

# Announcements

- Re-grade request for Exam 2 should be initiated at Prof. Guan's office hours.
- Syllabus and schedule updated.
- Pop quiz on April 26 class time, covering Chapter 9, 11, 14.

# Today's class

## Solid state physics

- Crystal structures
- Heat capacity

## in-class quiz (5 min)

H<sub>2</sub> molecule has a vibrational frequency of  $1.3 \times 10^{14}$  Hz. What is the corresponding vibrational frequency of HD. The Deuterium (D) atom, an isotope of H, has twice the mass of H atom.

- A.  $0.65 \times 10^{14}$  Hz
- B.  $1.1 \times 10^{14}$  Hz
- C.  $1.3 \times 10^{14}$  Hz
- D.  $1.8 \times 10^{14}$  Hz
- E.  $2.6 \times 10^{14}$  Hz

# in-class quiz (5 min)

H<sub>2</sub> molecule has a vibrational frequency of  $1.3 \times 10^{14}$  Hz. What is the corresponding vibrational frequency of HD. The Deuterium (D) atom, an isotope of H, has twice the mass of H atom.

A.  $0.65 \times 10^{14}$  Hz

B.  $1.1 \times 10^{14}$  Hz

C.  $1.3 \times 10^{14}$  Hz

D.  $1.8 \times 10^{14}$  Hz

E.  $2.6 \times 10^{14}$  Hz

$$\omega = 2\pi f = \sqrt{\frac{k}{m}} \rightarrow \underline{f \propto \sqrt{\frac{1}{m}}}$$

$$m = \frac{m_1 m_2}{m_1 + m_2}$$

$$m_{H_2} = \frac{m_H m_H}{m_H + m_H} = \frac{m_H}{2}$$

$$m_{HD} = \frac{m_H m_D}{m_H + m_D} = \frac{2 m_H m_H}{m_H + 2 m_H} = \frac{2}{3} m_H$$

$$\frac{f_{HD}}{f_{H_2}} = \sqrt{\frac{m_{H_2}}{m_{HD}}} = \sqrt{\frac{m_H/2}{2m_H/3}} = \sqrt{\frac{3}{4}} \approx 0.866 \Rightarrow f_{HD} = 0.866 \cdot f_{H_2} = 1.1 \times 10^{14} \text{ Hz}$$

# Crystal structure affects physical properties

- What determines the physical properties of solids?

density, ductility, m.p., conductivity, resistivity  
magnetic, color, strength, etc.....

① the type of atoms

② how the atoms are joined together to form the solid.

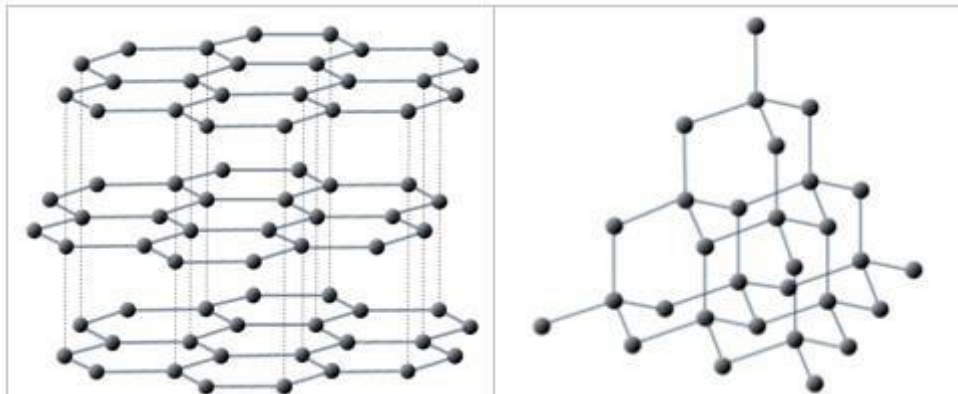
# Crystal structure



Graphite (the same as pencil tips) and diamond are all made of pure C atoms.

