

Chapter 2: Atomic structure and interatomic bonding

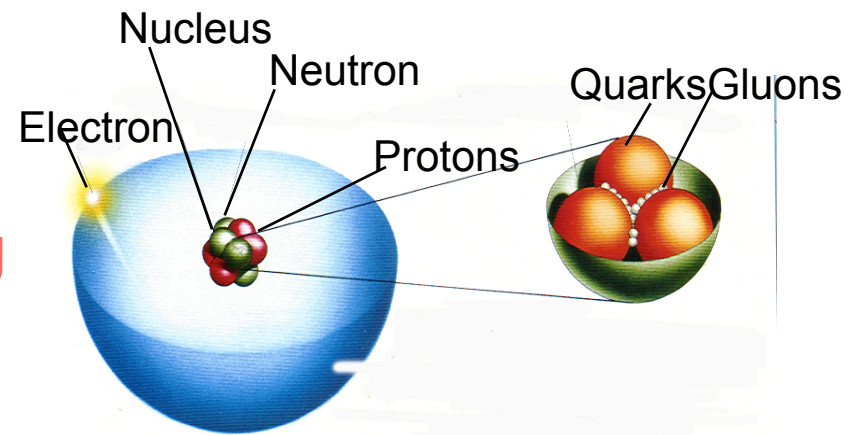
- ❑ Fundamental concepts
- ❑ Electrons in atoms
- ❑ Periodic table
- ❑ Bonding forces and energies



Chapter 2: Atomic structure and interatomic bonding

❑ Fundamental concepts

- Proton and electron
Charge: $1.60 \times 10^{-19} \text{ C}$
- Mass of electron $9.11 \times 10^{-31} \text{ kg}$
- Mass of protons and neutrons
→ $1.67 \times 10^{-27} \text{ kg}$
- Atomic number: the number of protons
- Atomic mass = protons + neutrons
- Isotopes
- Atomic mass unit (amu): $1 \text{ amu} = 1/12 \text{ C}$
- 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

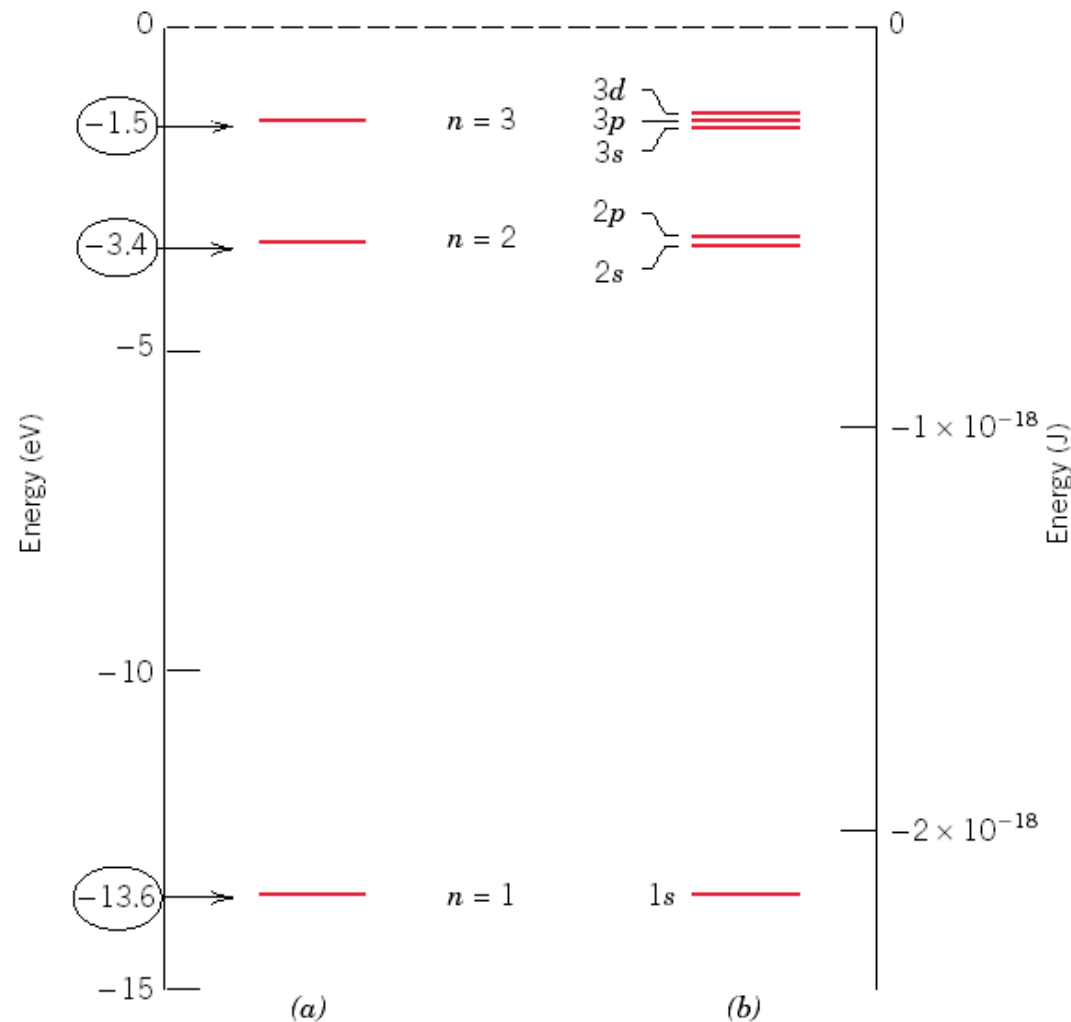
- Principal quantum number $n=1, 2 \dots$; K, L, M, N, O
- Orbital quantum number $l=0, \dots, n-1$; subshell, s, p, d, or f; the shape of the electron subshell
- $M_l = -l, \dots, 0, \dots, +l$
- Spin moment m_s 1/2 or -1/2

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



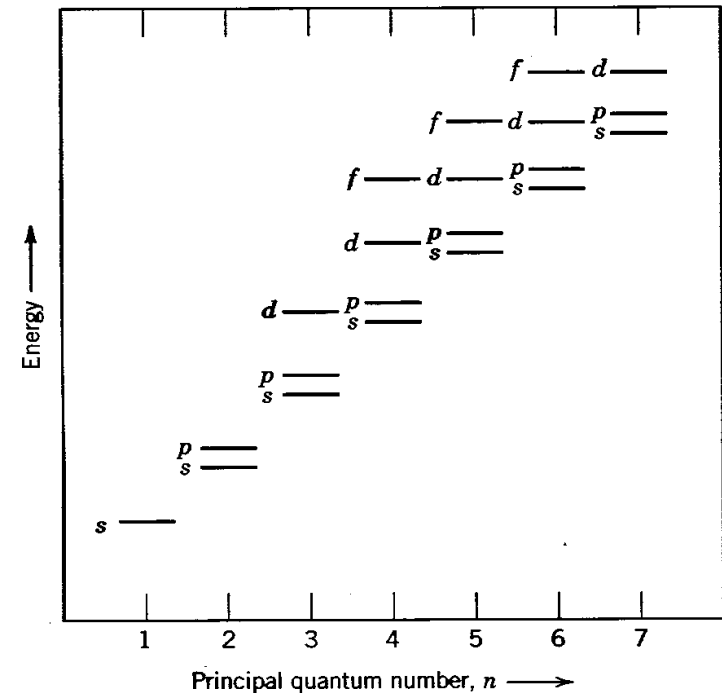
Bohr hydrogen model

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

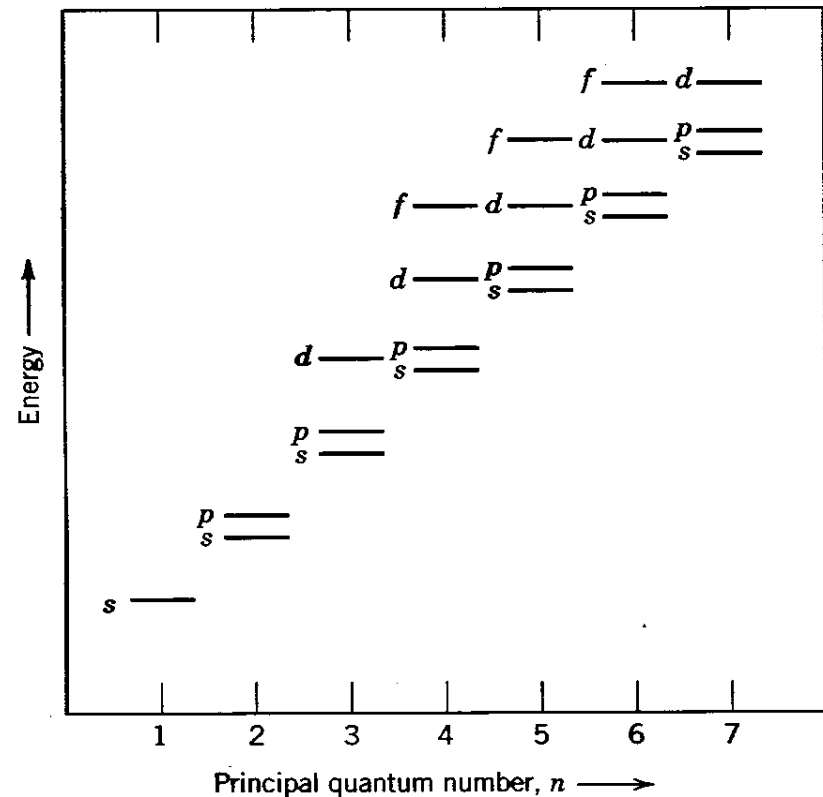


**Relative energies of the electrons
for various shells and subshells**



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

columns: Similar Valence Structure

The periodic table is color-coded to show valence electron configurations. Groups 1 and 2 are highlighted in red, with labels 'give up 1e' and 'give up 2e' respectively. Groups 13-18 are highlighted in blue, with labels 'accept 2e', 'accept 1e', and 'inert gases' respectively. The transition metals (groups 3-10) are highlighted in light blue, with a label 'Metal'. The metalloids (groups 11-12) are highlighted in light blue, with a label 'Nonmetal'. The noble gases (groups 17-18) are highlighted in light blue, with a label 'Intermediate'.

IA	IIA	IIIB	IVB	VB	VIB	VII B	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H	2 He									3 B	4 C	5 N	6 O	7 F	8 Ne
3 Li	4 Be									13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
11 Na	12 Mg									31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	49 In	50 Sn	51 Sb	52 Te
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	81 Tl	82 Pb	83 Bi	84 Po
55 Cs	56 Ba	Rare earth series	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po
87 Fr	88 Ra	Actinide series	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds						

Legend:

- Metal
- Nonmetal
- Intermediate

Valence electron configurations:

- give up 1e
- give up 2e
- give up 3e
- accept 2e
- accept 1e
- inert gases

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																	0
H																	He
2.1																	-
Li	Be											III A	IV A	VA	VIA	VII A	Ne
1.0	1.5											2.0	2.5	3.0	3.5	4.0	-
Na	Mg											Al	Si	P	S	Cl	Ar
0.9	1.2											1.5	1.8	2.1	2.5	3.0	-
		IIIB	IVB	VB	VIB	VII B	VIII			IB	IIB						
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.6	1.6	1.8	2.0	2.4	2.8	-
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5	-
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
0.7	0.9	1.1-1.2	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2	-
Fr	Ra	Ac-No															
0.7	0.9	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	$1s^2 2s^1$
Beryllium	4	$1s^2 2s^2$
Boron	5	$1s^2 2s^2 2p^1$
Carbon	6	$1s^2 2s^2 2p^2$
...
Neon	10	$1s^2 2s^2 2p^6$ (stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
...
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$ (stable)
...
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ (stable)

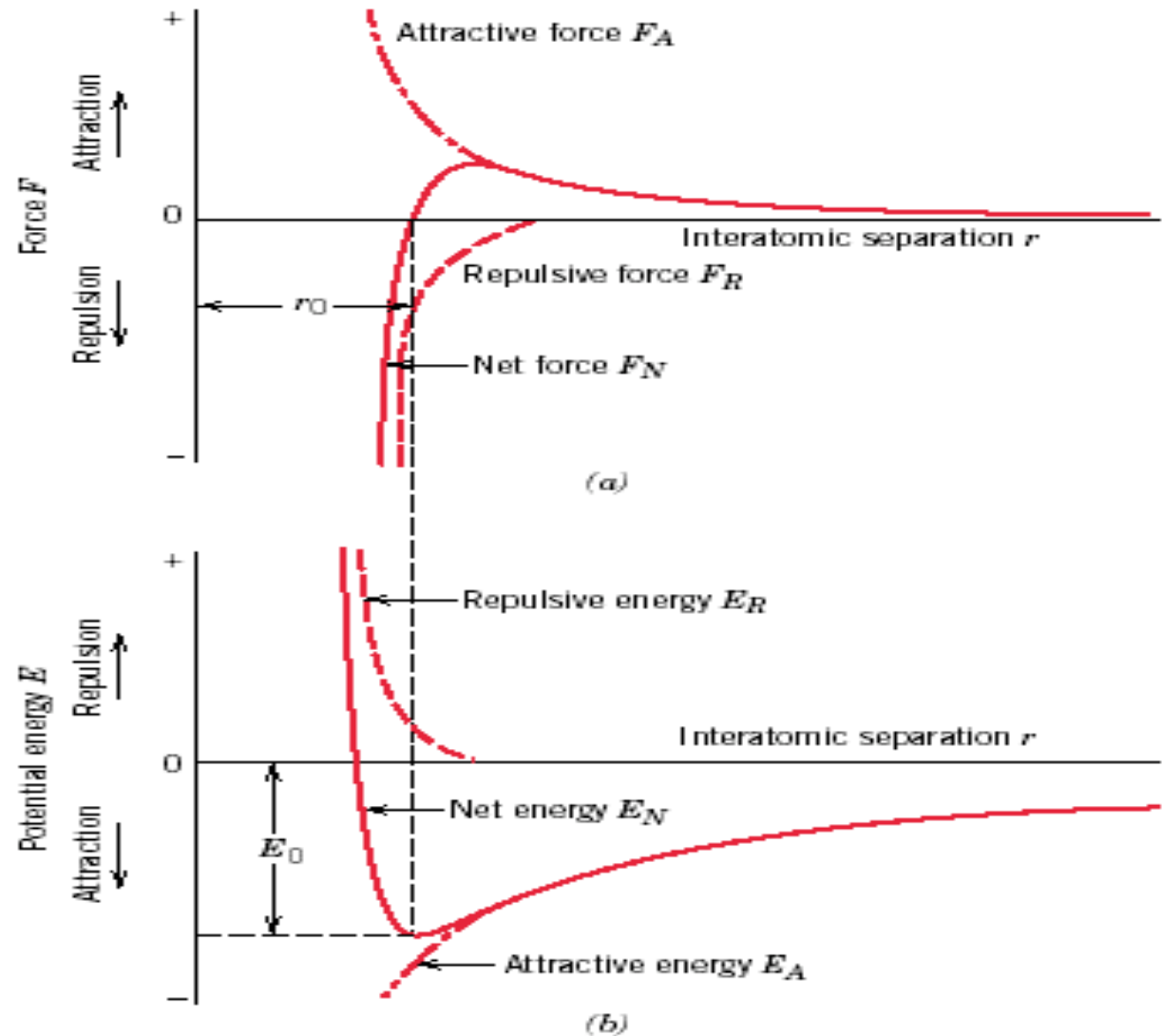
Adapted from Table 2.2,
Callister 7e.

- 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



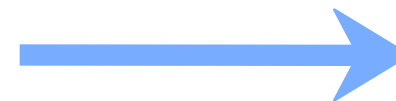
Examples: Ionic Bonding

- Predominant bonding in **Ceramics**

IA																	0
H																	He
2.1	IIA											IIIA	IVA	VA	VIA	VIIA	-
Li	Be											B	C	N	O	F	Ne
1.0	1.5											2.0	2.5	3.0	3.5	4.0	-
Na	Mg											Al	Si	P	S	Cl	Ar
0.9	1.2	IIIB	IVB	VB	VIB	VII B	VIII				IB	IIB					-
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.6	1.6	1.8	2.0	2.4	2.8	-
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5	-
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
0.7	0.9	1.1-1.2	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2	-
Fr	Ra	Ac-No															
0.7	0.9	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 \therefore share electrons
- bonds determined by valence – s & p orbitals dominate bonding
- Example: CH₄



Covalent Bonding

IA																	0
H 2.1																	He -
	IIA											IIIA	IVA	VA	VIA	VIIA	
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 -
		IIIB	IVB	VB	VIB	VII B	VIII				IB	IIB					
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

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

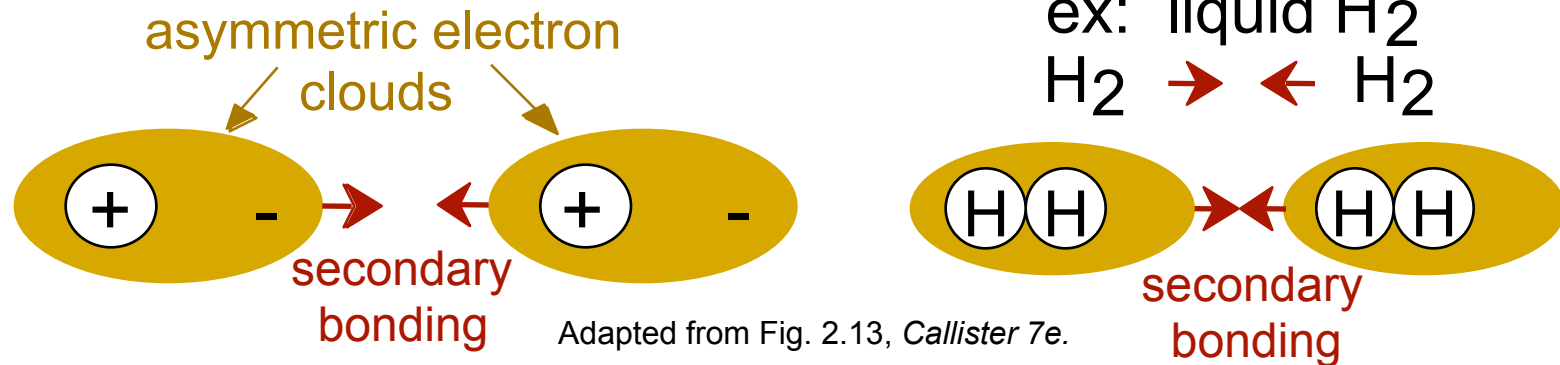
where X_A & X_B are Pauling electronegativities



SECONDARY BONDING

Arises from interaction between dipoles

- Fluctuating dipoles



- 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

