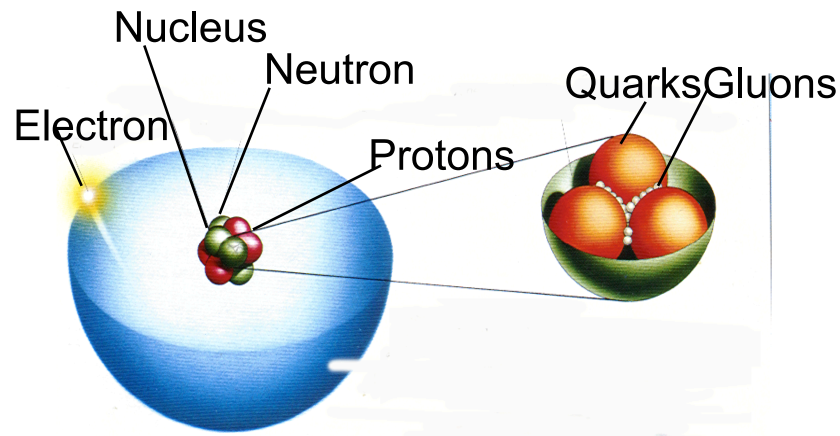
Chapter 2: Atomic structure and interatomic bonding

- Fundamental concepts
- Electrons in atoms
- Periodic table
- Bonding forces and energies

Chapter 2: Atomic structure and interatomic bonding

- Fundamental concepts
  - Proton and electron
    Charge: 1.60×10^{-19} C
  - Mass of electron 9.11×10^{-31} kg
  - Mass of protons and neutrons
    ➡ 1.67×10^{-27} kg
  - Atomic number: the number of protons
  - Atomic mass =protons+neutrons
  - Isotopes
  - Atomic mass unit (amu): 1amu=1/12 C
  - One mole = 6.023×10^{23} atoms (Avogadro's)



Electrons in atoms

- Atomic models
  - Bohr

    electrons revolve around the atomic nucleus in discrete orbitals and the energies of electrons are quantized

  - Wave-mechanical

    electrons exhibits both wavelike and particle-like characteristics, its position is considered to be a probability distribution

Electrons in atoms (*continued*)

- **Comparison of the (a) Bohr and (b) wave -mechanical atom models**

  In terms of electron distribution

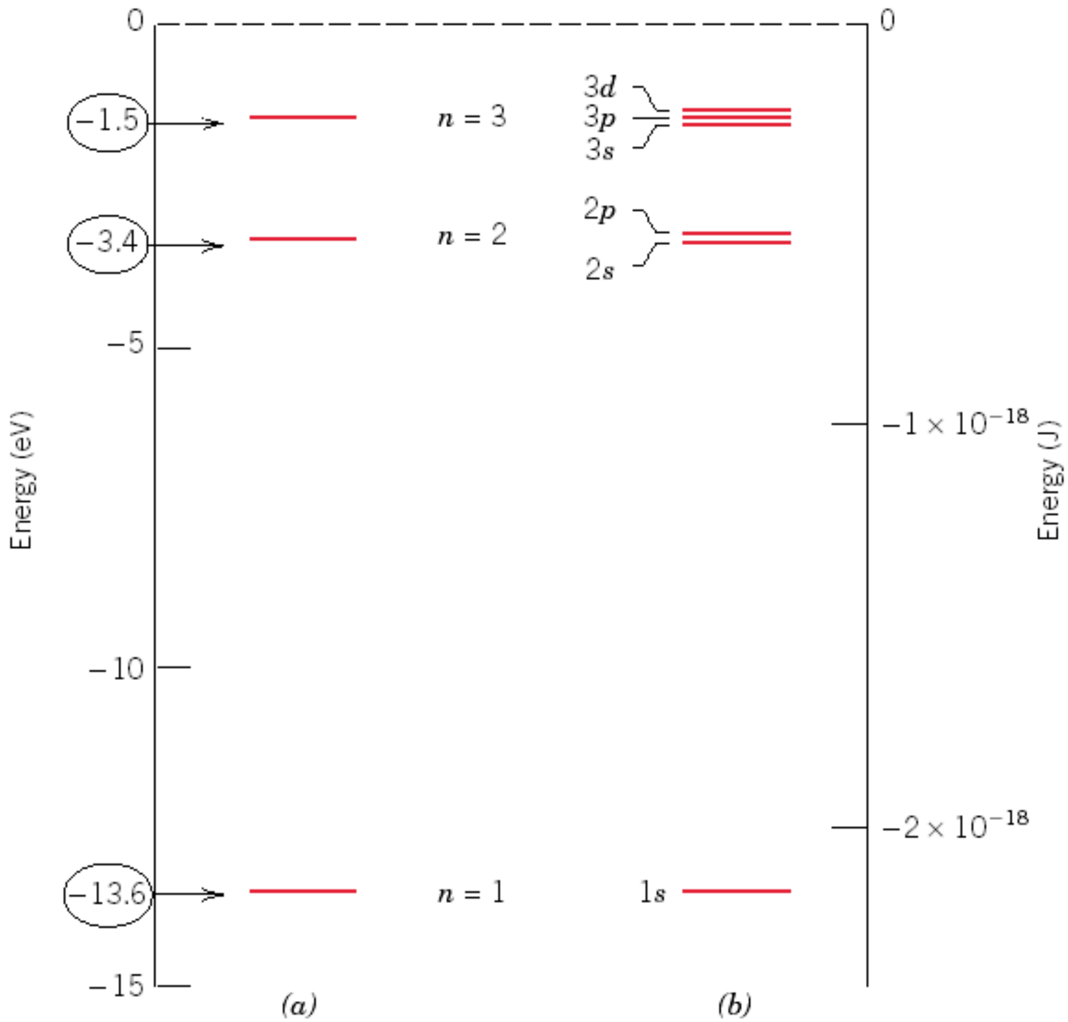
Quantum numbers

- Principal quantum number n=1, 2 ..; K, L, M, N, O
- Orbital quantum number l=0, ..n-1; subshell, s, p, d, or f; the shape of the electron subshell
- M_l= -l,…,0,…,+l
- Spin moment m_s 1/2 or -1/2

Table 2.1 The Number of Available Electron States in Some of the Electron Shells and Subshells

Principal Quantum Number n	*Shell Designation*	*Subshells*	*Number of States*	*Number of Electrons*	
				Per Subshell	*Per Shell*
1	*K*	*s*	1	2	2
2	*L*	*s*	1	2	8
		p	3	6	
3	*M*	*s*	1	2	18
		p	3	6	
		d	5	10	
4	*N*	*s*	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	

Electron energy states

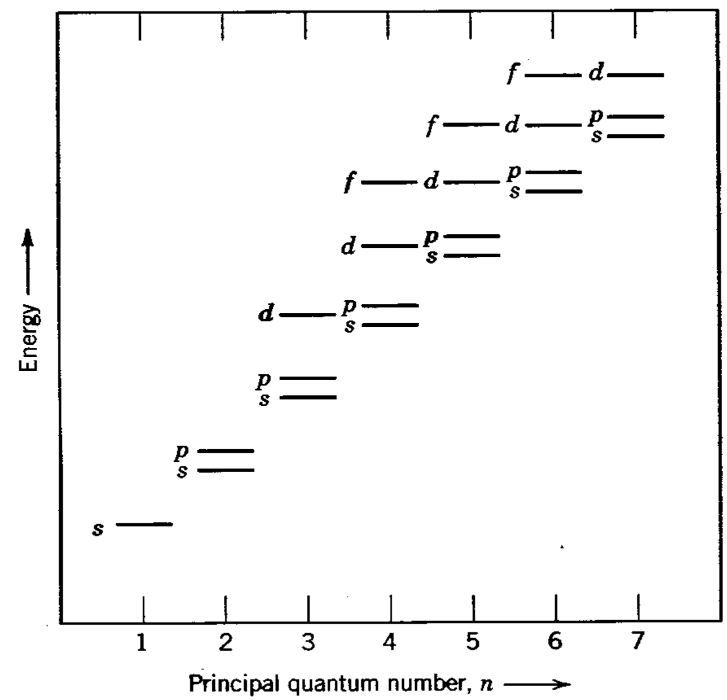


Bohr hydrogen model

Wave-mechanical hydrogen

Quantum Numbers

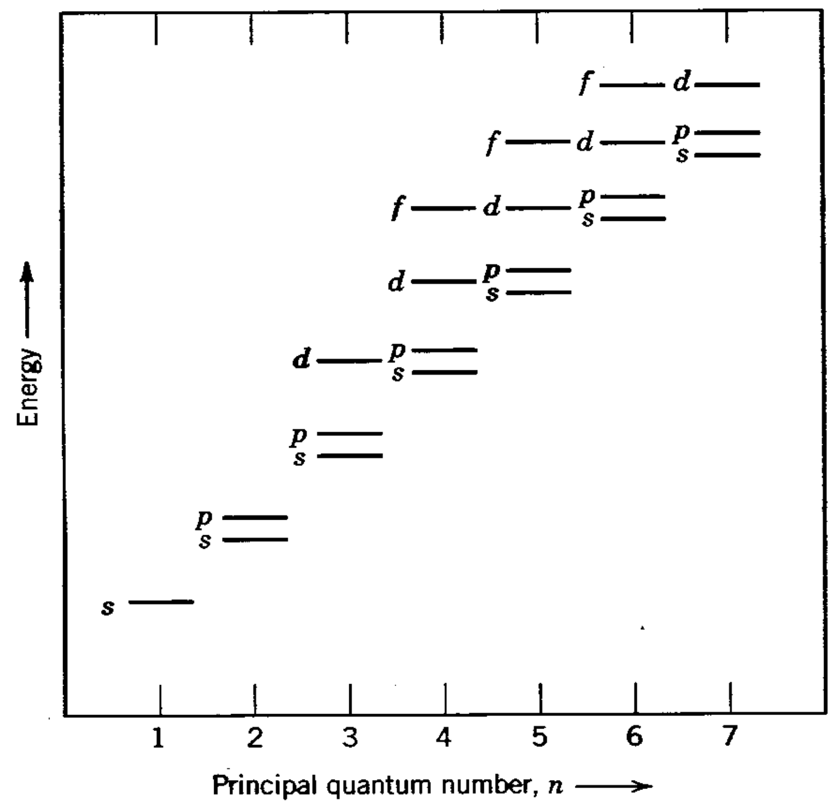
- The smaller n, the lower energy
- The smaller l, the lower energy
- There are some overlaps in energy, especially for d and f states



Relative energies of the electrons for various shells and subshells

Electron configurations

- Energy minimum rule
- Pauli exclusion principle
- Hund's rule: as many unpaired electrons as possible
- Ground state
- Valence electrons



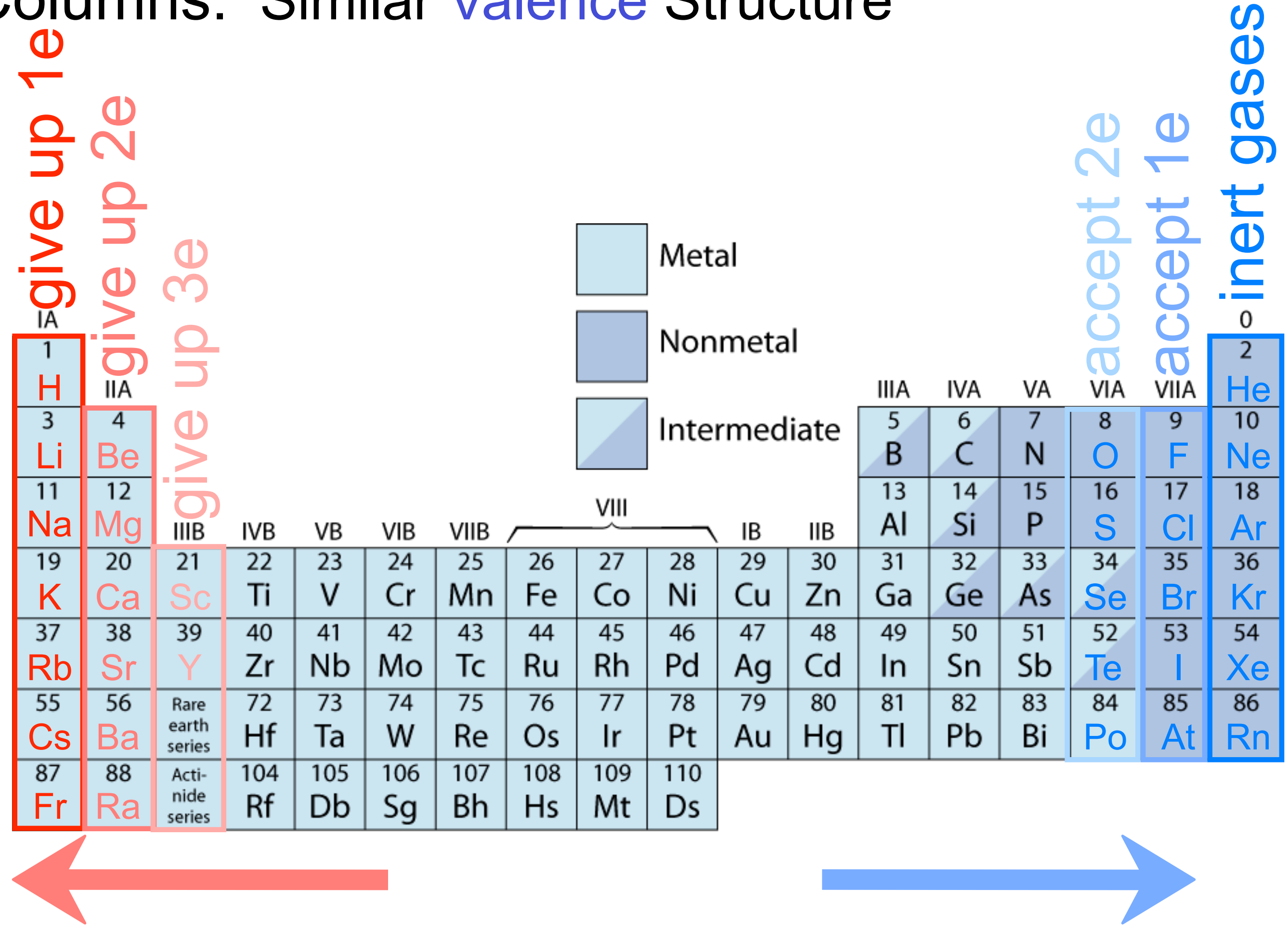
Relative energies of the electrons for various shells and subshells

Electronic Configurations

ex: Fe - atomic # = 26

The Periodic Table

- Columns: Similar Valence Structure



Adapted from Fig. 2.6, *Callister 7e.*

Electropositive elements: Readily donate electrons to become + ions.

Electronegative elements: Readily acquire electrons to become - ions.

Electronegativity

- Ranges from 0.7 to 4.0,
- Large values: tendency to acquire electrons.

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

Smaller electronegativity

Larger electronegativity

Adapted from Fig. 2.7, *Callister 7e.* (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.

The periodic table(*continued*)

SURVEY OF ELEMENTS

- Most elements: Electron configuration not stable.

