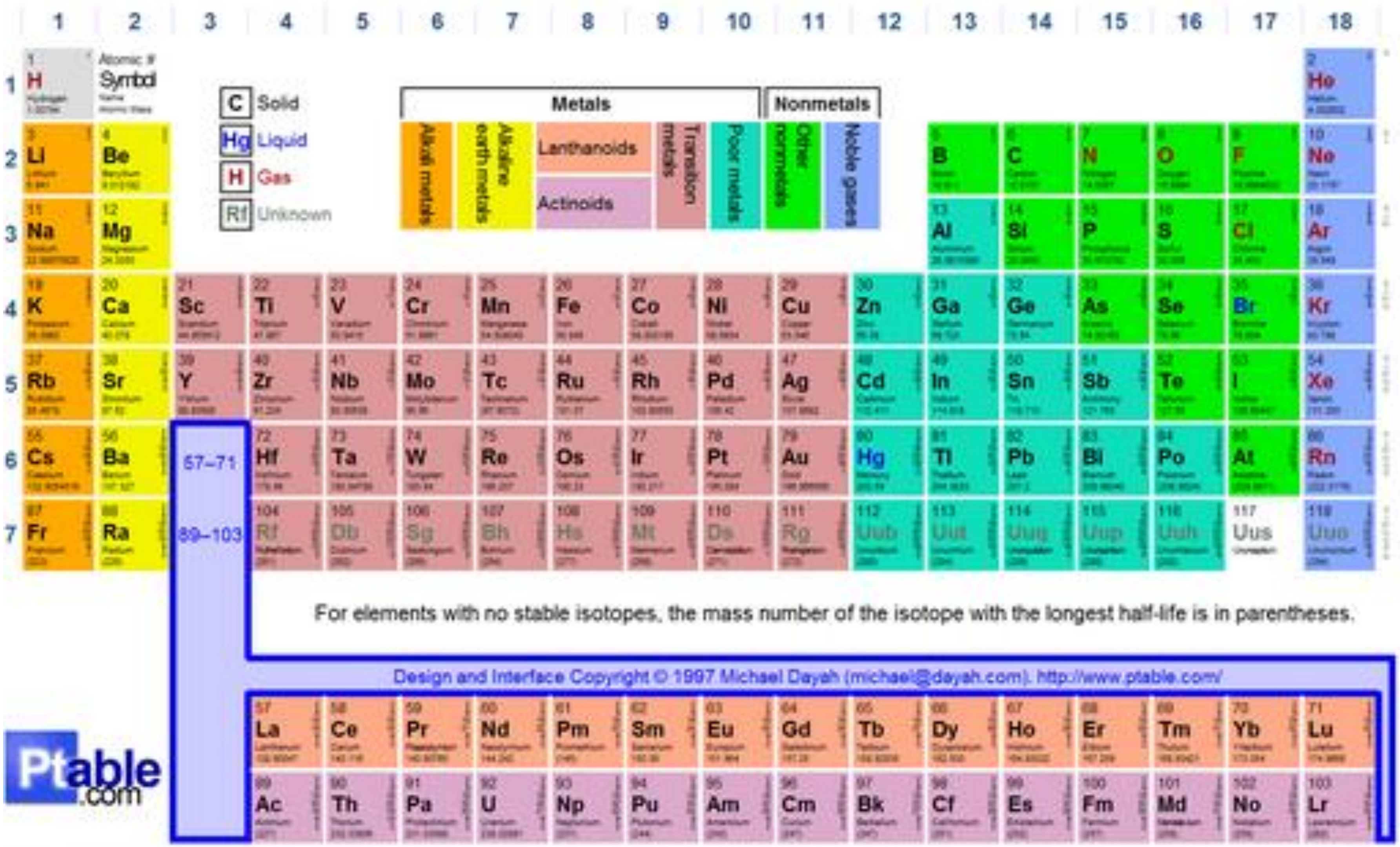
CHEMICAL BONDING

Periodic Table of Elements



Bonding

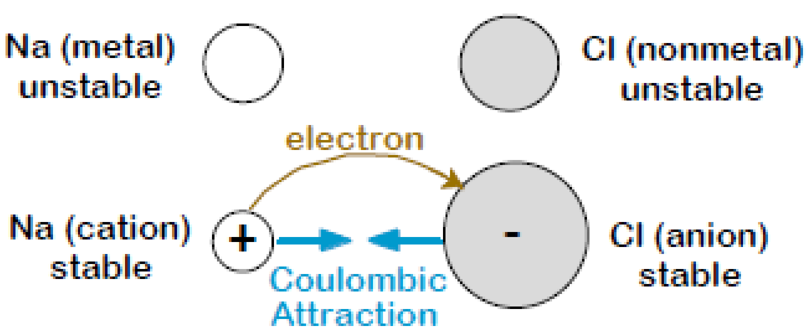
Primary bonding:

