Materials Science

Atomic Structures and Bonding

Atomic Structure

Fundamental concepts

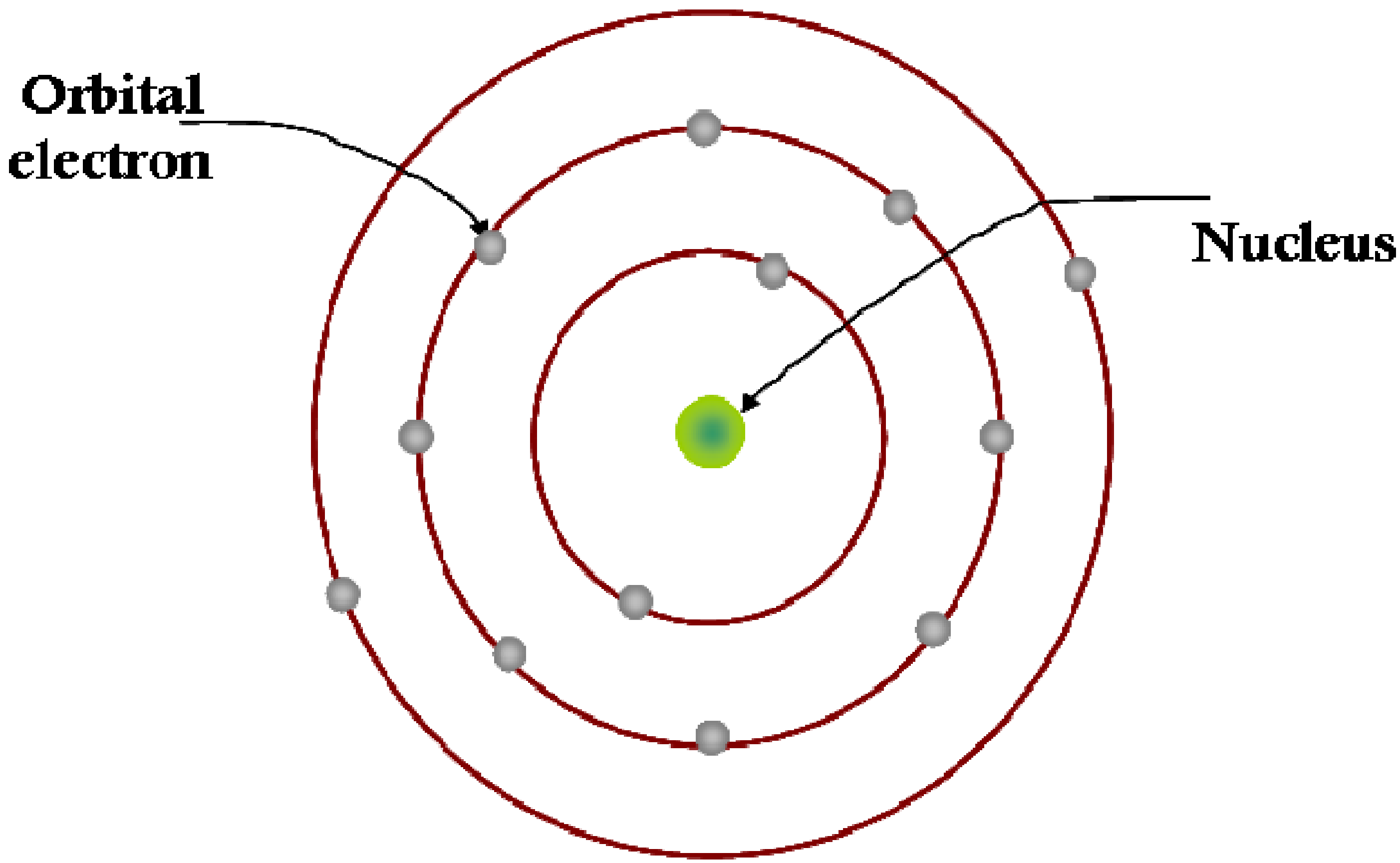
- Each atom consists of a nucleus composed of protons and neutrons which are encircled by electrons.
- Protons and electrons are electrically charged, the charge magnitude is 1.60×10^{-19}C.
- Protons are positively charged and electrons are negatively charged.
- Neutrons are electrically neutral.
- Protons and neutrons have approximately the same mass at 1.67×10^{-27} kg.
- The mass of an electron is 9.11×10^{-31}kg.

