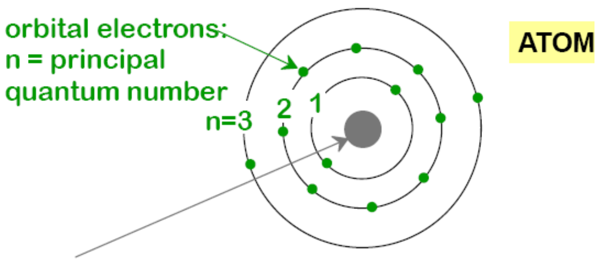
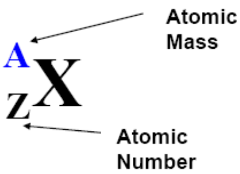
Atomic structure



Nucleus (Proton + Neutron):
• Z (atomic number) = # protons
[1 for hydrogen to 94 for plutonium]
• N = # neutrons
Atomic mass (A) ≈ Z + N

The mass and charge of Proton, Neutron, and Electron

	Mass (g)	Charge (C)
Proton	1.673×10^{-24}	$+1.602 \times 10^{-19}$
Neutron	1.675×10^{-24}	0
Electron	9.109×10^{-28}	-1.602×10^{-19}

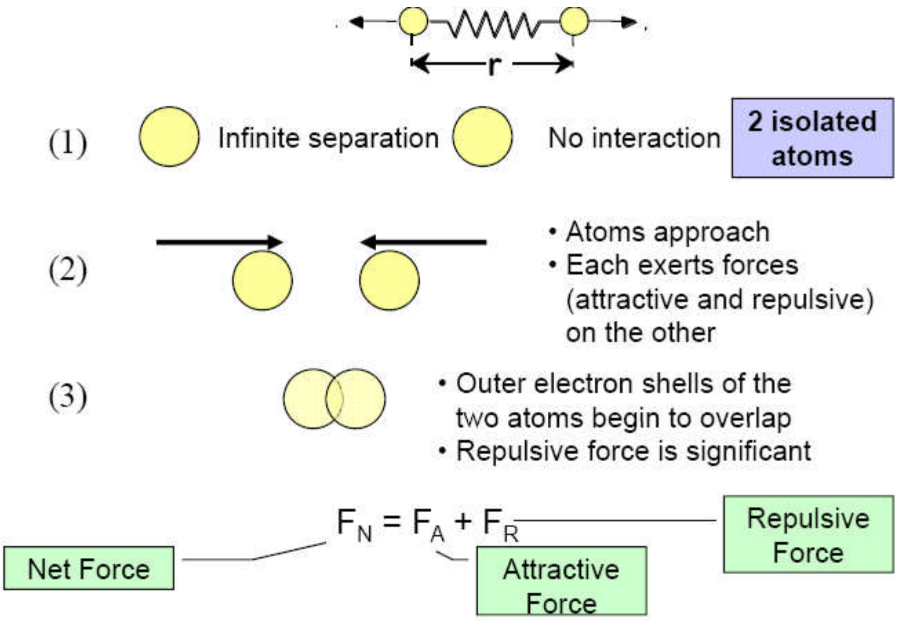


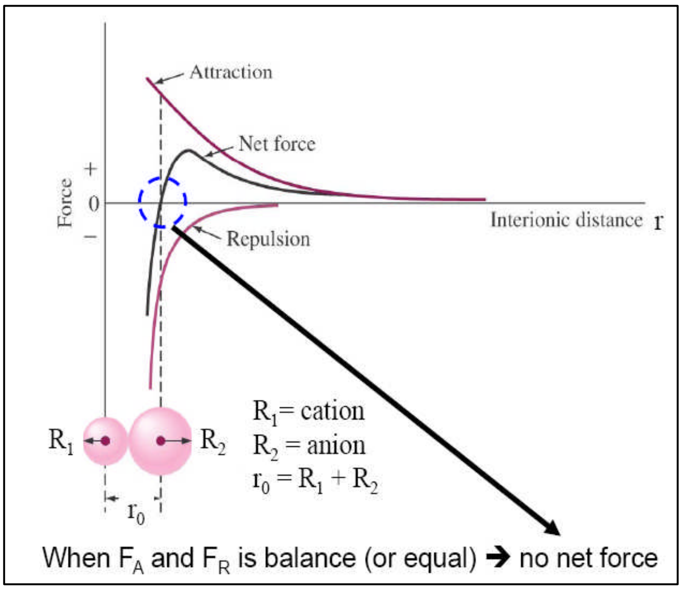
Bonding Forces & Energies

