## Second Lecture

# Atomic Structure and Interatomic Bonding

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# WHY STUDY Atomic Structure and Interatomic Bonding?

**to explain a material's properties.**

# 1. Atomic Structure

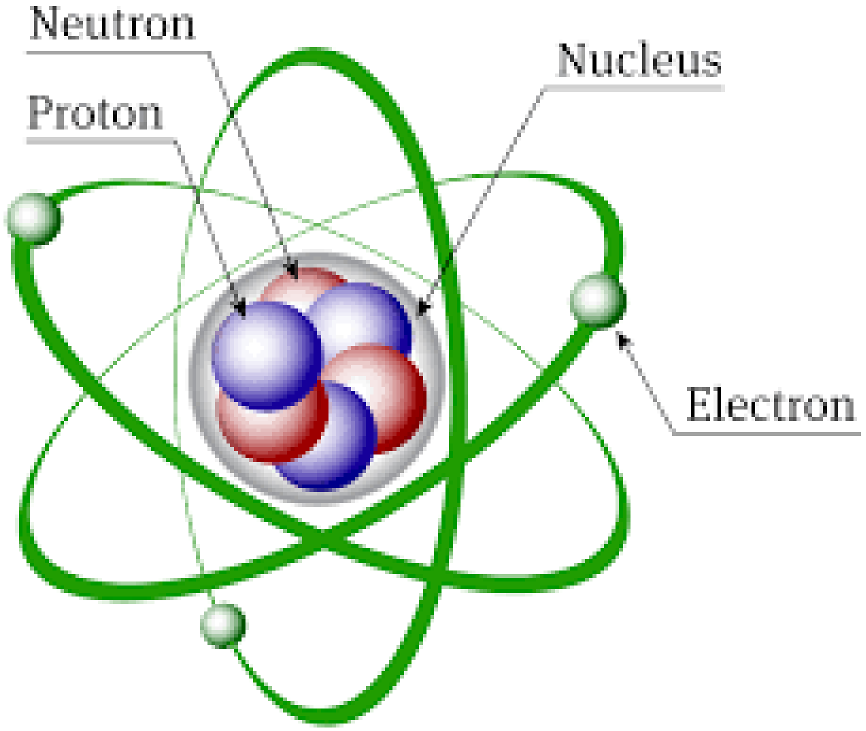
- Each **atom** consists of a very small nucleus (protons and neutrons), which is encircled by moving electrons.
- The **protons** have a positive electric charge

(1.602 10-$^{19}$ C)

- The **electrons** have a negative electric charge
- The **neutrons** have no electric charge
- More than 99.94% of an atom's mass is in the nucleus
- The **protons** and neutrons have approximately

The same mass is 1.67 $10^{-27}$ kg

- The **electron** mass is 9.11 $10^{-31}$ kg



# 1. Atomic Structure

- **Atomic number (Z)** the number of protons in the nucleus.
- This atomic number ranges in integral units from 1 for hydrogen to 92 for uranium.
- **The atomic mass** (A) of a specific atom may be expressed as the sum of the masses of protons and neutrons within the nucleus.
- **Isotopes** (النظائر) are variants of a particular chemical element which differ in neutron number.
- For example, **carbon-12**, **carbon-13** and **carbon-14** are three isotopes of the element carbon with mass numbers 12, 13 and 14 respectively. The atomic number of carbon is 6, which means that every carbon atom has 6 protons, so that the neutron numbers of these isotopes are 6, 7 and 8 respectively

# 1. Atomic Structure

- Although the number of protons (Z) is the same for all atoms of a given element, the number of neutrons (N) may be variable.
- Atomic mass $A \approx Z + N$
- The **atomic mass unit (amu)** may be used to compute atomic weight.
- atomic mass unit = amu = 1/12 mass of $^{12}C$
- 1 amu / atom = 1 g / mol
- 1mol of substance = $6.022 \times 10^{23}$ molecules or atoms
- For example, the atomic weight of iron is 55.85 amu/atom, or 55.85 g/mol

# 2. Bohr atomic model

- The Bohr model shows that the electrons in atoms are in orbits of differing energy around the nucleus (think of planets orbiting around the sun).
- Bohr used the term *energy levels* (or *shells*) to describe these orbits of differing energy. He said that the energy of an electron is *quantized*, meaning electrons can have one energy level or another but nothing in between.
- The energy level an electron normally occupies is called its *ground state*. But it can move to a higher-energy, less-stable level, or shell, by absorbing energy. This higher-energy, less-stable state is called the electron's *excited state*.
- After it's done being excited, the electron can return to its original ground state by releasing the energy it has absorbed, as shown in the diagram below.

# 2. Bohr atomic model

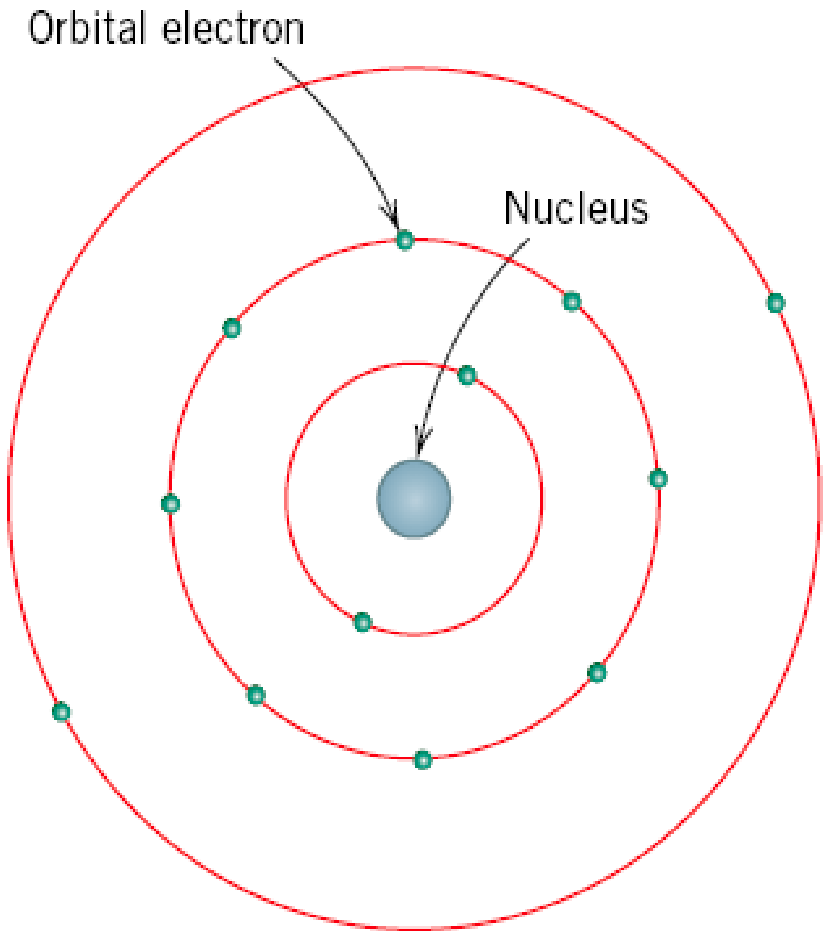



**Figure 2.1** Schematic representation of the Bohr atom.

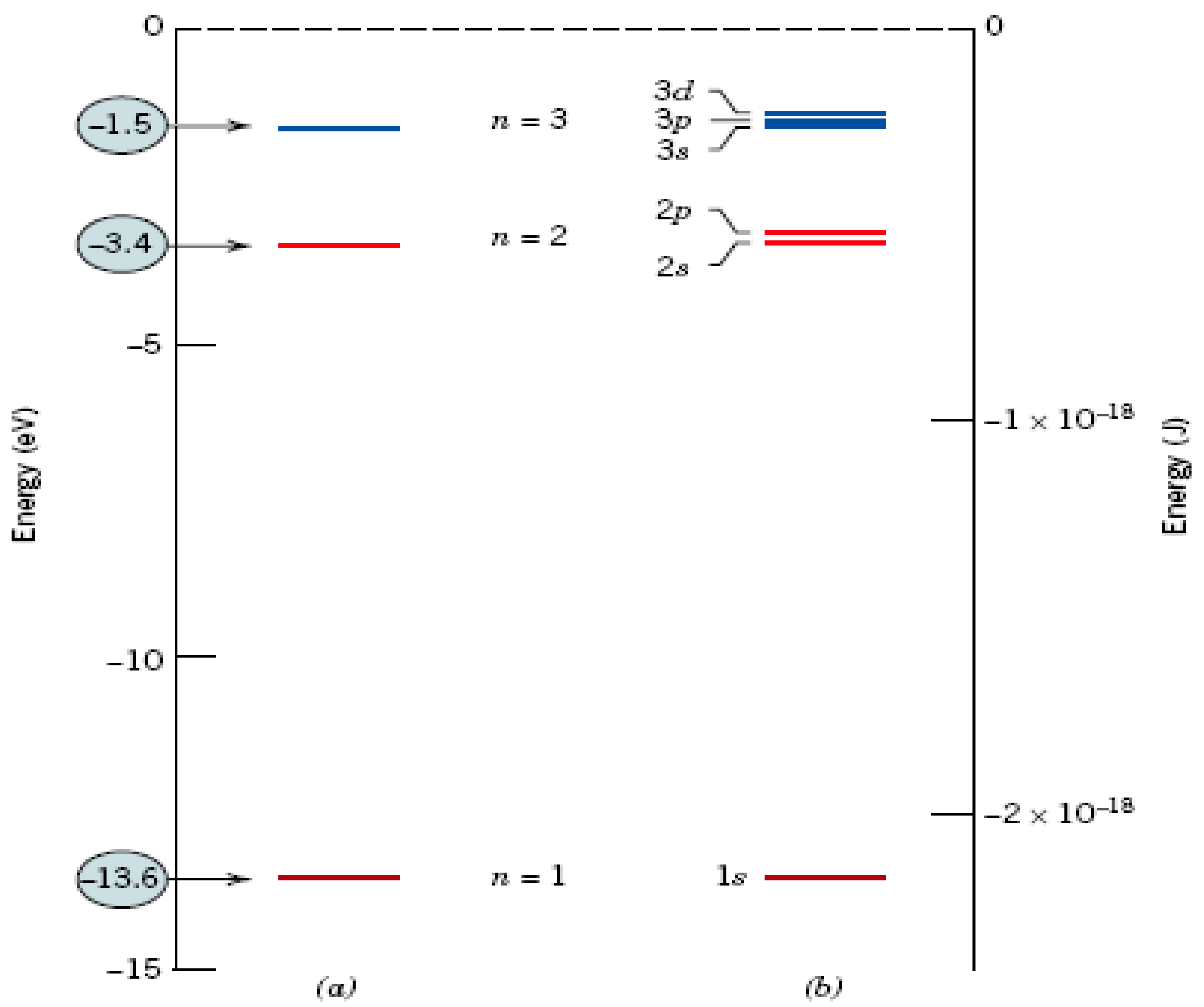



**Figure 2.2** (*a*) The first three electron energy states for the Bohr hydrogen atom. (*b*) Electron energy states for the first three shells of the wave-mechanical hydrogen atom. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 10. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