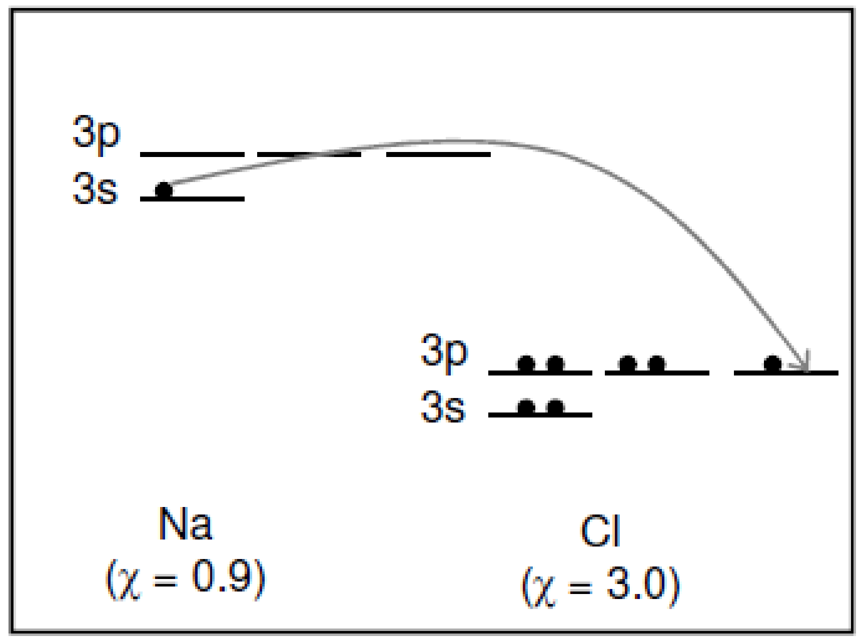
Ionic (transfer of valence electrons)
Covalent (sharing of valence electrons, directional)
Metallic (delocalization of valence electrons)

Secondary or van der Waals Bonding:
(Common, but weaker than primary bonding)
Dipole-dipole
H-bonds
Polar molecule-induced dipole
Fluctuating dipole (weakest)

Ionic Bonding

- Occurs between + and - ions.
- Requires electron transfer.
- Large difference in electronegativity required.
- Example: NaCl
- Nondirectional





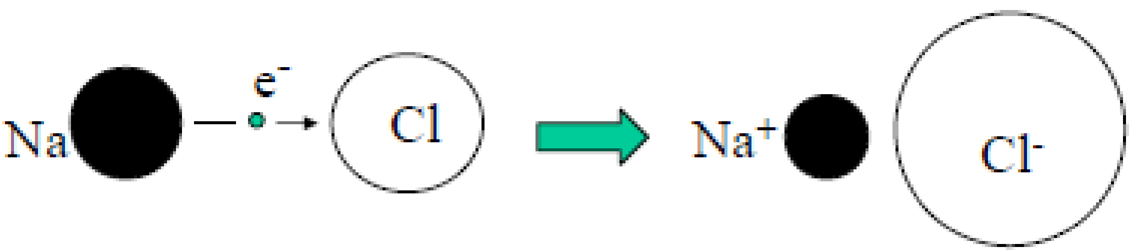
Example: table salt (NaCl)

Na has 11 electrons, 1 more than needed for a full outer shell (Neon)

11 Protons <u>Na</u>	$1S^2\ 2S^2\ 2P^6\ 3S^1$	**donates e^-**
11 Protons <u>Na^+</u>	$1S^2\ 2S^2\ 2P^6$	**10 e^- left**

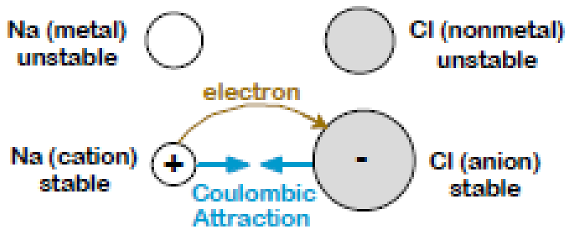
Cl has 17 electron, 1 less than needed for a full outer shell (Argon)

17 Protons <u>Cl</u>	$1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^5$	**receives e^-**
17 Protons <u>Cl^-</u>	$1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^6$	**18 e^-**



- Electron transfer reduces the energy of the system of atoms, that is, electron transfer is energetically favorable
- Note relative sizes of ions: Na shrinks and Cl expands

Ionic Bonding



$$E_A = \frac{z_1 z_2 e^2}{4\pi\varepsilon_o r}$$

Since z_1 = +1 for Na^+ and z_2 = -1 for Cl^-

$$\varepsilon_o = 8.854 \times 10^{-12} \frac{C^2}{N\text{-}m^2}$$

$$E_A = -\frac{e^2}{4\pi\varepsilon_o r} = -\frac{A}{r}$$

Negative energy means attraction only.
Will the atoms collapse on themselves?

No, there is also repulsive energy (e.g. steric repulsion, e-e repulsion)

$$E_R = \frac{B}{r^n}$$

B and *n* depend on atoms involved.
In many cases *n* ~ *8*.

