

Lecture 22

Chemical Bonding and Intermolecular forces- Part 2

Textbooks:

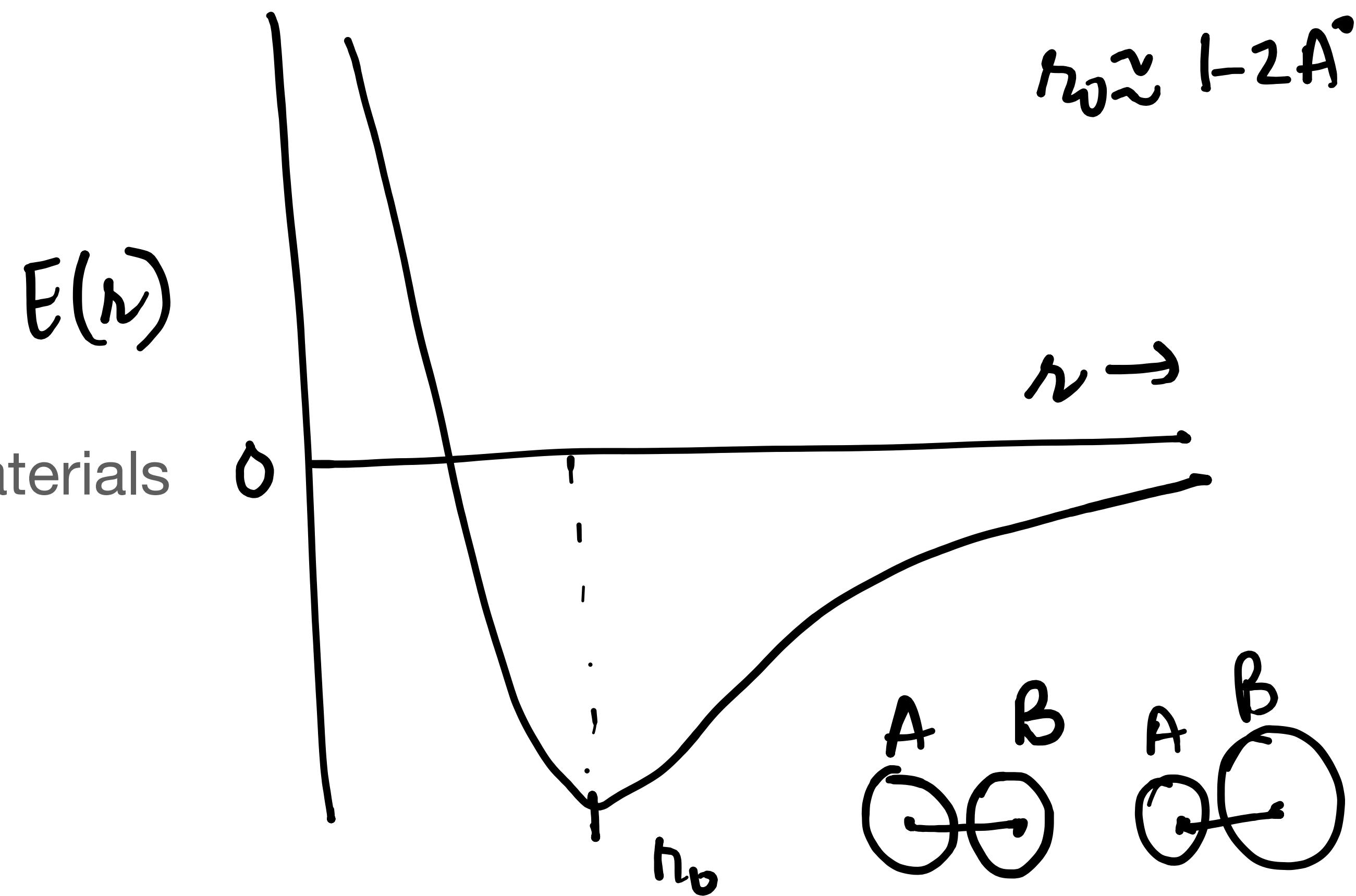
- Introduction to materials science and Engineering: V. Raghavan
- Materials Science and Engineering: Callister and Rethwisch

Recap

- Why intermolecular forces/chemical bonding are important to understand?
- Differences between chemical bonding and intermolecular forces
- The net force and net energy of interaction between atoms: attraction and repulsion