# 2. Bohr atomic model

- Bohr's theory was successful in that:
  1. It provided a physical model of the atom, whose internal energy levels matched those of the observed hydrogen spectrum.
  2. It accounted for the stability of atoms.
  3. It applied equally well to other one electron atoms such as a singly ionized helium ion.
- Bohr's theory failed in that:
  1. It broke down when applied to many electron atoms, because it took no account of the interactions between electrons in orbit.
  2. With the development of more precise spectroscope techniques, it became apparent that each of the excited states was not a unique single energy level, but a group of finely separated levels

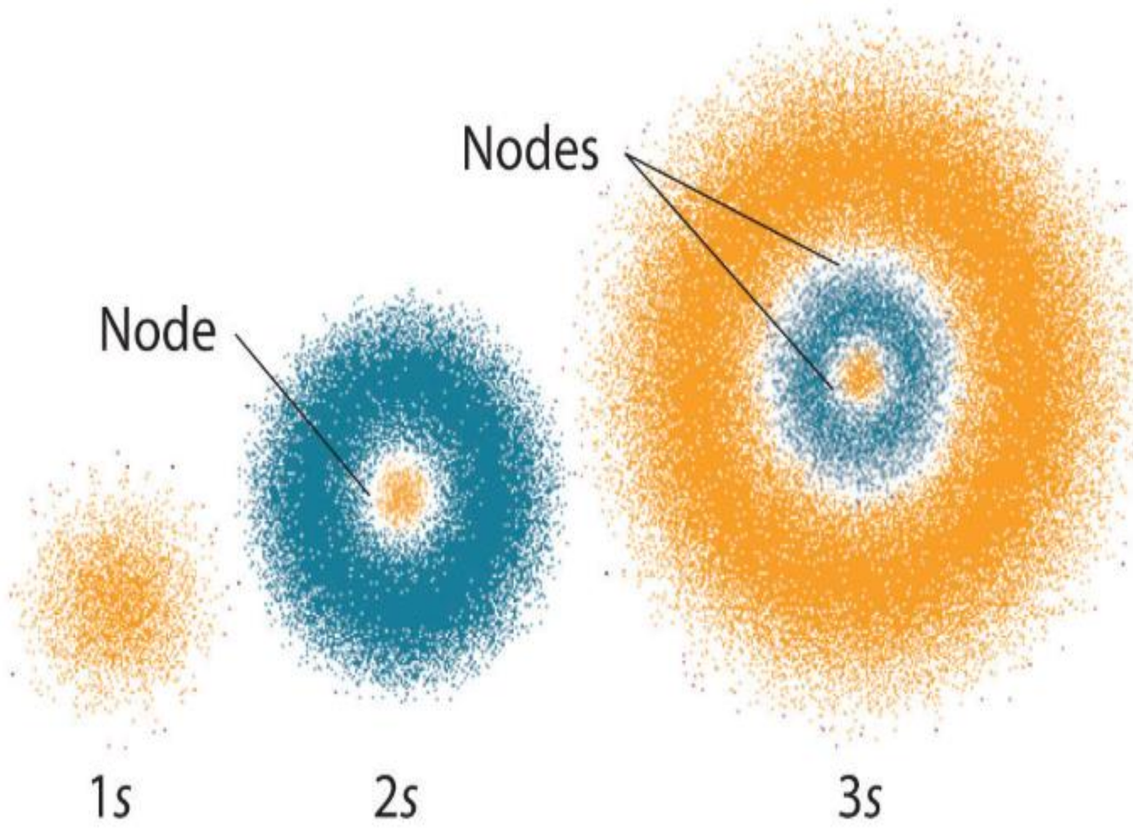
# 3. Wave-mechanical model Quantum Mechanical model

1. -Electrons are NOT in circular orbits around nucleus.
2. -Electrons are in a 3-D region around the nucleus called atomic orbitals.
3. -The atomic orbital describes the probable location of the electron
4. The quantum mechanical model describes the probable location of electrons in atoms by describing:

- Principal energy level [n] -------------- (1,2,3,4,5,6,7)
- Energy sublevel (angular moment quantum number) [L]----(0 =s,1 =p,2= d,3 =f)
- Orbital in each sublevel ($m_l$) (magnetic quantum number)---- (-L,L)

L= 0 ($m_l$ =0) L= 1 ($m_l$ =-1,0,1) ) L= 2 ($m_l$ =-2,-1,0,1,2) L= 3 ($m_l$ =-3,-2,-1,0,1,2,3)

- Spin ($m_s$) = (-1/2,1/2)




Probability distributions for 1s, 2s, and 3s orbitals. Greater color intensity indicates regions where electrons are more likely to exist. Nodes indicate regions where an electron has zero probability of being found. Image credit:

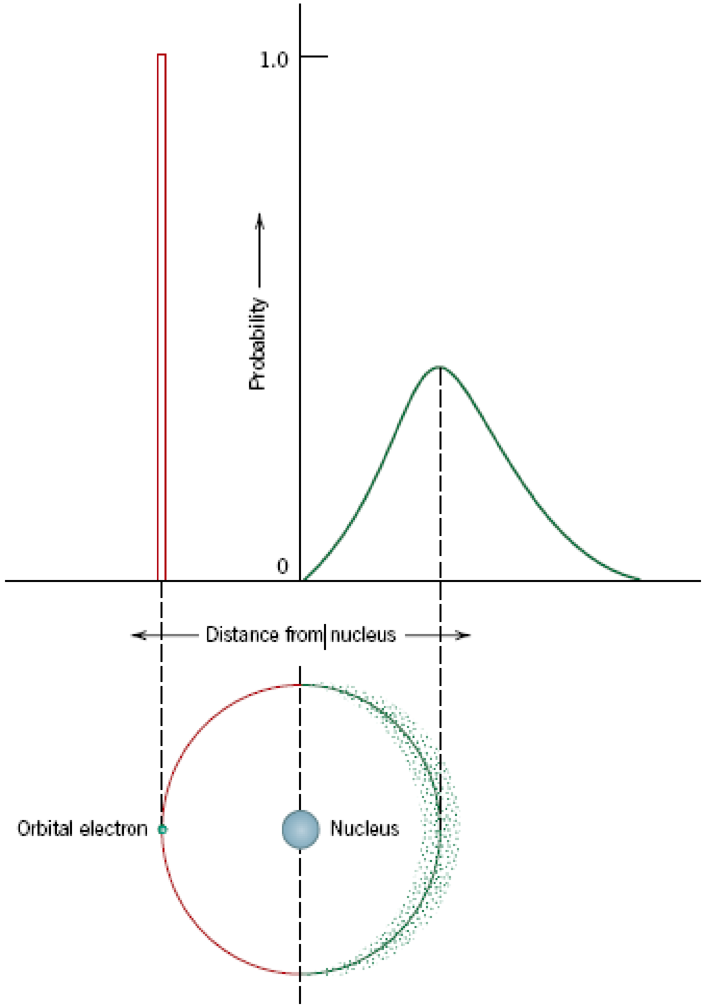



**Figure 2.3** Comparison of the (*a*) Bohr and (*b*) wave-mechanical atom models in terms of electron distribution. (Adapted from Z. D. Jastrzebski, *The Nature and Properties of Engineering Materials*, 3rd edition, p. 4. Copyright © 1987 by John Wiley & Sons, New York. Reprinted by permission of John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

# 4. ELECTRONS IN ATOMS

**Principal Energy Level (n) (**principal quantum number**)** "shells"

Indicates the relative size and energy of atomic orbitals.

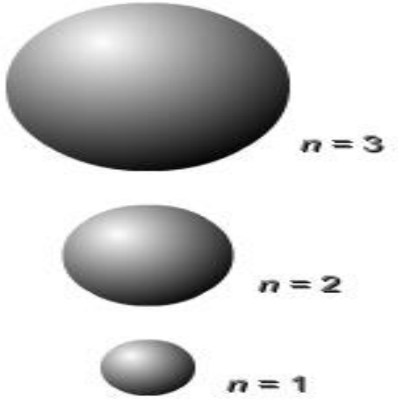
**n=integers:** n= 1, 2, 3, etc.

- As n increases:

> orbital becomes larger

> electron spends more time farther away from nucleus

➢ atom's energy level increases




As the principle quantum number *n* increases, the size and energy of the orbital both increase, but the shape remains essentially the same.

The general formula is that the *n*th shell can in principle hold up to 2($n^2$)
2($n^2$) electrons

The shells are labeled K, L, M, N, O, P, and Q; or 1, 2, 3, 4, 5, 6, and 7

# 4. ELECTRONS IN ATOMS

**Energy sublevel (*l*)** (The second quantum number)

Principal energy levels are broken down into sublevels.

