- In terms of potential energy, where:

$$E = \int F dr$$

$$E_N = \int_{\infty}^{r} F_N dr$$

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

$$= E_A + E_R$$

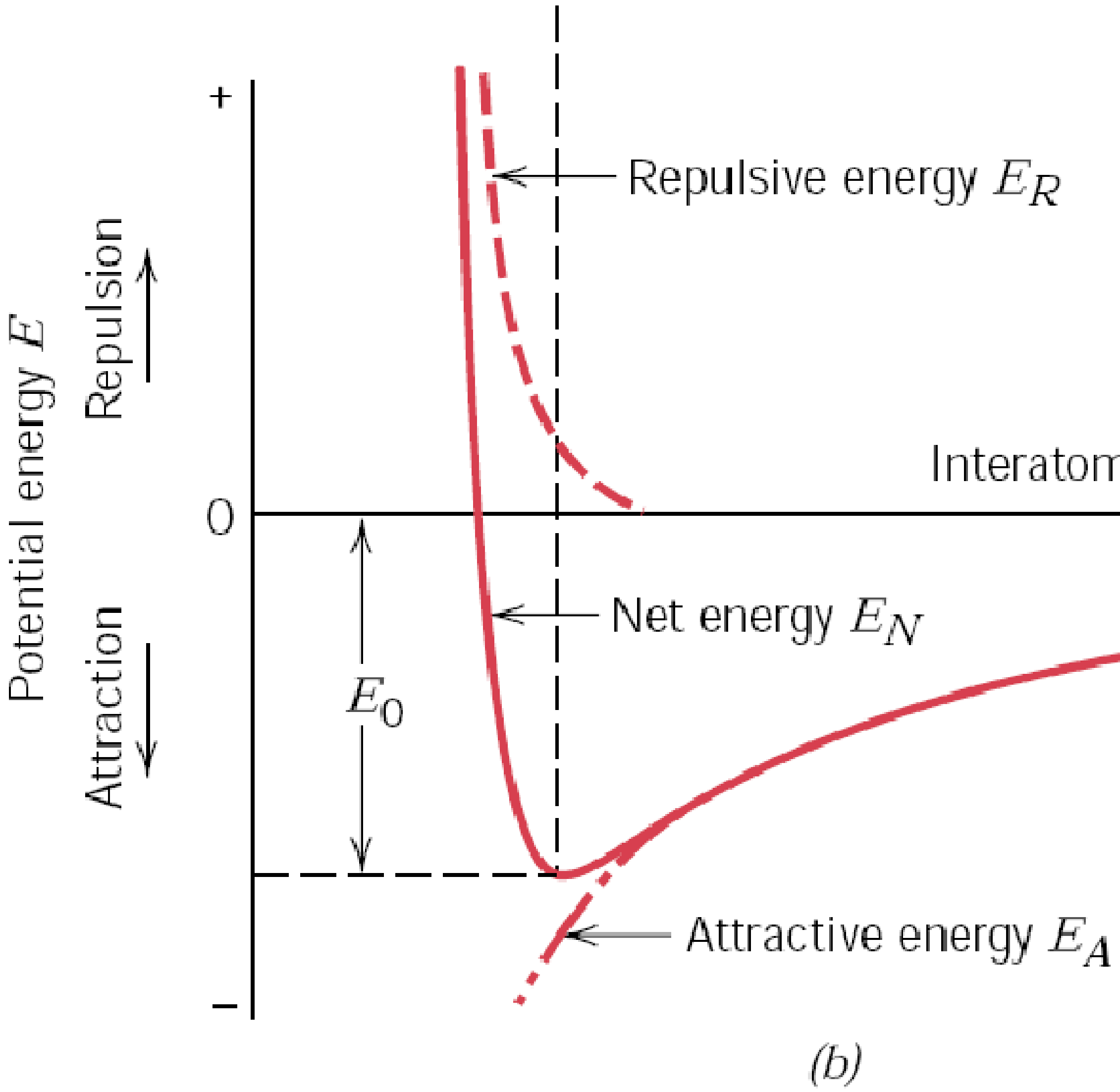
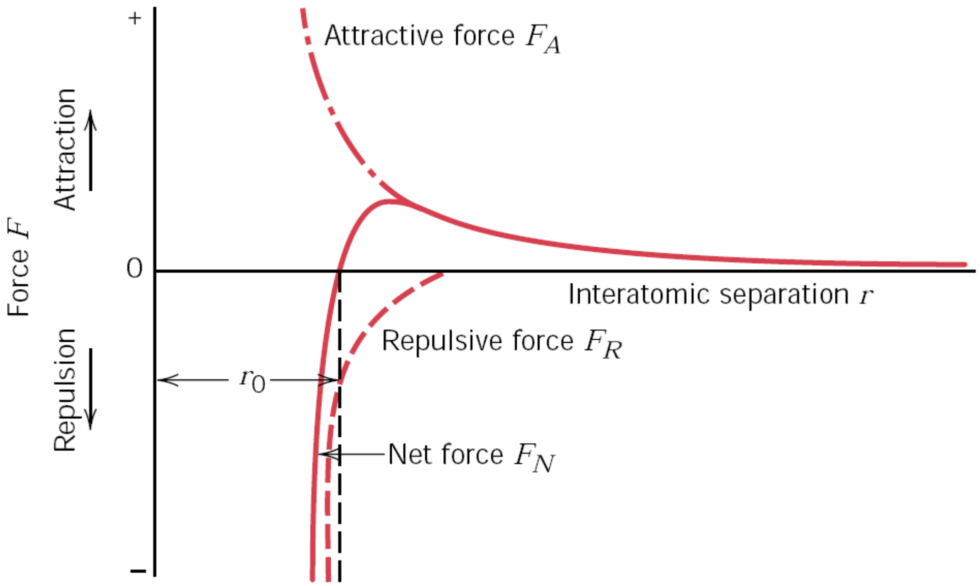