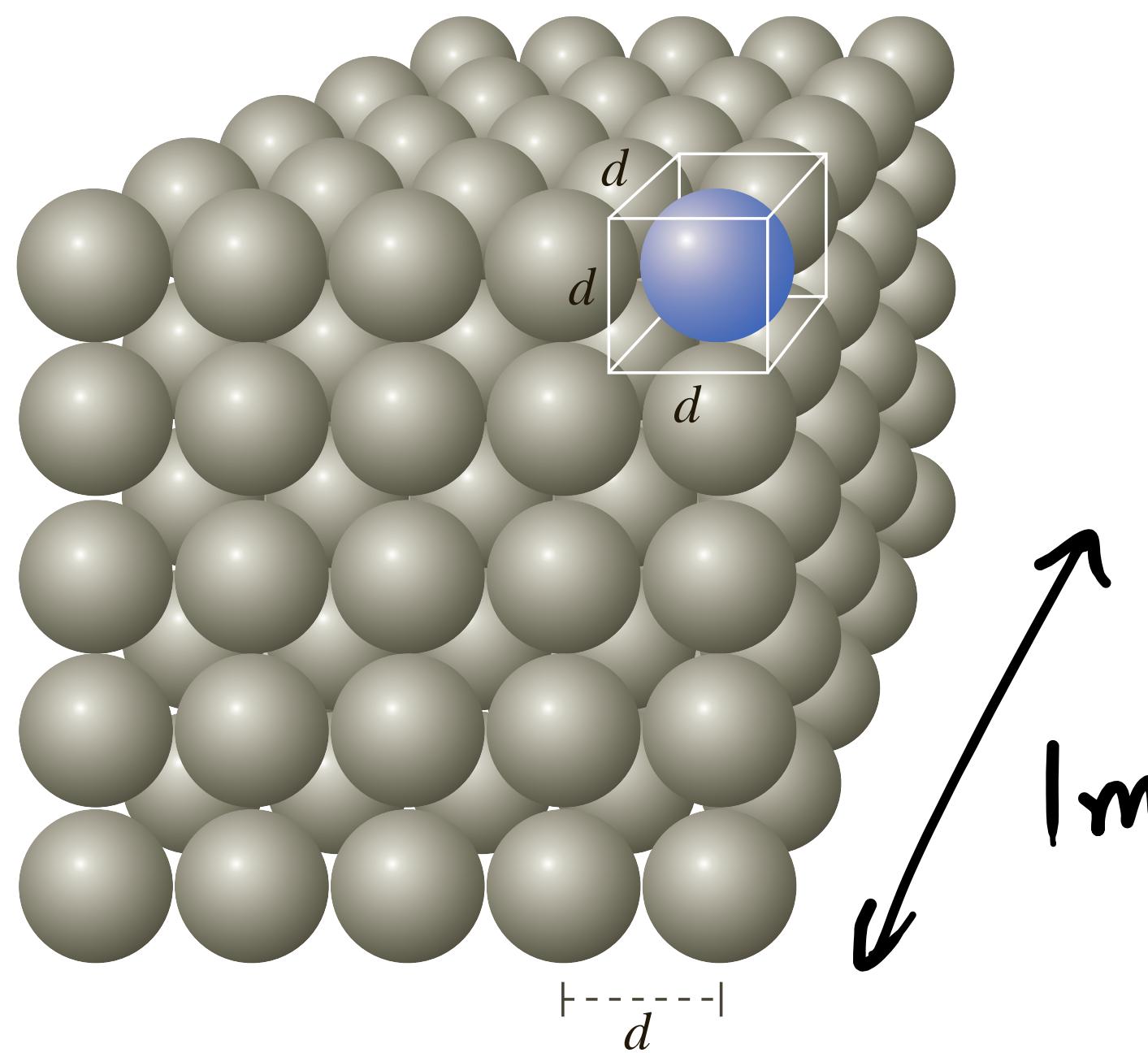
Pre-cap

- Different types of chemical bonding
- Different types of intermolecular forces
- Effect of these forces on properties of materials



Problem: Computing the diameter of a Copper Atom (Length of a Bond in Copper)

One mole of copper (6.02×10^{23} atoms) has a mass of 64 g. The density of copper is 8.94 g/cm^3 . What is the approximate diameter, in meters, of a copper atom in solid copper?



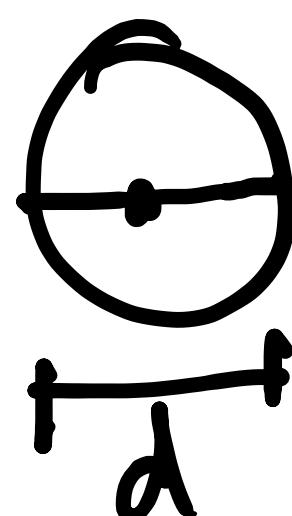