- Sublevels define the orbital shape (s, p, d, f)

> n=1, 1 sublevel (s)

> n=2, 2 sublevels (s, p)

> n=3, 3 sublevels (s, p, d)

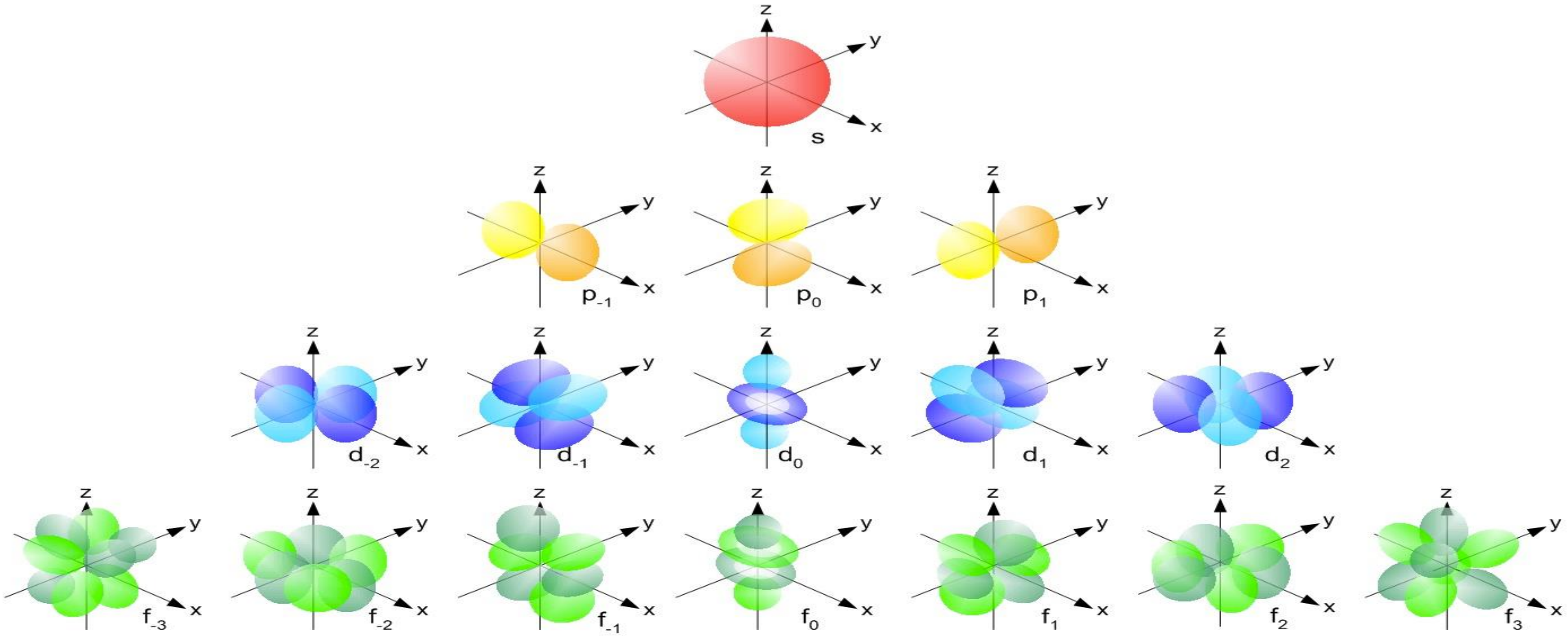
> n=4, 4 sublevels (s, p, d, f)

# 4. ELECTRONS IN ATOMS

**Orbitals** (in each sublevel) (third quantum number) $m_l$

Each sublevel has a different number of orbitals.

- s: 1 orbital
- p: 3 orbitals
- d: 5 orbitals
- f: 7 orbitals




•Forth quantum number $m_s$: spin moment of an electron Associated with each electron is a *spin moment*, which must be oriented either up or down

# 4. ELECTRONS IN ATOMS

**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 | Number of Electrons 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 | |

# 4. Electron configurations

Electron configurations are a simple way of writing down the locations of all of the electrons in an atom.

**Aufbau Principle**– Electrons enter orbit alsof lowest energy first.

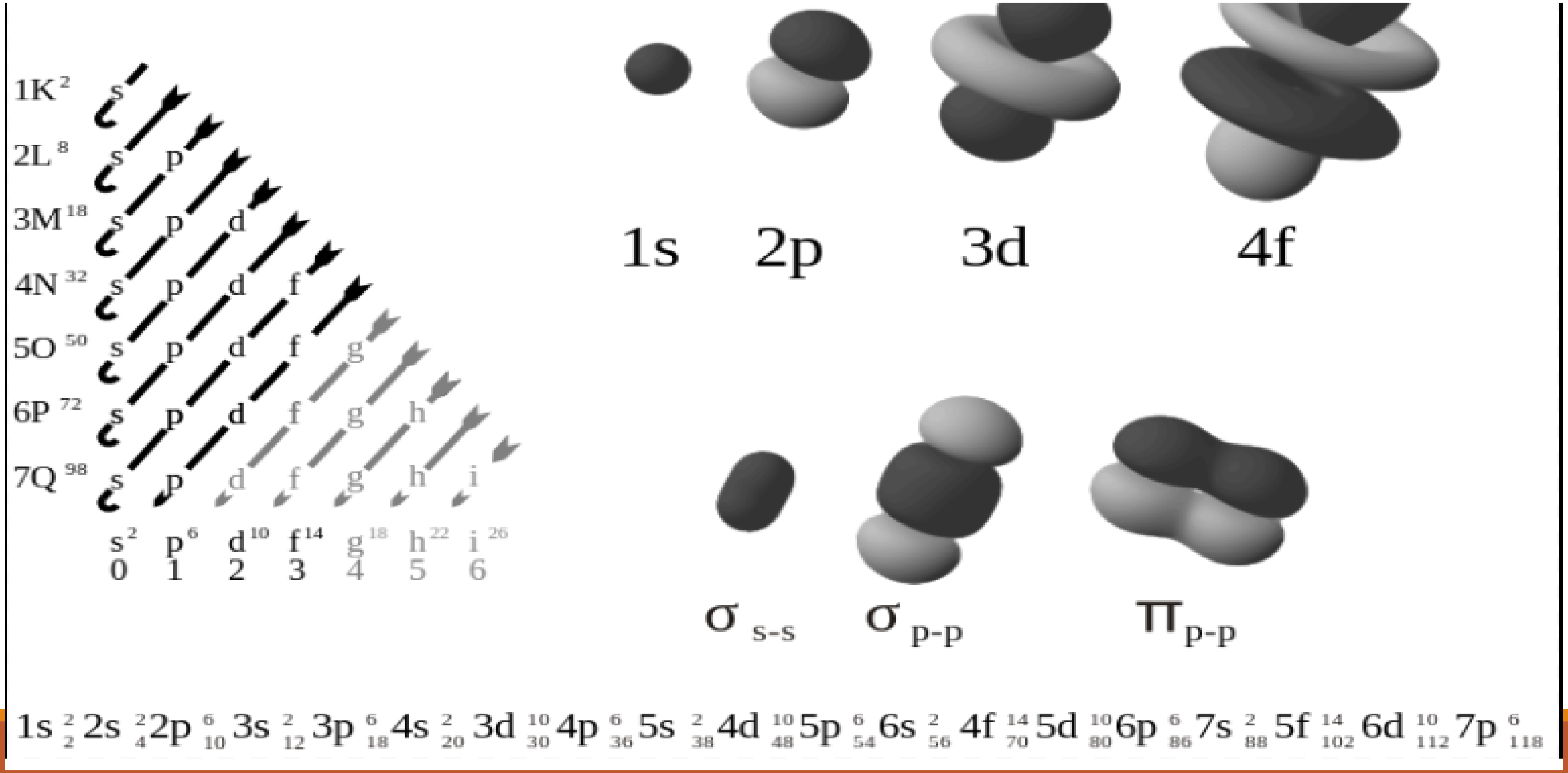


**Table 2.2 A Listing of the Expected Electron Configurations for Some of the Common Elements**[a]

| *Element* | *Symbol* | *Atomic Number* | *Electron Configu* |
|---|---|---|---|
| Hydrogen | H | 1 | $1s^1$ |
| Helium | He | 2 | $1s^2$ |
| Lithium | Li | 3 | $1s^22s^1$ |
| Beryllium | Be | 4 | $1s^22s^2$ |
| Boron | B | 5 | $1s^22s^22p^1$ |
| Carbon | C | 6 | $1s^22s^22p^2$ |
| Nitrogen | N | 7 | $1s^22s^22p^3$ |
| Oxygen | O | 8 | $1s^22s^22p^4$ |
| Fluorine | F | 9 | $1s^22s^22p^5$ |
| Neon | Ne | 10 | $1s^22s^22p^6$ |
| Sodium | Na | 11 | $1s^22s^22p^63s^1$ |
| Magnesium | Mg | 12 | $1s^22s^22p^63s^2$ |
| Aluminum | Al | 13 | $1s^22s^22p^63s^23p^1$ |
| Silicon | Si | 14 | $1s^22s^22p^63s^23p^2$ |
| Phosphorus | P | 15 | $1s^22s^22p^63s^23p^3$ |
| Sulfur | S | 16 | $1s^22s^22p^63s^23p^4$ |
| Chlorine | Cl | 17 | $1s^22s^22p^63s^23p^5$ |
| Argon | Ar | 18 | $1s^22s^22p^63s^23p^6$ |
| Potassium | K | 19 | $1s^22s^22p^63s^23p^64s^1$ |
| Calcium | Ca | 20 | $1s^22s^22p^63s^23p^64s^2$ |
| Scandium | Sc | 21 | $1s^22s^22p^63s^23p^63d^14s^2$ |
| Titanium | Ti | 22 | $1s^22s^22p^63s^23p^63d^24s^2$ |
| Vanadium | V | 23 | $1s^22s^22p^63s^23p^63d^34s^2$ |
| Chromium | Cr | 24 | $1s^22s^22p^63s^23p^63d^54s^1$ |
| Manganese | Mn | 25 | $1s^22s^22p^63s^23p^63d^54s^2$ |
| Iron | Fe | 26 | $1s^22s^22p^63s^23p^63d^64s^2$ |
| Cobalt | Co | 27 | $1s^22s^22p^63s^23p^63d^74s^2$ |
| Nickel | Ni | 28 | $1s^22s^22p^63s^23p^63d^84s^2$ |
| Copper | Cu | 29 | $1s^22s^22p^63s^23p^63d^{10}4s^1$ |
| Zinc | Zn | 30 | $1s^22s^22p^63s^23p^63d^{10}4s^2$ |
| Gallium | Ga | 31 | $1s^22s^22p^63s^23p^63d^{10}4s^24p^1$ |
| Germanium | Ge | 32 | $1s^22s^22p^63s^23p^63d^{10}4s^24p^2$ |
| Arsenic | As | 33 | $1s^22s^22p^63s^23p^63d^{10}4s^24p^3$ |
| Selenium | Se | 34 | $1s^22s^22p^63s^23p^63d^{10}4s^24p^4$ |
| Bromine | Br | 35 | $1s^22s^22p^63s^23p^63d^{10}4s^24p^5$ |
| Krypton | Kr | 36 | $1s^22s^22p^63s^23p^63d^{10}4s^24p^6$ |

[a] When some elements covalently bond, they form *sp* hybrid bonds. This is especially true for C, Si, and Ge.