- Each chemical element is characterised by the number of protons called the atomic number (*Z*).
- A neutral atom has the same number of protons and electrons.
- The atomic mass (*A*) is the sum of the masses of protons and neutrons.
- The number of protons is the same for all atoms of an element but the number of neutrons (*N*) may vary.
- Some elements have two or more different atomic masses which are called isotopes.
- The atomic weight of an elements is the weighted average of the atomic masses of the atom’s naturally occurring isotopes.

- The atomic mass unit (amu) is used in the computation of atomic weight where $1\ amu = 1.66 \times 10^{-24}\ g$
- The atomic weight or molecular weight of a compound may be expressed on the basis of amu per atom (molecule) or mass per mole of material.
- 1 mole of a substance has 6.023×10^{23} *atoms / molecules*. This is called the Avogadro's number.
- Thus, *1 amu/atom (molecule) =1 g/mole*
- In the periodic table the atomic weight is given in terms of *amu/atom* or *g/mole*.

Electrons in atoms – atomic models

- Bohr atomic model (See following slide)
  - Electrons revolve around the atomic nucleus in discrete orbitals
  - Position of electron is well defined in terms of orbitals
  - Electrons permitted to have specific values of energy (quantized) depending on its position – called energy levels or states
  - Electrons may change energy but in doing do so, it must make a quantum jump to either an allowed higher energy (with energy absorption) or a lower energy (with energy emission)



The Bohr's atomic model

- Wave-mechanical model
  - Electron particles do not move in discrete orbitals
  - There is a probability of electrons being in various locations around the nucleus.
  - Electron position is describe by a probability distribution or an electron cloud.
  - See following slides