FIGURE 2.8 (*a*) The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms. (*b*) The dependence of repulsive, attractive, and net potential energies on interatomic separation for two isolated atoms.

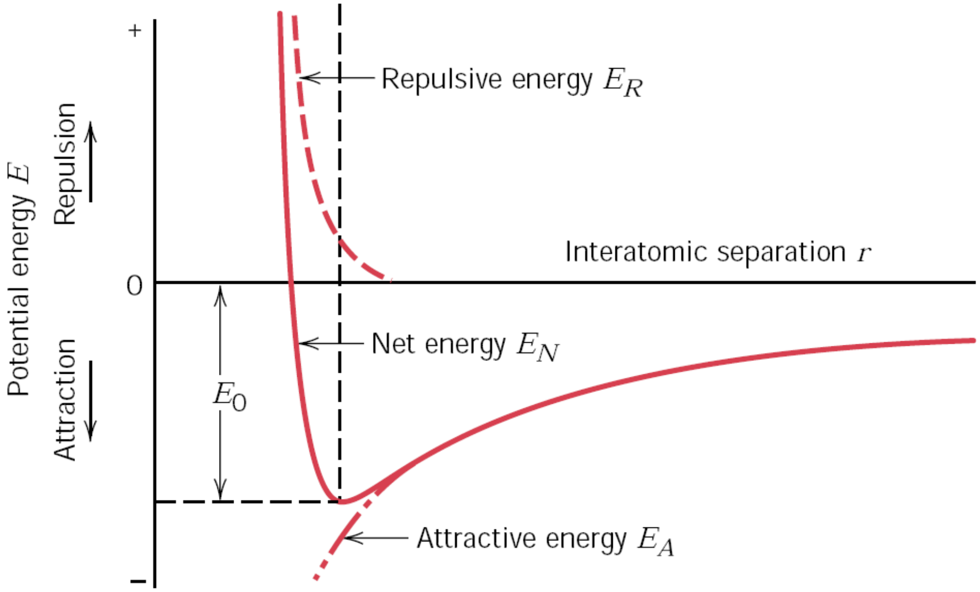
- Looking at the graph, r_0 corresponds to the minimum of the potential energy curve.
- The bonding energy for these two atoms, E_0, corresponds to the energy at this minimum point; it represents the energy that would be required to separate these two atoms to an infinite separation.
- This is an ideal situation between two atoms, in reality the condition is more complex with more than two atoms interacting with each other.
- Bonding energy and the shape of the energy curve is different from material to material.
- Material properties depends on E_0 e.g. melting temperature

Force vs. Separation Distance



(a)

Energy vs. Separation Distance



(b)

Categories of material bonds

Primary bonds:

1. Ionic bond
2. Covalent bond
3. Metallic bond

Secondary bonds, between:

1. Induced dipoles
2. Induced dipoles and polar molecules
3. Polar molecules (permanent bonds)
    - Hydrogen bonding

Ionic bonding

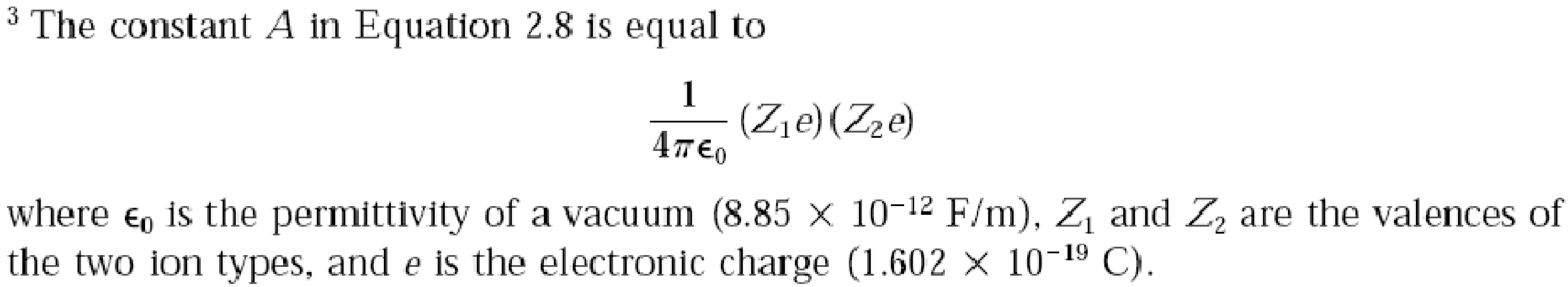
- Compounds composed of metallic and non metallic elements.
- Metallic atoms gives up valence electrons to non-metallic atoms.
- All atoms acquire stable electron configuration and an electric charge – they become ions.
- The attractive bonding force between positive and negative atoms are called coulombic force.
- For two isolated atoms, the attractive energy is given by the following equations respectively:

$$E_A = -\frac{A}{r} \qquad E_R = \frac{B}{r^n}$$

The value of n is approximately 8

Ionic bonding (cont.)

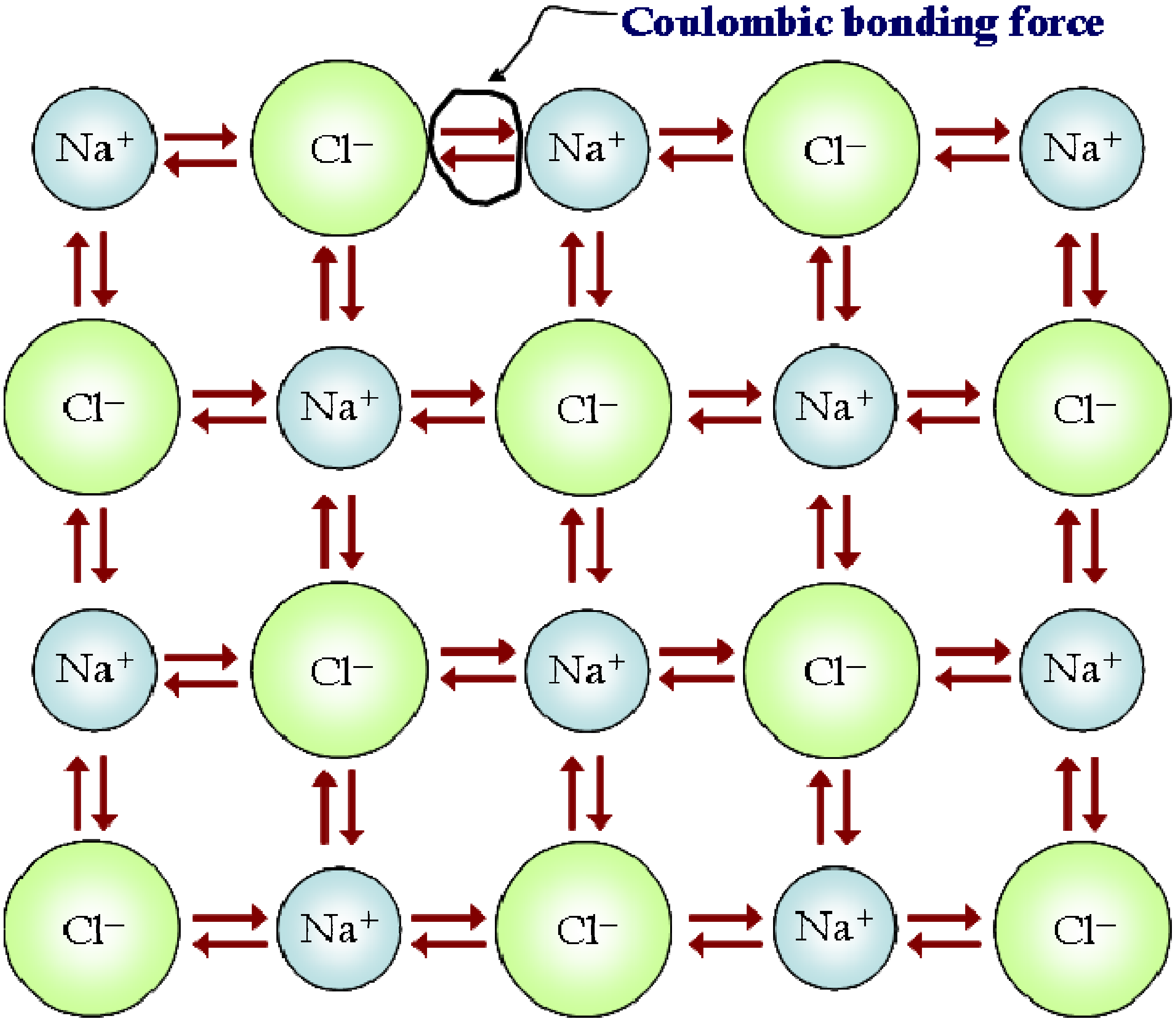
- Bonding energies generally range from 600 and 1500 kJ/mol (3 and 8 eV/atom) are relatively large, as reflected in high melting temperatures.
- Ionic material are hard and brittle and, they are good electrically and thermally insulation.
- Ceramics are mostly ionic.
- Magnitude of the bond is equal in all directions – they are non-directional.



