Chapter 2: Atomic structure and interatomic bonding

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

- Columns: Similar Valence Structure

Electropositive elements: Readily give up electrons to become + ions.

Electronegative elements: Readily acquire electrons to become - ions.
Chapter 2: Atomic structure and interatomic bonding

- **Fundamental concepts**
  - Proton and electron, charged $1.60 \times 10^{-19}$ C
  - Mass of electron $9.11 \times 10^{-31}$ kg
  - Mass of protons and neutrons $1.67 \times 10^{-27}$ kg
  - Atomic number: the number of protons
  - Atomic mass = protons + neutrons
  - Isotope
  - Atomic mass unit (amu): $1$ amu = $1/12$ 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

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

**Table 2.1** The Number of Available Electron States in Some of the Electron Shells and Subshells

<table>
<thead>
<tr>
<th>Principal Quantum Number $n$</th>
<th>Shell Designation</th>
<th>Subshells</th>
<th>Number of States</th>
<th>Number of Electrons Per Subshell</th>
<th>Number of Electrons Per Shell</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>K</td>
<td>s</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>s</td>
<td>1</td>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>p</td>
<td>3</td>
<td>6</td>
<td>8</td>
</tr>
<tr>
<td>2</td>
<td>L</td>
<td>s</td>
<td>1</td>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>p</td>
<td>3</td>
<td>6</td>
<td>18</td>
</tr>
<tr>
<td></td>
<td></td>
<td>d</td>
<td>5</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>s</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>M</td>
<td>p</td>
<td>3</td>
<td>6</td>
<td>18</td>
</tr>
<tr>
<td></td>
<td></td>
<td>d</td>
<td>5</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>f</td>
<td>7</td>
<td>14</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>N</td>
<td>p</td>
<td>3</td>
<td>6</td>
<td>32</td>
</tr>
</tbody>
</table>
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

Relative energies of the electrons for various shells and subshells
Electronic Configurations

ex: Fe - atomic # = 26 1s² 2s² 2p⁶ 3s² 3p⁶ 3d⁶ 4s²

K-shell  n = 1
L-shell  n = 2
M-shell  n = 3
N-shell  n = 4

Adapted from Fig. 2.4, Callister 7e.
# The Periodic Table

- **Columns:** Similar Valence Structure

## Electropositive Elements:
- Readily give up electrons to become + ions.

## Electronegative Elements:
- Readily acquire electrons to become - ions.

### Metal

<table>
<thead>
<tr>
<th>Element</th>
<th>Group</th>
<th>Period</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Li</td>
<td>1A</td>
<td>2</td>
</tr>
<tr>
<td>Na</td>
<td>1A</td>
<td>3</td>
</tr>
<tr>
<td>K</td>
<td>1A</td>
<td>4</td>
</tr>
<tr>
<td>Rb</td>
<td>1A</td>
<td>5</td>
</tr>
<tr>
<td>Cs</td>
<td>1A</td>
<td>6</td>
</tr>
<tr>
<td>Fr</td>
<td>1A</td>
<td>7</td>
</tr>
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</table>

### Nonmetal

<table>
<thead>
<tr>
<th>Element</th>
<th>Group</th>
<th>Period</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Ne</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>Ar</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>Kr</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>Xe</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>Rn</td>
<td>0</td>
<td>6</td>
</tr>
</tbody>
</table>

### Intermediate

<table>
<thead>
<tr>
<th>Element</th>
<th>Group</th>
<th>Period</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Be</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Mg</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Al</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Si</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>P</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>S</td>
<td>3</td>
<td>7</td>
</tr>
<tr>
<td>Cl</td>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>Ar</td>
<td>18</td>
<td>8</td>
</tr>
</tbody>
</table>

### Inert Gases

<table>
<thead>
<tr>
<th>Element</th>
<th>Group</th>
<th>Period</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ne</td>
<td>0</td>
<td>2</td>
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<tr>
<td>Ar</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>Kr</td>
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<td>Xe</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>Rn</td>
<td>0</td>
<td>6</td>
</tr>
</tbody>
</table>

## Adapted from Fig. 2.6, *Callister 7e.*
### Electronegativity

- Ranges from **0.7** to **4.0**,
- Large values: tendency to 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.)
The periodic table (continued)

- **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**
SURVEY OF ELEMENTS

- Most elements: Electron configuration **not stable**.