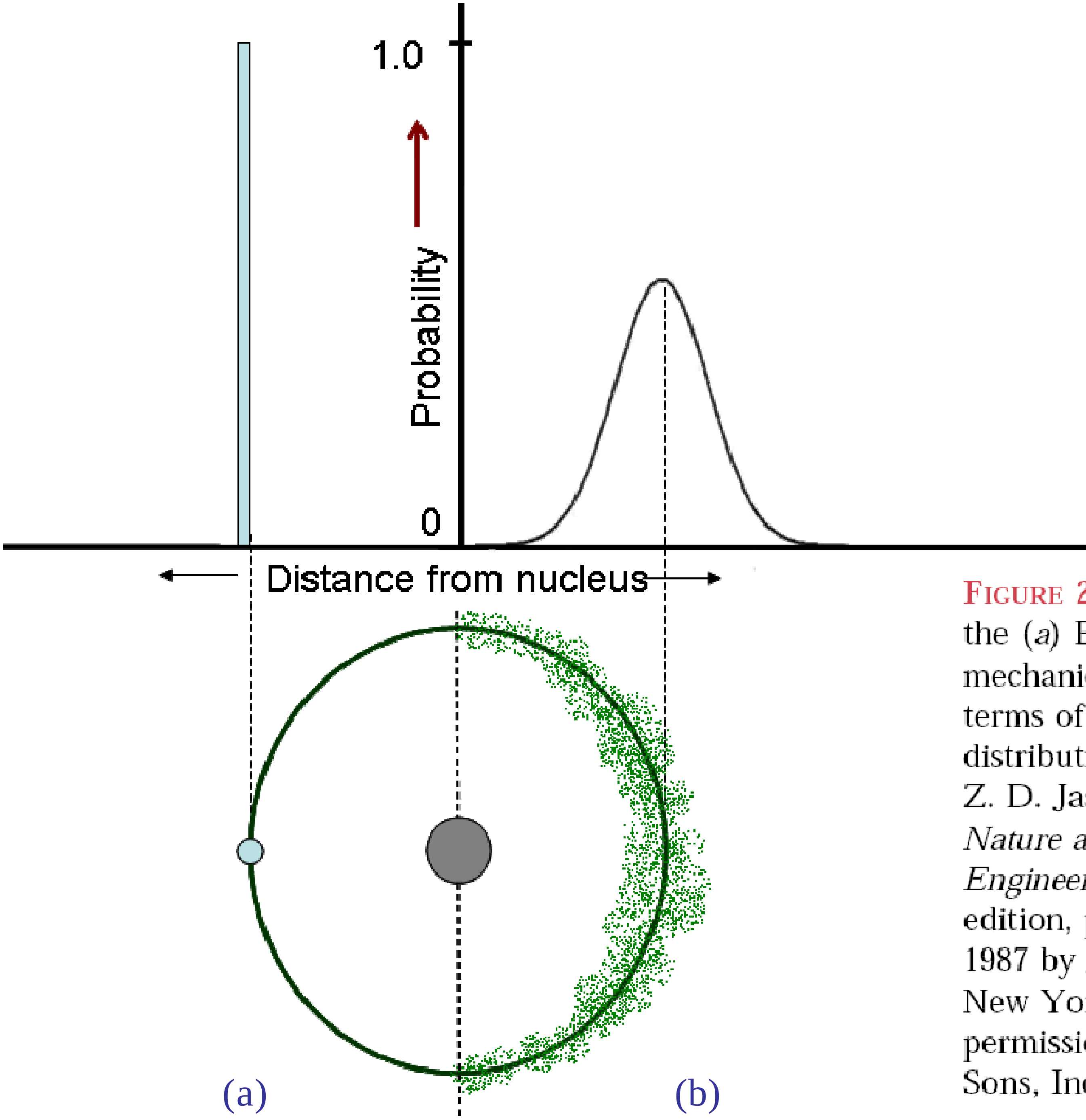


FIGURE 2.3 Comparison of the (*a*) Bohr and (*b*) wave-mechanical atom models in terms of electron distribution. (Adapted from Z. D. Jastrzebski, *The Nature and Properties of Engineering Materials,* 3rd edition, p. 4. Copyright © 1987 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

Quantum numbers

Every electron in an atom is characterised by four parameters called quantum numbers.

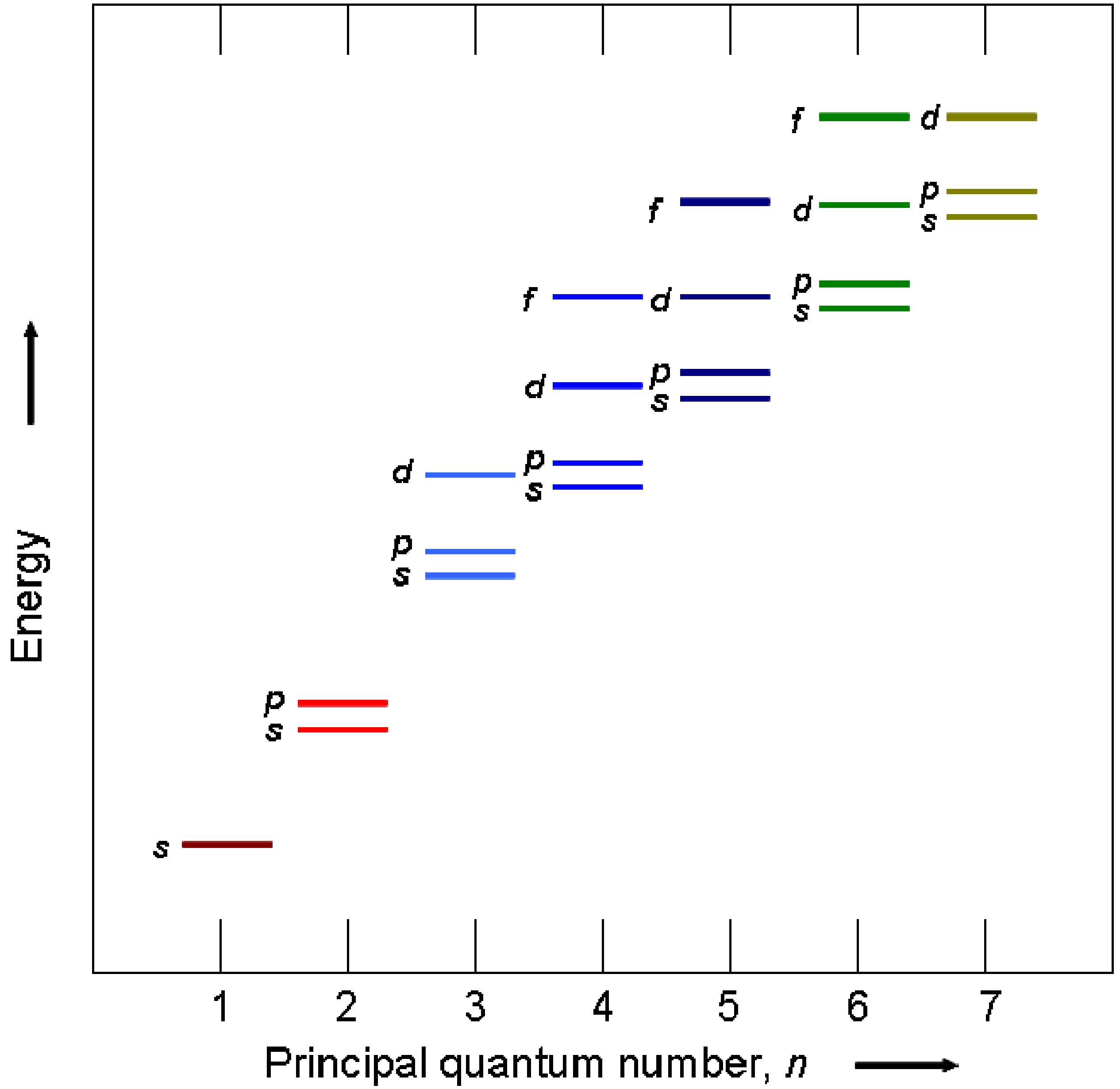
1. Principle quantum number, n: specifies the shells i.e. relates the distance form the nucleus where electron can be found. It also determines the major energy level. The maximum number of electrons allowed at any one level is $2n^2$.