[3] The constant A in Equation 2.8 is equal to

$$\frac{1}{4\pi\epsilon_0}(Z_1 e)(Z_2 e)$$

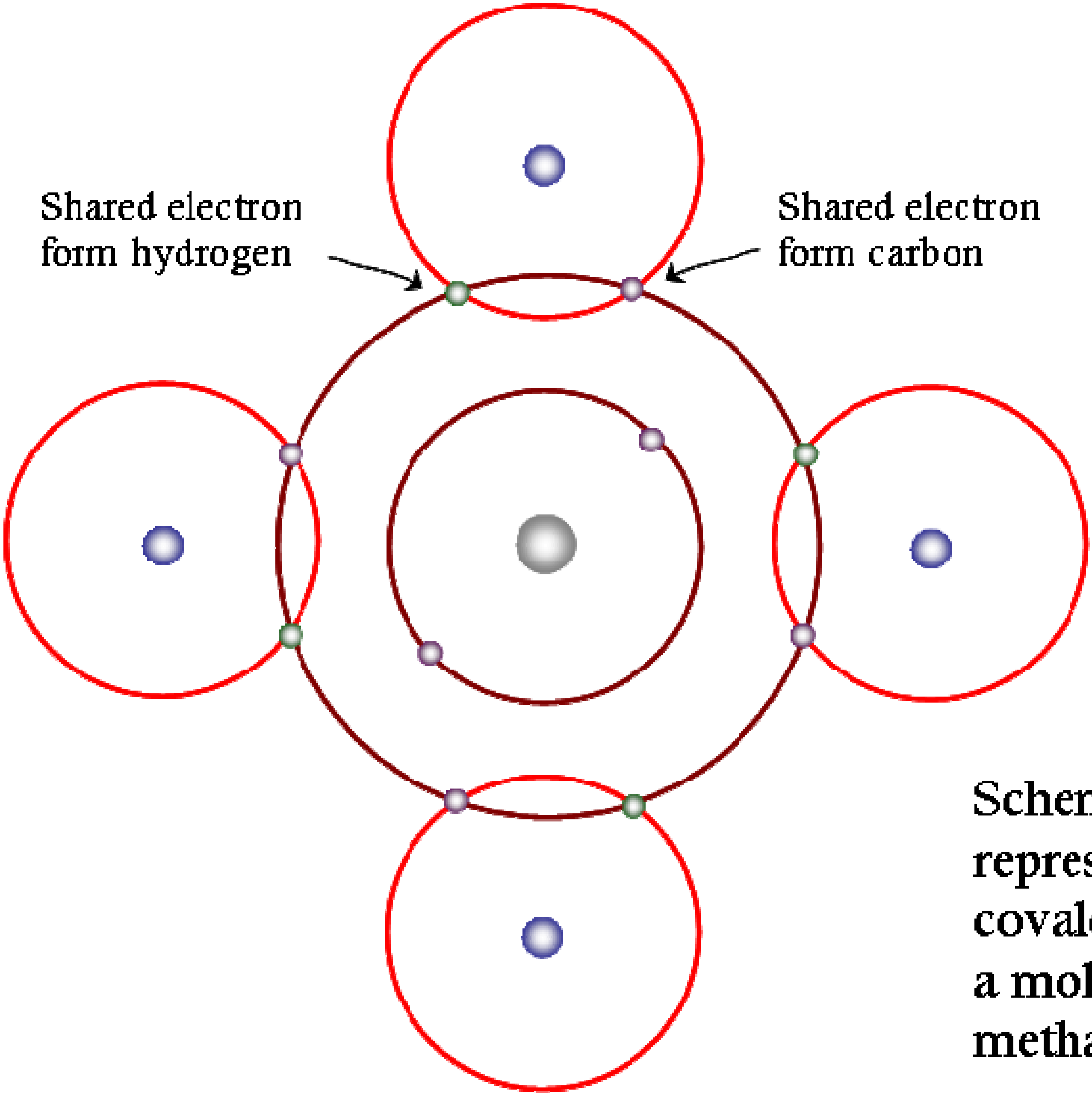
where ϵ_0 is the permittivity of a vacuum (8.85×10^{-12} F/m), Z_1 and Z_2 are the valences of the two ion types, and e is the electronic charge (1.602×10^{-19} C).