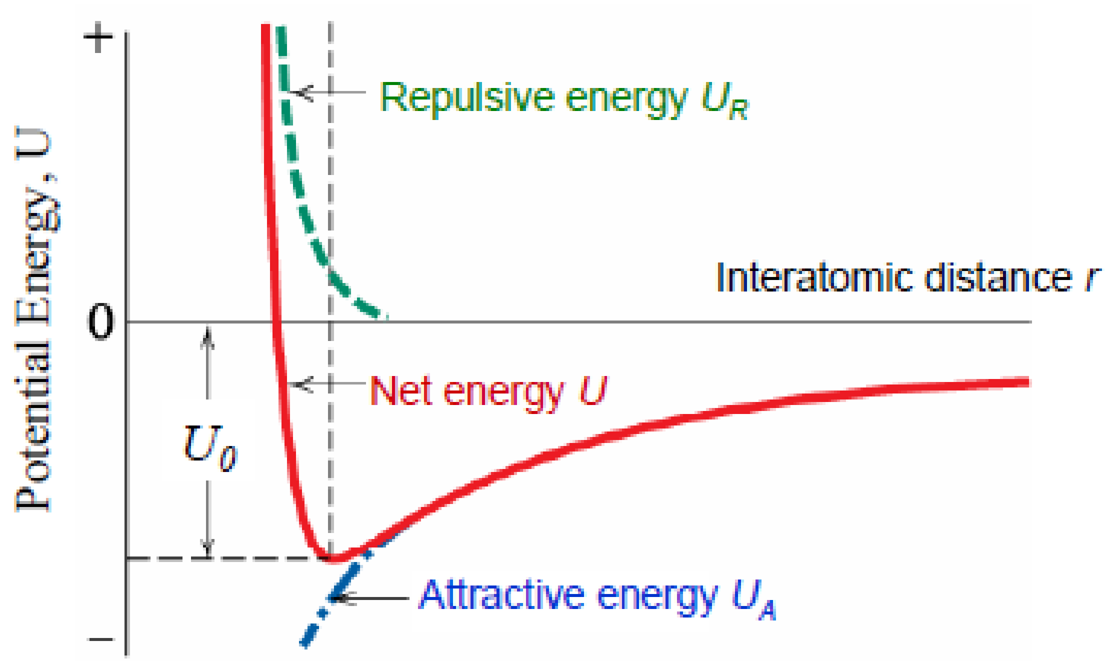
Attractive coulomb interaction between charges of opposite sign:

$$U_A = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r} = -\frac{A}{r}$$

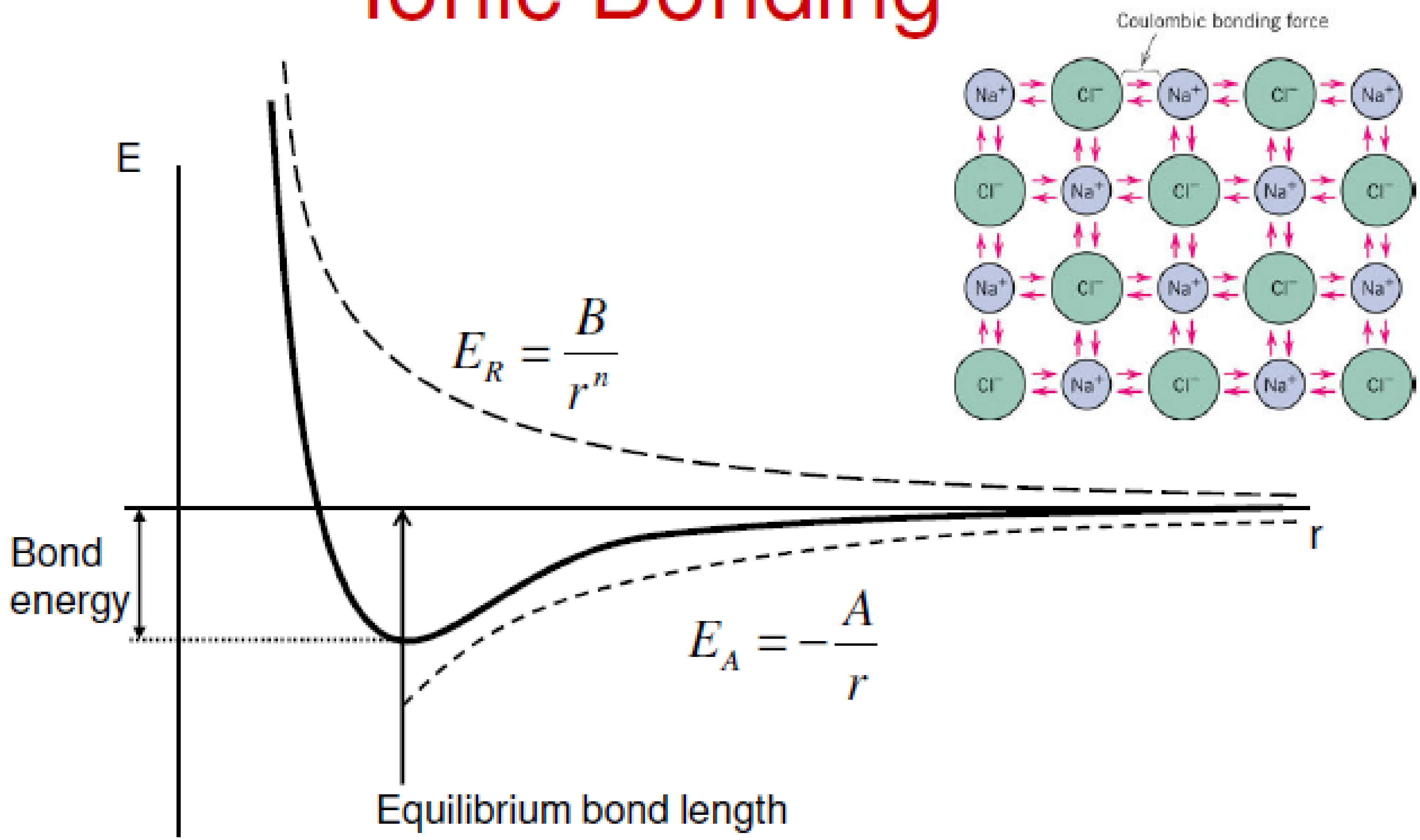
Repulsion due to the overlap of electron clouds at close distances (Pauli principle of QM):