   $n = 1, 2, 3, 4, \ldots$
2. Angular momentum quantum number, l: signifies the subshell and it describes the shape of the shell.

   $l = 0, 1, 2, 3, \ldots (n-1)$

   $l = s, p, d, f, \ldots (n-1)$

   these may hold up to 2,6,10 and 14 electrons, respectively.
3. Magnetic quantum number, m_l: determines the number of energy states for each subshell and $m_l = -l$ to l
4. Electron spin number m_s: two electrons can exist in a single energy state of a subshell and this number relates the up or down orientation of an electron within the energy state.



Schematic representation of the relative energies of the electrons for the various shells and subshells

- The smaller the quantum number the smaller the energy level
- Within each shell the energy of a subshell level increases with the value of the *l* quantum number.
- There may be overlap in energy state in one shell with energy states in adjacent shell

- Pauli exclusion principle stipulates that each electron state can hold no more that two electrons which must have opposite spins.
- It also states that no two electron in an atom can have the same set of quantum numbers. Refer to the table in the next slide.
- Electrons fill up the lowest possible energy states in the electron shells and subshells first. The second following slide is an example of sodium atom. Sodium is said to be in the ground state.

Electron configuration

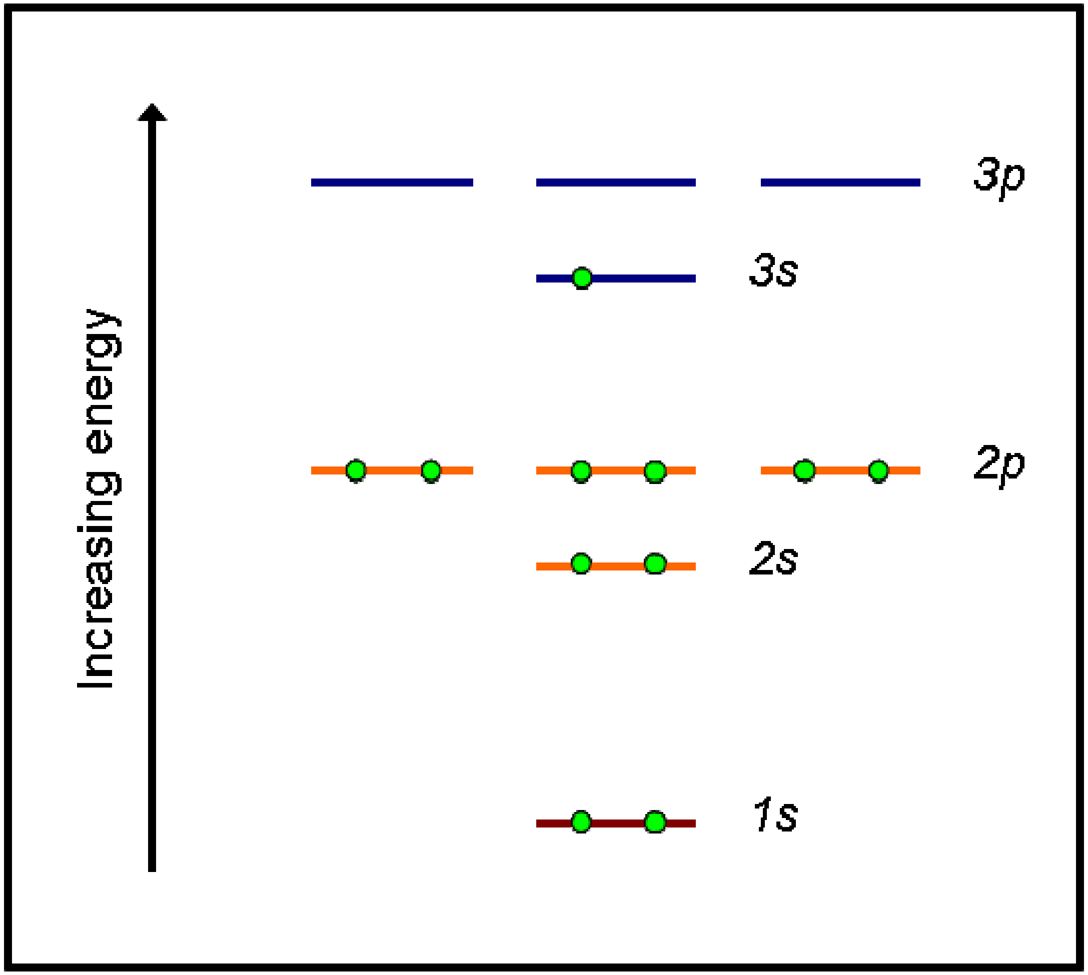
- The electron configuration of an atom represents the manner in which these states are occupied.