# 4. ELECTRONS IN ATOMS

- the **valence electrons** are those that occupy the outermost shell. These electrons are extremely important; as will be seen, they participate in the bonding between atoms to form atomic and molecular aggregates. Furthermore, many of the physical and chemical properties of solids are based on these valence electrons.
- some atoms have what are termed stable electron configurations; that is, the states within the outermost or valence electron shell are completely.
- Normally this corresponds to the occupation of just the s and p states for the outermost shell by a total of eight electrons, as in neon, argon, and krypton; one exception is helium, which contains only two 1s electrons .These elements

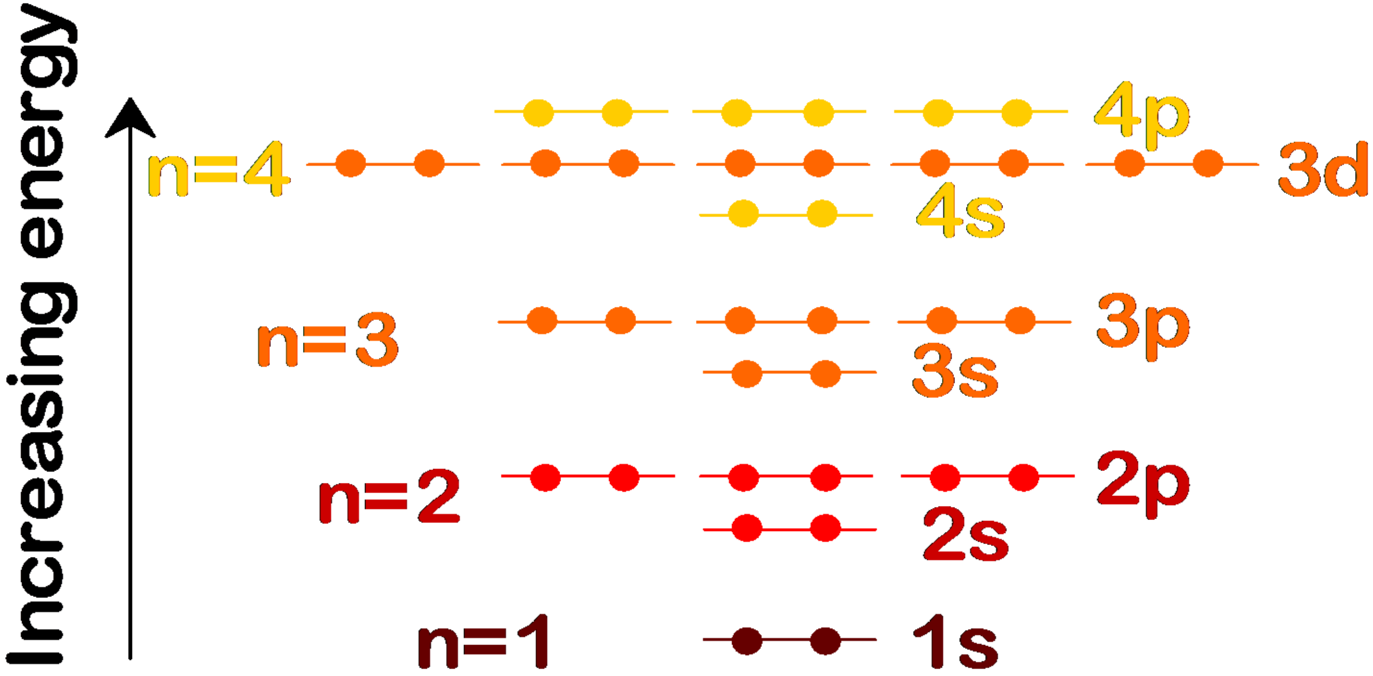
(Ne, Ar, Kr, and He) are the inert, or noble, gases, which are virtually unreactive chemically.

| 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 | $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ |

# 4. ELECTRONS IN ATOMS

have discrete energy states

- tend to occupy lowest available energy state



# 4. ELECTRONS IN ATOMS

**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 | $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ |

# 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 | $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4^6$ | (stable) |

Adapted from Table 2.2, *Callister 6e.*

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

# 5. THE PERIODIC TABLE

- All the elements have been classified according to electron configuration in the periodic table.
- the elements are situated, with increasing atomic number, in seven horizontal rows called periods. The arrangement is such that all elements arrayed in a given column or group have similar valence electron structures.
- The elements positioned in Group 0, the rightmost group, are the inert gases, noble gases
- **electropositive elements,** indicating that they are capable of giving up their few valence electrons to become positively charged ions
- **electronegative elements**, they readily accept electrons to form negatively charged ions, or sometimes they share electrons with other atoms

C Solid
Hg Liquid
H Gas
Rf Unknown

**Metals**: Alkali metals, Alkaline earth metals, Lanthanoids, Actinoids, Transition metals, Post-transition metals, Metalloids

**Nonmetals**: Other nonmetals, Noble gases

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 Pnictogens | 16 Chalcogens | 17 Halogens | 18 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 H Hydrogen 1.008 | Atomic Sym Name Weight | | | | | | | | | | | | | | | | 2 He Helium 4.0026 |
| 2 | 3 Li Lithium 6.94 | 4 Be Beryllium 9.0122 | | | | | | | | | | | 5 B Boron 10.81 | 6 C Carbon 12.011 | 7 N Nitrogen 14.007 | 8 O Oxygen 15.999 | 9 F Fluorine 18.998 | 10 Ne Neon 20.180 |
| 3 | 11 Na Sodium 22.990 | 12 Mg Magnesium 24.305 | | | | | | | | | | | 13 Al Aluminium 26.982 | 14 Si Silicon 28.085 | 15 P Phosphorus 30.974 | 16 S Sulfur 32.06 | 17 Cl Chlorine 35.45 | 18 Ar Argon 39.948 |
| 4 | 19 K Potassium 39.098 | 20 Ca Calcium 40.078 | 21 Sc Scandium 44.956 | 22 Ti Titanium 47.867 | 23 V Vanadium 50.942 | 24 Cr Chromium 51.996 | 25 Mn Manganese 54.938 | 26 Fe Iron 55.845 | 27 Co Cobalt 58.933 | 28 Ni Nickel 58.693 | 29 Cu Copper 63.546 | 30 Zn Zinc 65.38 | 31 Ga Gallium 69.723 | 32 Ge Germanium 72.630 | 33 As Arsenic 74.922 | 34 Se Selenium 78.971 | 35 Br Bromine 79.904 | 36 Kr Krypton 83.798 |
| 5 | 37 Rb Rubidium 85.468 | 38 Sr Strontium 87.62 | 39 Y Yttrium 88.906 | 40 Zr Zirconium 91.224 | 41 Nb Niobium 92.906 | 42 Mo Molybdenur 95.95 | 43 Tc Technetium (98) | 44 Ru Ruthenium 101.07 | 45 Rh Rhodium 102.91 | 46 Pd Palladium 106.42 | 47 Ag Silver 107.87 | 48 Cd Cadmium 112.41 | 49 In Indium 114.82 | 50 Sn Tin 118.71 | 51 Sb Antimony 121.76 | 52 Te Tellurium 127.60 | 53 I Iodine 126.90 | 54 Xe Xenon 131.29 |
| 6 | 55 Cs Caesium 132.91 | 56 Ba Barium 137.33 | 57–71 | 72 Hf Hafnium 178.49 | 73 Ta Tantalum 180.95 | 74 W Tungsten 183.84 | 75 Re Rhenium 186.21 | 76 Os Osmium 190.23 | 77 Ir Iridium 192.22 | 78 Pt Platinum 195.08 | 79 Au Gold 196.97 | 80 Hg Mercury 200.59 | 81 Tl Thallium 204.38 | 82 Pb Lead 207.2 | 83 Bi Bismuth 208.98 | 84 Po Polonium (209) | 85 At Astatine (210) | 86 Rn Radon (222) |
| 7 | 87 Fr Francium (223) | 88 Ra Radium (226) | 89–103 | 104 Rf Rutherfordiu (267) | 105 Db Dubnium (268) | 106 Sg Seaborgiur (269) | 107 Bh Bohrium (270) | 108 Hs Hassium (277) | 109 Mt Meitnerium (278) | 110 Ds Darmstadtiu (281) | 111 Rg Roentgeniu (282) | 112 Cn Copernicium (285) | 113 Nh Nihonium (286) | 114 Fl Flerovium (289) | 115 Mc Moscovium (290) | 116 Lv Livermoriur (293) | 117 Ts Tennessine (294) | 118 Og Oganesson (294) |

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

Periodic Table Design & Interface Copyright © 1997 Michael Dayah. Ptable.com Last updated Jun 16, 2017