- The nature of various states of matter (except plasma) can be explained by using atomic forces (bonding forces) and potential energy of interatomic distance.
- There are 2 forces (attractive and repulsive) that act on a collection of atoms, depending on the relative distances between various atoms.
- Attractive forces acting on atoms ⟶ pull them together (would they collide?).
- Repulsive forces (short range force) acting between nuclei and electrons of individual atoms.

Forces between 2 atoms

Bond length, r, = interatomic distance





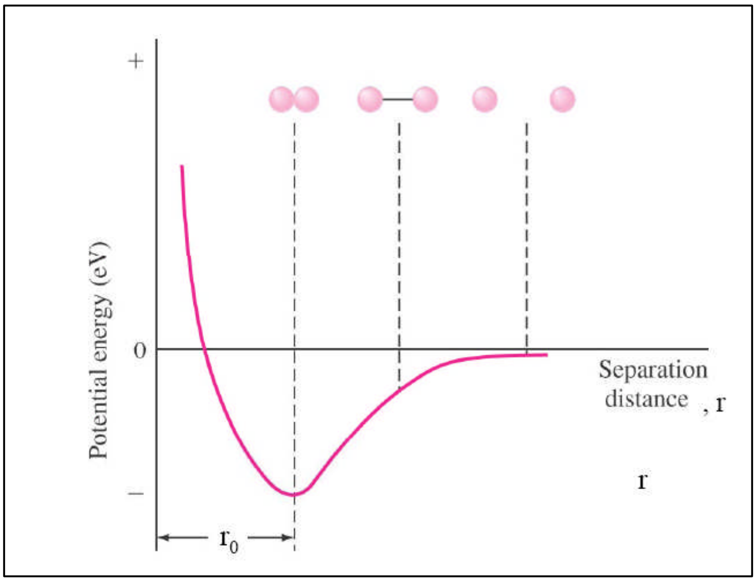
Energy (E) ←→ Force (F)