Table 2.2 A Listing of the Expected Electron Configurations for Some of the Common Elements[a]

Element	*Symbol*	*Atomic Number*	*Electron Configuration*
Hydrogen	H	1	$1s^1$
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^2 2s^1$
Beryllium	Be	4	$1s^2 2s^2$
Boron	B	5	$1s^2 2s^2 2p^1$
Carbon	C	6	$1s^2 2s^2 2p^2$
Nitrogen	N	7	$1s^2 2s^2 2p^3$
Oxygen	O	8	$1s^2 2s^2 2p^4$
Fluorine	F	9	$1s^2 2s^2 2p^5$
Neon	Ne	10	$1s^2 2s^2 2p^6$
Sodium	Na	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	Mg	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	Al	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
Silicon	Si	14	$1s^2 2s^2 2p^6 3s^2 3p^2$
Phosphorus	P	15	$1s^2 2s^2 2p^6 3s^2 3p^3$
Sulfur	S	16	$1s^2 2s^2 2p^6 3s^2 3p^4$
Chlorine	Cl	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Argon	Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$

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	



Schematic representation of the filled and lowest unfilled energy states for a sodium atom.

Important facts:

- Valence electrons are those that occupy the outermost shell.
- An atom with its outermost shell filled it is said to have a "stable electron configuration", inert or noble gases.
- Other atoms loose or gain electron or share electrons to assume stable electron configuration.

The periodic table

- Elements situated with increasing atomic number, seven horizontal rows called periods.
- Elements in a given column or group have similar valence electron structure, as well as chemical and physical properties.
- Group zero (right most) – inert gases
- Group VIIA – halogens
- Group IA – alkali metals
- Group IIA – alkaline earth metals
- Group IIIB to IIB – transition metals partially filled d electron states in some cases one or two electrons in the next higher energy shell
- Most elements come under metal classification.

Metal

Nonmetal

Intermediate

Key

29 ← Atomic number
Cu ← Symbol
63.54 ← Atomic weight

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 1.0080																	2 He 4.0026
3 Li 6.939	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.183
11 Na 22.990	12 Mg 24.312											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
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	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.98	84 Po (210)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	Acti-nide series															

Rare earth 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
Actinide series	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 Lw (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.

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 2.1																	2 He –
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne –
11 Na 0.9	12 Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar –
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr –
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe –
55 Cs 0.7	56 Ba 0.9	57–71 La–Lu 1.1–1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn –
87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7															

FIGURE 2.7 The electronegativity values for the elements. (Adapted from Linus Pauling, *The Nature of the Chemical Bond,* 3rd edition. Copyright 1939 and 1940, 3rd edition copyright © 1960, by Cornell University. Used by permission of the publisher, Cornell University Press.)

Electropositive elements indicate that they are capable of giving up their few valence electrons to become positively charge ions. Electronegative elements readily accept electrons to form negatively charged ions, or sometimes they share electrons with other atoms

Atomic Bonding

Bonding forces and energies

- When the atoms are at large inter-atomic separation distance, the atoms do not exert any force on each other.
- When the distance is decreased, an attractive force F_A starts to pull the atoms closer.
- F_A increases as the atoms gets closer.
- But as the atoms get closer a repulsive force F_R begin to act.
- The net force F_N between the two atoms is given by:

$$F_N = F_A + F_R$$

- At some inter-atomic distance $r_{o,}$ F_R exactly equals F_A and F_N becomes Zero

$$F_N = 0 = F_A + F_R$$

- r_o is called the equilibrium inter-atomic separation distance at which atoms enter into bonding

$$r_o \approx 0.3 \text{ nm}$$

- At r_0, the two atoms will counteract any attempt to separate them by an attractive force, or to push them together by a repulsive force.