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 57 La Lanthanum 138.91 | 58 Ce Cerium 140.12 | 59 Pr Praseodymi 140.91 | 60 Nd Neodymiur 144.24 | 61 Pm Promethiur (145) | 62 Sm Samarium 150.36 | 63 Eu Europium 151.96 | 64 Gd Gadolinium 157.25 | 65 Tb Terbium 158.93 | 66 Dy Dysprosium 162.50 | 67 Ho Holmium 164.93 | 68 Er Erbium 167.26 | 69 Tm Thulium 168.93 | 70 Yb Ytterbium 173.05 | 71 Lu Lutetium 174.97 |
| 89 Ac Actinium (227) | 90 Th Thorium 232.04 | 91 Pa Protactiniur 231.04 | 92 U Uranium 238.03 | 93 Np Neptunium (237) | 94 Pu Plutonium (244) | 95 Am Americium (243) | 96 Cm Curium (247) | 97 Bk Berkelium (247) | 98 Cf Californium (251) | 99 Es Einsteinium (252) | 100 Fm Fermium (257) | 101 Md Mendeleviu (258) | 102 No Nobelium (259) | 103 Lr Lawrencìur (266) |

alkaline earth metals

Key

| 29 Cu 63.55 |
|---|

- 29 — Atomic number
- Cu — Symbol
- 63.55 — Atomic weight

- Metal
- Nonmetal
- Intermediate

the inert gases

halogens

transition metals

d

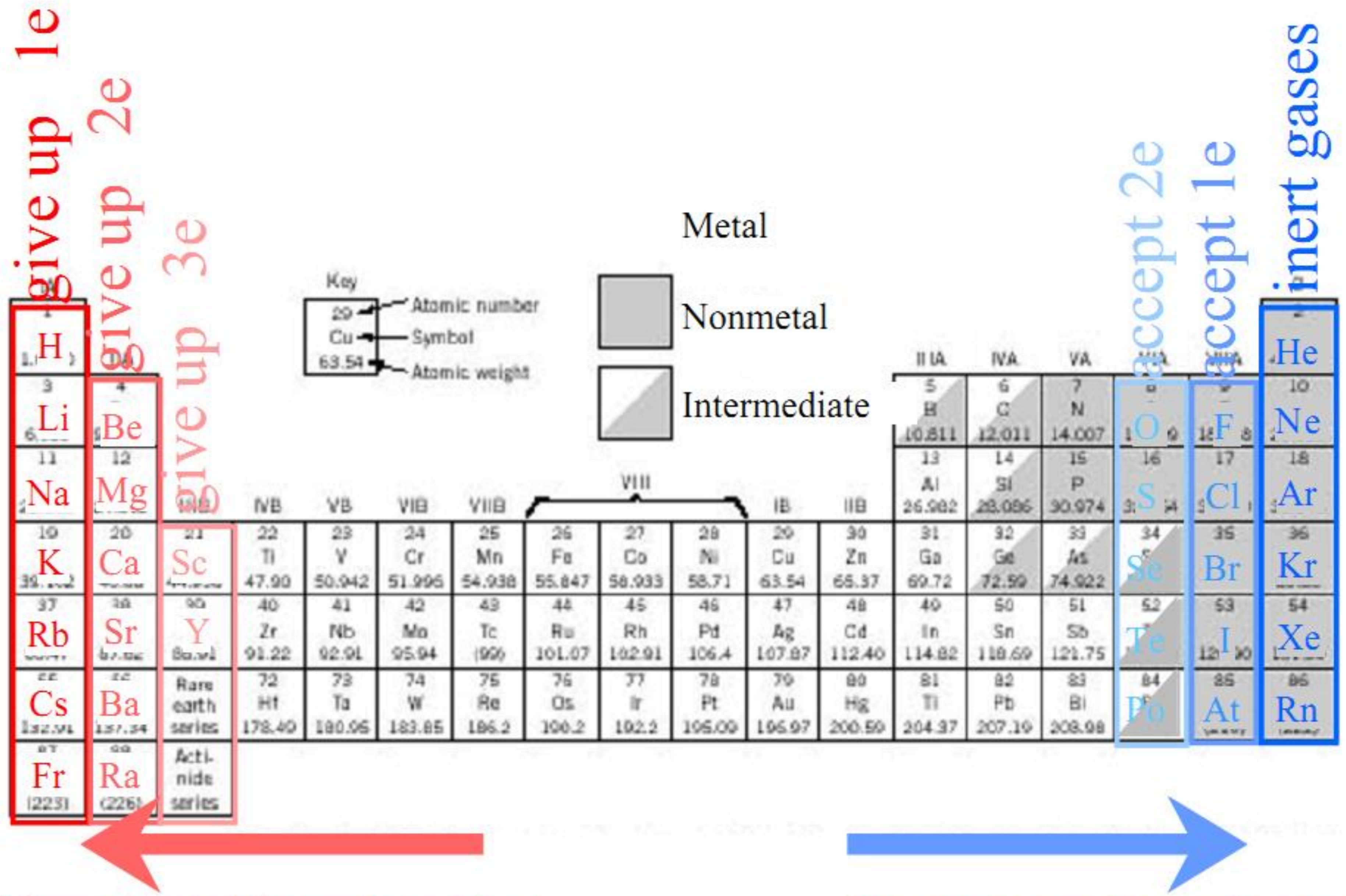
| IA | IIA | IIIB | IVB | VB | VIB | VIIB | | VIII | | IB | IIB | IIIA | IVA | VA | VIA | VIIA | 0 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 H 1.0080 | | | | | | | | | | | | | | | | | 2 He 4.0026 |
| 3 Li 6.941 | 4 Be 9.0122 | | | | | | | | | | | 5 B 10.811 | 6 C 12.011 | 7 N 14.007 | 8 O 15.999 | 9 F 18.998 | 10 Ne 20.180 |
| 11 Na 22.990 | 12 Mg 24.305 | | | | | | | | | | | 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 39.098 | 20 Ca 40.08 | 21 Sc 44.956 | 22 Ti 47.87 | 23 V 50.942 | 24 Cr 51.996 | 25 Mn 54.938 | 26 Fe 55.845 | 27 Co 58.933 | 28 Ni 58.69 | 29 Cu 63.55 | 30 Zn 65.41 | 31 Ga 69.72 | 32 Ge 72.64 | 33 As 74.922 | 34 Se 78.96 | 35 Br 79.904 | 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 (98) | 44 Ru 101.07 | 45 Rh 102.91 | 46 Pd 106.4 | 47 Ag 107.87 | 48 Cd 112.41 | 49 In 114.82 | 50 Sn 118.71 | 51 Sb 121.76 | 52 Te 127.60 | 53 I 126.90 | 54 Xe 131.30 |
| 55 Cs 132.91 | 56 Ba 137.33 | Rare earth series | 72 Hf 178.49 | 73 Ta 180.95 | 74 W 183.84 | 75 Re 186.2 | 76 Os 190.23 | 77 Ir 192.2 | 78 Pt 195.08 | 79 Au 196.97 | 80 Hg 200.59 | 81 Tl 204.38 | 82 Pb 207.19 | 83 Bi 208.98 | 84 Po (209) | 85 At (210) | 86 Rn (222) |
| 87 Fr (223) | 88 Ra (226) | Acti-nide series | 104 Rf (261) | 105 Db (262) | 106 Sg (266) | 107 Bh (264) | 108 Hs (277) | 109 Mt (268) | 110 Ds (281) | | | | | | | | |

S

P

F

| | 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 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 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 231.04 | 92 U 238.03 | 93 Np (237) | 94 Pu (244) | 95 Am (243) | 96 Cm (247) | 97 Bk (247) | 98 Cf (251) | 99 Es (252) | 100 Fm (257) | 101 Md (258) | 102 No (259) | 103 Lr (262) |