$$\text{Density} = 8.94 \text{ g cm}^{-3} = 8.94 \times 10^3 \text{ kg m}^{-3}$$

In a cube of edge length 1m, the no. of Cu atoms is,

$$8.94 \times 10^3 \frac{\text{kg}}{\text{m}^3} \times \frac{1 \text{ mol}}{0.064 \text{ kg}} \times \frac{6.023 \times 10^{23} \text{ atoms}}{1 \text{ mol}}$$

$$= 8.41 \times 10^{28} \text{ atoms in } 1\text{m}^3$$

$$\text{In } 1\text{ m length, no. of Cu atoms} = (8.41 \times 10^{28}) \\ = 4.38 \times 10^9 \text{ atoms}$$

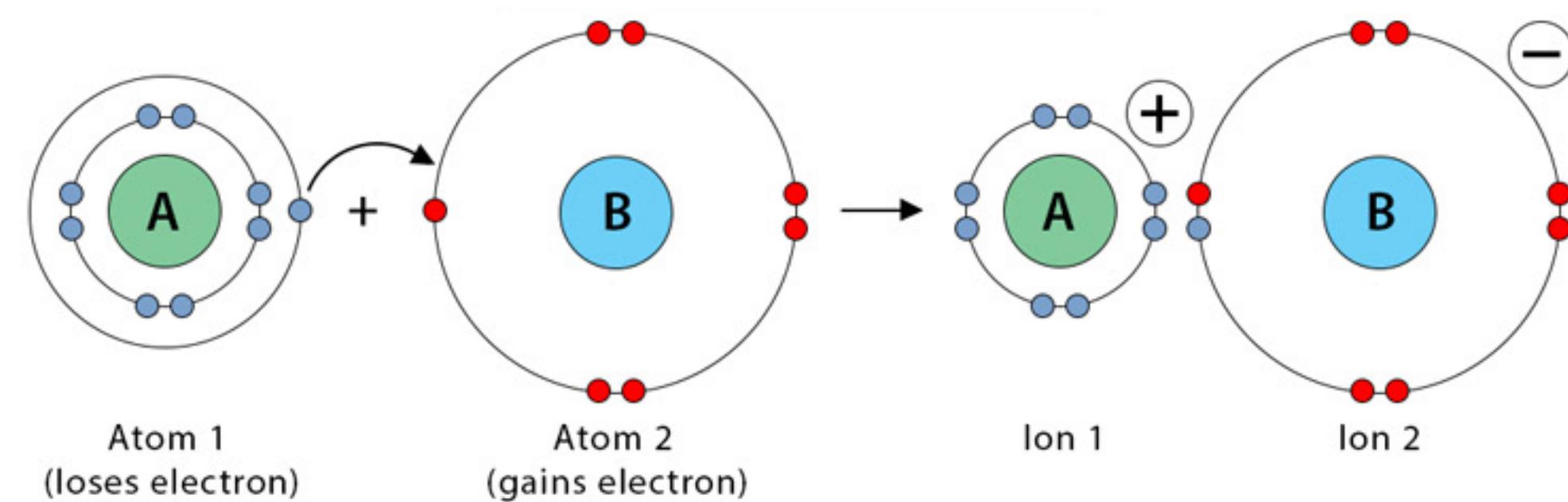
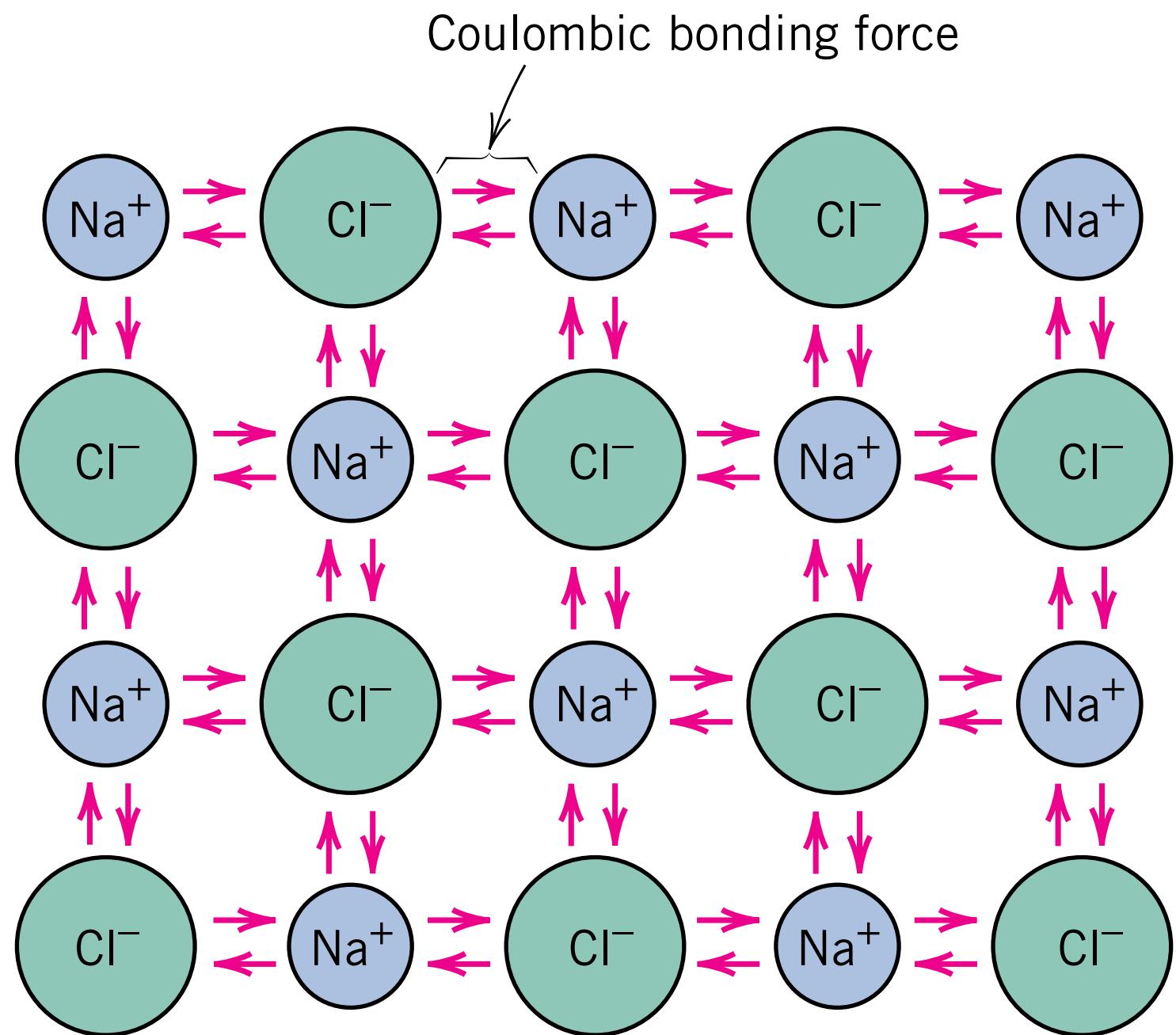