$$U_R = \frac{B}{r^n}$$

$$U = U_A + U_R = -\frac{A}{r} + \frac{B}{r^n}$$



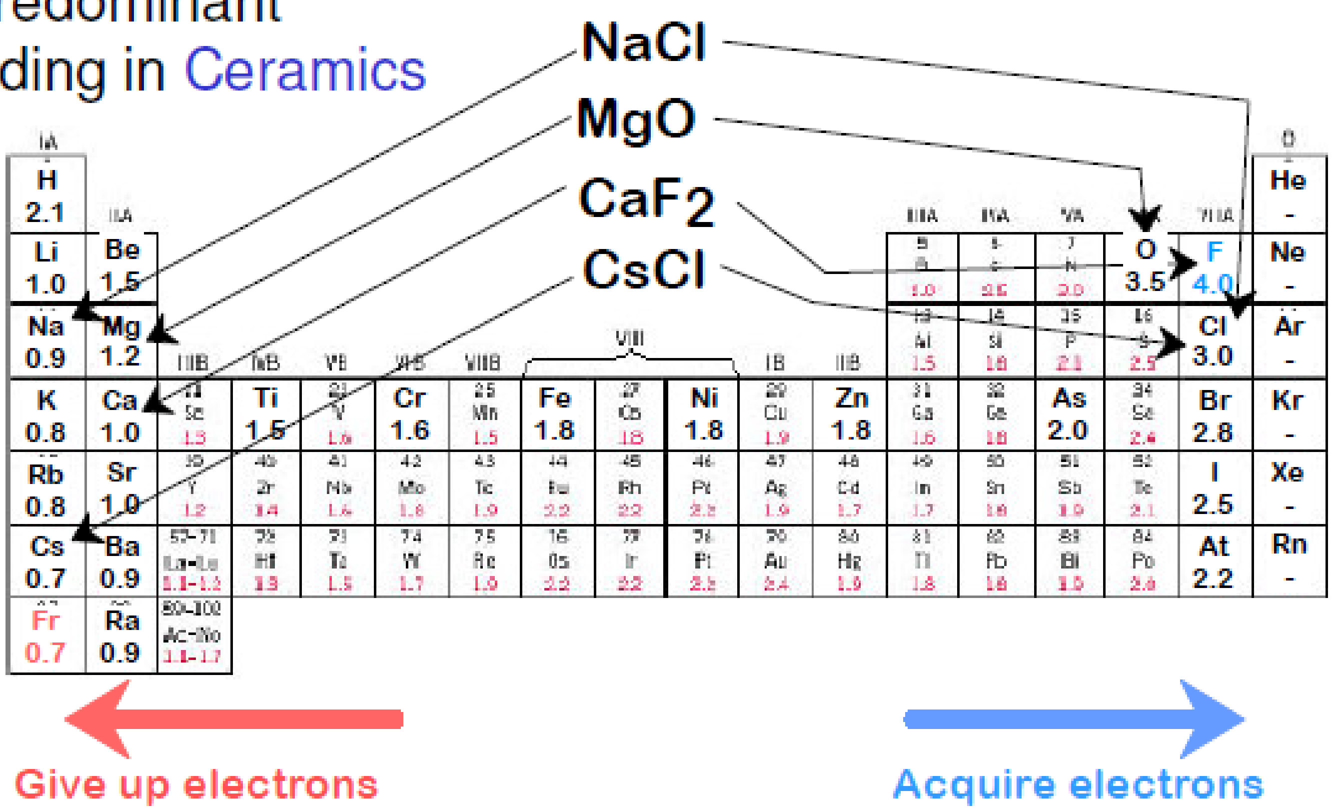
Ionic Bonding



Note: Other types of bonds can also be described in a similar manner

Ionic Bonding: examples

- Predominant bonding in Ceramics



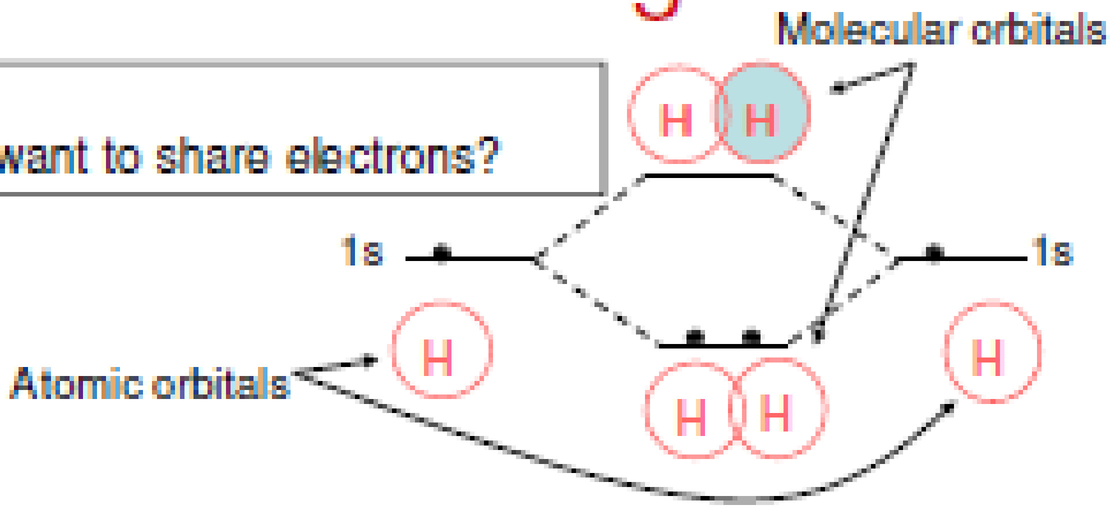
Adapted from Fig. 2.7, *Callister 6e*. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

From Callister 6e resource CD.

Covalent Bonding

- "Sharing" of electrons
- Why do some atoms want to share electrons?