<table>
<thead>
<tr>
<th>Element</th>
<th>Atomic #</th>
<th>Electron configuration</th>
<th>Atomic #</th>
<th>Electron configuration</th>
<th>Atomic #</th>
<th>Electron configuration</th>
<th>Atomic #</th>
<th>Electron configuration</th>
<th>Atomic #</th>
<th>Electron configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>1</td>
<td>$1s^1$</td>
<td>Sodium</td>
<td>$1s^22s^22p^63s^1$</td>
<td>11</td>
<td>$1s^22s^22p^63s^1$</td>
<td>11</td>
<td>$1s^22s^22p^63s^1$</td>
<td>11</td>
<td>$1s^22s^22p^63s^1$</td>
</tr>
<tr>
<td>Helium</td>
<td>2</td>
<td>$1s^2$ (stable)</td>
<td>Magnesium</td>
<td>$1s^22s^22p^63s^2$</td>
<td>12</td>
<td>$1s^22s^22p^63s^2$</td>
<td>12</td>
<td>$1s^22s^22p^63s^2$</td>
<td>12</td>
<td>$1s^22s^22p^63s^2$</td>
</tr>
<tr>
<td>Lithium</td>
<td>3</td>
<td>$1s^22s^1$</td>
<td>Aluminum</td>
<td>$1s^22s^22p^63s^23p^1$</td>
<td>13</td>
<td>$1s^22s^22p^63s^23p^1$</td>
<td>13</td>
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<td>13</td>
<td>$1s^22s^22p^63s^23p^1$</td>
</tr>
<tr>
<td>Beryllium</td>
<td>4</td>
<td>$1s^22s^2$</td>
<td>Argon</td>
<td>$1s^22s^22p^63s^23p^6$</td>
<td>18</td>
<td>$1s^22s^22p^63s^23p^6$</td>
<td>18</td>
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<td>18</td>
<td>$1s^22s^22p^63s^23p^6$</td>
</tr>
<tr>
<td>Boron</td>
<td>5</td>
<td>$1s^22s^22p^1$</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Carbon</td>
<td>6</td>
<td>$1s^22s^22p^2$</td>
<td>Neon</td>
<td>$1s^22s^22p^6$ (stable)</td>
<td>10</td>
<td>$1s^22s^22p^6$ (stable)</td>
<td>10</td>
<td>$1s^22s^22p^6$ (stable)</td>
<td>10</td>
<td>$1s^22s^22p^6$ (stable)</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Krypton</td>
<td>36</td>
<td>$1s^22s^22p^63s^23p^63d^{10}4s^24p^6$ (stable)</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

- Why? **Valence** (outer) shell usually not filled completely.
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
Ionic bond – metal + nonmetal

↑
donates electrons

↑
accepts electrons

Dissimilar electronegativities

ex: MgO

Mg 1s² 2s² 2p⁶ 3s²
[Ne] 3s²

O 1s² 2s² 2p⁴

Mg²⁺ 1s² 2s² 2p⁶
[Ne]

O²⁻ 1s² 2s² 2p⁶
[Ne]
Ionic Bonding

- Occurs between + and - ions.
- Requires electron transfer.
- Large difference in electronegativity required.
- Example: NaCl

Na (metal) unstable

Cl (nonmetal) unstable

Na (cation) stable

Coulombic Attraction

electron

Cl (anion) stable
Examples: Ionic Bonding

- Predominant bonding in Ceramics

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 ∴ share electrons
- bonds determined by valence – s & p orbitals dominate bonding
- Example: CH$_4$

  C: has 4 valence e$^-$, needs 4 more
  H: has 1 valence e$^-$, needs 1 more

Electronegativities are comparable.

Adapted from Fig. 2.10, *Callister 7e.*
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

Ex: MgO

\[
\begin{align*}
X_{\text{Mg}} &= 1.3 \\
X_{\text{O}} &= 3.5
\end{align*}
\]
SECONDARY BONDING

Arises from interaction between dipoles

- Fluctuating dipoles
  - asymmetric electron clouds

- Permanent dipoles - molecule induced
  - general case:
  - ex: liquid HCl
  - ex: polymer

Adapted from Fig. 2.13, *Callister 7e.*

Adapted from Fig. 2.14, *Callister 7e.*
# Summary: Bonding

<table>
<thead>
<tr>
<th>Type</th>
<th>Bond Energy</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionic</td>
<td>Large!</td>
<td>Nondirectional (ceramics)</td>
</tr>
<tr>
<td>Covalent</td>
<td>Variable</td>
<td>Directional</td>
</tr>
<tr>
<td></td>
<td>large-Diamond</td>
<td>(semiconductors, ceramics)</td>
</tr>
<tr>
<td></td>
<td>small-Bismuth</td>
<td>polymer chains</td>
</tr>
<tr>
<td>Metallic</td>
<td>Variable</td>
<td>Nondirectional (metals)</td>
</tr>
<tr>
<td></td>
<td>large-Tungsten</td>
<td></td>
</tr>
<tr>
<td></td>
<td>small-Mercury</td>
<td></td>
</tr>
<tr>
<td>Secondary</td>
<td>smallest</td>
<td>Directional</td>
</tr>
<tr>
<td></td>
<td></td>
<td>inter-chain (polymer)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>inter-molecular</td>
</tr>
</tbody>
</table>
Summary

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

- Wear goggles & gloves and/or any other safety wear required for your project.
- Wear long pants and closed toed shoes.
- Know where the MSDS’s are located and read them for the chemicals you use.
- Know where the chemical emergency wash and Fire extinguishers are located.
What’s the big deal?

• Injuries occur when you least expect it.

• The safety glasses are required to prevent you from experiencing this:
EQUIPMENT SAFETY

Cold Rolling

Instron

Charpy

Furnaces
General Housekeeping

- Clean up after yourself.
- Wash, Dry, and put away your glassware or any supplies.
- Put trash in the trash receptacles.
- Broken glass or sharps do not go in the trash.
- Don’t leave completed experiments or projects for someone else to pick up.
- Have the proper tools and materials before you start.
SEWER, GLASS, & TRASH

- Be aware of what can and cannot go in the sink.
- Put glass waste in glass waste containers only.
- Be aware of what can and cannot go in the trash. Razors and other sharp objects must go in a sharps container, not the trash.
- Lists are available in the lab safety notebook and online.
• If you don’t know, ASK!

• No eating or drinking in the labs.

• Especially MUE 166