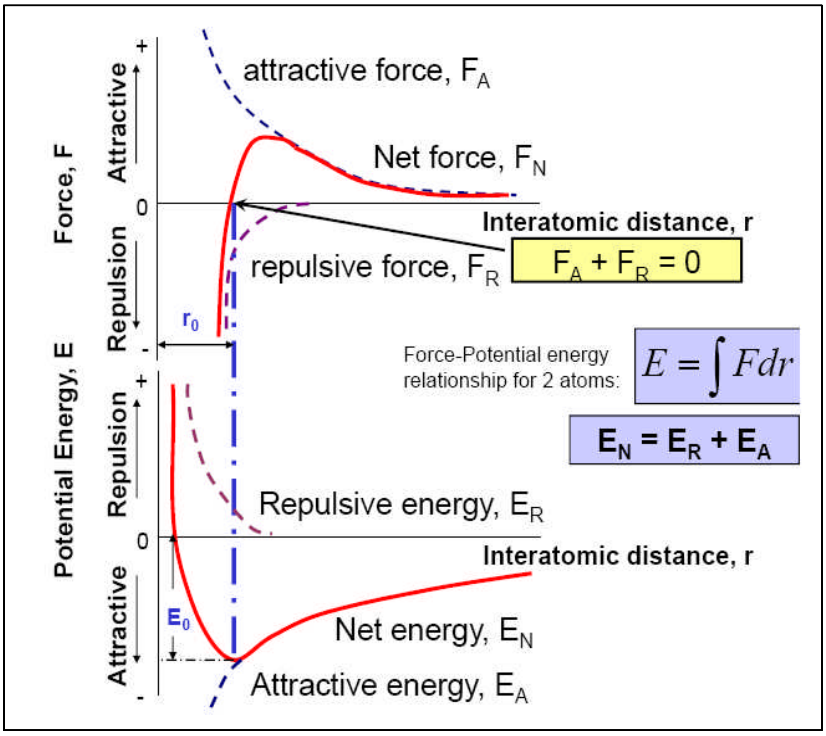
$$E = \int F dr$$

$$E_{net} = \int_{\infty}^{r} F_{net} dr$$

$$E_{net} = \int_{\infty}^{r} F_A dr + \int_{\infty}^{r} F_R dr$$

$$E_{net} = E_A + E_R$$





Interatomic Bonds

Primary bonding

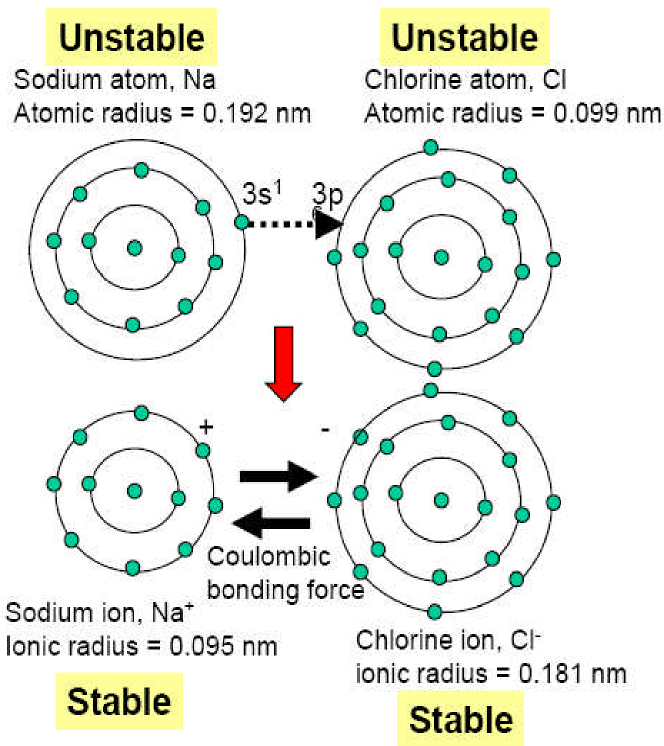
- Ionic
- Covalent
- Metallic

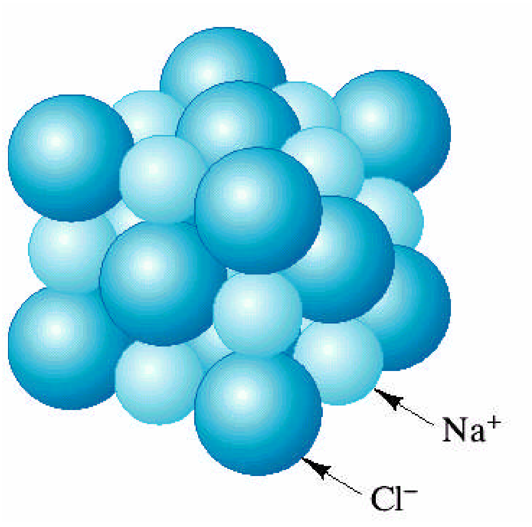
Secondary Bonding

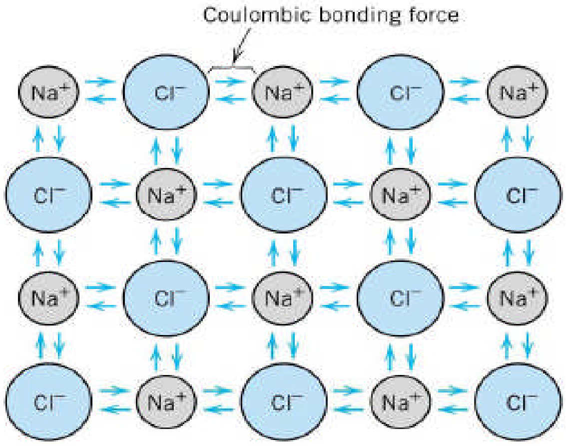
- Van der Waals bonds

Ionic Bonding

- Formed between highly electropositive (metallic) elements and highly electronegative (nonmetallic) elements → large difference in electronegativity.
- Ionization: electrons are transferred from atoms of electropositive elements to atoms of electronegative elements, producing positively charged cations and negatively charge anions.
- Ionic bonding: due to **electrostatic** or **Coulombic force** attraction of oppositely charged ions.
- **Nondirectional bonding** → magnitude of the bond is equal in all directions around an ion.
- **Binding energy** → large → high melting temp.
- Ionic material → hard, brittle, electrically and thermally insulative







Schematic representation of ionic bonding in sodium chloride(NaCl)

Covalent Bonding

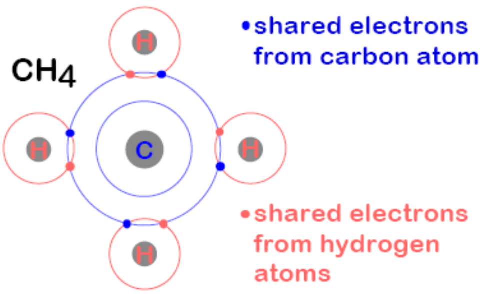
- In covalent bonding stable electron configurations are assumed by **sharing of electrons** between adjacent atoms.