But they are completely different in *e.g.*, electrical conductivity, strength and light transmission.

Because the C atoms are organized differently, having different **crystal structures**.



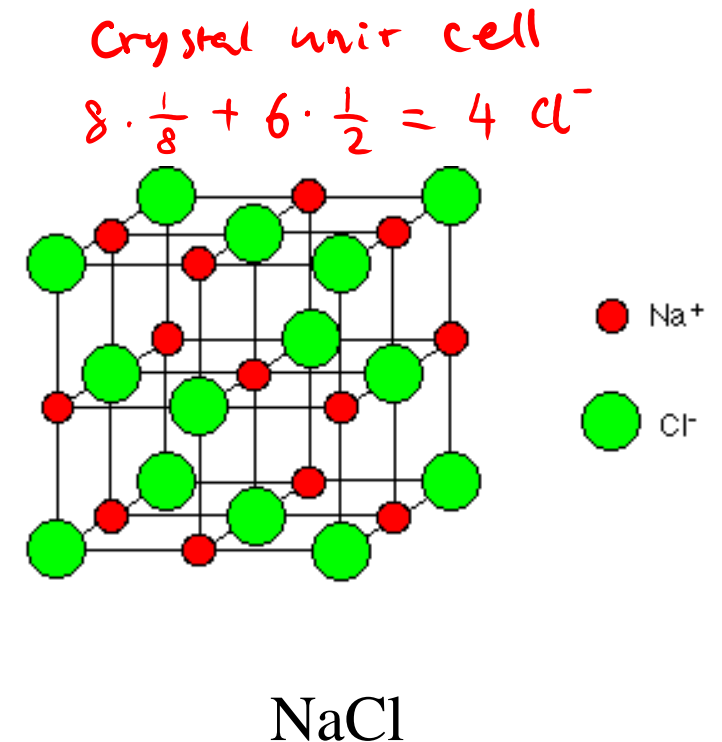
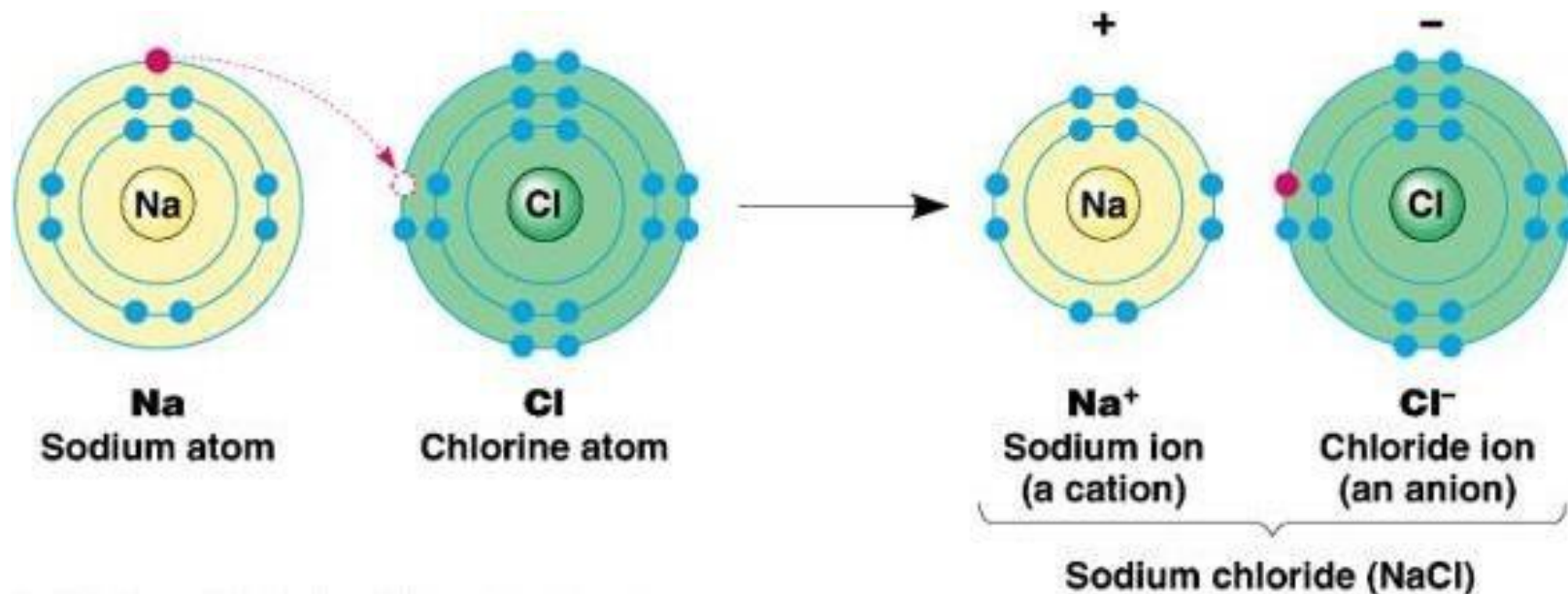
# Atomic bonds inside solids