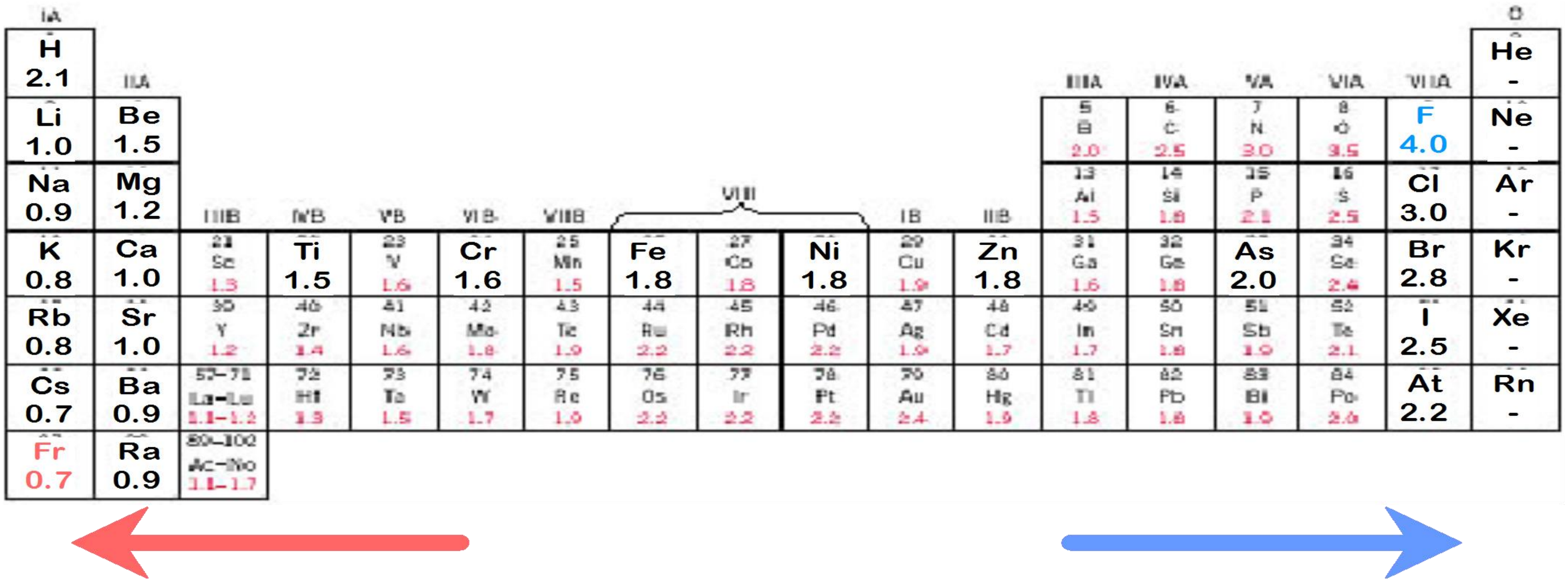



Electropositive elements:
Readily give up electrons

Electronegative elements:
Readily acquire electrons

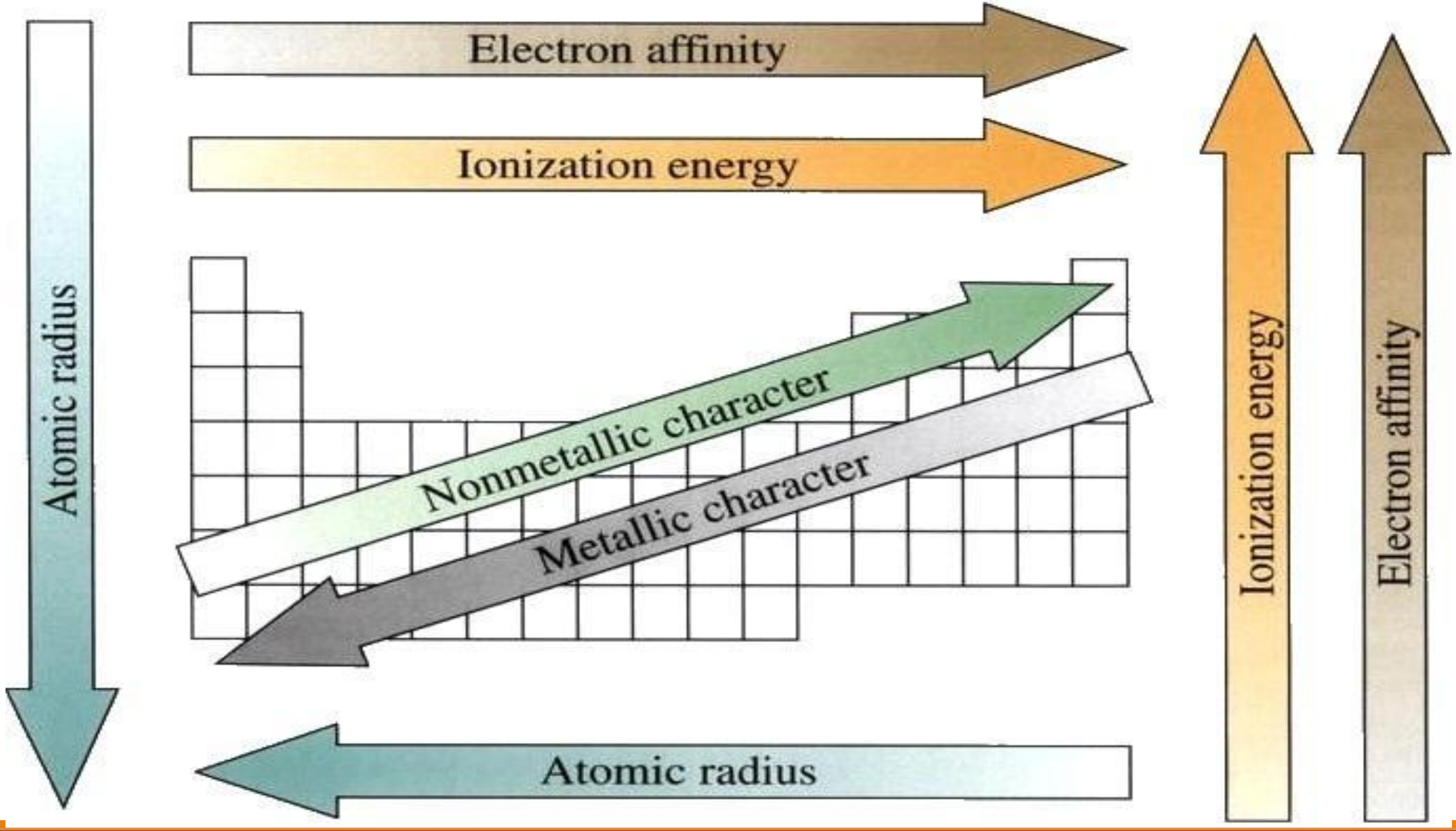
# ELECTRONEGATIVITY

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




Smaller electronegativity Larger electronegativity

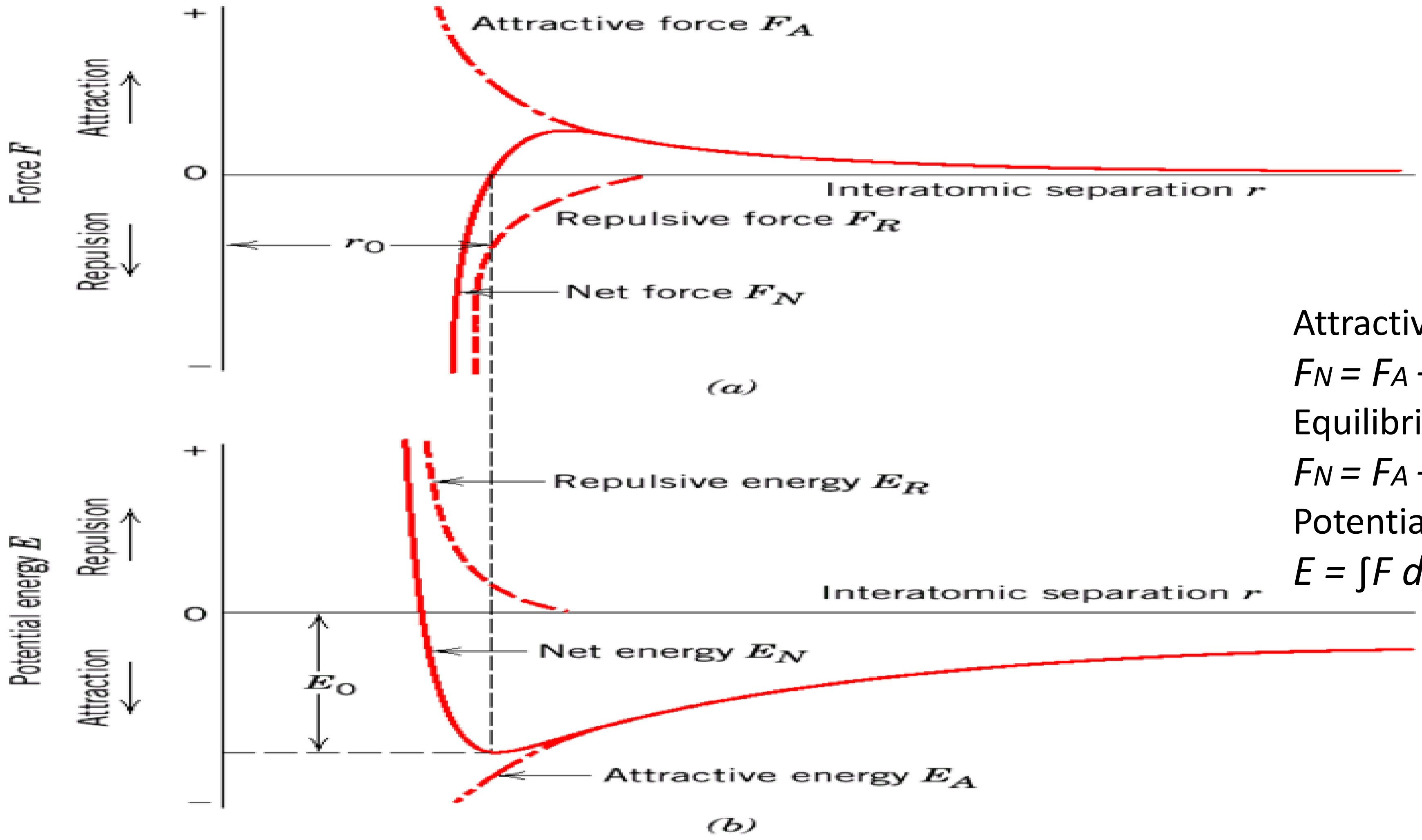
Adapted from Fig. 2.7, *Callister 6e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.


Electron affinity
Ionization energy
Nonmetallic character
Metallic character
Atomic radius
Atomic radius
Ionization energy
Electron affinity

# 6. MOLECULES

- Many of the common molecules are composed of groups of atoms that are bound together by strong covalent bonds; these include elemental diatomic molecules ($F_2$, $O_2$, $H_2$, etc.) as well as a host of compounds ($H_2O$, $CO_2$, $HNO_3$, $C_6H_6$, $CH_4$, etc.).
- In the condensed liquid and solid states, bonds between molecules are weak secondary ones. Consequently, molecular materials have relatively low melting and boiling temperatures. Most of those that have small molecules composed of a few atoms are gases at ordinary, or ambient, temperatures and pressures.
- On the other hand, many of the modern polymers, being molecular materials composed of extremely large molecules, exist as solids

# 7. BONDING FORCES AND ENERGIES




Attractive force and repulsive force

$F_N = F_A + F_R$

Equilibrium State

$F_N = F_A + F_R = 0$

Potential Energy

$E = \int F\,dr E_N = E_A + E_R$

# 7. BONDING FORCES AND ENERGIES

## A. Primary interatomic bonds

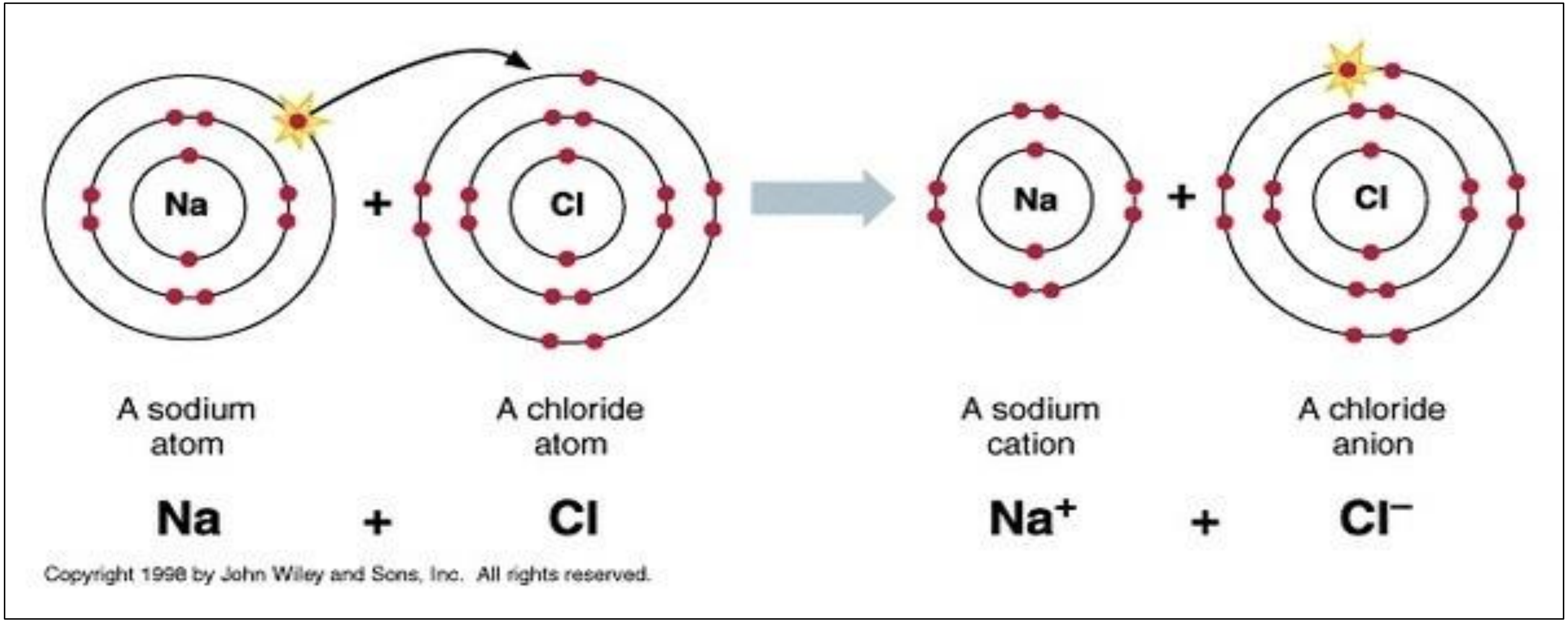
### (1) Ionic Bonding

- It is always found in compounds that are composed of both metallic and nonmetallic elements.
- Atoms of a metallic element easily give up their valence electrons to the nonmetallic atoms
- In the process all the atoms acquire stable or inert gas configurations and, in addition, an electrical charge; that is, they become ions
- Large difference in electronegativity required (>2)