- Two atoms that are covalently bonded will each contribute at least one electron to the bond, and the shared electrons may be considered to belong to both atoms.

- **Example: CH_4**

  C: has 4 valence e, needs 4 more

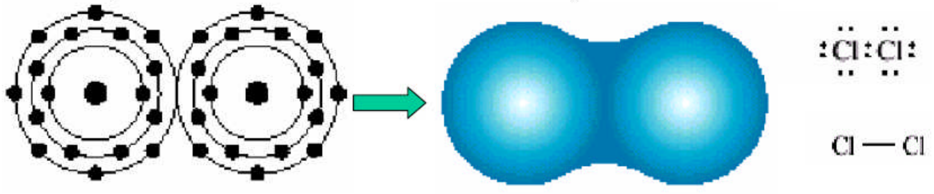
  H: has 1 valence e, needs 1 more

  Electronegativities are comparable.



- Many nonmetallic elemental molecules (H_2, Cl_2, F_2, etc)
- Molecules containing dissimilar atoms (CH_4, H_2O, HNO_3, HF, etc)
- Other elemental solids: diamond (carbon), silicon, germanium
- Other solid compounds composed (GaAs, InSb, SiC)
- Number of covalent bonds in an atom is determined by number of **valence electron**.
- N' valence electron ⟶ an atom can covalently bond with at most **8-N'** other atoms

Example: Cl_2 molecule. Z_{Cl} =17 ($1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^5$)
N' = 7, 8 - N' = 1 $\rightarrow$ can form only one covalent bond



- **Highly directional type of bonding**.
- Binding energy & melting temp for covalently bonded materials ⟶ very high (diamond) to very weak (bismuth, polymeric material)
- Very few compounds exhibit pure covalent bonding (or ionic bonding).
- Possible of having interatomic bonds (partially ionic and partially covalent).

Metallic Bonding

Valence electrons are detached from atoms, and spread in an 'electron sea' that "glues" the positive ions together.