$$\therefore d = \text{Diameter of } 1 \text{ Cu atom} = \frac{1 \text{ m}}{4.38 \times 10^9} = 2.28 \times 10^{-10} \text{ m} \\ = 2.28 \text{ Å}$$

Ionization potential, electronegativity and electron affinity

- **Ionization potential:** the energy required to remove an electron from its outer orbital
- **Electron affinity:** the work done by the system when the extra electron is attracted from infinity to the outer orbital of the neutral atom
- **Electronegativity:** the tendency of the atom to attract electrons to itself during the formation of bonds with other atoms is measured by electronegativity.

Ionic bonding



- Atoms of metallic elements give up their valence electrons to non-metallic atoms - e.g. NaCl

Coulombic energy:

$$E_A = -\frac{A}{r} \quad \text{and} \quad E_R = \frac{B}{r^n}$$

A, B are constants, $n=8$

$$A = \frac{(z_1 e)(z_2 e)}{4\pi\epsilon_0} ; z_i = \text{valency of ion}$$

$e = \text{electronic charge}$

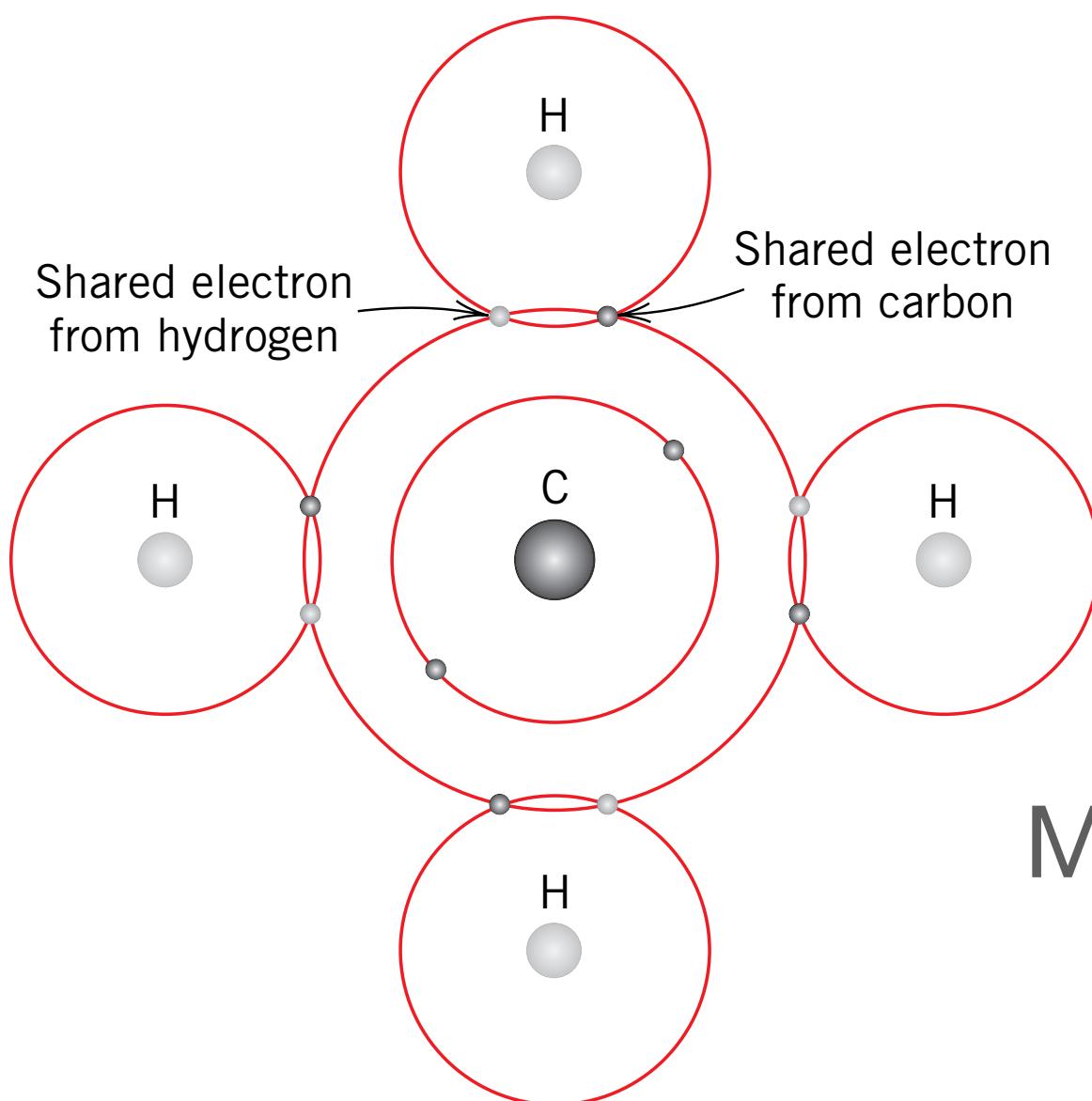
$(1.602 \times 10^{-19} \text{ C})$

$\epsilon_0 = \text{permittivity of vacuum}$

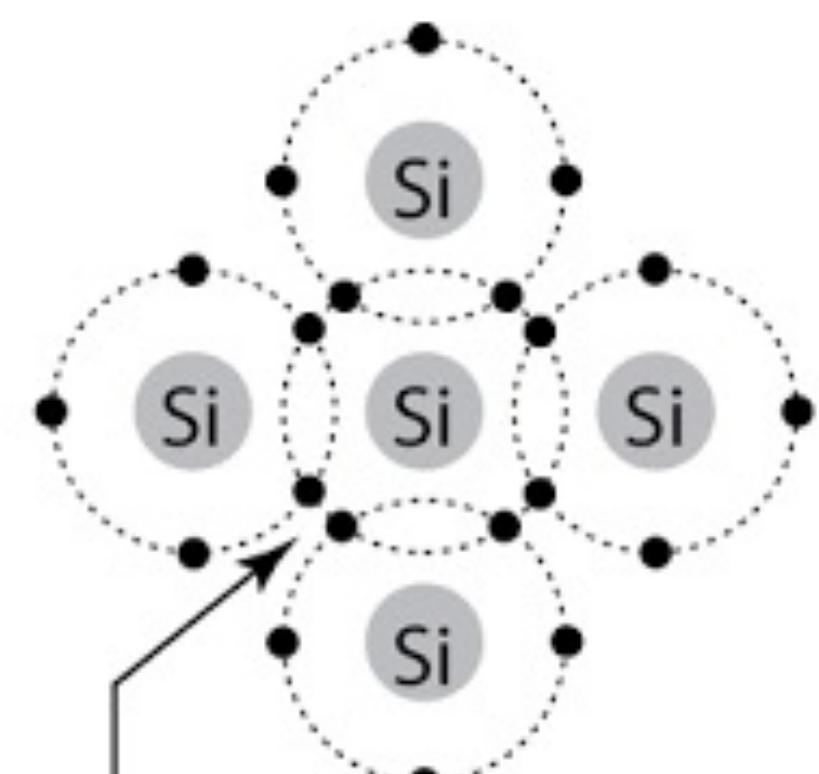
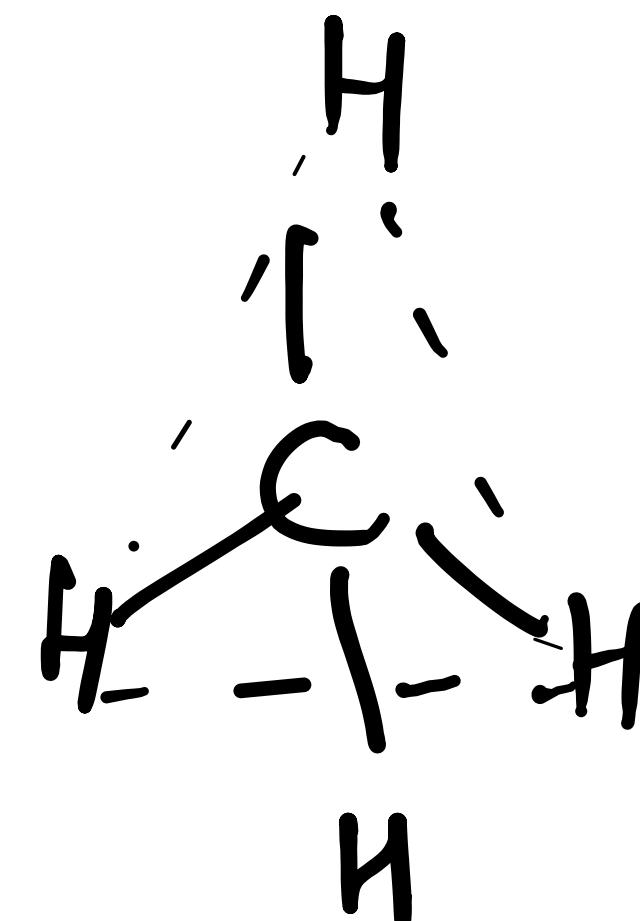
$$E \propto \frac{1}{r}$$

- long-range interaction
- Non-directional

Covalent bonding



Methane



Silicon

Shared electrons
of a covalent
bond.

- electrons are shared between the atoms

- Directional bonding

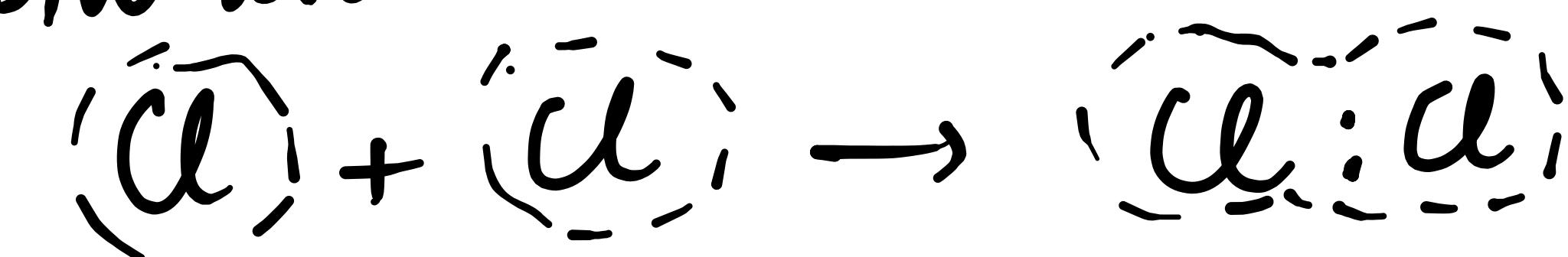
- Polar covalent bonding :