- Example1: H_2

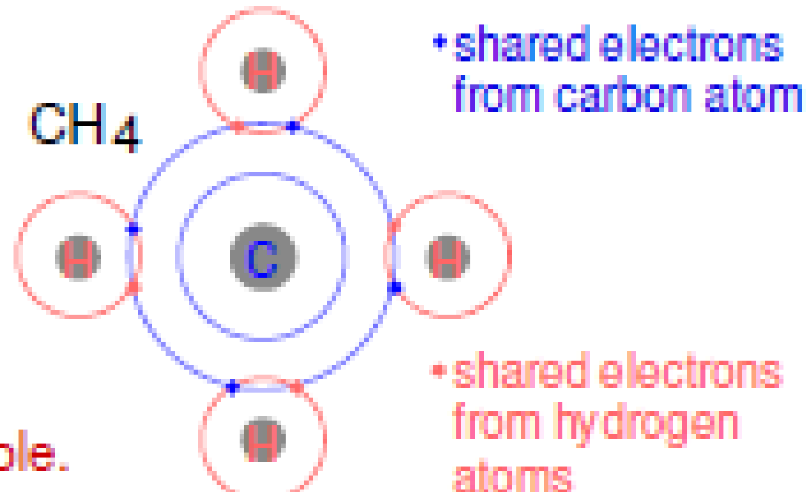


- Example2: CH_4

  C: has 4 valence e,
  needs 4 more

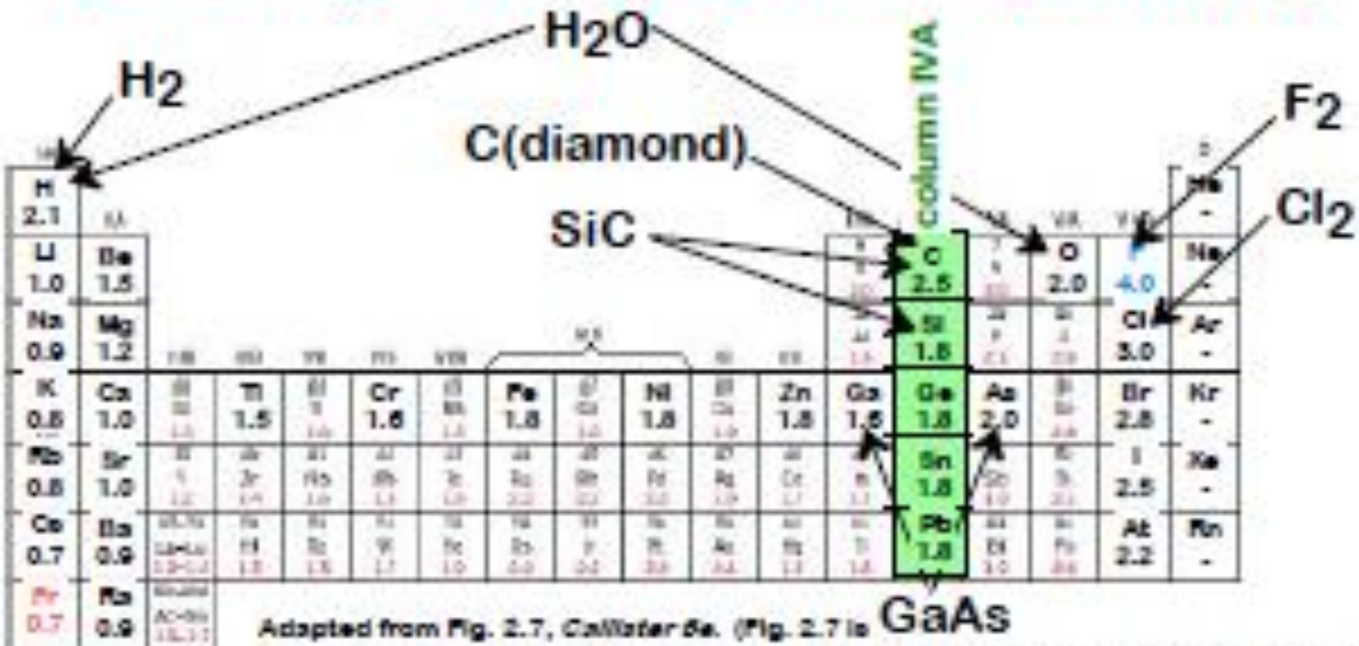
  H: has 1 valence e,
  needs 1 more

  Electronegativities
  are same or comparable.



Adapted from Fig. 2.10, Callister 6e.

Examples: Covalent Bonding



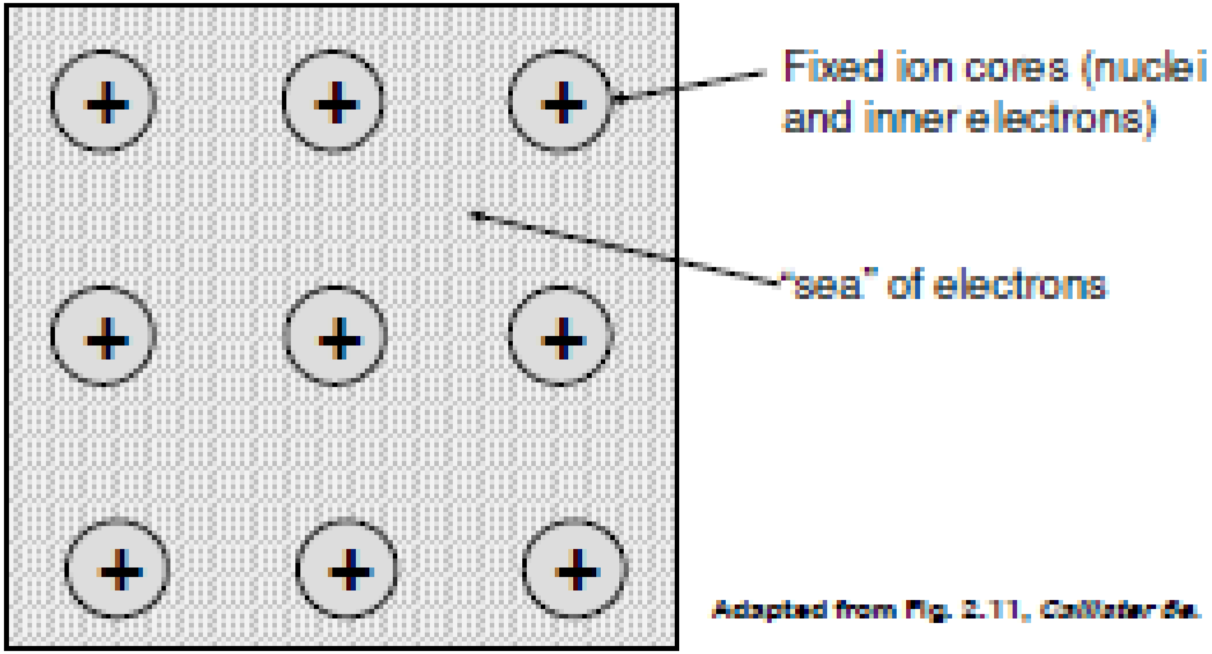
Adapted from Fig. 2.7, *Callister 6e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

From Callister 6e resource CD.