# 7. BONDING FORCES AND ENERGIES

## (1) Ionic Bonding Example

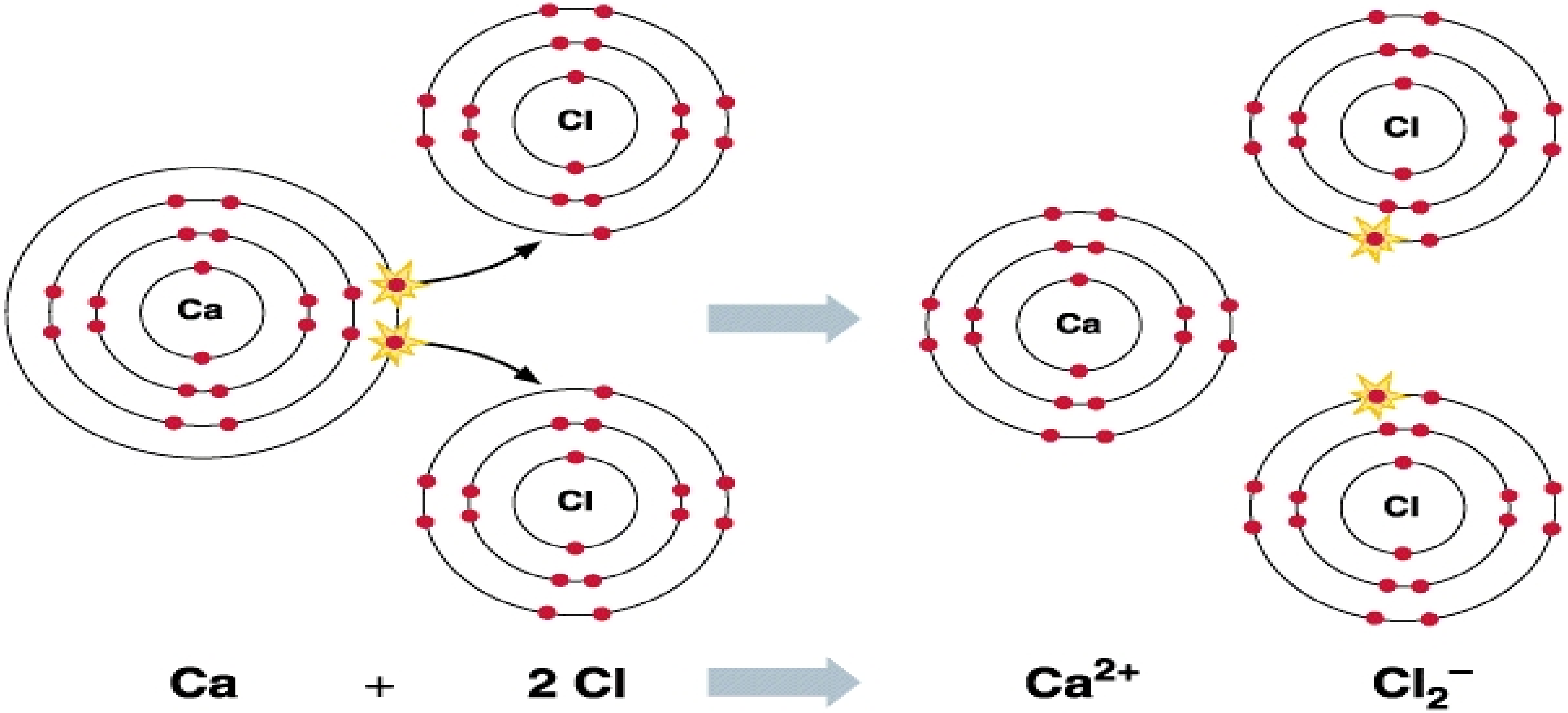
### Example 1: NaCl



# 7. BONDING FORCES AND ENERGIES

## (1) Ionic Bonding Example

**Example 2: $CaCl_2$**



# 7. BONDING FORCES AND ENERGIES

the attractive energy EA and the repulsion energy ER are function of the interatomic distance according to

$$E_A = \frac{A}{r} \qquad E_R = \frac{B}{r^n} \qquad where, A = \frac{1}{4\pi\epsilon_0}(Z_1 e)(Z_2 e)$$

where is the permittivity of a vacuum (8.85  $10^{-12}$ F/m), *Z*1 and *Z*2 are the valences of the two ion types, and *e* is the electronic charge (1.602  $10^{-19}$ C). In these expressions, *A*, *B*, and *n* are constants whose values depend on the particular ionic system. The value of *n* is approximately 8.

https://sciencenotes.org/valences-of-the-elements/

# 7. BONDING FORCES AND ENERGIES

## (2) Covalent Bonding

- A covalent bond, also called a molecular bond, is a chemical bond that involves the sharing of electron pairs between atoms. These electron pairs are known as shared pairs or bonding pairs.
- A covalent bond is constructed If the electronegativity is less than 1.7.
- Many nonmetallic elemental molecules ($H_2$, $Cl_2$, $F_2$, etc.) as well as molecules containing dissimilar atoms, such as $CH_4$, $H_2O$, $HNO_3$, and HF, are covalently bonded. Furthermore, this type of bonding is found in elemental solids such as diamond (carbon), silicon, and germanium and other solid compounds composed of elements that are located on the right-hand side of the periodic table, such as gallium arsenide (GaAs), indium antimonide (InSb), and silicon carbide (SiC).

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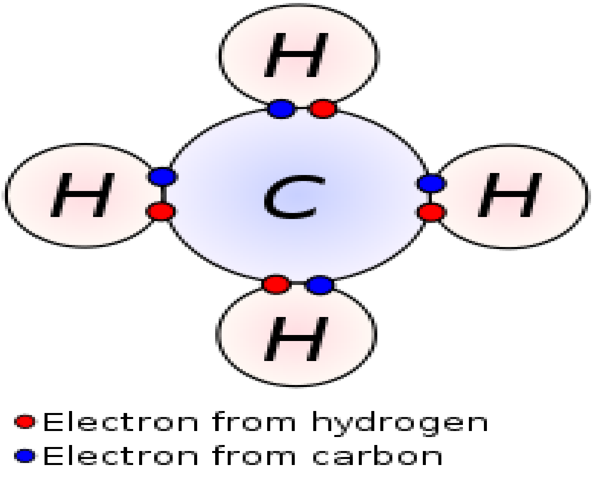
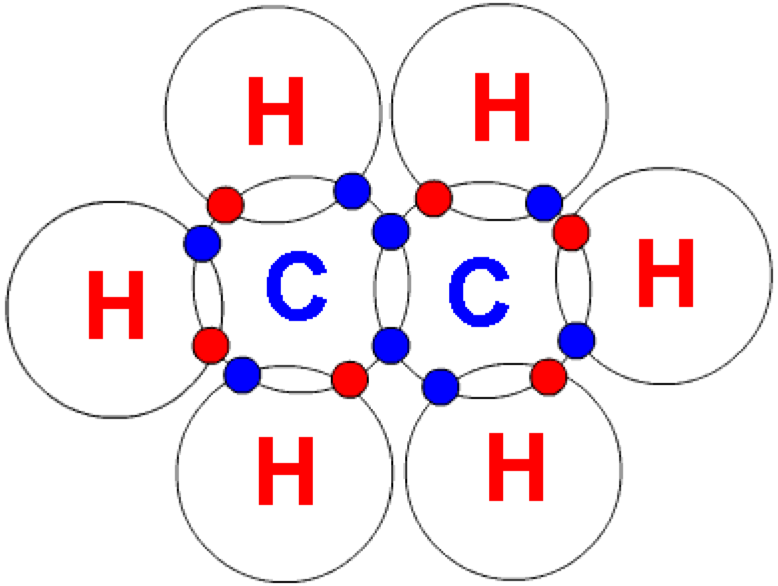
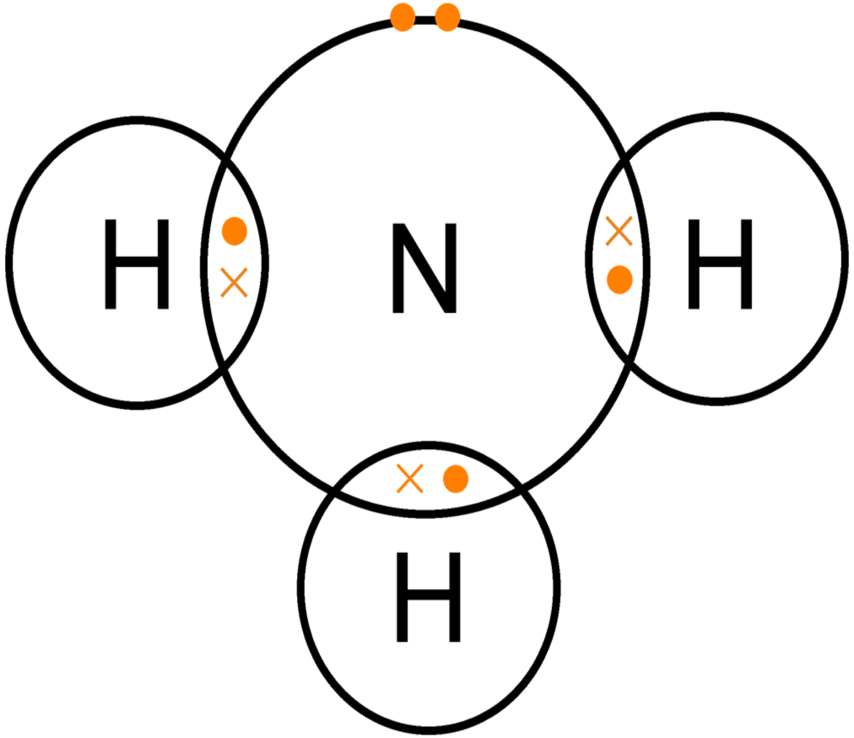
# 7. BONDING FORCES AND ENERGIES