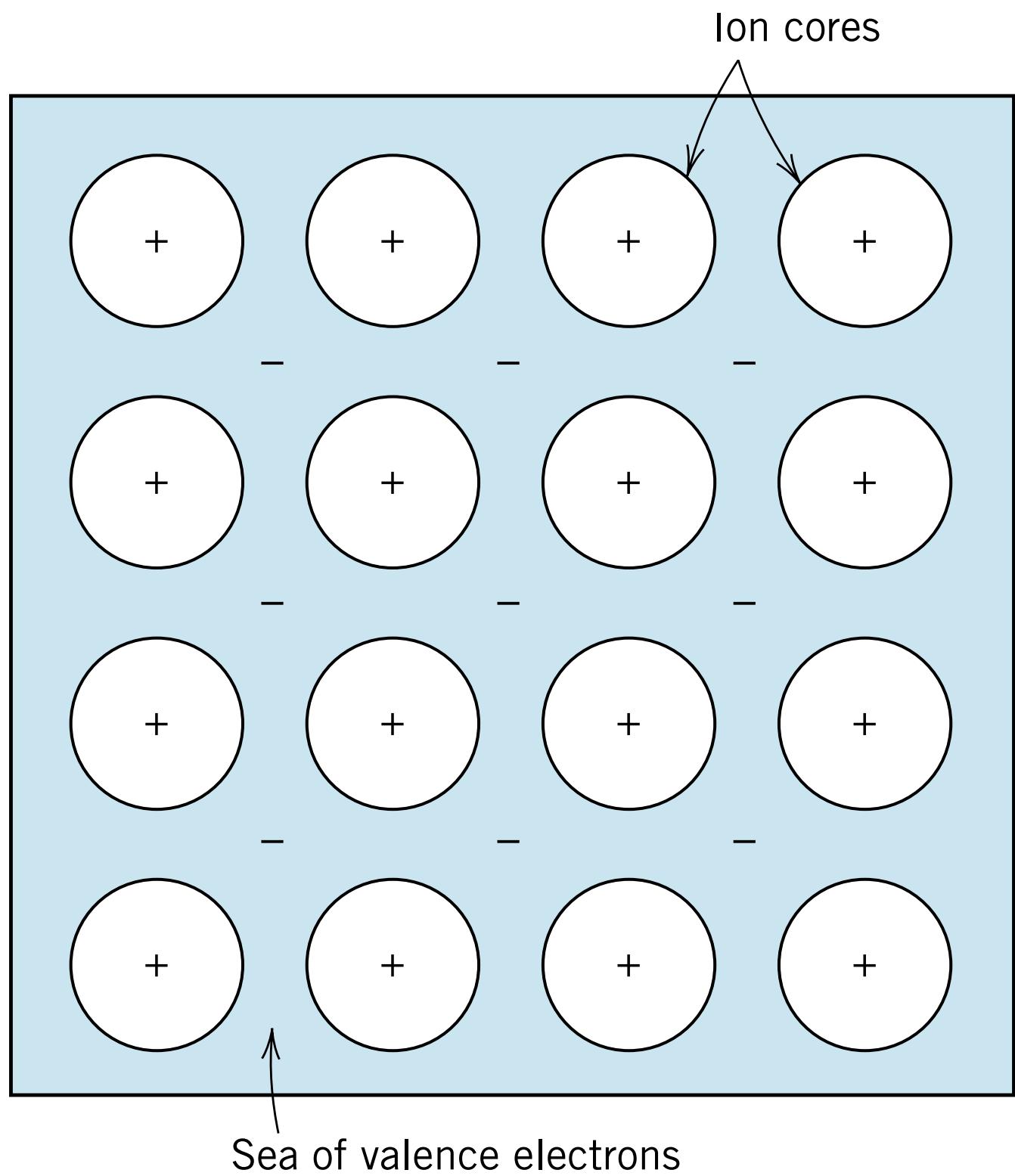
electronic charge distribution is unequal between the atoms

- Non-polar covalent bonding :

electronic charge dist. is equal b/w atoms



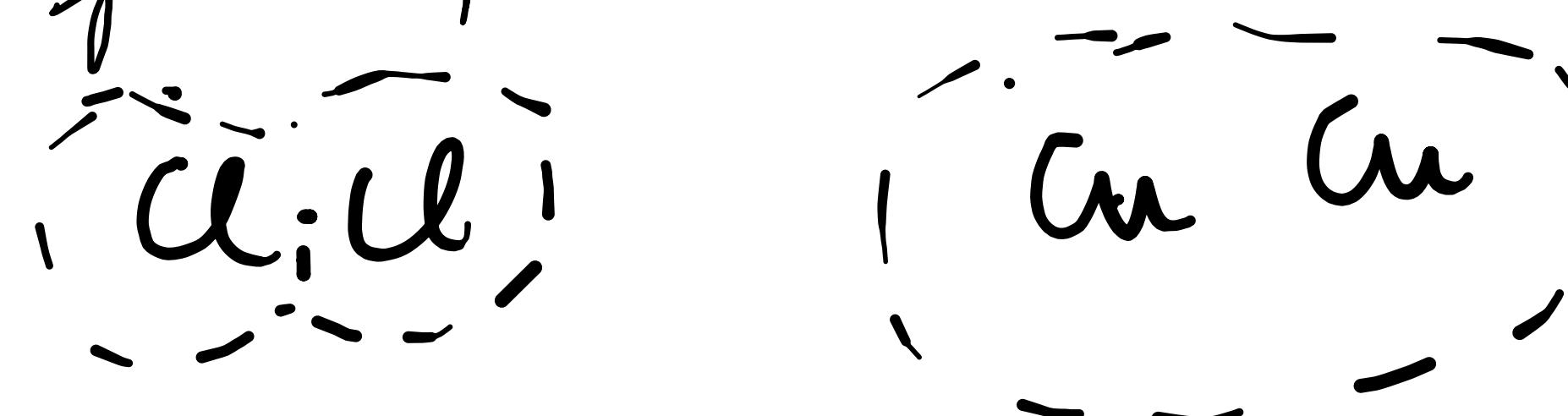
Metallic Bonding



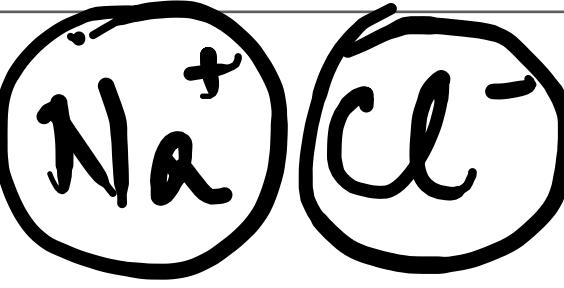
Cu, Fe, Zn

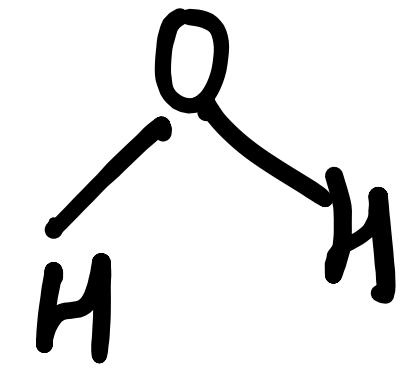
- Metals have a large no. of valence electrons that are delocalized over the atom. These e^- do not bound to any atom
- Non-directional bonding
- The e^- cloud shields positively charged nuclei from repulsion and act as glue to hold the nuclei together -

eg: Group I, II metals



Chemical Bonding- A summary

Bond	Attraction	Energy (kJ/mol)	Example	Model
Ionic	Cation-anion	400-4000	Na-Cl	
Non-polar covalent	Sharing of electrons	150-1000	Cl-Cl	
Polar covalent	Sharing of electrons	150-1000	H-Cl	