- **Ionic bonds**

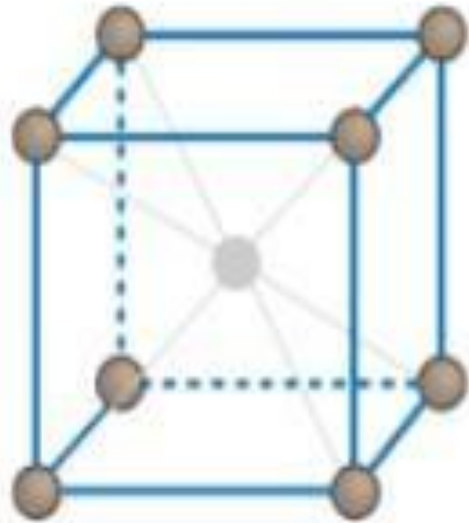
Crystalline – not amorphous – orderly packing of atoms

Bonding involving the Coulomb attraction of oppositely charged ions

Not in the form of molecules

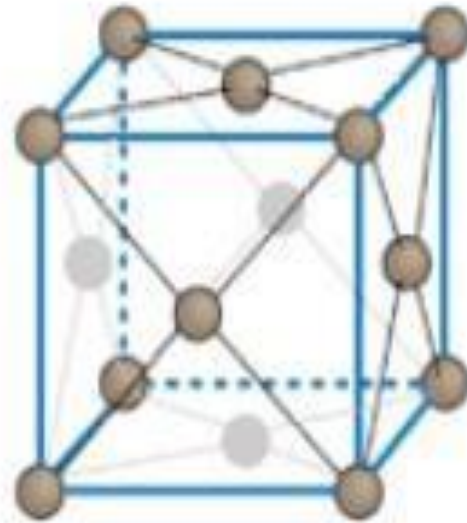


# Packing in ionic crystals



**Cubic body centered (bcc)**

CsCl

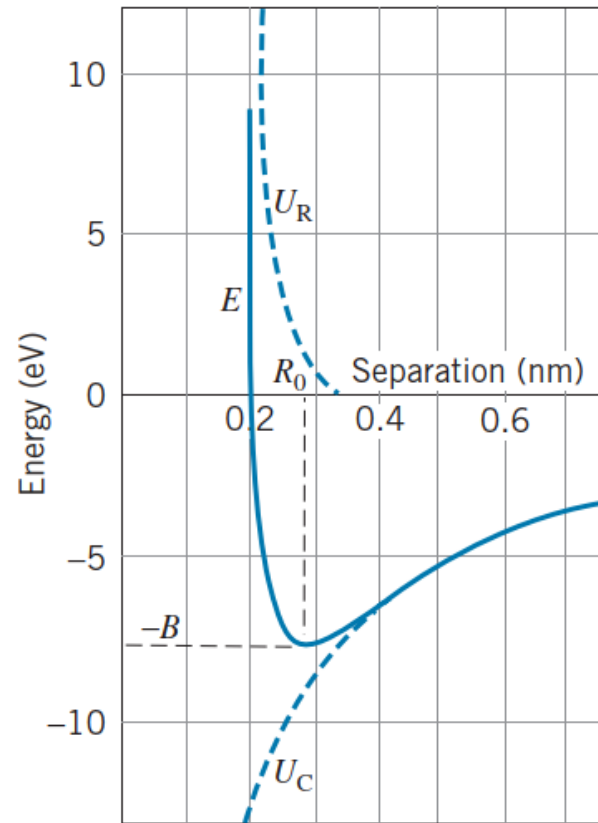


**Cubic face centered (fcc)**

NaCl

Different packing is due to the size of atoms.





Two contributions to the energy:

Coulomb attraction