Schematic representation of ionic bonding in sodium chloride (NaCl)

Covalent bonding

- Stable electron configurations are assumed by the sharing of electrons between adjacent atoms.
- Covalent bonds are directional according to the atom it is sharing with.
- The number of covalent bonds possible for an atom depends on the number of valence electron *N’* i.e. an atom can covalently bond with at most 8 - *N’* other atoms.
- Covalent bonds can be very strong as in diamond which is very hard and has a high melting point > 3550°C or it can be very week.
- Polymeric materials are covalent bonded.
- Most compounds are partially ionic and partially covalent
- The wider their separation (the greater the difference in electronegativity) in the periodic table the more ionic the bonds.



Shared electron
form hydrogen

Shared electron
form carbon

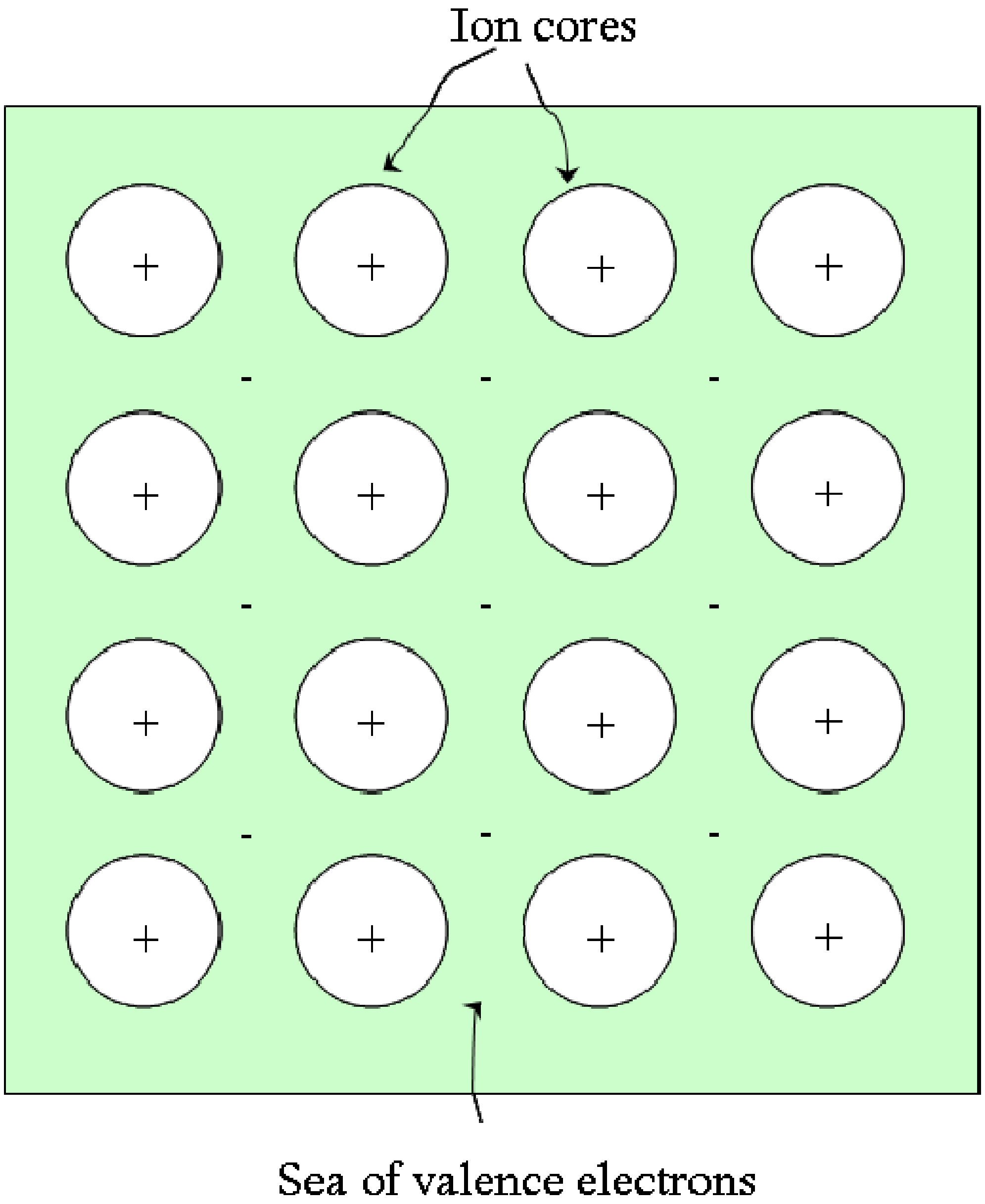
Schematic representation of covalent bonding in a molecule of methane (CH_4)

Metallic bonding

- Metallic bonding is primarily found in metals and their alloys.
- Metallic atoms have at most 3 valence electrons and these electrons are free to drift throughout the entire metal.
- The valence electron belongs to the metal as a whole forming a “sea of electrons”.
- The remaining non valence electrons and the atomic nuclei form ion cores, which are positively charged.