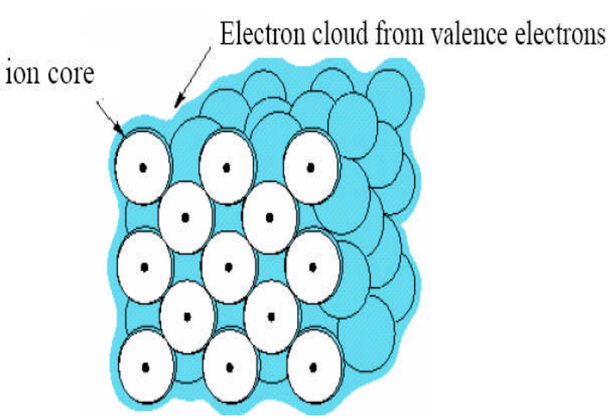
• A metallic bond is **non-directional** (bonds form in any direction) → atoms pack closely

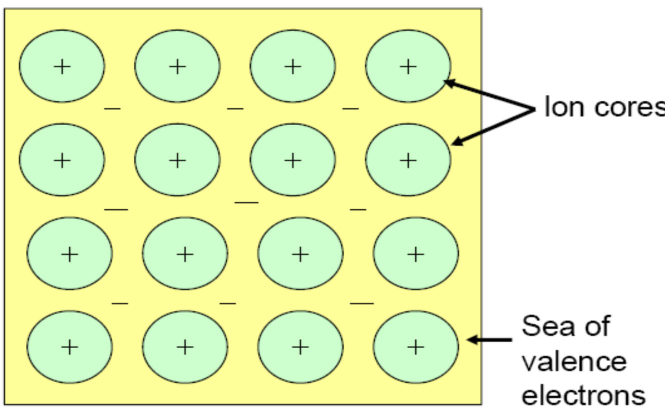
• The "bonds" do not "break" when atoms are rearranged – metals can experience a significant degree of plastic deformation.

• Binding energy & melting temp (wide range)

• All elemental metals, highly conductive, Ductile.

• Examples of typical metallic bonding: Cu, Al, Au, Ag, etc. Transition metals (Fe, Ni, etc.) form mixed bonds that are comprising of metallic bonds and covalent bonds involving their 3d-electrons. As a result the transition metals are more brittle (less ductile) that Au or Cu.





Schematic illustration of metallic bonding

Secondary Bonds

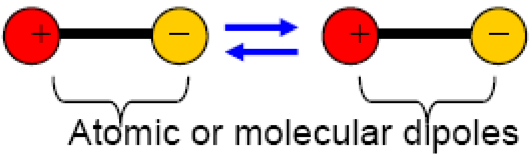
Van der Waals Bonds

- Van der Waals bond or physical bond
- Exist between virtually all atoms or molecules.
- The presence of any of the 3 primary bonding types may obscure it.
- This force arises from atomic or molecular dipoles → electric dipoles.
- Electric dipoles

  → Separation of positive and negative portions of an atom or molecule

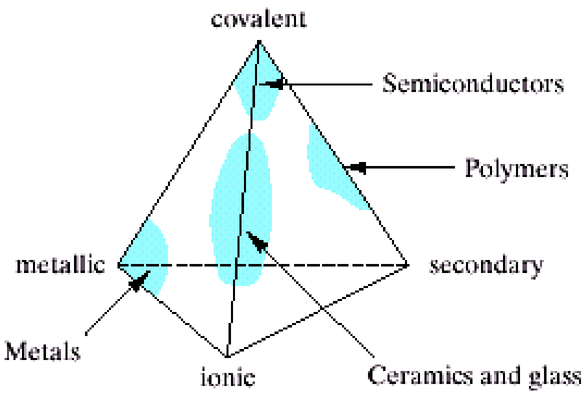
  → Coulombic attraction between +ve end of one dipole and –ve end dipole.

Schematic illustration of van der Waals bonding between two dipoles



Bonding in real materials

In many materials more than one type of bonding is involved (ionic and covalent in ceramics, covalent and secondary in polymers, covalent and ionic in semiconductors.



Correlation between bonding energy and melting temperature

Bonding Type	Substance	Bonding Energy		Melting Temperature (°C)
		kJ/mol	eV/atom, ion, molecule	
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covelent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
Metallic	Hg	68	0.7	-39
	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
Van der Waals	Ar	7.7	0.08	-189
	Cl_2	31	0.32	-101
Hydrogen	NH_3	35	0.36	-78
	H_2O	51	0.52	0

Summary

Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional semiconductors, ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular