

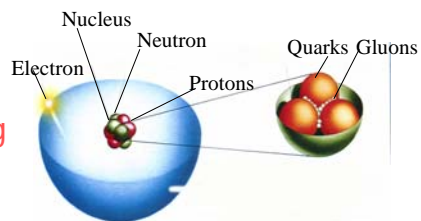
Chapter 2: Atomic structure and interatomic bonding

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

Chapter 2: Atomic structure and interatomic bonding

□ Fundamental concepts

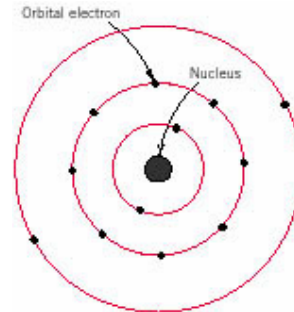
- Proton and electron, charged
 $1.60 \times 10^{-19} \text{ C}$
- Mass of electron $9.11 \times 10^{-31} \text{ kg}$
- Mass of protons and neutrons
 $1.67 \times 10^{-27} \text{ kg}$
- Atomic number: the number of protons
- Atomic mass = protons + neutrons
- Isotope
- Atomic mass unit (amu): $1 \text{ amu} = 1/12 \text{ C}$
- One mole = 6.023×10^{23} atoms (Avogadro's)



Electrons in atoms

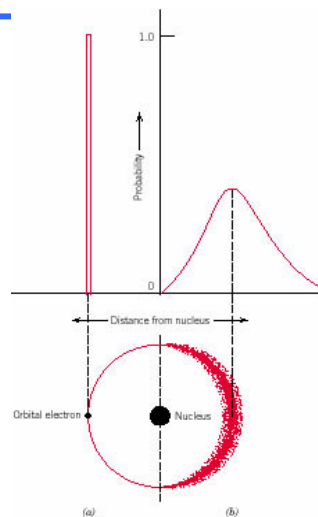
□ Atomic models

- Bohr atomic
electrons revolve around the atomic nucleus in discrete orbital and the energies of electrons are quantized
- Wave-mechanical
Electron exhibits both wavelike and particle-like characteristics, its position is considered to be a probability distribution



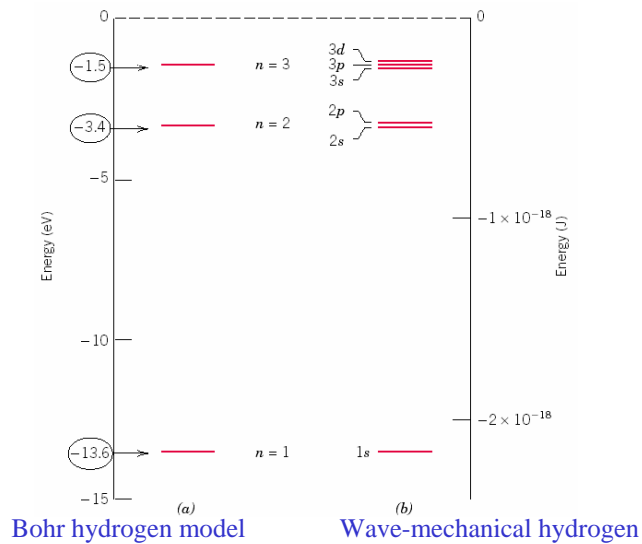
Electrons in atoms (*continue*)

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



In terms of electron distribution

Electron energy states



Quantum numbers

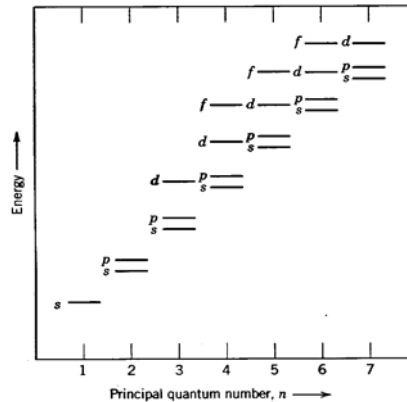
- Principle quantum number $n=1, 2 \dots$; K, L, M, N, O
- Orbital quantum number $l=0, \dots, n-1$; subshell, s, p, d, or f; the shape of the electron subshell
- Spin moment $m_s +1/2$ or $-1/2$

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	

Quantum Numbers

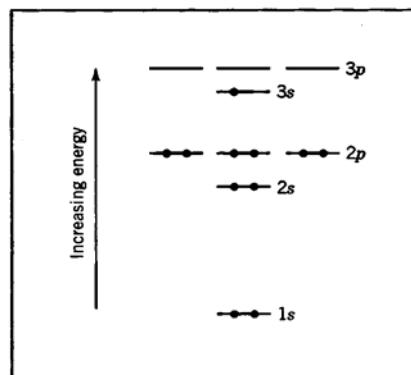
- The smaller n , the lower energy
- The smaller l , the lower energy
- There are some overlaps in energy, especially for d and f states



Relative energies of the electrons for various shells and subshells

Electron configurations

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

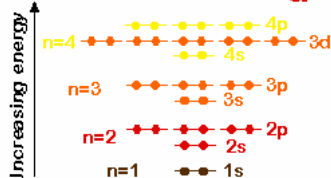


Filled energy states for a sodium atom

Electron configurations

□ Examples of expected electron configuration

Electrons have discrete energy states



Stable electron configurations...