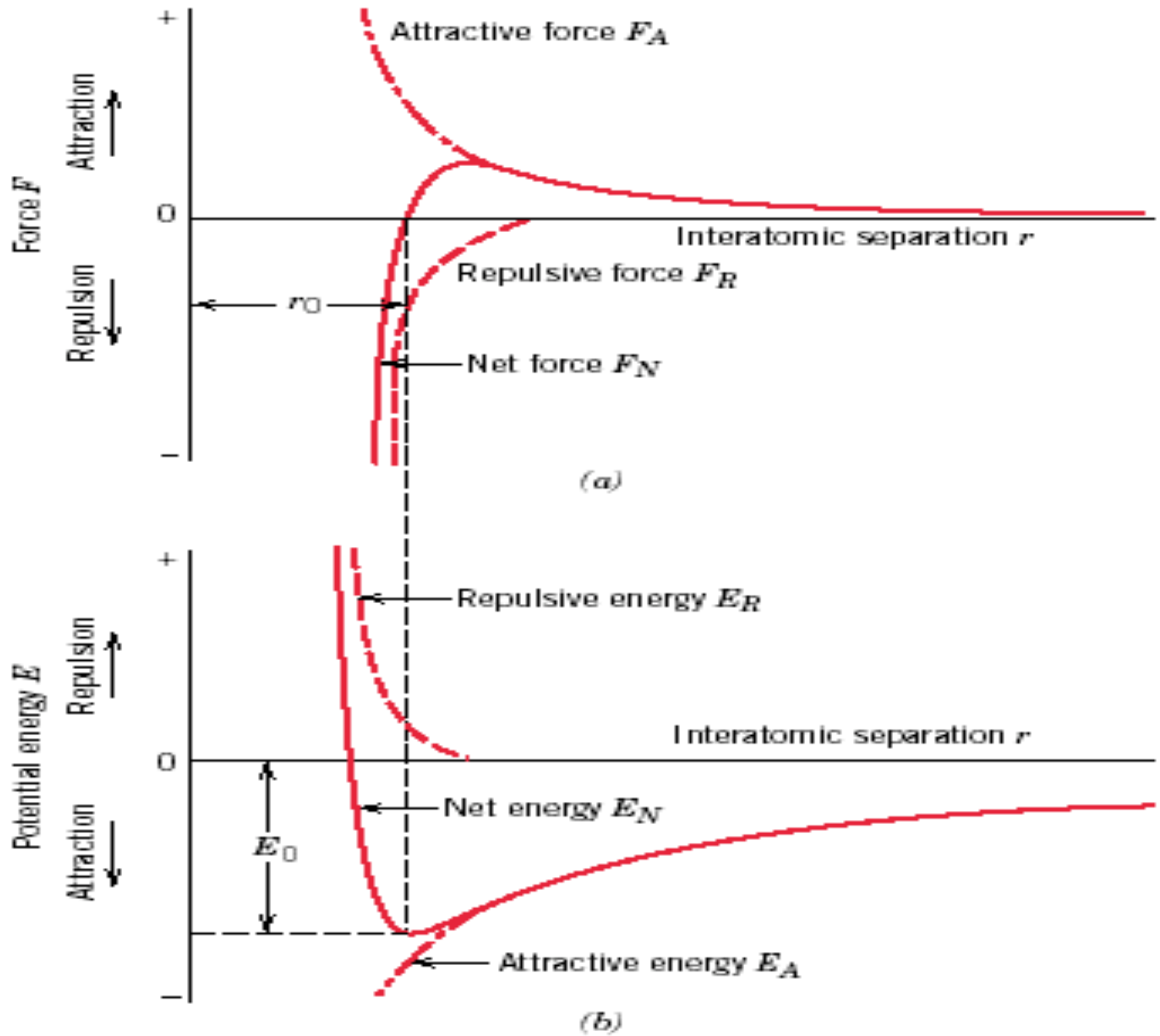
Element	Atomic #	Electron configuration	
Hydrogen	1	$1s^1$	
Helium	2	$1s^2$	(stable)
Lithium	3	$1s^22s^1$	
Beryllium	4	$1s^22s^2$	
Boron	5	$1s^22s^22p^1$	
Carbon	6	$1s^22s^22p^2$	
...		...	
Neon	10	$1s^22s^22p^6$	(stable)
Sodium	11	$1s^22s^22p^63s^1$	
Magnesium	12	$1s^22s^22p^63s^2$	
Aluminum	13	$1s^22s^22p^63s^23p^1$	
...		...	
Argon	18	$1s^22s^22p^63s^23p^6$	(stable)
...	...	...	
Krypton	36	$1s^22s^22p^63s^23p^63d^{10}4s^24p^6$	(stable)