## (2) Covalent Bonding

### Examples



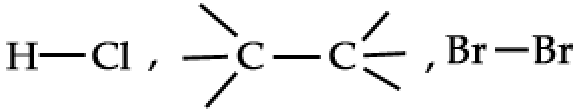
# 7. BONDING FORCES AND ENERGIES

## (2) Covalent Bonding

There are three types of covalent bond depending upon the number of shared electron pairs.

### (1) Single covalent bond

A covalent bond formed by the mutual sharing of one electron pair between two atoms is called a "single covalent bond.“




### (2) double covalent bond

A covalent bond formed between two atoms by the mutual sharing of two electron pairs is called a "double covalent bond“


### (3) triple covalent bond

A covalent bond formed by the mutual sharing of three electron pairs is called a "Triple covalent bond".

$N\equiv N$, $-C\equiv C-$

# 7. BONDING FORCES AND ENERGIES

## (4) Polar covalent bond

A covalent bond formed between two different atoms is known as Polar covalent bond. For example when a Covalent bond is formed between H and Cl , it is polar in nature because Cl is more electronegative than H atom . Therefore, electron cloud is shifted towards Cl atom. Due to this reason a partial -ve charge appeared on Cl atom and an equal +ve charge on H ------()

$H^{+\delta} - Cl^{-\delta}$

$H^{+\delta} - F^{-\delta}$

## (5) Non-polar bond

A covalent bond formed between two like atoms is known as Non-polar bond. Since difference of electro negativity is zero therefore, both atoms attract electron pair equally and no charge appears on any atom and the whole molecule becomes neutral.

H – H

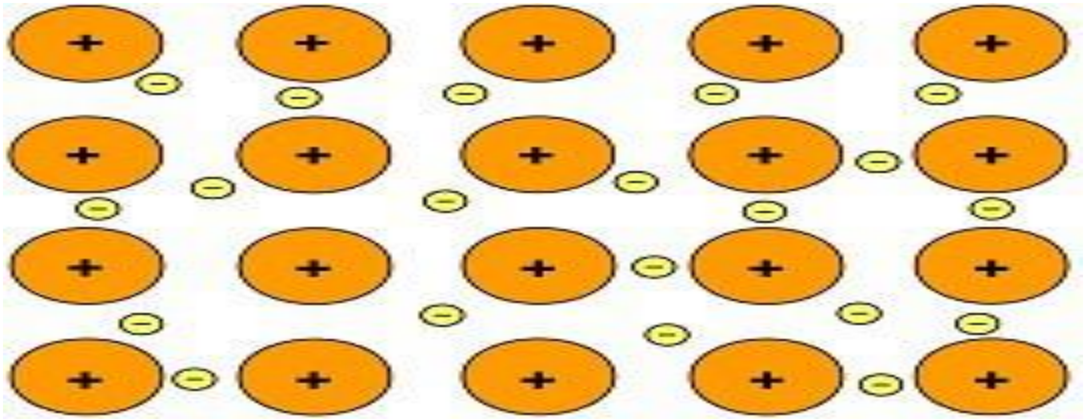
Cl – Cl

F – F

# 7. BONDING FORCES AND ENERGIES

## (3) Metallic Bonding

- **Metallic bonding,** the final primary bonding type, is found in metals and their alloys.
- **Metallic bonding** is a type of chemical bonding that arises from the electrostatic attractive force between conduction electrons (in the form of an electron cloud of delocalized electrons) and positively charged metal ions. It may be described as the sharing of free electrons among a lattice of positively charged ions (cations).
- Metallic bonding is found in the periodic table for Group IA and IIA elementsand, in fact, for all elemental metals



# 7. BONDING FORCES AND ENERGIES

## B. Secondary bonding or van der waals bonding

- **Secondary, van der Waals,** or physical **bonds** are weak in comparison to the primary or chemical ones; bonding energies are typically on the order of only 10 kJ/mol (0.1 eV/atom).
- Secondary bonds are weak in comparison to primary bonds
- They are found in most materials, but their effects are often overshadowed by the strength of the primary bonding.
- Secondary bonding is evidenced for the inert gases, which have stable electron structures, and, in addition, between molecules in molecular structures that are covalently bonded.

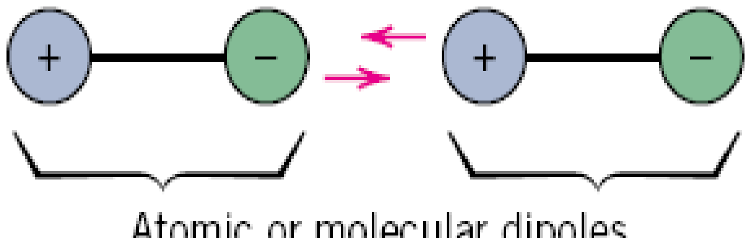


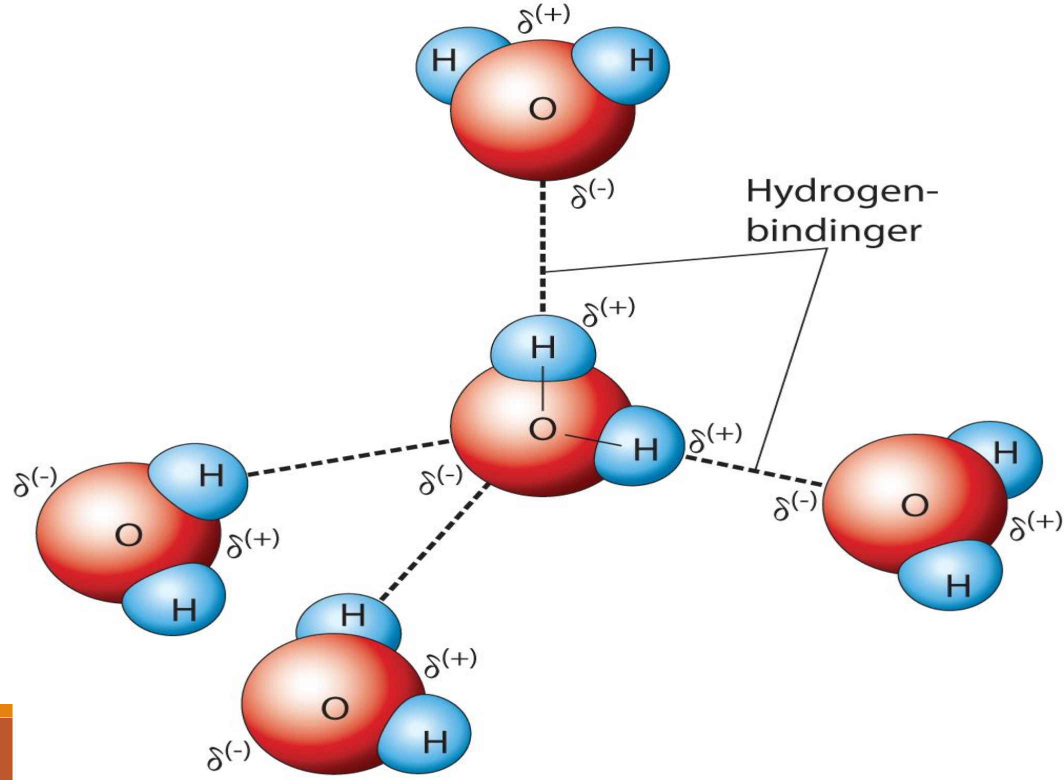

**Figure 2.12** Schematic illustration of van der Waals bonding between two dipoles.

# 7. BONDING FORCES AND ENERGIES

## Hydrogen bonding

- **Hydrogen bonding,** a special type of secondary bonding, is found to exist between some molecules that have hydrogen as one of the constituents
- hydrogen bond is a partially electrostatic attraction between a hydrogen (H) which is bound to a more

electronegative atom such as nitrogen (N),
oxygen (O), or fluorine (F),
and another adjacent atom bearing a lone
pair of electrons



# 7. BONDING FORCES AND ENERGIES

**Table 2.3** **Bonding Energies and Melting Temperatures for Various Substances**

| *Bonding Type* | *Substance* | *Bonding Energy* *kJ/mol* | *Bonding Energy* *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 |

**Table 2.3 Bonding Energies and Melting Temperatures for Various Substances**

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# 7. Important problems

**Problem 1**

## Average Atomic Weight Computation for Cerium

Cerium has four naturally occurring isotopes: 0.185% of $^{136}Ce$, with an atomic weight of 135.907 amu; 0.251% of $^{138}Ce$, with an atomic weight of 137.906 amu; 88.450% of $^{140}Ce$, with an atomic weight of 139.905 amu; and 11.114% of $^{142}Ce$, with an atomic weight of 141.909 amu. Calculate the average atomic weight of Ce.

# 7. Important problems

## Problem 2

### Computation of Attractive and Repulsive Forces between Two Ions

The atomic radii of $K^+$ and $Br^-$ ions are 0.138 and 0.196 nm, respectively.

**(a)** Using Equations 2.9 and 2.10, calculate the force of attraction between these two ions at their equilibrium interionic separation (i.e., when the ions just touch one another).

**(b)** What is the force of repulsion at this same separation distance?