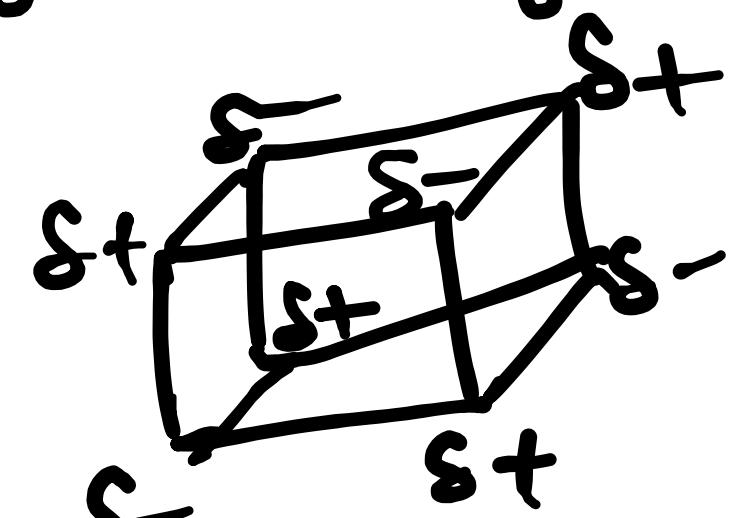
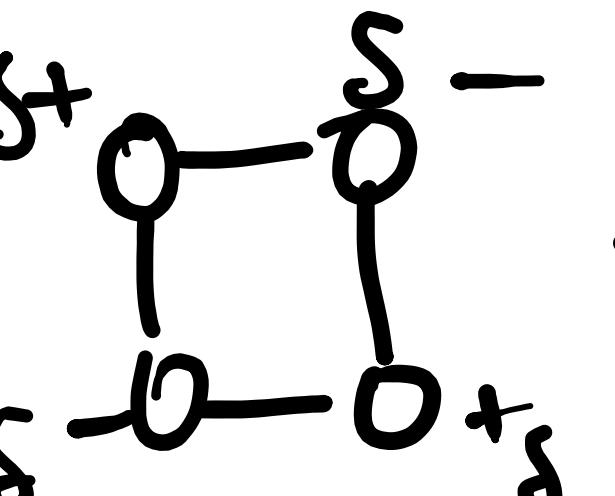
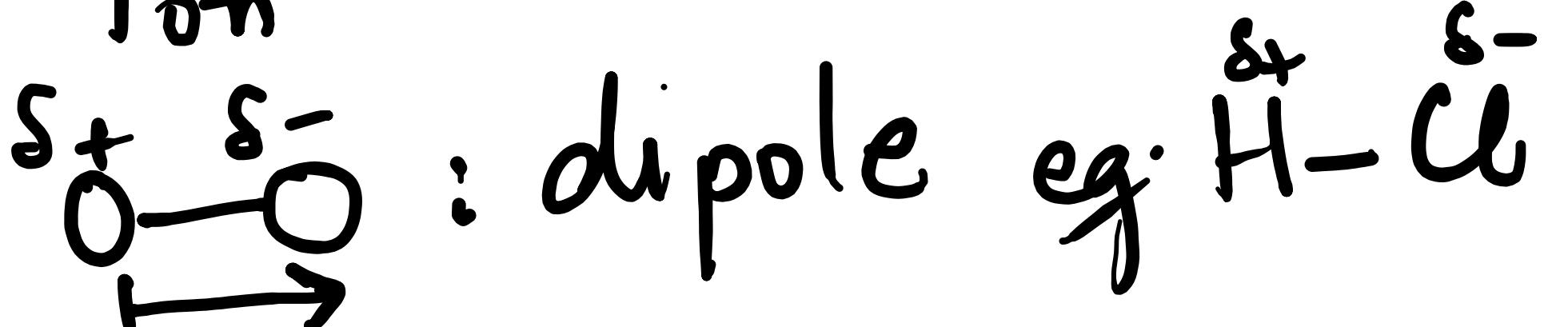


“Non-bonding” Intermolecular forces

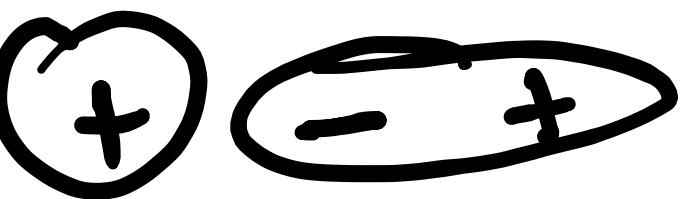
Electrostatic

Bond	Attraction	Energy (kJ/mol)	Example	Model
Ion-dipole	Ion-dipole	40-600	Na ⁺ ---- H-Cl	
Dipole-dipole	Dipole-dipole	5-25	H-Cl---- H-Cl	
Induction	ion-induced dipole	3-15	Na ⁺ ---- H-H	
Dipole-induced dipole	Dipole-polarizable electron cloud	2-10	H-Cl---Cl-Cl	
✓ London dispersion forces	Polarizable electron cloud	0.05-40	Cl-Cl---Cl-Cl	

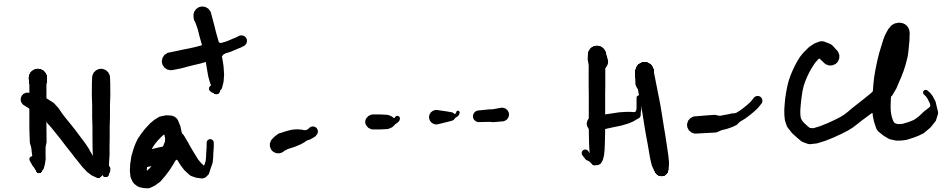
Multipoles: Set of partial charges arranged in a symmetric manner.