Adapted from Table 2.2, *Callister 7e.*

- Why? Valence (outer) shell usually not filled completely.

Atomic bonding in solids

- Bonding forces and energies



Ionic Bonding

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

Examples: Ionic Bonding

- Predominant bonding in Ceramics

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

← Donate electrons

Acquire electrons →

Adapted from Fig. 2.7, *Callister 7e.* (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.

Covalent Bonding

- similar electronegativity ∴ share electrons
- bonds determined by valence – *s* & *p* orbitals dominate bonding
- Example: CH_4

Covalent Bonding

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

← Donate electrons

Acquire electrons →

Primary Bonding

- Metallic Bond -- delocalized as electron cloud

- Ionic-Covalent Mixed Bonding

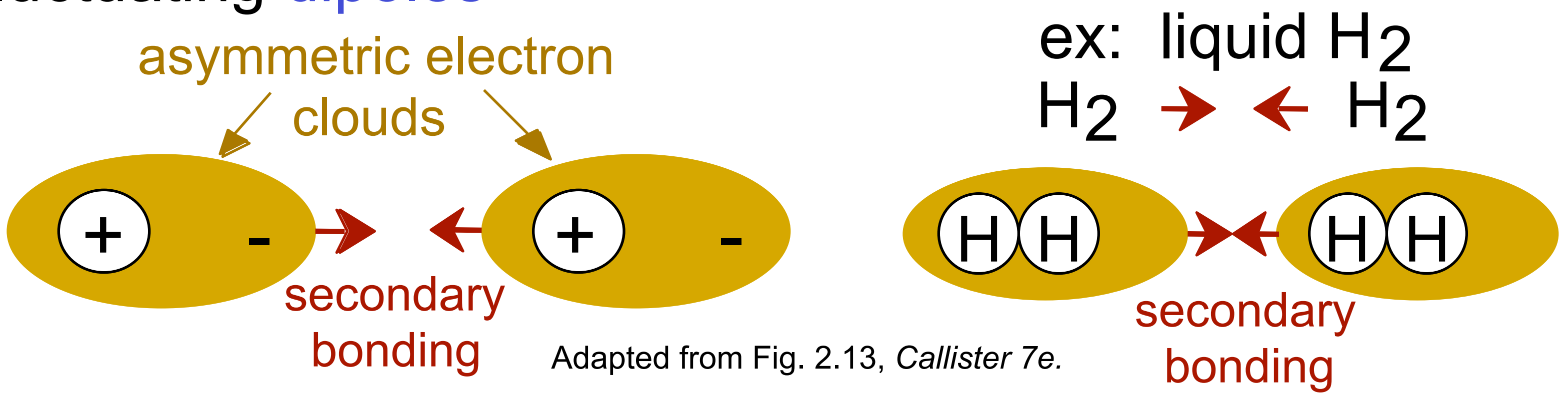
  % ionic character = $\left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \text{x} \, (100\%)$

  where X_A & X_B are Pauling electronegativities

SECONDARY BONDING

Arises from interaction between dipoles

- Fluctuating dipoles



Adapted from Fig. 2.13, *Callister 7e.*

- Permanent dipoles-molecule induced

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

Summary

- Atomic structure
- Electrons in atoms:
  - Bohr atomic and wave-mechanical model
  - Quantum numbers
  - Electron configuration
- Periodic table
- Bonding forces and energies
- Bondings