Repulsion due to the Pauli principle – filled subshells don't overlap

# Properties of ionic solids

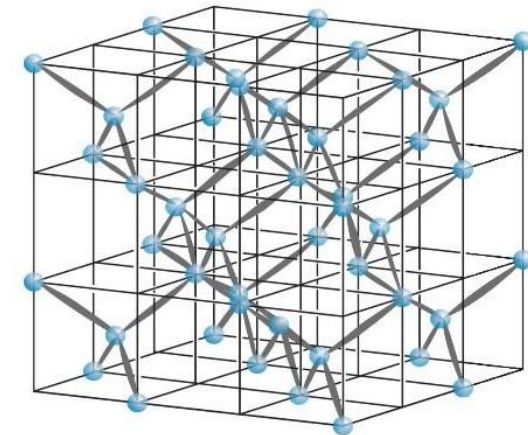
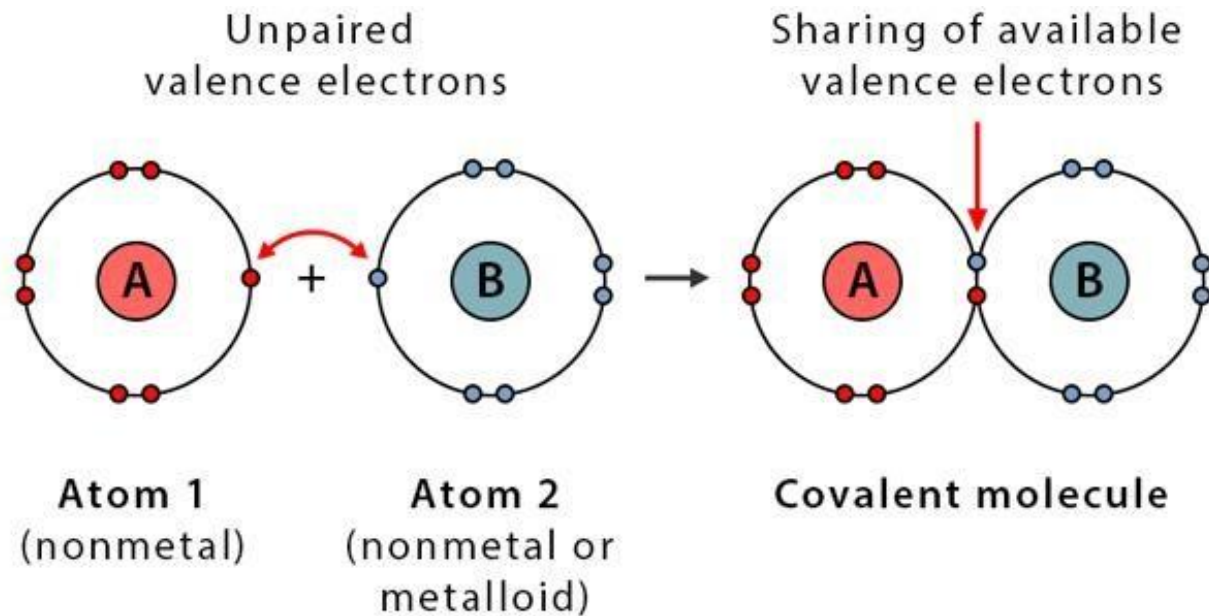
- Example NaCl crystal (not powder form)
- hard, with high melting and vaporization temperatures
- soluble in polar liquids such as water
- poor electrical conductors and not strongly magnetic – no free or valence electrons
- transparent to visible light, and absorb strongly in the infrared – atomic vibration on lattice.

# Atomic bonds inside solids

- **Covalent bonds**

Highly directional bonding because of sharing or overlap of electron wave functions

Recall: hybrid orbits



Diamond

# Properties of covalent solids

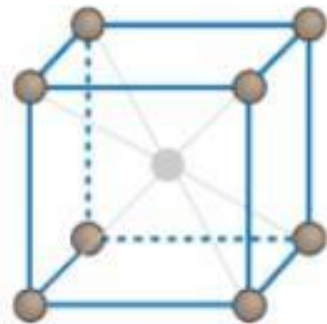
- Diamond, silicon, ...

No generalization. Depends on bonds and atoms.

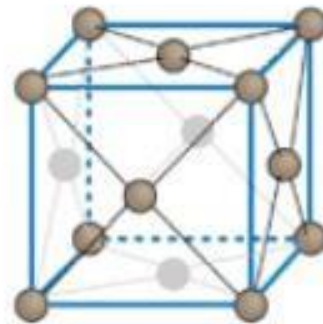
- { Diamond – hard, transparent to visible light, poor electrical conductor
- { Silicon – semiconductor.

# Atomic bonds inside solids

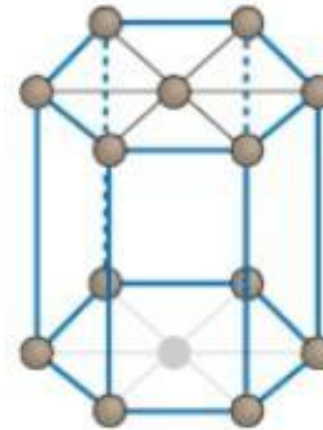
- **Metallic bonds**
- The valence electrons - loosely bound, and the electronic shells are only partially filled.
- 1–4 eV/atom, weaker than ionic and covalent bonds. Lower m.p.; not transparent in visible.
- free electron - high electrical and thermal conductivity
- Alloy - a “sea” or “gas” of approximately free electrons surrounding a lattice of positive ions. The identity of atoms are less relevant.