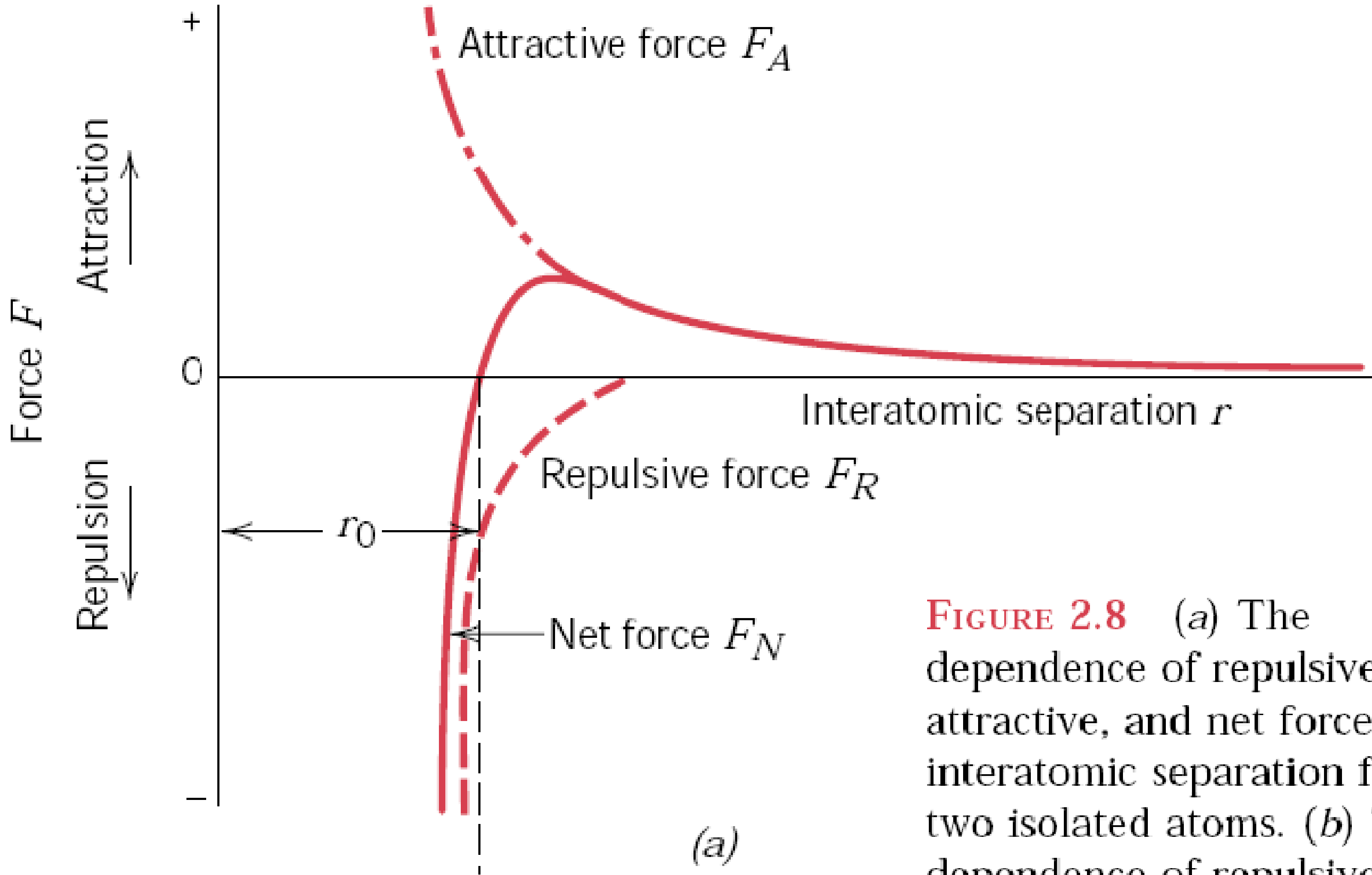


Figure 2.8 (*a*) The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms. (*b*) The dependence of repulsive, attractive, and net potential energies on interatomic separation for two isolated atoms.