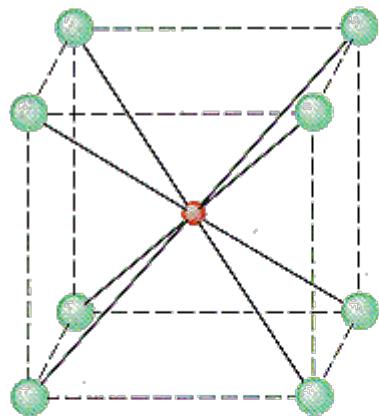
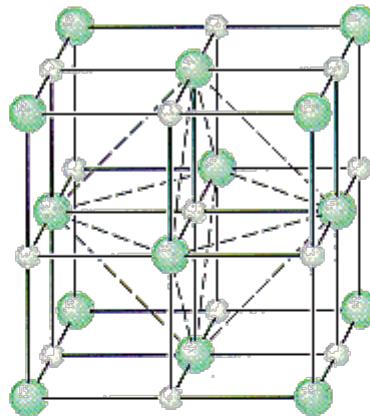


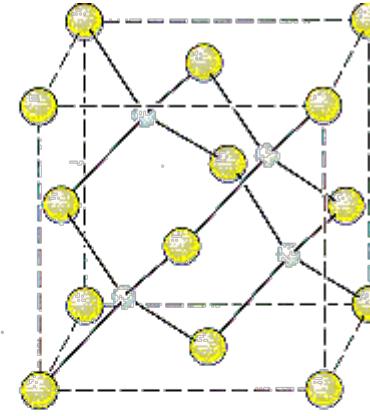
# Crystal Structures



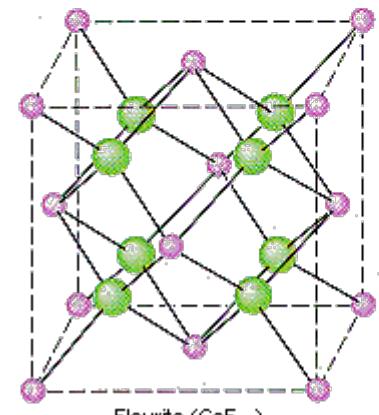
CsCl



NaCl

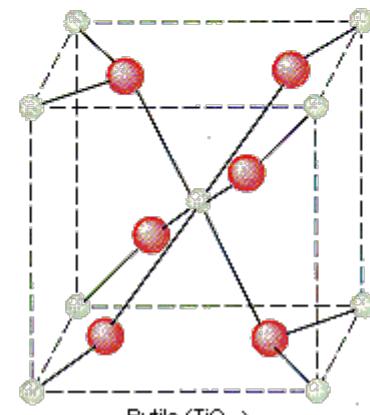


Zinc blende (cubic ZnS)



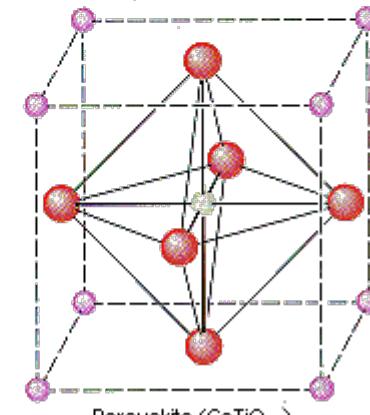
Flourite (CaF<sub>2</sub>)

● = Ca<sup>2+</sup>



Rutile (TiO<sub>2</sub>)

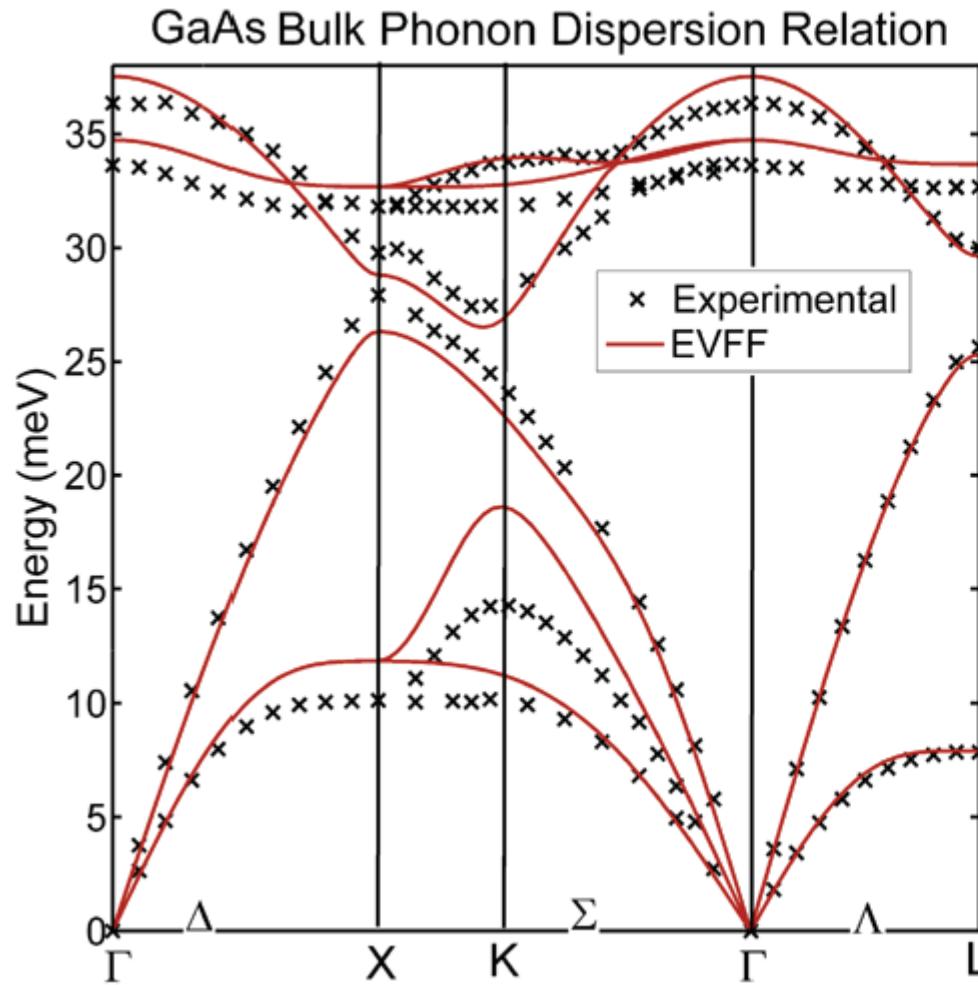
● = Ti<sup>IV</sup>



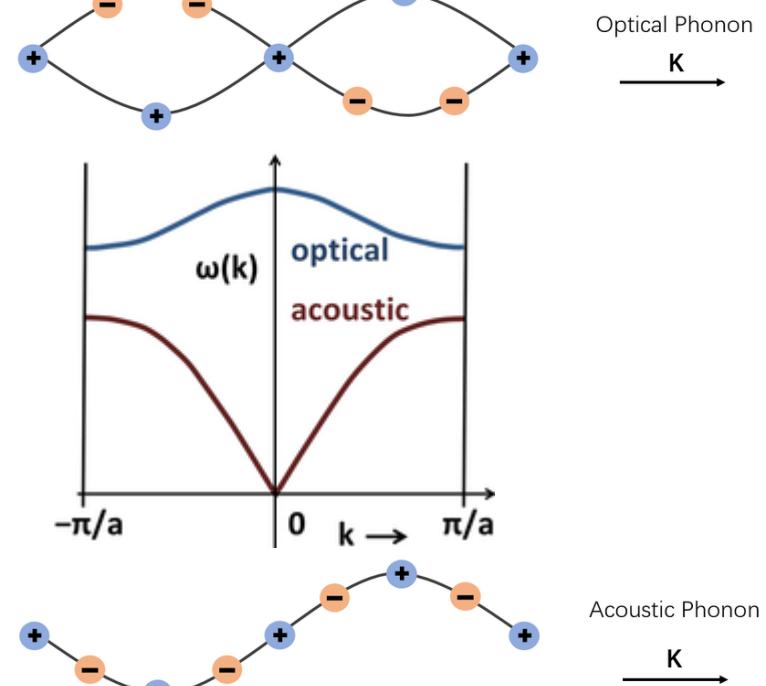
Perovskite (CaTiO<sub>3</sub>)

● = Ti<sup>IV</sup>   ● = Ca<sup>2+</sup>   ● = O<sup>2-</sup>

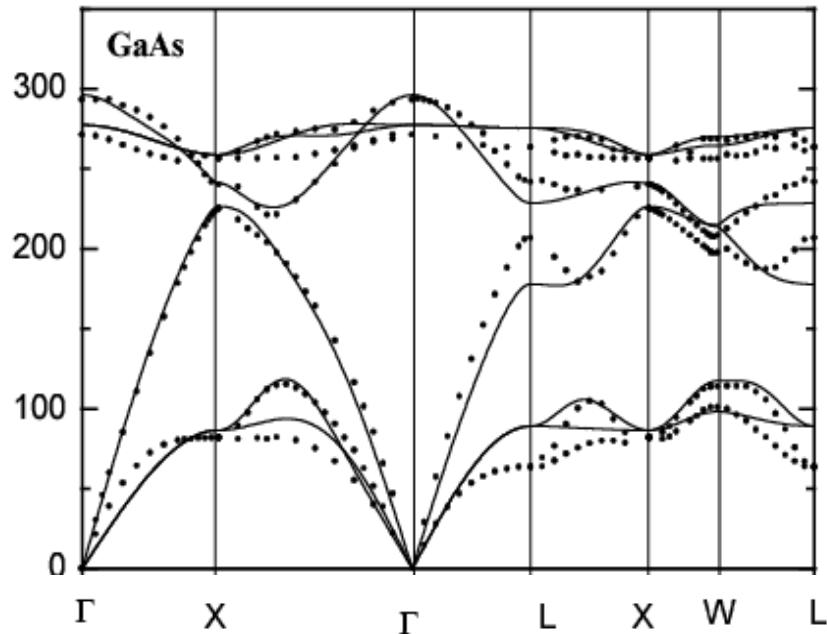
# Crystal Structures



EVFF = Enhanced Valence Force Field

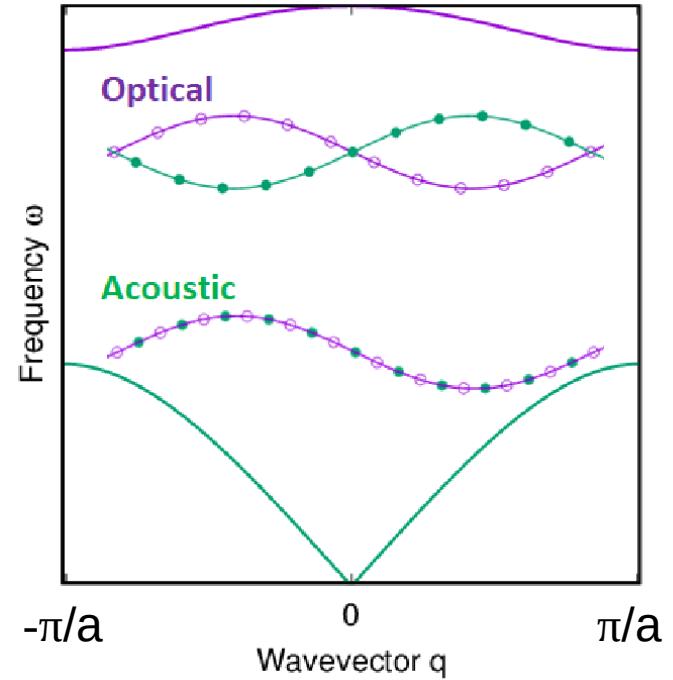


# Crystal Structures



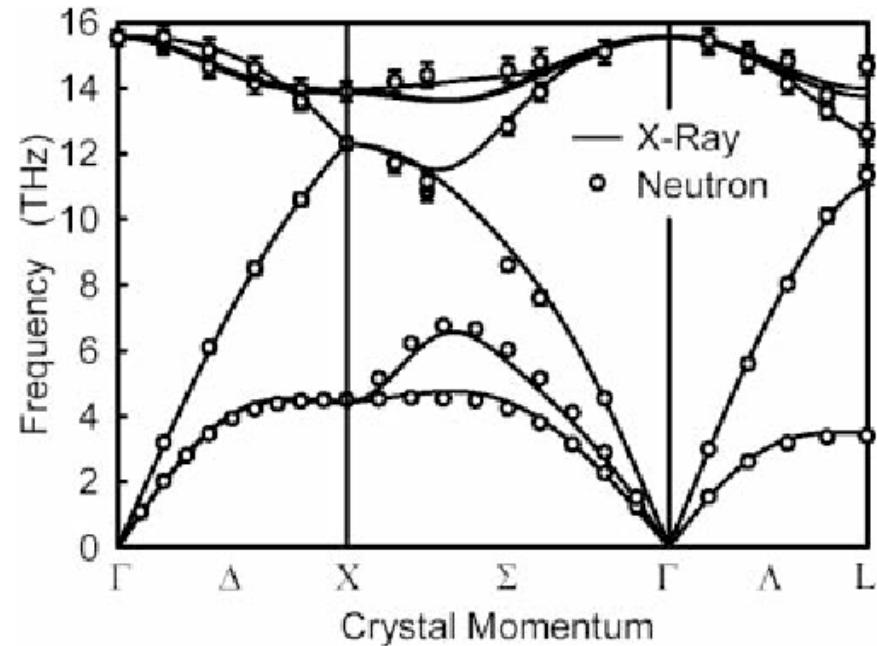
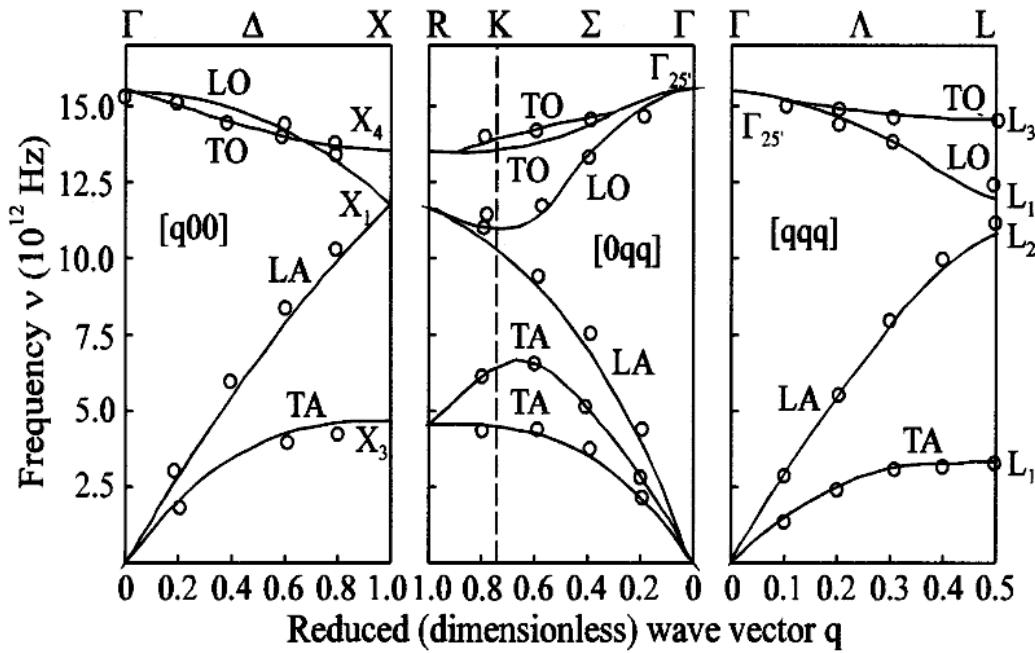
● experimento

— cálculo teórico (ab-initio)



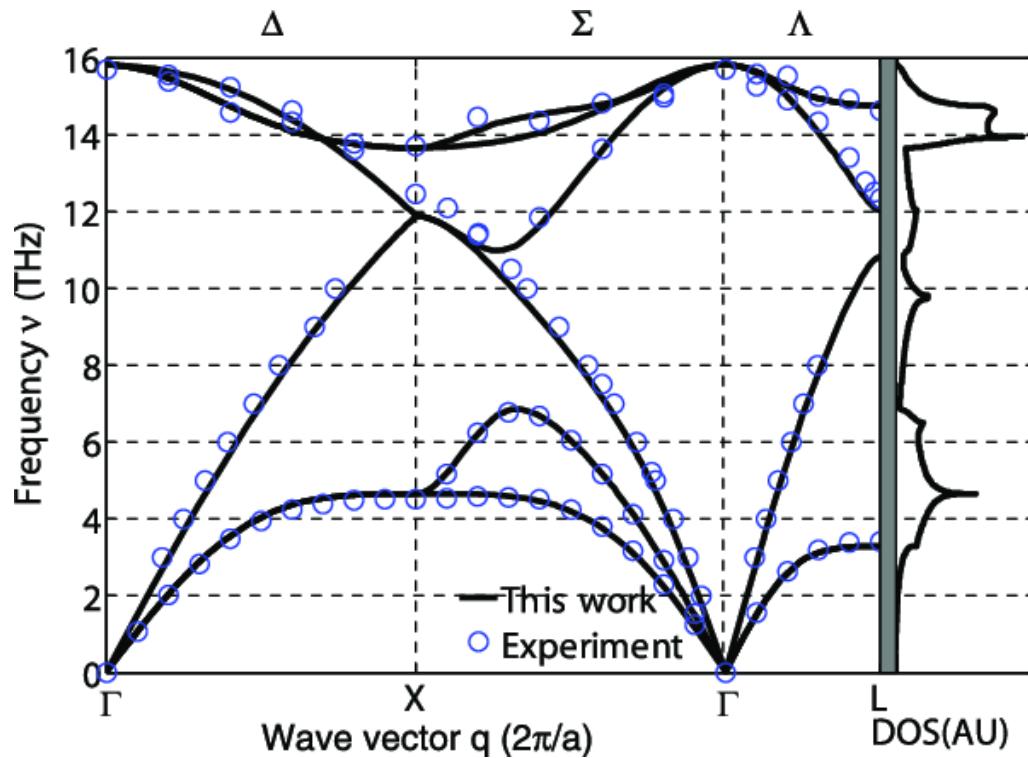
# Crystal Structures

Phonon dispersion curves of Si.



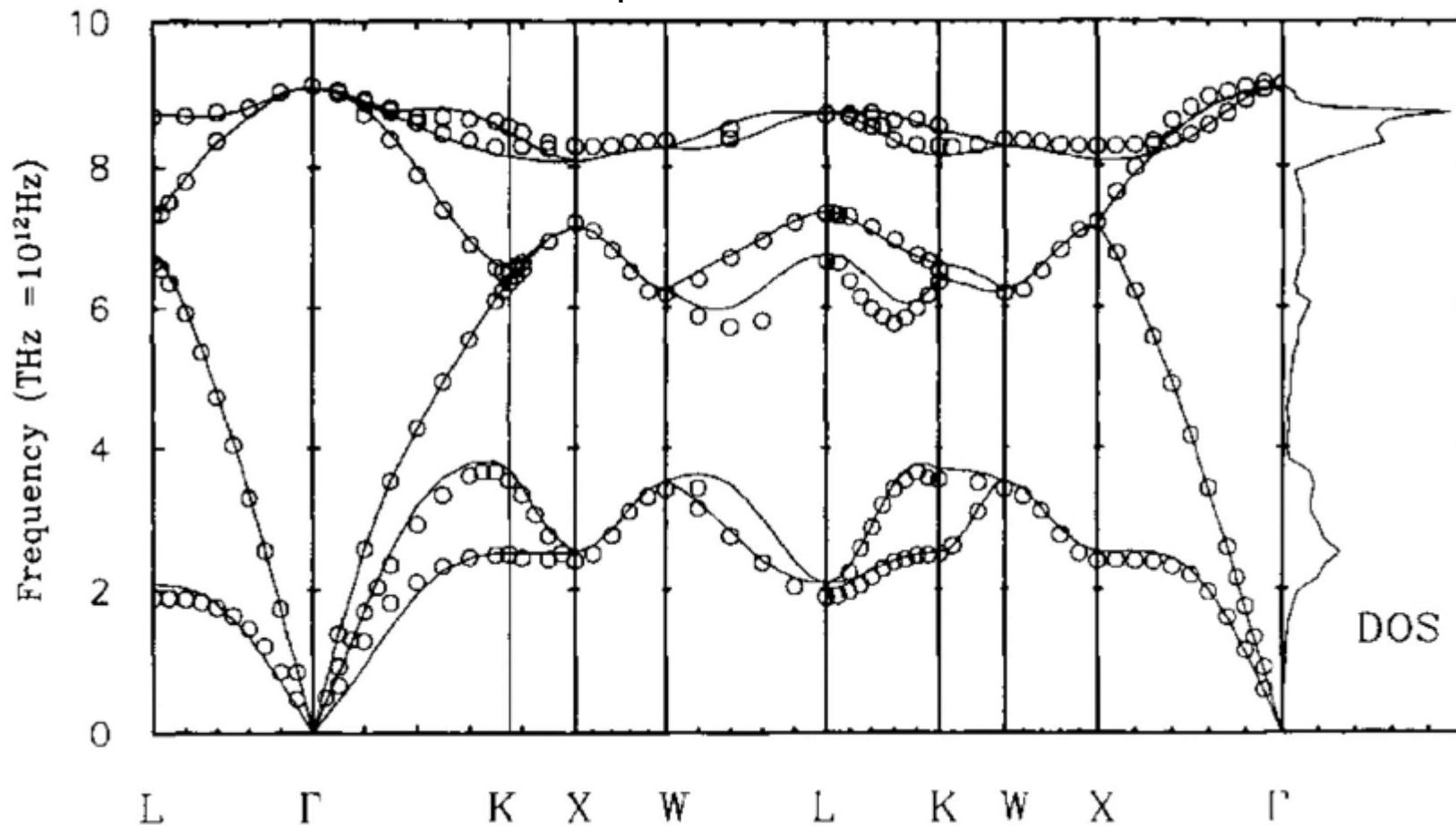
# Crystal Structures

Phonon dispersion curves of Si.

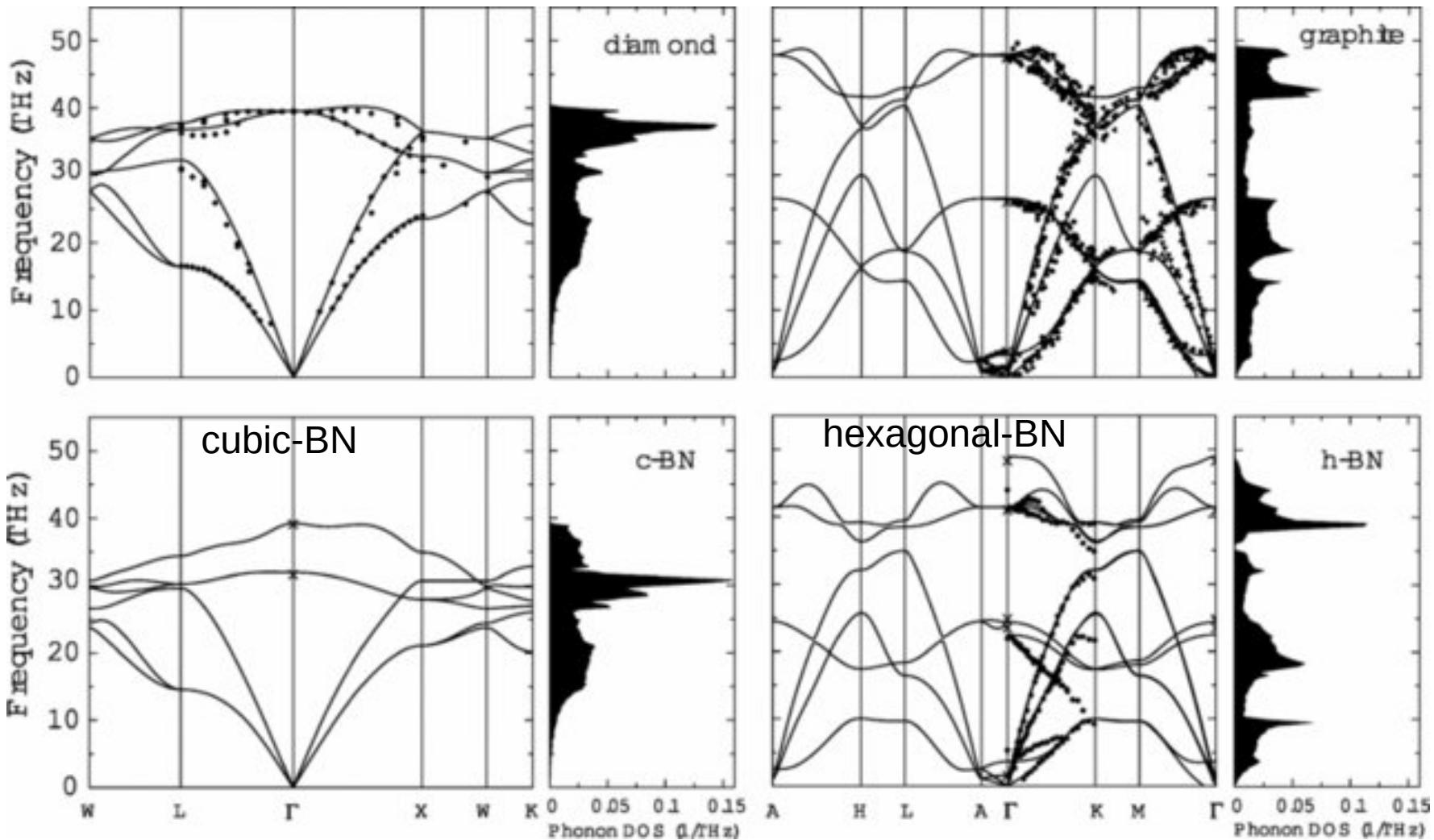


# Crystal Structures

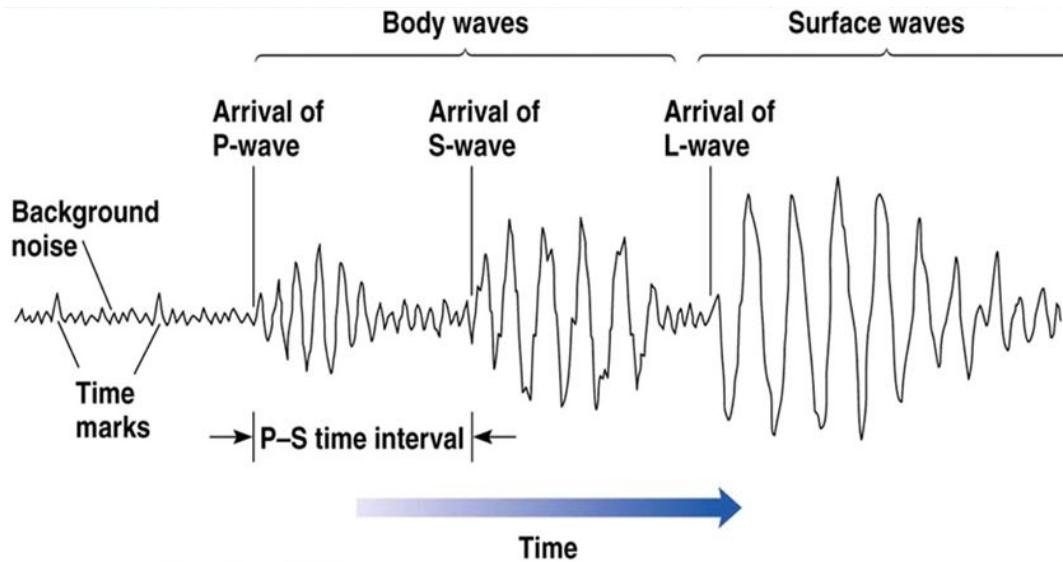
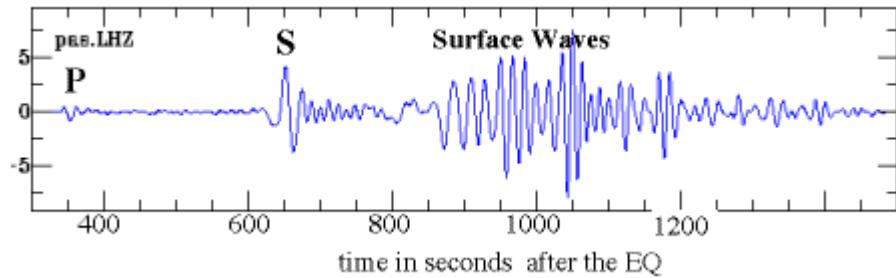
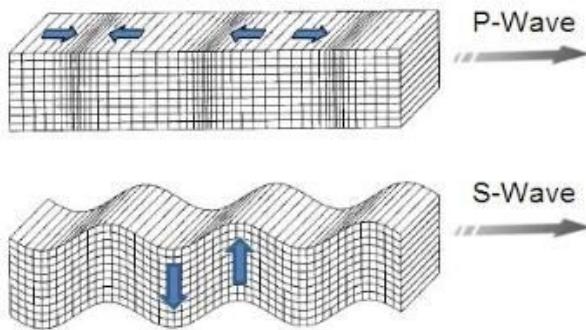
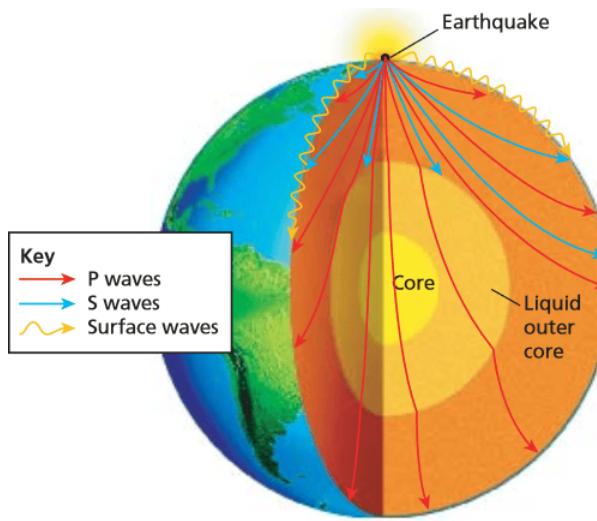
Phonon dispersion curves of Ge.



# Crystal Structures



# Velocity of Earthquake Waves



# First Solvay Conference - 1911



Notes on Fig. 2. Left to right seated: Walter Nernst; Marcel-Louis Brillouin; E. Solvay; Hendrik Lorentz; Emil Warburg; Jean-Baptiste Perrin; Wilhelm Wien; Marie Curie; Henri Poincaré. Left to right standing: Robert Goldschmidt; Max Planck; Heinrich Rubens; Arnold Sommerfeld; Frederick Lindemann; Maurice de Broglie; Martin Knudsen; Friedrich Hasenöhrl; G. Hostelet; E. Herzen; Sir James Jeans; Ernest Rutherford; Heike Kamerlingh-Onnes; Albert Einstein; Paul Langevin. Further remarks: M. de Broglie (the elderly brother of Louis de Broglie), F. Lindemann

# First Solvay Conference - 1911

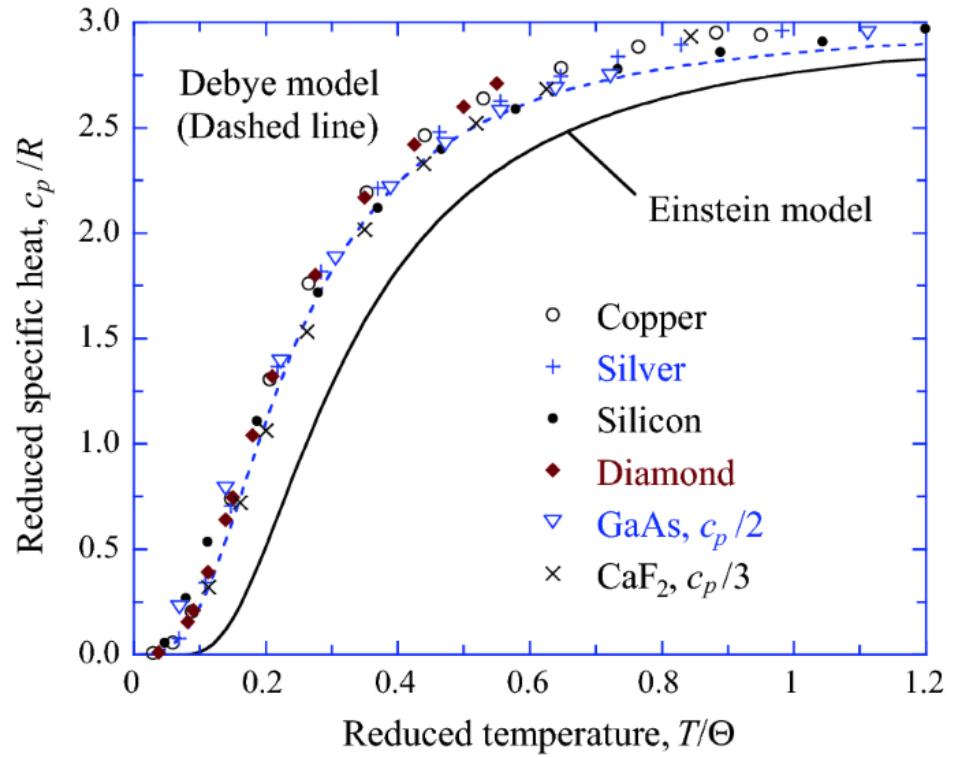
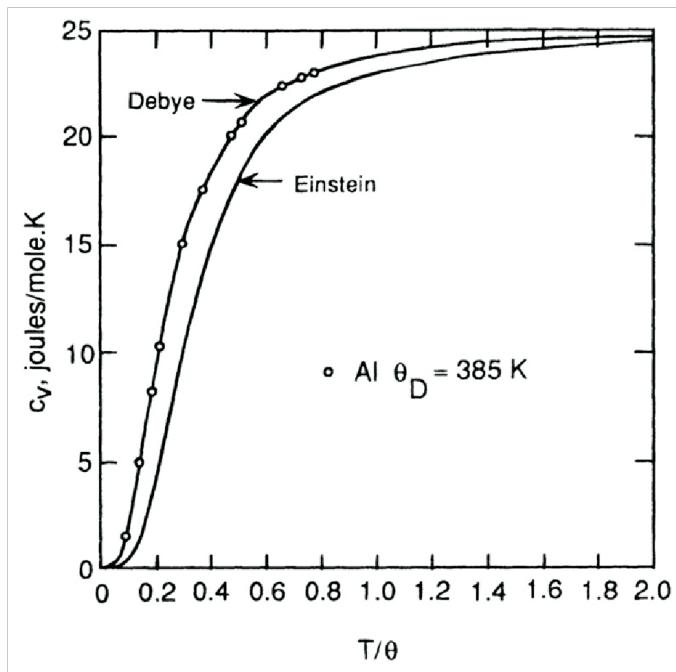


Notes on Fig. 2. Left to right seated: Walter Nernst; Marcel-Louis Brillouin; E. Solvay; Hendrik Lorentz; Emil Warburg; Jean-Baptiste Perrin; Wilhelm Wien; Marie Curie; Henri Poincaré. Left to right standing: Robert Goldschmidt; Max Planck; Heinrich Rubens; Arnold Sommerfeld; Frederick Lindemann; Maurice de Broglie; Martin Knudsen; Friedrich Hasenöhrl; G. Hostelet; E. Herzen; Sir James Jeans; Ernest Rutherford; Heike Kamerlingh-Onnes; Albert Einstein; Paul Langevin. Further remarks: M. de Broglie (the elderly brother of Louis de Broglie), F. Lindemann

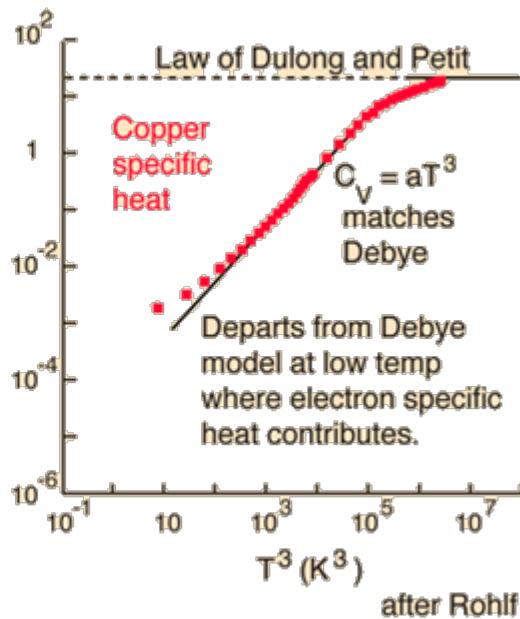
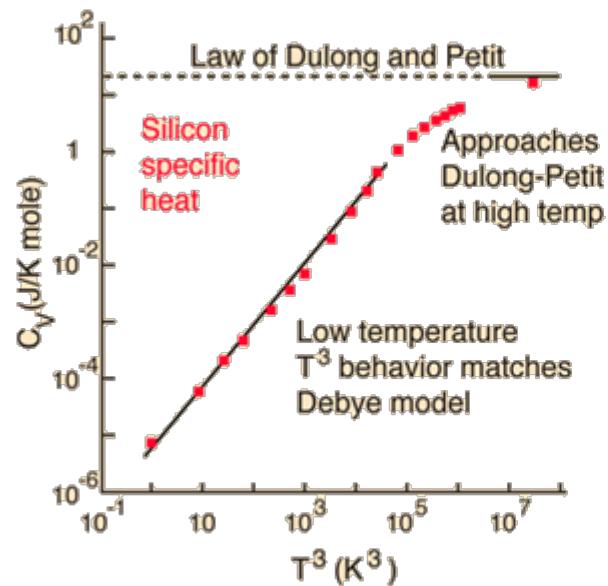
Einstein's report:

“On the Present State of the Problem of Specific Heats”

# Specific Heat of Solids



# Specific Heat of Solids



$$C = C_{\text{el}} + C_{\text{vib}}$$

Para um metal (Al, Ag, Au, etc.)

$$C = \alpha T + \beta T^3$$

Para um dielétrico (Si, diamante)

$$C = \beta T^3$$

# Effects of Electron-Phonon Interaction

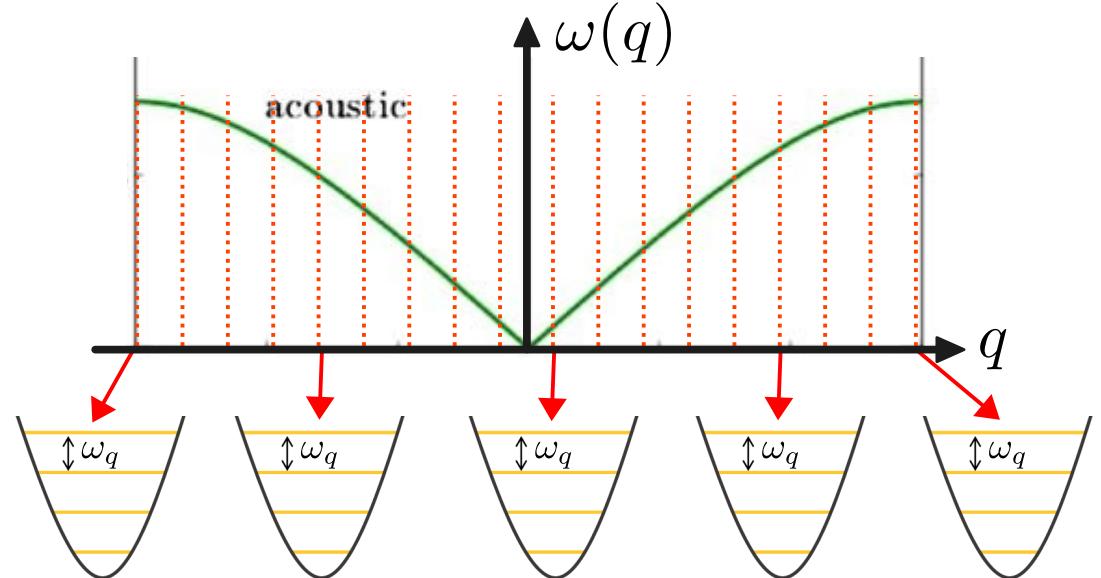
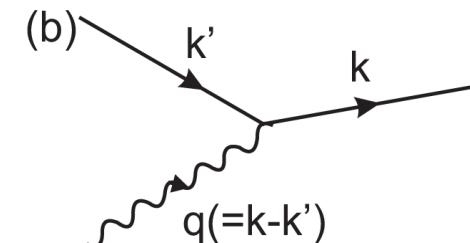
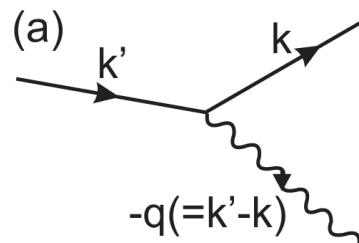
$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$

$$\hat{H}_{ph} = \hbar\omega_q \left( a_q^+ a_q + \frac{1}{2} \right)$$

$$a_q = \sqrt{\frac{M\omega_q}{2\hbar}} \left( \hat{x} + \frac{i}{M\omega_q} \hat{p} \right)$$

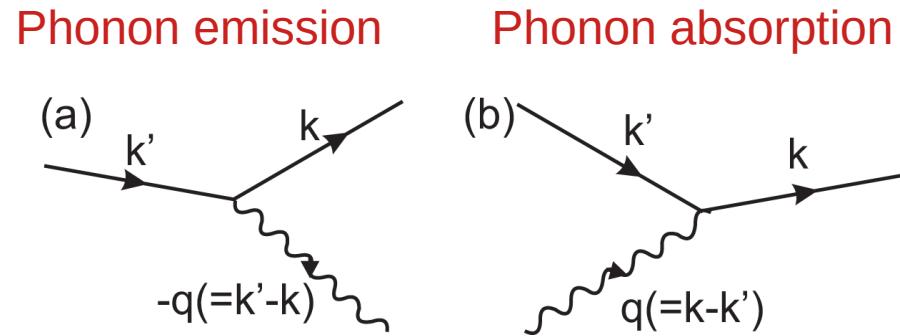
$$a_q^+ = \sqrt{\frac{M\omega_q}{2\hbar}} \left( \hat{x} - \frac{i}{M\omega_q} \hat{p} \right)$$

Phonon emission      Phonon absorption

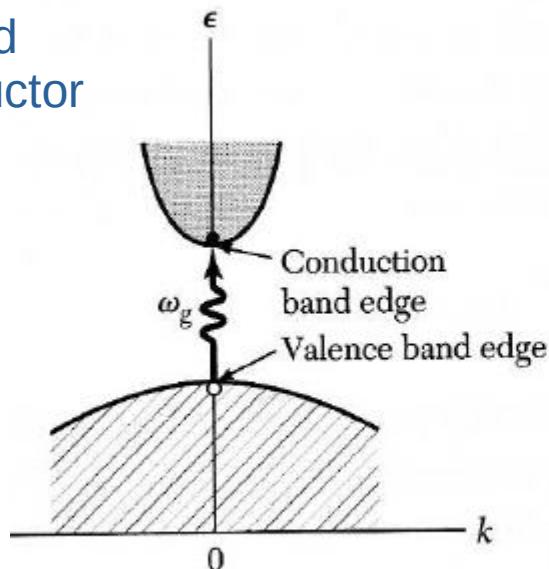


# Effects of Electron-Phonon Interaction

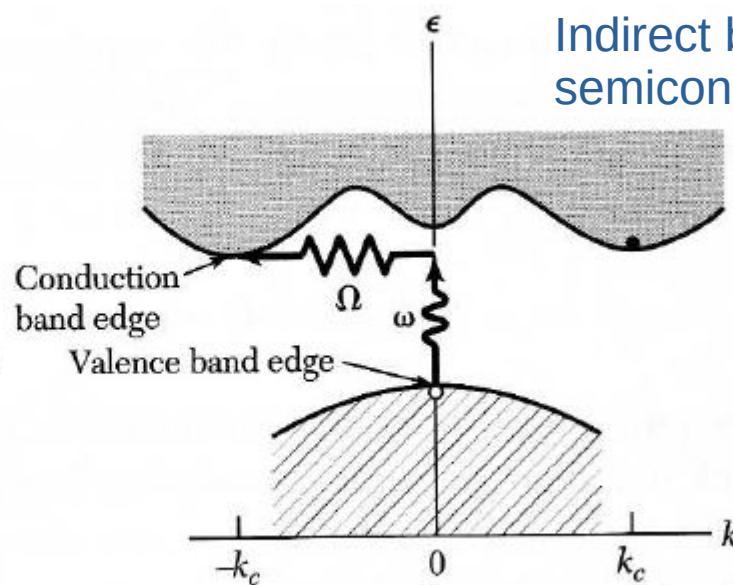
$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$



Direct band semiconductor



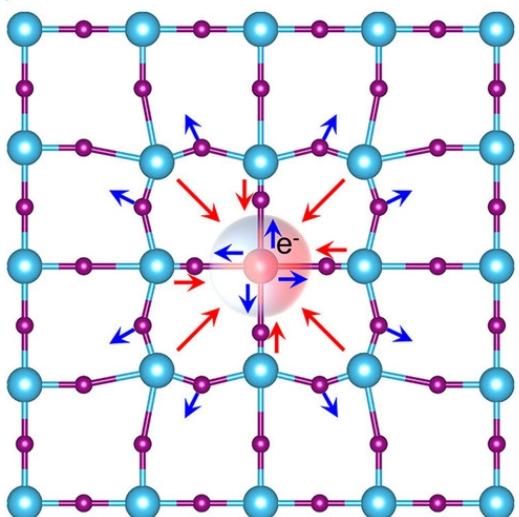
Indirect band semiconductor



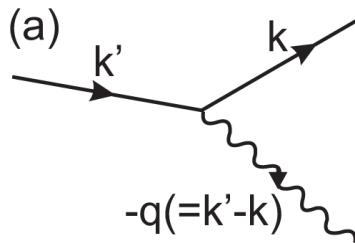
# Effects of Electron-Phonon Interaction

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$

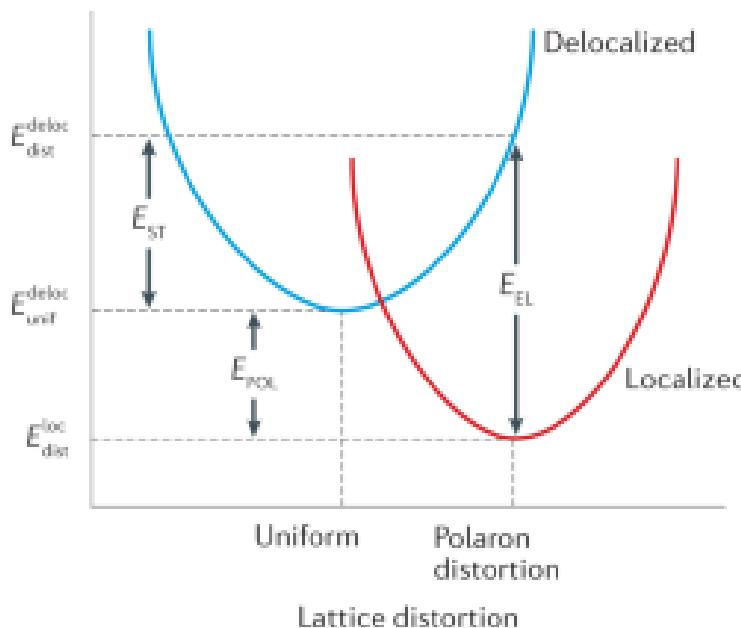
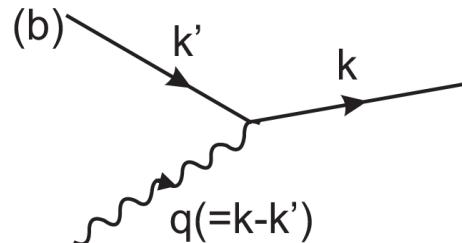
POLARON



Phonon emission



Phonon absorption

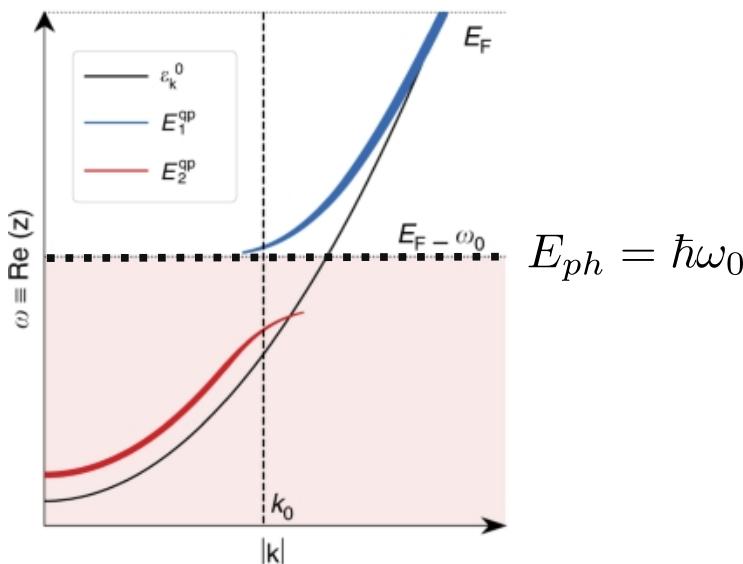
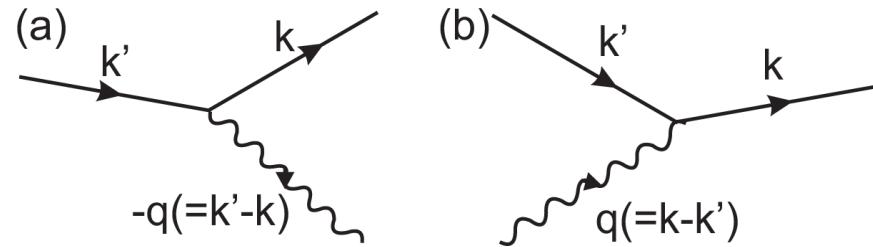


Polarons in Materials  
Nature Rev. Materials vol. 6,  
p. 560–586 (2021)

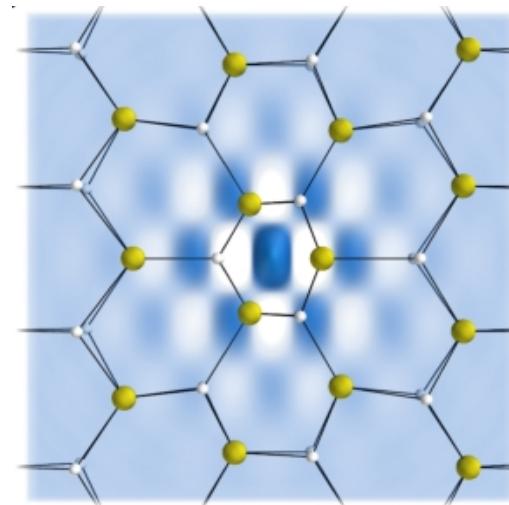
# Effects of Electron-Phonon Interaction

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$

Phonon emission      Phonon absorption

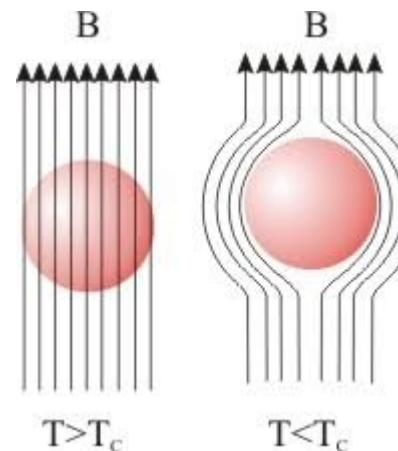
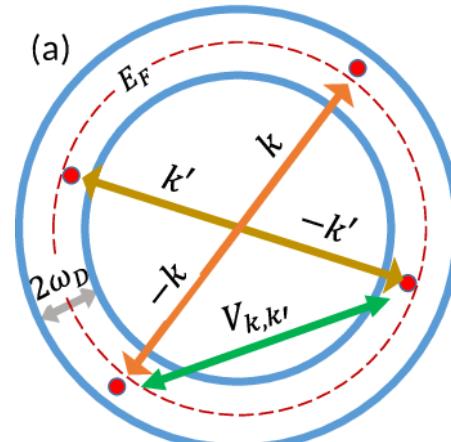
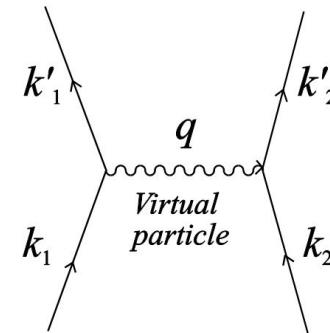
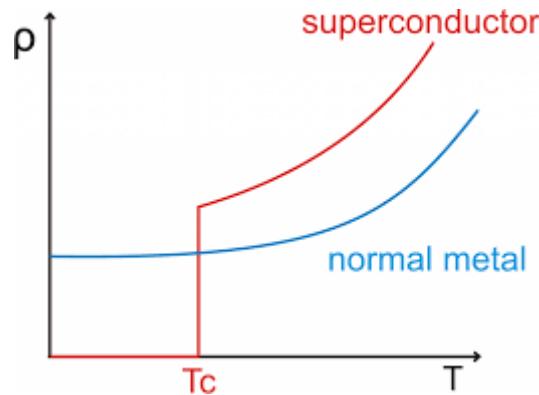
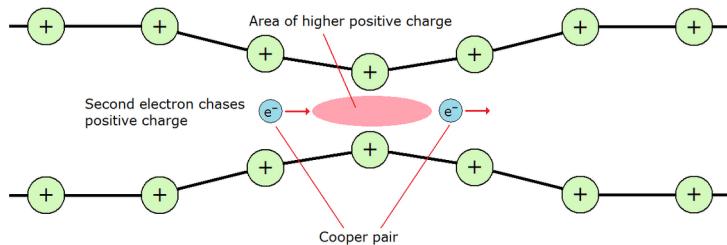


$$E_{ph} = \hbar\omega_0$$

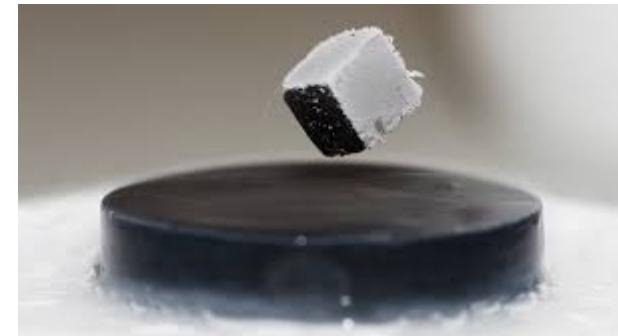


# Effects of Electron-Phonon Interaction

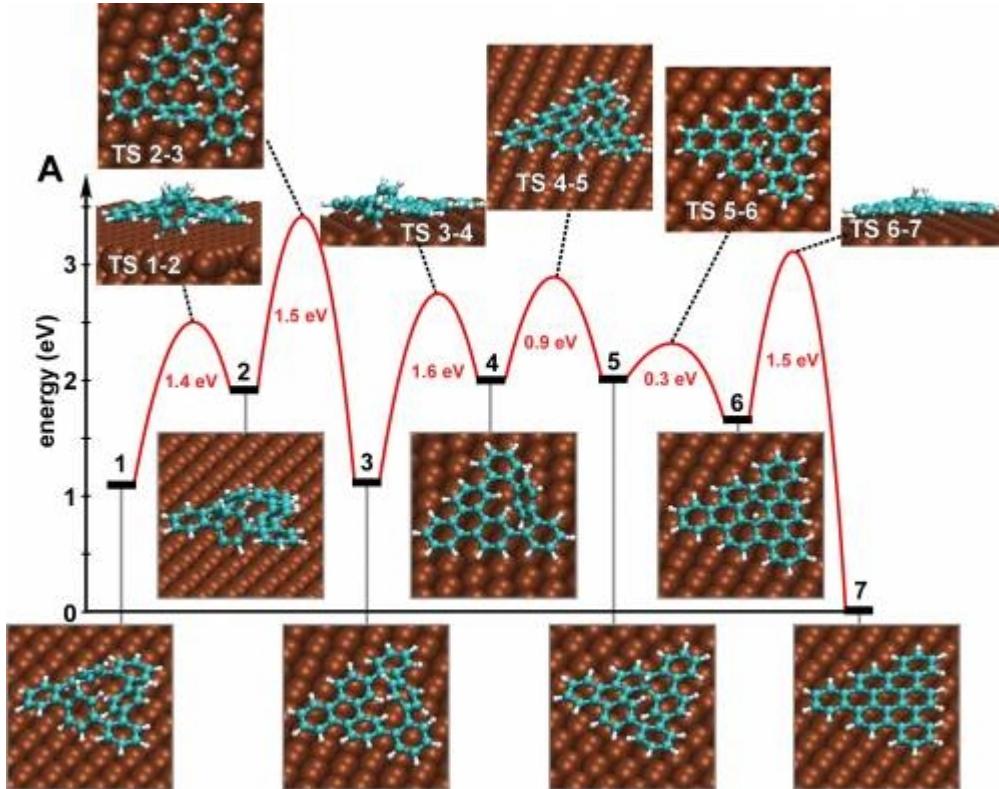
$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$



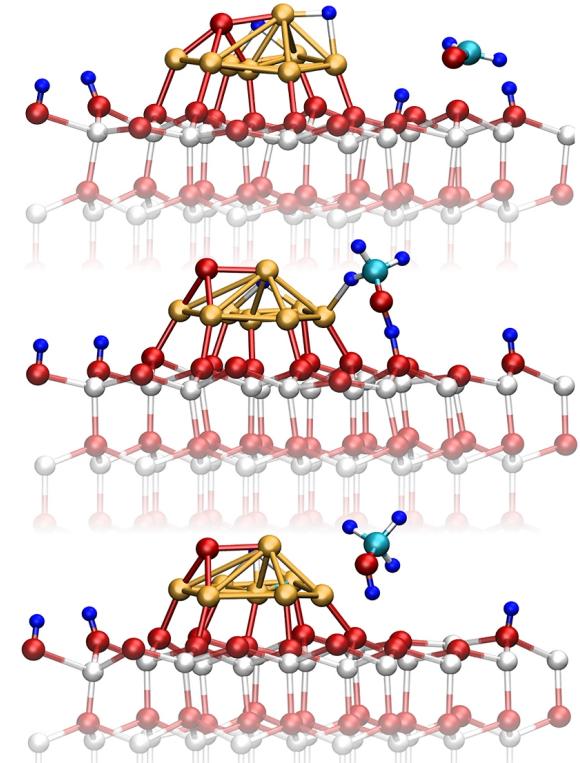
Meissner Effect



## Nanostructures and adsorption on metallic surfaces

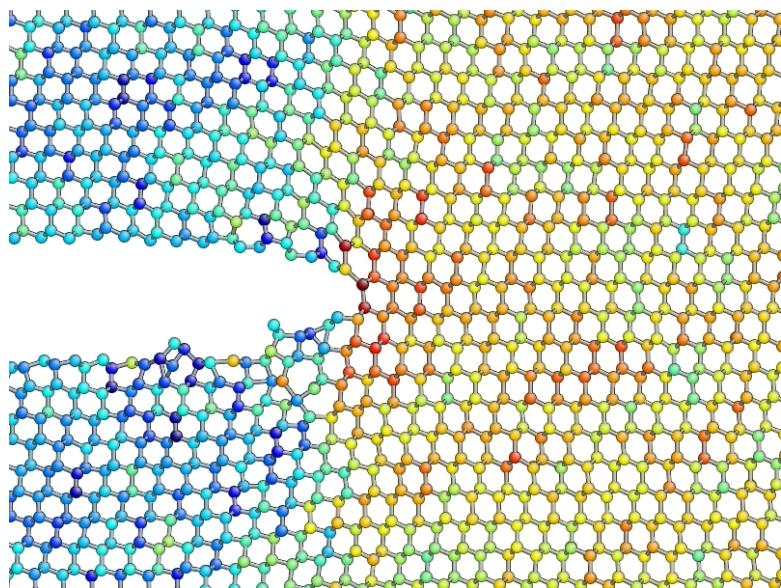


## Heterogeneous Catalysis

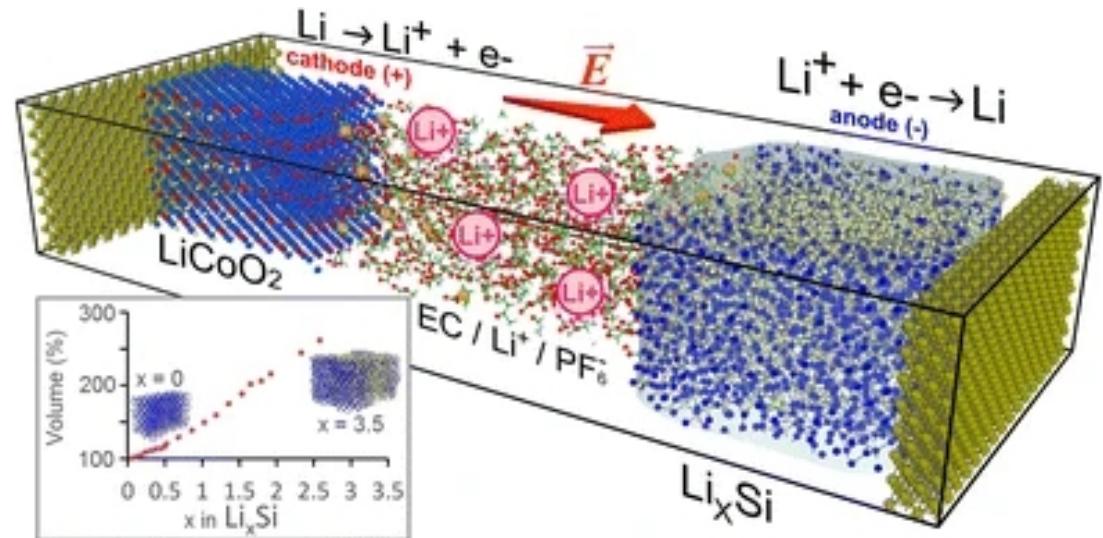


# Nuclear Dynamics

Simulation of fracture in Si

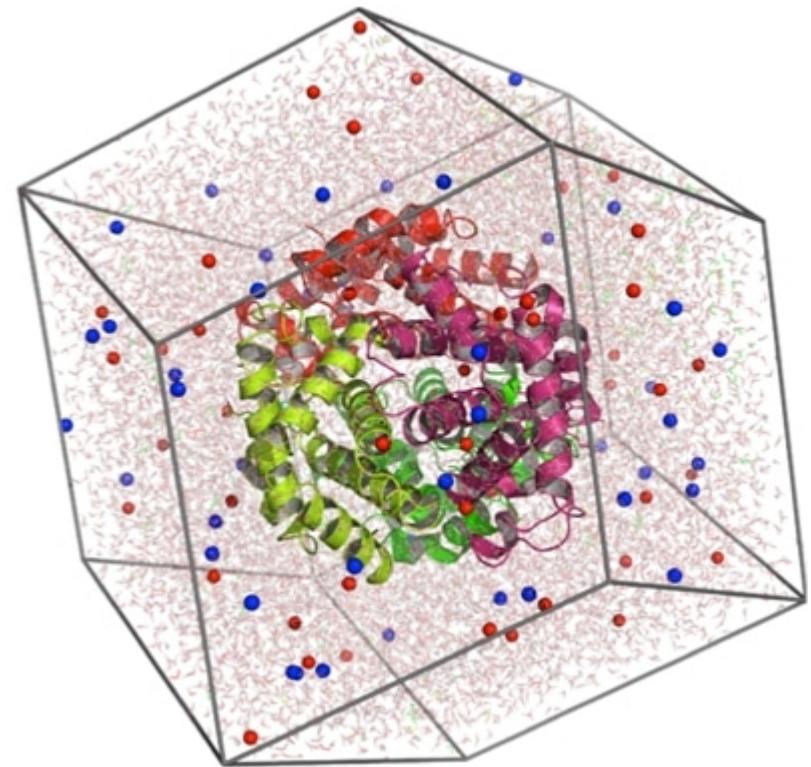
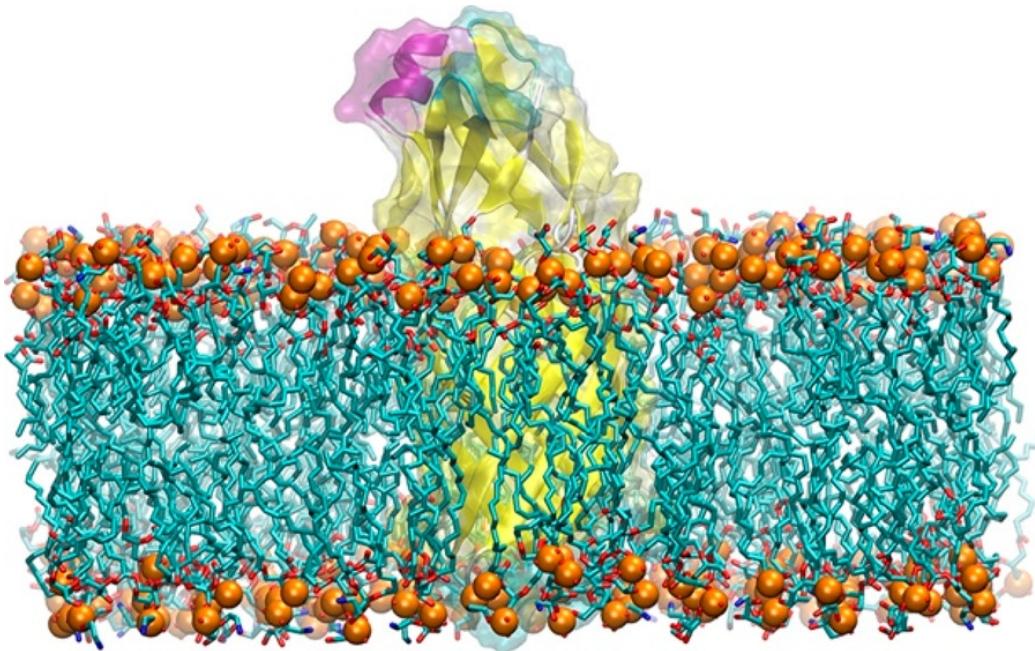


Simulation of Li ion nanobattery



# Nuclear Dynamics

## Biophysics: Membranes and Proteins



# Nuclear Dynamics

## Molecular Dynamics solution:

Because of the heavy mass of the nuclei one can assume that they behave like classical particles, above cryogenic temperatures.

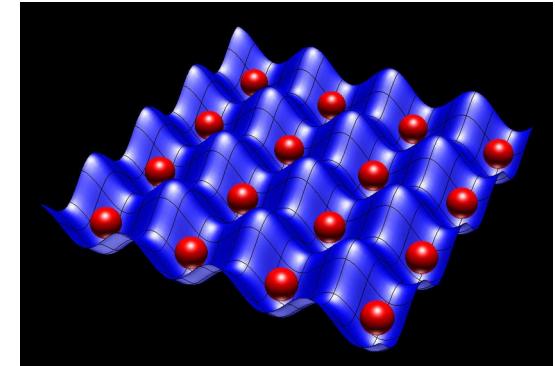
The Schrödinger equation is substituted by the classical dynamical equations

$$\sum_n \frac{P_n^2}{2M_n} \nabla_n^2 + U_a(R) = E \quad U_a(R) = \varepsilon_a^{el}(R) - V_{NN}$$

The harmonic approximation can be dropped.

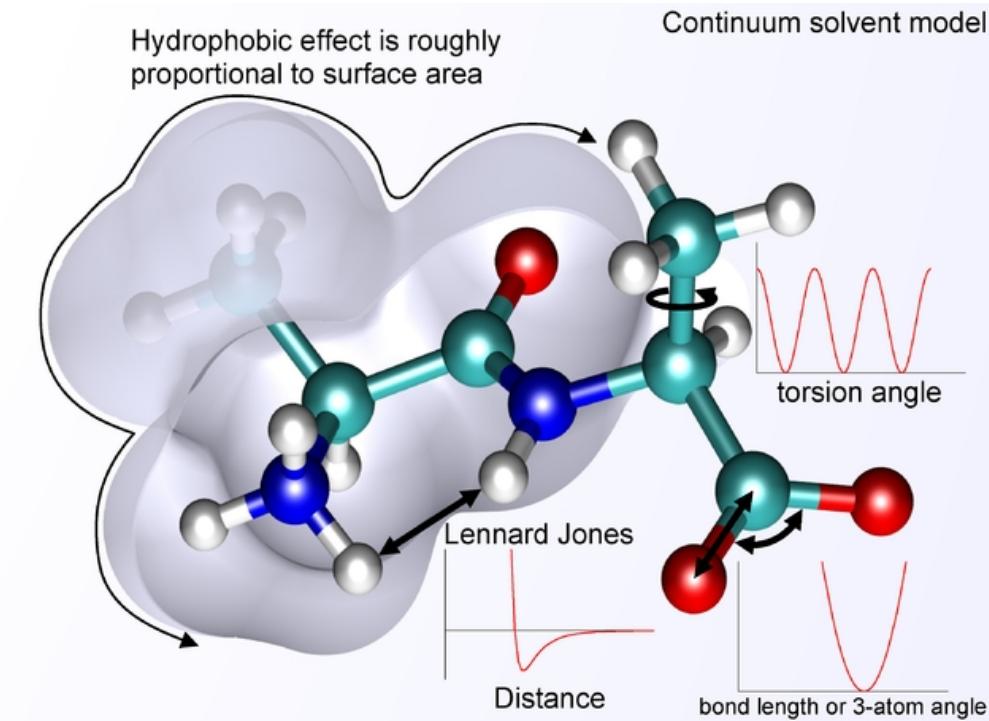
The classical equations of motion can be written as

$$M_n \frac{d^2 \vec{R}_n}{dt^2} = -\vec{\nabla}_n U_a(R) \quad \vec{F}_n = -\vec{\nabla}_n U_a(R)$$



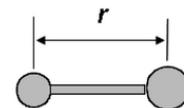
# Nuclear Dynamics

## Molecular Mechanics with Force-Fields

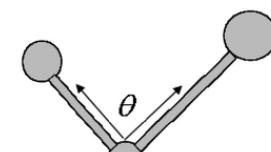


### Physical model for the AMBER force field

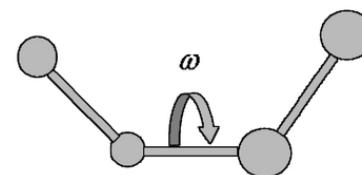
$$V_{total} = V_{bond} + V_{angle} + V_{torsion} + V_{non-bond}$$



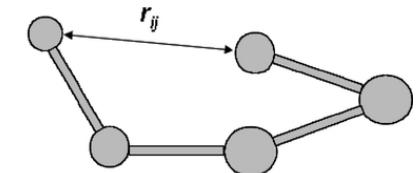
$$V_{bond} = k_{bond} (r - r_0)^2$$



$$V_{angle} = k_{angle} (\theta - \theta_0)^2$$



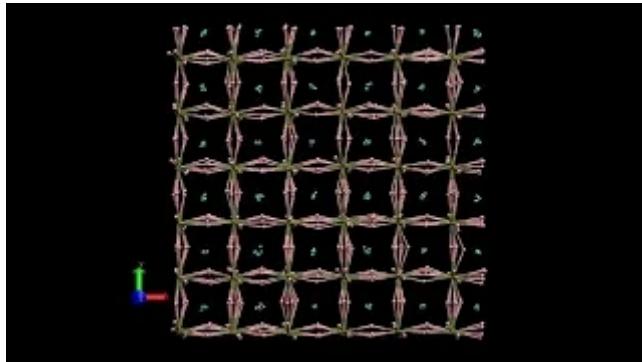
$$V_{torsion} = \frac{1}{2} k_{torsion} \{1 + \cos(n\omega - \omega_0)\}$$



$$V_{non-bond} = \frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^6} + \frac{q_i q_j}{\epsilon r_{ij}}$$

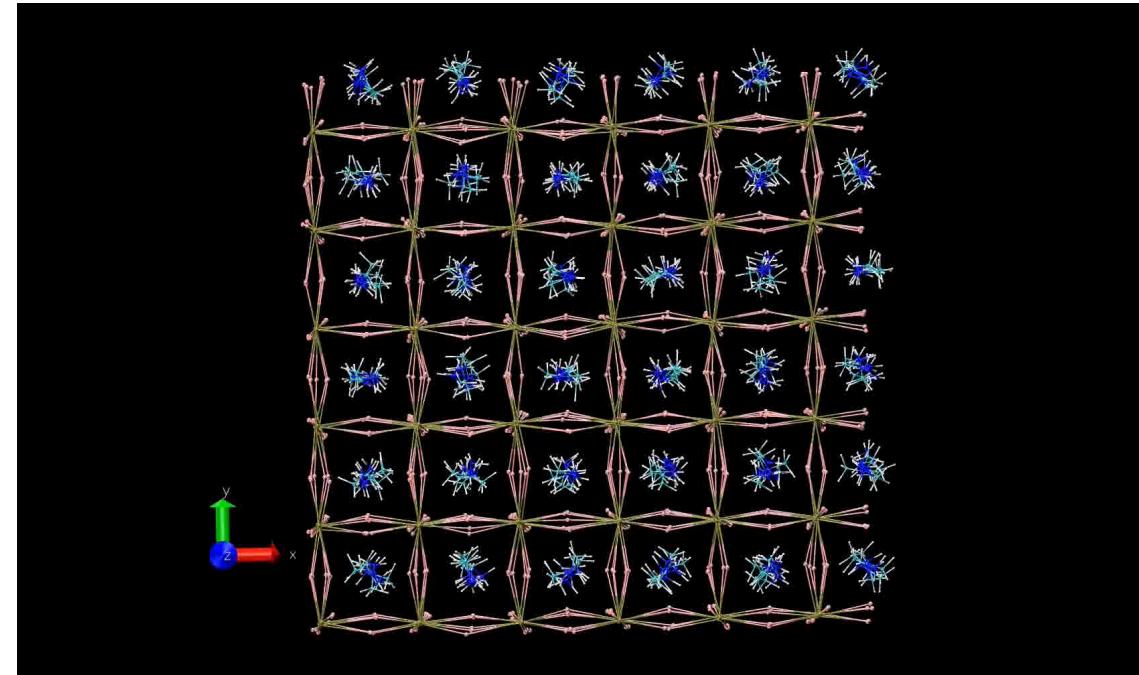
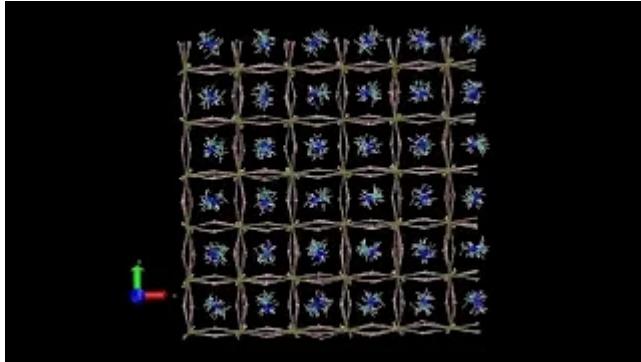
# Nuclear Dynamics

CsPbI<sub>3</sub> perovskite



# Nuclear Dynamics

$\text{CH}_3\text{NH}_3\text{-PbI}_3$  hybrid perovskite



# Nuclear Dynamics and Density of Vibrational States

velocity power spectrum (**VelPS.dat**) for stationary state:

$$\sum_i^N |\mathbf{v}_i(\omega)|^2 = \sum_i^N \int_{-\infty}^{\infty} \left( \int_{-\infty}^{\infty} \mathbf{v}_i(\tau + t) \cdot \mathbf{v}_i(\tau) d\tau \right) e^{i\omega t} dt$$

$$\text{VelPS}(\omega) \equiv \sum_i^N |\mathbf{v}_i(\omega)|^2 = \sum_i^N \int_{-\infty}^{\infty} \langle \mathbf{v}_i(\tau + t) \cdot \mathbf{v}_i(\tau) \rangle_{\tau} e^{i\omega t} dt$$

Vibrational Density of States (**VDOS.dat**):

$$VACF_{mw}(t) = \frac{\sum_i m_i \langle \mathbf{v}_i(t) \cdot \mathbf{v}_i(0) \rangle}{\sum_i m_i \langle \mathbf{v}_i(0) \cdot \mathbf{v}_i(0) \rangle} = \frac{\sum_i m_i \langle \mathbf{v}_i(t) \cdot \mathbf{v}_i(0) \rangle}{3Nk_B T}$$

$$\dot{\mathbf{r}}_k(t) = \mathbf{v}_k = \sum_s^{modes} \mathbf{Q}_{sk}(-i\omega_s) e^{-i\omega_s t} \xrightarrow{\text{thermal equil. + eqiupartition}} m_k |\mathbf{Q}_{sk}|^2 \omega_s^2 = 3k_B T$$

$$\sum_i^N m_i |\mathbf{v}_i(\omega)|^2 = \sum_s \sum_{k=1}^N \int_{-\infty}^{\infty} m_k |\mathbf{Q}_{sk}|^2 \omega_s^2 e^{i(\omega + \omega_s)t} dt = 3Nk_B T \sum_s \delta(\omega + \omega_s)$$