- Molecules with nonmetals
- Molecules with metals and nonmetals
- Elemental solids (RHS of Periodic Table)
- Compound solids (about column IVA)

Metallic Bonding

- Arises from a sea of donated valence electrons



Adapted from Fig. 2.11, *Callister 6e.*

- Primary bond for metals and their alloys.
- Large atomic radius and small IP will more likely lead to metallic bonding.

Metallic Bonding

- Valence electrons are completely delocalized to form an electron cloud, in which positive ionic cores are embedded.

- The remaining nonvalence electrons and atomic nuclei form "ion cores", which posses a net positive charge equal in magnitude to the total valence electron charge per atom.

- The metallic bond is nondirectional.

- Metallic bonding is found in the periodic table for Group IA and IIA elements.

- Electron delocalization is the origin of good electrical and thermal conductivities in metals. (Ionically and covalently bonded materials are typically electrical and thermal insulators, due to the absence of large numbers of free electrons) .

Secondary Bonds: Intermolecular Forces

- **Secondary, Van der Waals, or physical bonds** are weak in comparison to the primary bonds.

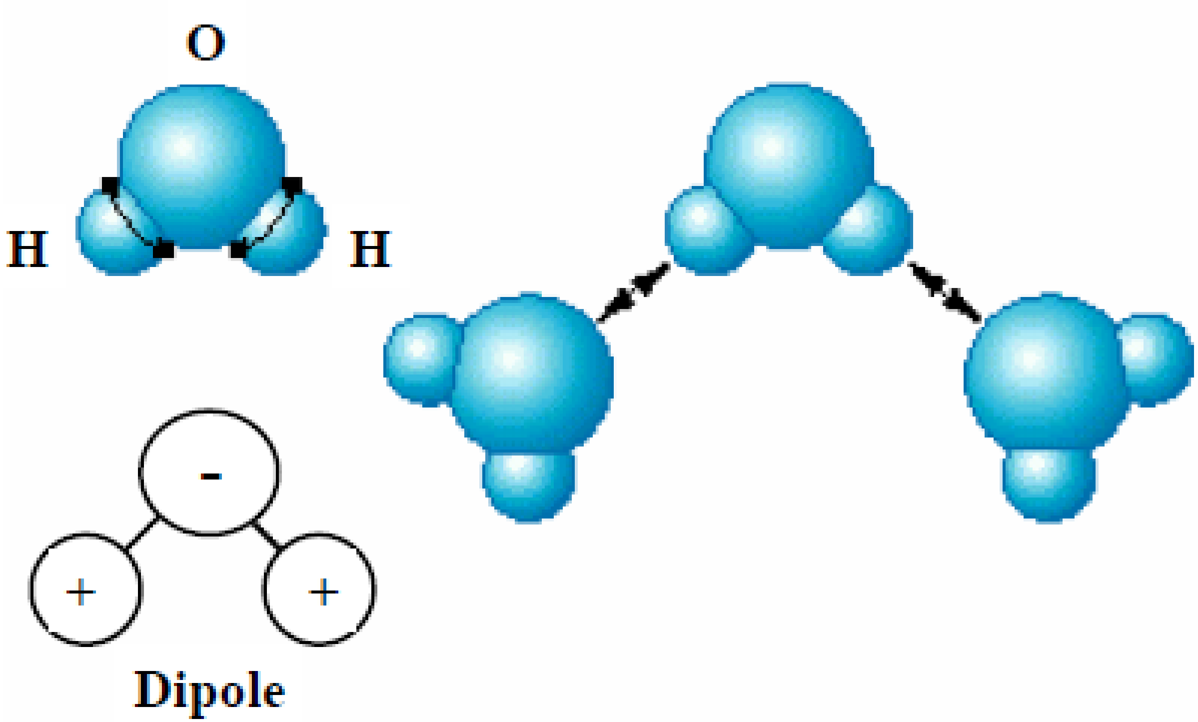
- Secondary bonding exists between virtually all atoms or molecules, but its presence may be obscured if any of the three primary bonding types is present.

- Secondary bonding forces arise from atomic or molecular dipoles. An electric dipole exists whenever there is some separation of positive and negative portions of an atom or molecule.

- Dipole interactions occur between induced dipoles, between induced dipoles and polar molecules (which have permanent dipoles), and between polar molecules.

- Hydrogen bonding, a special type of secondary bonding, is found to exist between some molecules that have hydrogen as one of the constituents.

Example: hydrogen bond in water. The H end of the molecule is positively charged and can bond to the negative side of another H_2O molecule (the O side of the H_2O dipole)



"Hydrogen bond" – secondary bond formed between two **permanent dipoles** in adjacent water molecules.

Secondary Bonds: Intermolecular Forces

- **Dipole-dipole interaction**: secondary bond between molecules with permanent dipole moments

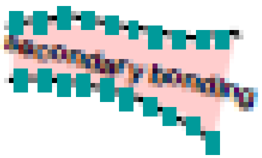
-general case:

Adapted from Fig. 2.14, Callister 6e.

