Chapter 2: Atomic structure and interatomic bonding

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

- 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 = $6.023 \times 10^{23}$ 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

Bohr hydrogen model

Wave-mechanical hydrogen

Quantum numbers

- Principle quantum number $n=1, 2, \ldots; K, L, M, N, O$
- Orbital quantum number $l=0, \ldots, n-1$; subshell, $s, p, d, \text{or } f$; 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 Shell | Number of States | Number of Electrons | Per Subshell | Per Shell |
| $n=1$ | $K$ | $s$ | 1 | 2 | 2 |
| | | $p$ | 3 | 6 | 8 |
| $n=2$ | $L$ | $s$ | 1 | 2 | 8 |
| | | $p$ | 3 | 6 | 18 |
| | | $d$ | 5 | 10 | |
| | | $f$ | 7 | 14 | |
| $n=3$ | $M$ | $s$ | 1 | 2 | |
| | | $p$ | 3 | 6 | 18 |
| | | $d$ | 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

- n=4
- n=3
- n=2
- n=1

Stable electron configurations...
- have complete s and p subshells
- tend to be unreactive

Z Element Configuration

2 He $1s^2$
10 Ne $1s^22s^22p^6$
18 Ar $1s^22s^22p^63s^23p^6$
36 Kr $1s^22s^22p^63s^23p^64s^23d^{10}4p^6$

The periodic table

alkaline
Alkaline-earth

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
  - $E_A = -A/r, E_r = B/r^n, n \sim 8$

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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

- **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