**Cubic body centered (bcc)**  
*Fe, V, Nb, Cr*



**Cubic face centered (fcc)**  
*Al, Ni, Ag, Cu, Au*



**Hexagonal**  
*Ti, Zn, Mg, Cd*

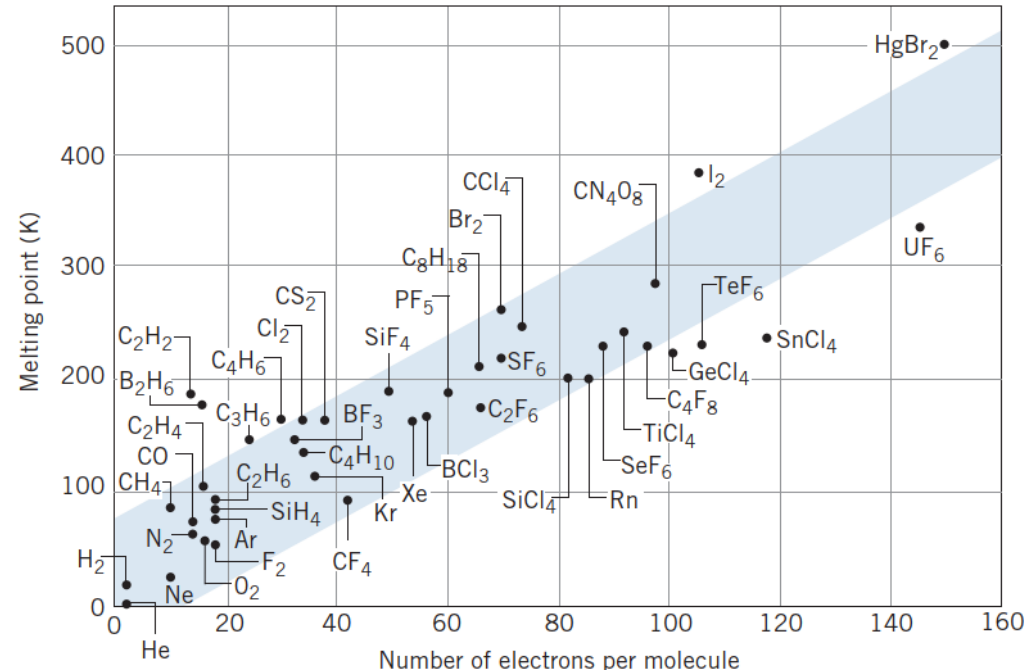
# Atomic bonds inside solids

- van der Waals bonds

Attraction between molecules. They exist in the form of molecules.

Permanent or transient electric dipole moment,

weaker than ionic, covalent, and metallic bonds.



# classical prediction for the heat capacity of a solid

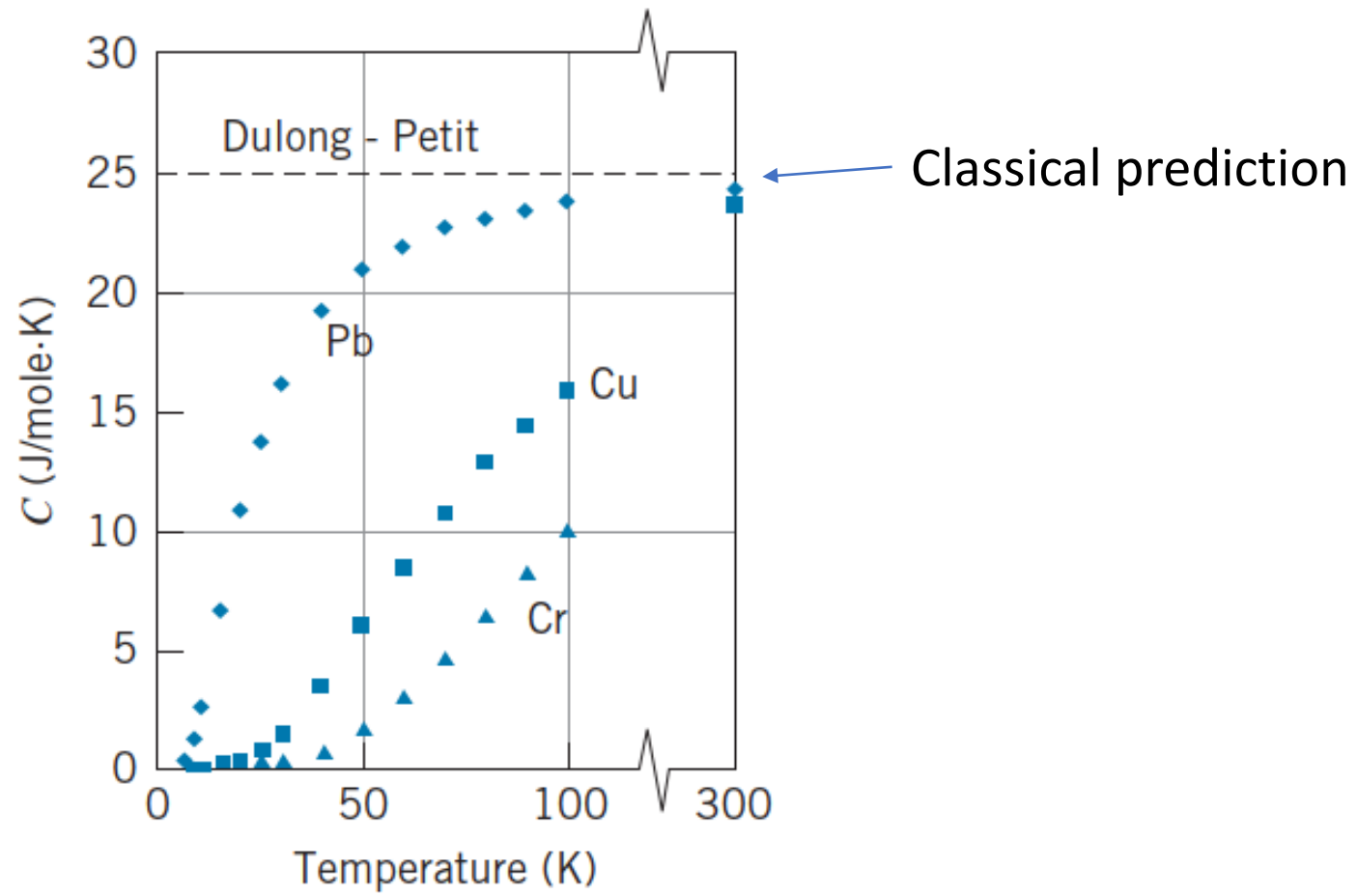
Atoms vibrate on lattice.

Vibrational potential and kinetic energy in  $x, y, z$  3D.  
6 degrees of freedom

the average energy per atom  $6 \cdot \frac{1}{2} kT = 3kT$

the average energy per mole  $3RT$   $R$ : universal gas constant

molar heat capacity  $C = \frac{\Delta E}{\Delta T} = 3R$



Only valid for high T ( $\sim$ room temperature)



Electron contribution to the heat capacity:

Assumptions: treat electrons in a metal as a Fermi gas; one valence electron per atom.

$$C = \frac{\pi^2 k^2 N_A T}{2E_F} = \frac{\pi^2 RkT}{2 E_F}$$

Einstein theory of heat capacity:

Assumptions: contribution from both electron and **lattice vibration**;

“phonon” – quantization of vibration energy;  $E = \hbar\omega$

Phonons follow Bose-Einstein distribution.

$$C = 3R \left( \frac{T_E}{T} \right)^2 \frac{e^{T_E/T}}{(e^{T_E/T} - 1)^2}$$

$T_E$ : Einstein temperature

Debye theory of heat capacity:

Assumption: **a distribution of frequencies**.

$$C = \frac{12\pi^4}{5} R \left( \frac{T}{T_D} \right)^3$$

$T_D$ : Debye temperature

At lowest temperatures,  $C = aT + bT^3$ , contribution from electron gas and lattice vibration.

# Debye theory is successful across materials and temperatures

**TABLE 11.4 Heat Capacities of Common Metals\***

Metal	$T = 300 \text{ K}$		$T = 100 \text{ K}$	$T = 25 \text{ K}$
	J/kg · K	J/mole · K	J/mole · K	J/mole · K
Al	0.904	23.4	12.8	0.420
Ag	0.235	24.3	20.0	3.05
Au	0.129	23.4	21.1	5.11
Cr	0.461	23.8	10.0	0.199
Cu	0.387	23.9	16.0	0.971
Fe	0.450	24.6	12.0	0.398
Pb	0.128	24.7	23.8	14.0
Sn	0.222	23.8	22.0	6.80