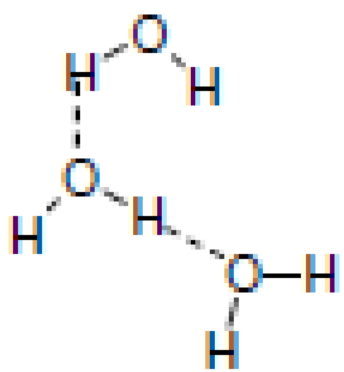
-ex: liquid HCl

Adapted from Fig. 2.14, Callister 6e.

-ex: polymer

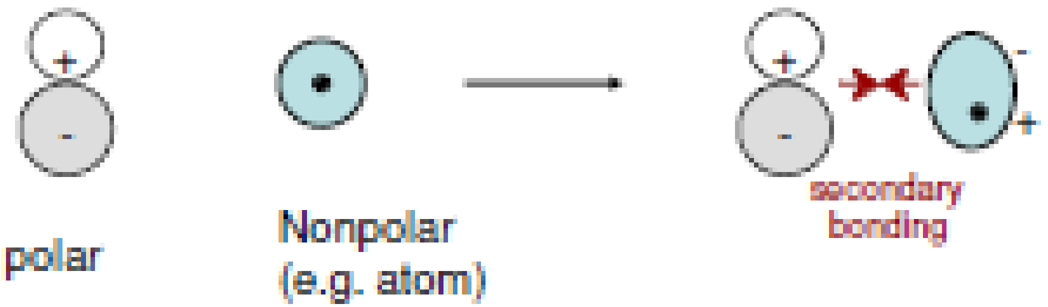


- **Hydrogen bonding**



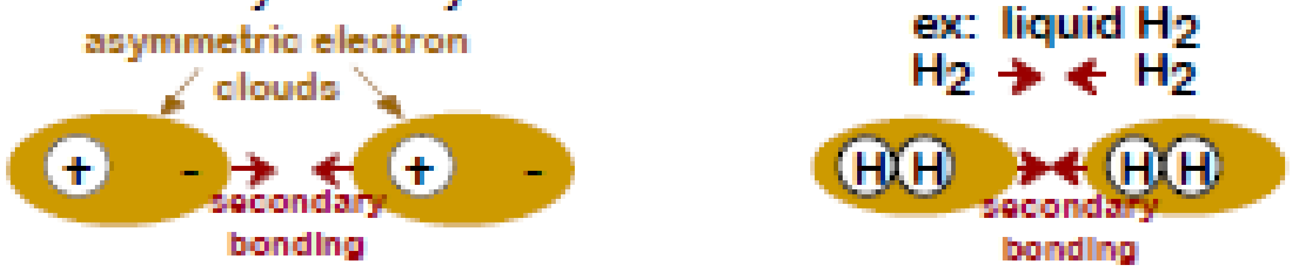
- **Polar molecule-induced dipole interaction:**

  Polar molecules (with asymmetric arrangement of positively and negatively charged regions) can induce dipoles in adjacent nonpolar molecules



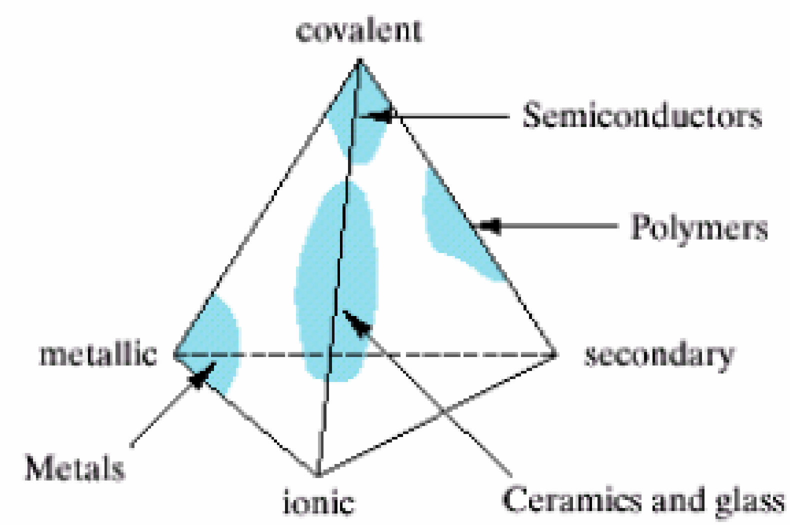
- **Fluctuating dipoles**

  Constant vibrational motion can cause distortions of electrical symmetry



Adapted from Fig. 2.13, Callister 6e.

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.



Examples of bonding in Materials:

Metals: Metallic

Ceramics: Ionic / Covalent

Polymers: Covalent and Secondary

Semiconductors: Covalent or Covalent / Ionic

Bonding Energies and Melting Temperatures for Various Substances

		Bonding Energy		
Bonding Type	***Substance***	***kJ/mol***	***eV/Atom, Ion, Molecule***	***Melting Temperature (°C)***
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covalent	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: BONDING

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