- The sea of electrons act as glue to hold the ion cores together and shield the positively charged ion cores from mutually repulsive electrostatic forces.
- Metallic bonds may be strong or weak with energies ranging from 68 kJ/mole (0.7 eV/atom) to 850 kJ/mole (8.8 eV/atom)

Metallic bonding cont…

- Metals are good conductors of electricity and heat (as a consequence of their free electrons).
- Metals are ductile as compared to ionic materials which are brittle.



Schematic illustration of metallic bonding

Secondary or van der Waals bonding

- Secondary bonds are weaker bonds compared to permanent bonds.
- They exist between all atoms or molecules.
- Evidence of secondary bonds are bonds between inert gases and molecules of covalent bonds.
- It has very small bonding energy however, permanent dipoles have greater energies than induced dipoles.
- Secondary bonding attraction depends on uneven distribution of positive and negative charge – referred to as dipole.

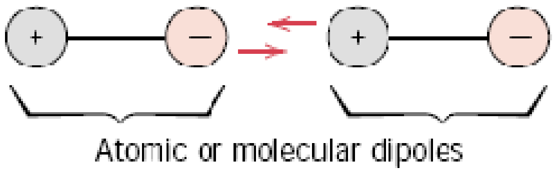


FIGURE 2.12 Schematic illustration of van der Waals bonding between two dipoles.

Secondary bonds cont…

- Secondary bonds exist between
  - Fluctuating induced dipole bonds
  - Induced dipoles and polar molecules
  - Polar molecules (permanent bonds)
  - Hydrogen bonding

Fluctuating induced dipole bonds

- A dipole may be created or induced in an atom or molecule that is normally electrically symmetric.