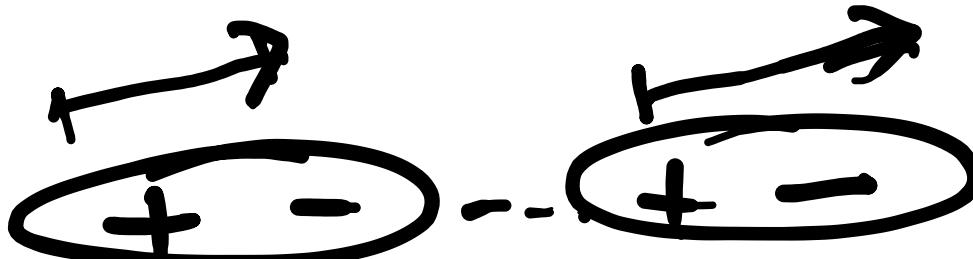
Ion-dipole:



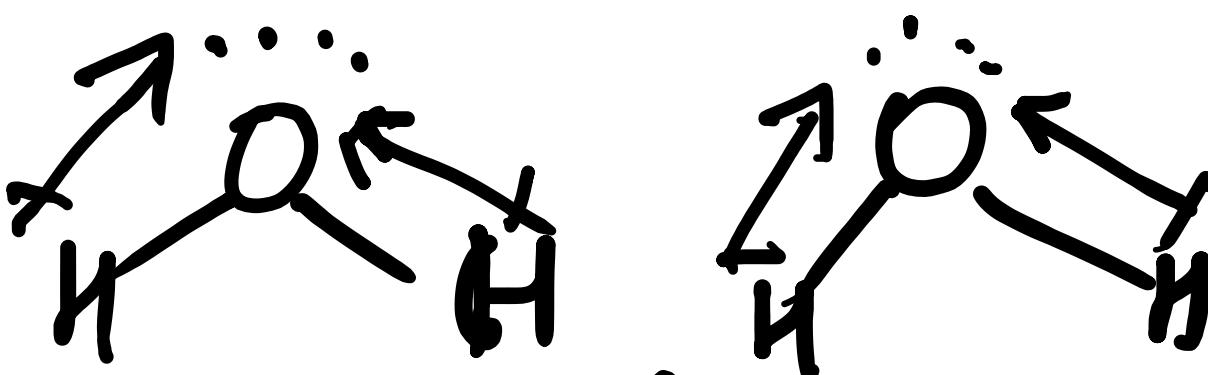
$$E \propto -\frac{1}{r^2}$$



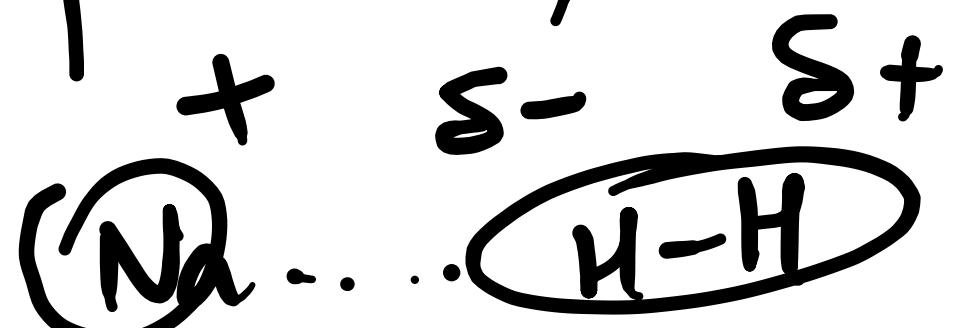
Dipole-Dipole:



$$E \propto -\frac{1}{r^3}$$



Induction interaction: multipole
another molecule depending on
molecule.

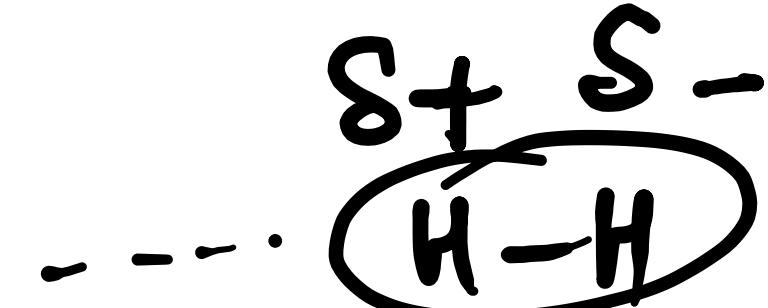


$$E \propto -\frac{1}{r^6}$$

Ion-induced dipole:



Dipole-induced dipole:

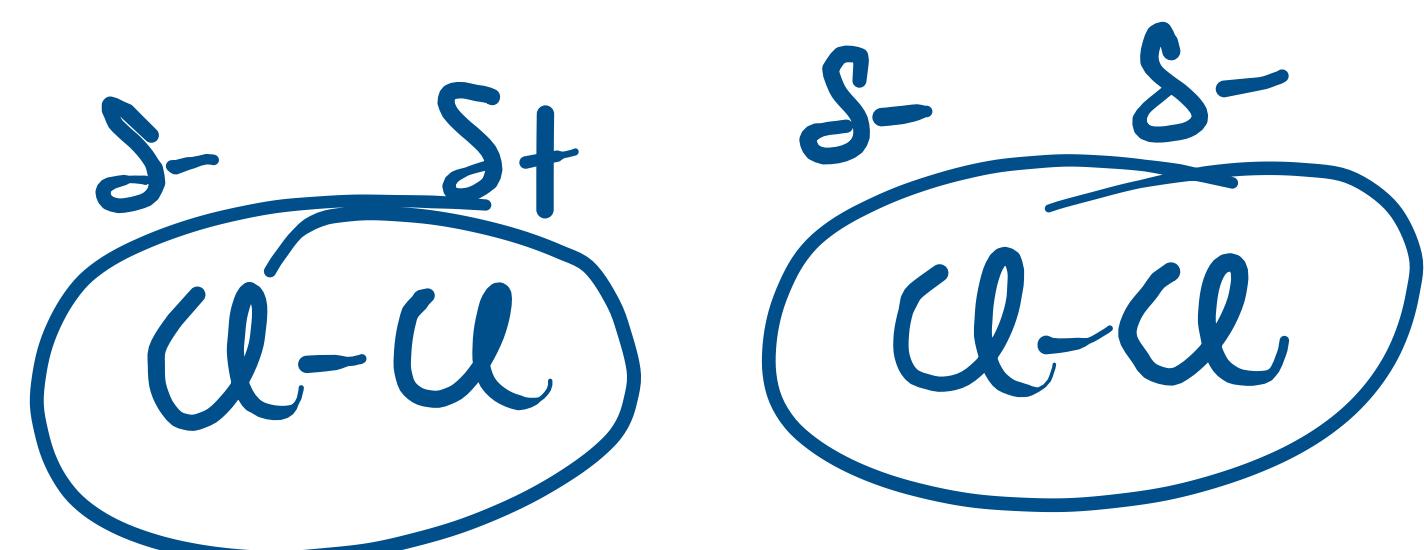


induces interaction in
polarizability of that
transient dipole
"Distortion in
e⁻ charge distribution"

Dispersion interaction:
(van der Waals)



$$\epsilon(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$



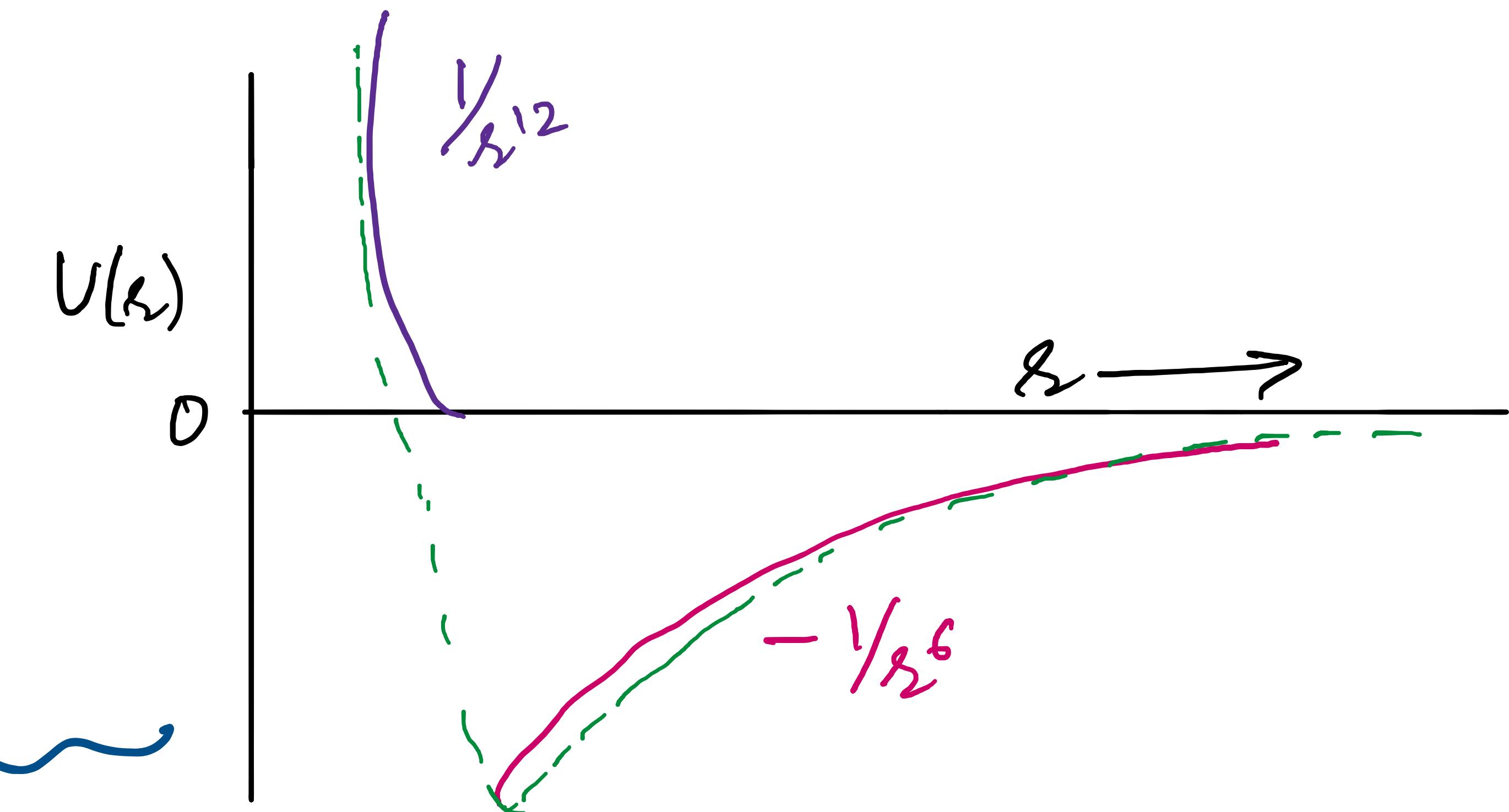
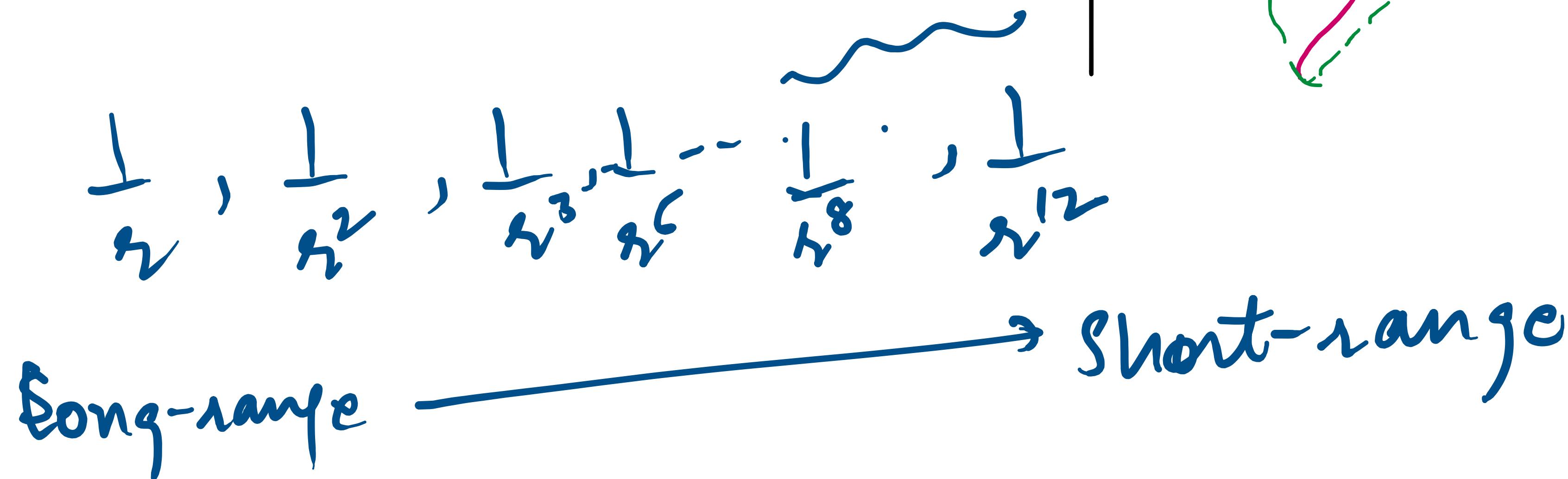
"Fluctuation" in charge distribution
repulsion attraction

General functional form of the van der Waals energy

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

Lennard-Jones Potential

- Weak interactions
- Ubiquitous in nature
- Non-directional bonding



$$\frac{1}{r^{12}}$$

$$-\frac{1}{r^6}$$