- have complete s and p subshells
- tend to be unreactive

Z	Element	Configuration
2	He	$1s^2$
10	Ne	$1s^2 2s^2 2p^6$
18	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$
36	Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

The periodic table

alkaline

Alkaline-earth

Key

- Atomic number
- Symbol
- Atomic weight

Metal

Nonmetal

Intermediate

1 H 1.0080	2 He 4.0026																
3 Li 6.939	4 Be 9.0122																
11 Na 22.990	12 Mg 24.312																
19 K 39.102	20 Ca 40.08	21 Sc 44.956	22 Ti 47.90	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.71	29 Cu 63.54	30 Zn 65.37	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.91	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.40	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.34	Rare earth series															
87 Fr (223)	88 Ra (226)	Actinide series															
		57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97	
		89 Ac (227)	90 Th 232.04	91 Pa (231)	92 U 238.03	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lr (257)	

FIGURE 2.6 The periodic table of the elements. The numbers in parentheses are the atomic weights of the most stable or common isotopes.

Electropositive elements: the ability to give up electrons

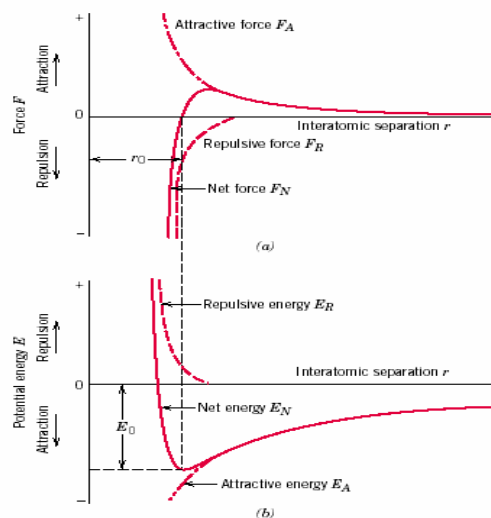
Electronegative elements: the ability to accept electrons (-ions)

The periodic table(*continue*)

- Period: horizontal rows
- Group and column
 - Same group, same valence electrons, similar properties
 - Group 0, inert gas
 - Group IA, IIA, 1 or 2 excess electrons from stable structure
 - Transition metals (IVB and IIB).
 - III A, IVA and VA, semiconductor
- Electropositive and electronegative
- Electronegativity

Atomic bonding in solids

- Bonding forces and energies
 - $F_n = F_A + F_R$
 - E_0 -- bonding energy
 - large bonding E, high melting point
 - stiffness -- shape of f-r curve
 - thermal expansion -- E-r curve

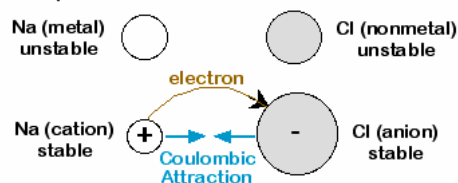


Primary interatomic bonds

□ Ionic bonding

- An ionic bond is formed when an atom loses or gains one or more electrons from its outer shell
- Between metallic and nonmetallic
- Attractive bonding force--coulombic
- Non-directional
- $E_A = -A/r$, $E_R = B/r^n$, $n \sim 8$

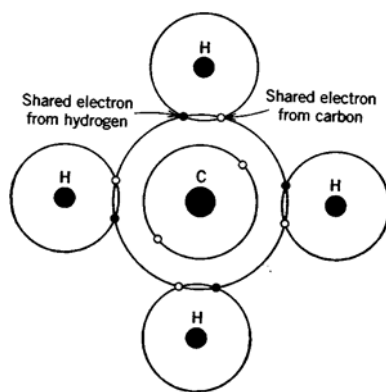
Example: NaCl



Primary interatomic bonds (*continue*)

□ Covalent bonding

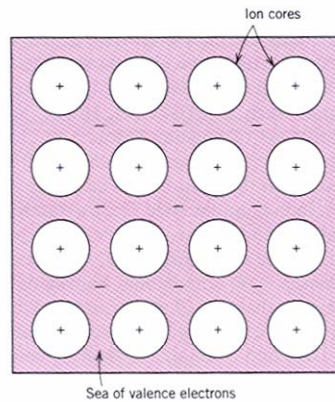
- stable electron configurations are assumed by sharing electrons between adjacent atoms
- directional
- many non-metallic elements
- % ionic character = $\{1 - \exp[-(0.25)(X_A - X_B)^2]\} \times 100$



Primary interatomic bonds (*continue*)

□ Metallic bonding

- sea of valence electrons floating on ion cores
- non-directional
- metal and alloys
- electrons are balanced with ion cores in charge



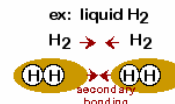
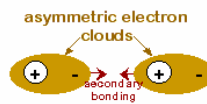
Secondary bonding

□ Van der Waals bonding

- bonding energy 10kJ/mol (0.1 eV/atom)
- existing in all atoms
- arise from fluctuating and permanent dipoles
- forces are temporary and fluctuating with time

Arises from interaction between dipoles

• Fluctuating dipoles



• Permanent dipoles - molecule induced:

in general:



ex: liquid HCl



ex: polymer



□ Hydrogen bonding 51kJ/mol (0.52eV/molecule): H-F, H-O, H-N

Summary

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