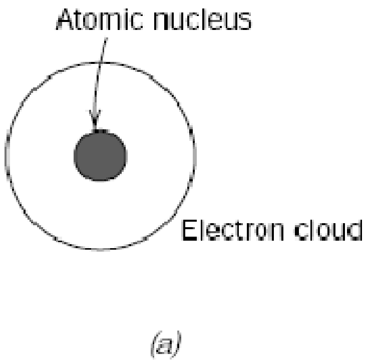


FIGURE 2.13 Schematic representations of (*a*) an electrically symmetric atom and (*b*) an induced atomic dipole.

- All atoms experience constant vibrational motion that can cause a short-lived distortion of this electrical symmetry for some atoms or molecules. Hence a small electric dipole is created

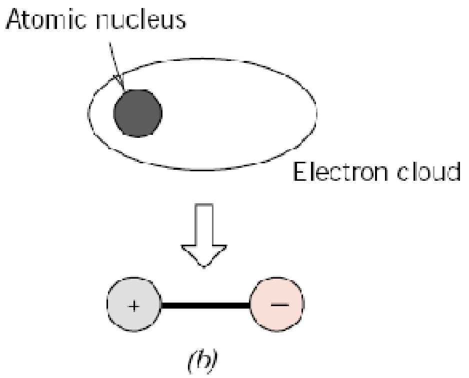


FIGURE 2.13 Schematic representations of (*a*) an electrically symmetric atom and (*b*) an induced atomic dipole.

- The induced dipole above will turn a neighbouring atom or molecule into a dipole. Causing them to attract one another and bond.
- These attractive forces exist between large amounts of atoms and molecules and these forces are temporary and fluctuate with time.
- These bonds are weak hence materials where these bonds are predominant have low melting and boiling points.

Polar molecule – Induced Dipole Bonds

- Permanent dipoles or polar molecules exist in some molecules due to its inter-molecular arrangement.

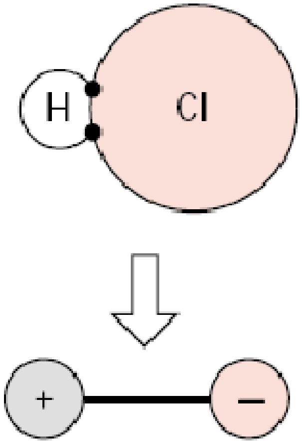


FIGURE 2.14 Schematic representation of a polar hydrogen chloride (HCl) molecule.

- Polar molecules can also induce adjacent non-polar molecules and bond.
- The magnitude of these bonds are great than for fluctuating induced dipoles.

Permanent dipole bonds

- Van der Waals force can also exist between adjacent polar molecules.
- Hydrogen bond is a special case of permanent dipole bonds
  - It occurs between molecules in which hydrogen in covalently bonded to fluorine (HF), oxygen (H_2O), and nitrogen (NH_3)
  - The magnitude of a hydrogen bond is greater than other secondary bonds.

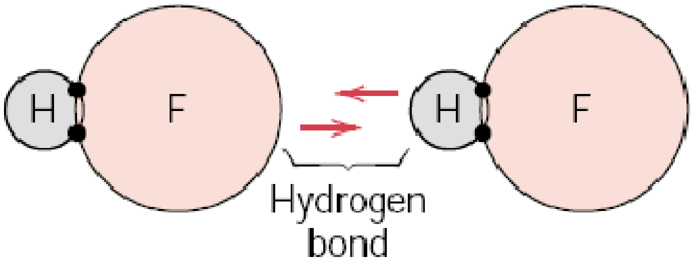


FIGURE 2.15 Schematic representation of hydrogen bonding in hydrogen fluoride (HF).

Bonding Energies and Melting Temperature for Various Substances

Bonding Type	Substance	Bonding Energy		Melting Temperature (°C)
		kJ/mol	eV/Atom, Ion, Molecule	
Ionic	NaCl	640	3.3	801
	MgO	1,000	5.2	2,800
Covalent	Si	450	4.7	1,410
	C (diamond)	713	7.4	> 3,550
	Hg	68	0.7	-39
Metallic	Al	324	3.4	660
	Fe	406	4.2	1,538
	W	849	8.8	3,410
van der Waals	Ar	7.7	0.08	-189
	Cl_2	31	0.32	-101
Hydrogen	NH_3	35	0.36	-78
	H_20	51	51	0

The End