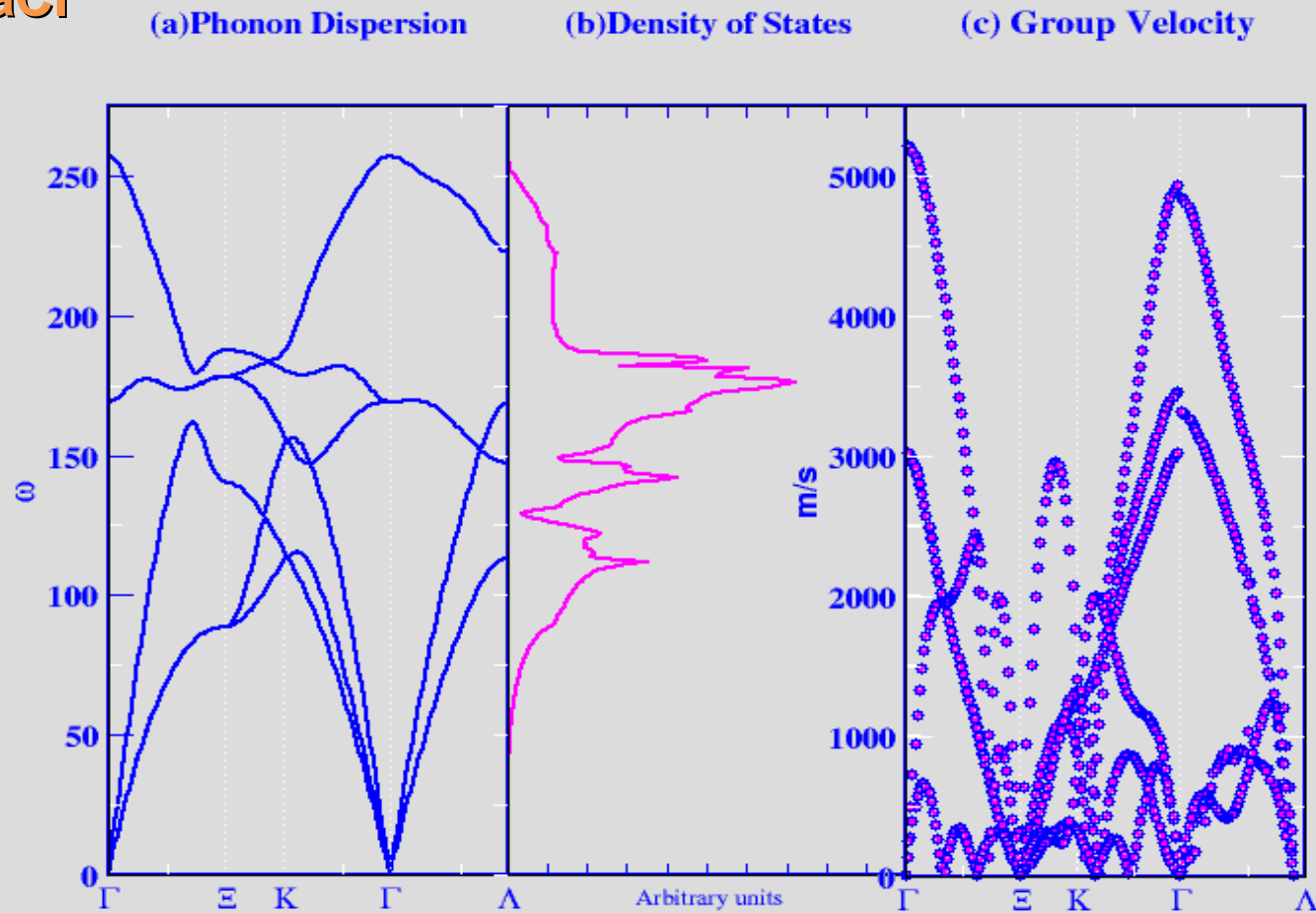
# Preliminary Results: NaCl v.s. MgO

MgO

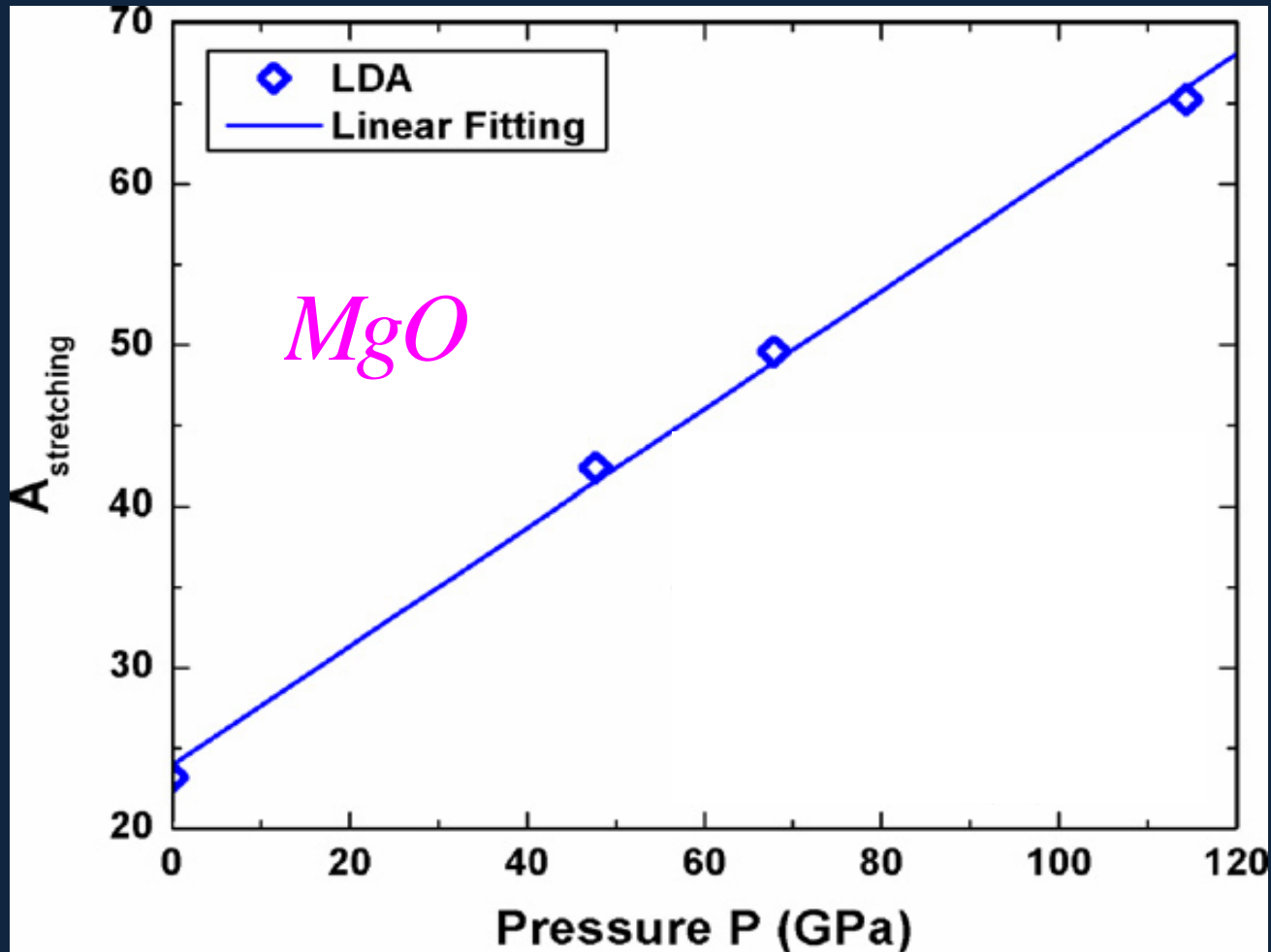


# Preliminary Results: NaCl v.s. MgO

NaCl

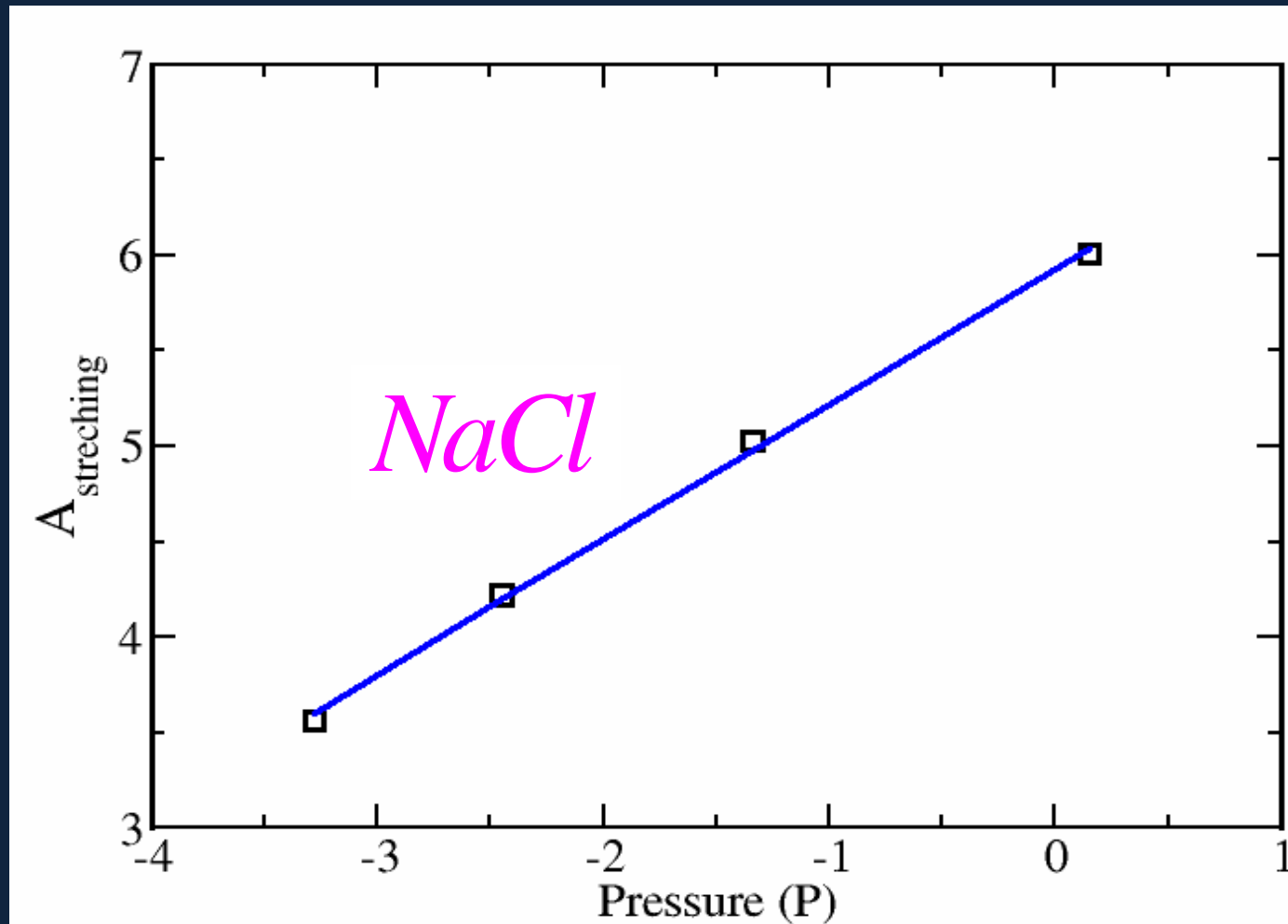


## Preliminary Results: NaCl v.s. MgO



$$A_{stretch}(P) = A_{stretch}(P = 0) \times (1 + .0153P)$$

## Preliminary Results: NaCl v.s. MgO



$$A_{stretch}(P) = A_{stretch}(P = 0) \times (1 + .11967P)$$

# Summary and Future Work

## ➤ MgO:

- First-principles calculation of phonon spectra and 3<sup>rd</sup> order lattice anharmonicity
- A density-temperature model for thermal conductivity over a wide range of (T, P) conditions.
- Good agreement with measurements at ambient conditions.

## ➤ NaCl:

- First-principles calculation of phonon spectra and 3<sup>rd</sup> order lattice anharmonicity
- Direct calculation of phonon scattering rates (**ongoing**)
- A general model for the B1-structured crystals (**future**)



# Thanks!



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