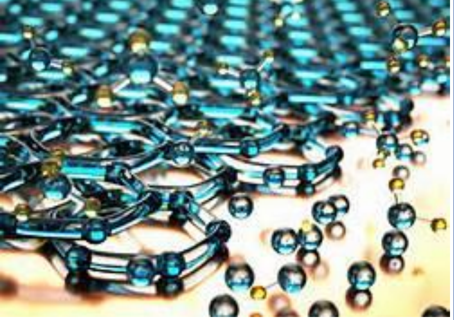

Materials Science

Lecture 3

Lebanese University - Faculty of Engineering – Branch 3

Fall 2022

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Contents

Lecture 3:

Chap2: Atomic Structure & Bonding

Introduction

- Some of the important **properties of solid materials depend on geometric atomic arrangements** and also the **interactions** that exist among constituent atoms or molecules.

- **One basis of the materials' classification** system is found in the **nature of atomic bonding.**

- Atomic bonding falls into **two general categories**. **Primary bonding** involves the transfer or sharing of electrons and produces a relatively strong joining of adjacent atoms**. Ionic, covalent, and metallic bonds** are in this category.

- **Secondary bonding** involves a relatively **weak attraction** between atoms in which **no electron transfer or sharing occurs**. **Van der Waals** bonds are in this category.

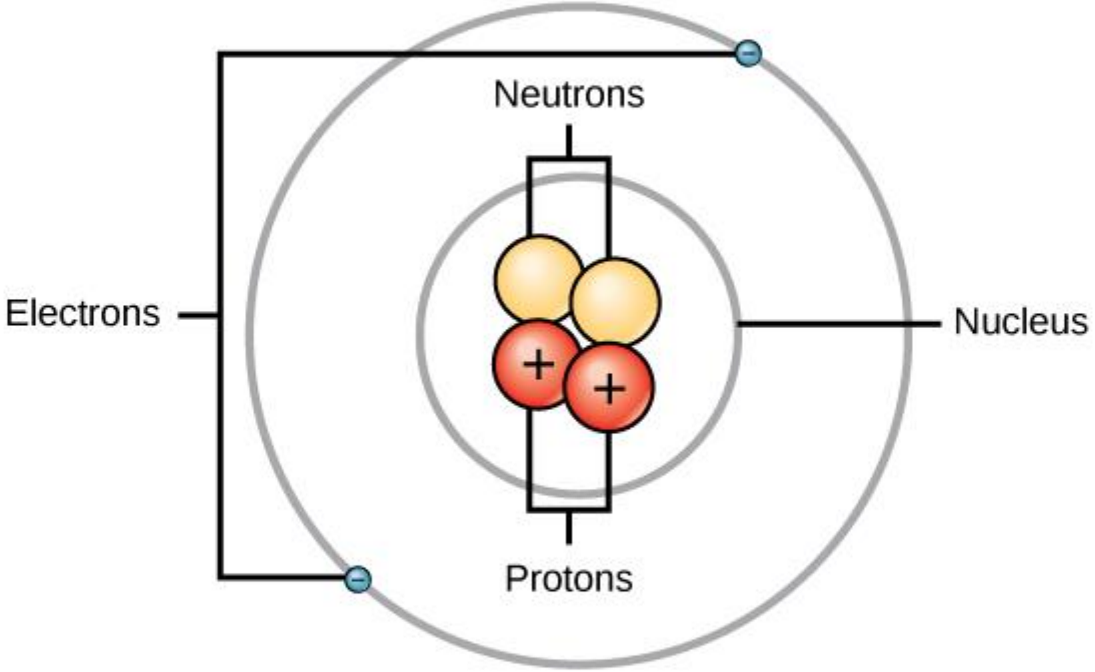
- In order to understand bonding between atoms, we must appreciate the structure within the individual atoms.

2.1. Atomic Structure

Reminder of Fundamental Concepts

- Each atom consists of a **very small nucleus** composed of **protons** and **neutrons** and is **encircled by moving electrons**.
- Both **electrons and protons are electrically charged**, the charge magnitude being **1.602×10^{-19}C**, which is **negative** in sign for electrons and **positive** for protons.
- Neutrons are electrically neutral.

- **Masses** for these subatomic particles are **extremely small.**
- **Protons and neutrons** have approximately the same mass, **1.67×10^{-27} kg**, which is significantly **larger than that of an electron**, **9.11×10^{-31} kg**.



2.1. Atomic Structure

Reminder of Fundamental Concepts

Particle	Symbol	Mass (kg)	Relative Mass (proton =1)	Relative Charge
Proton	p^+	1.673×10^{-27}	1	+1
Neutron	n^0	1.675×10^{-27}	1	0
Electron	e^-	9.109×10^{-31}	0.00055	-1

Properties of subatomic particles

2.1. Atomic Structure

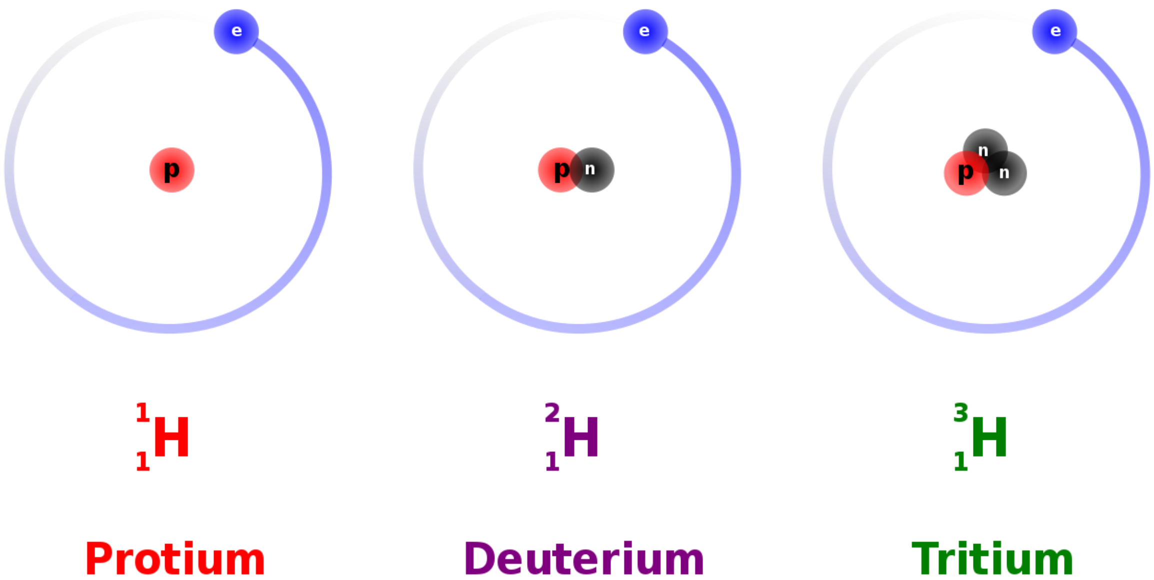
Reminder of Fundamental Concepts

- Each chemical element is characterized by the **number of protons in the nucleus**, or the **atomic number (Z).**
- **For an electrically neutral or complete atom**, **the atomic number also equals the number of electrons.**
- This atomic number ranges in integral units from **1 for hydrogen to 92 for uranium, the highest of the naturally occurring elements.**
- **The atomic mass (A)** of a specific atom may be expressed as the **sum of the masses of protons and neutrons within the nucleus**.
- Although the number of protons is the same for all atoms of a given element, the **number of neutrons (N)** may be variable.
- Thus **atoms of some elements have two or more different atomic masses**, which are called **isotopes**.

2.1. Atomic Structure

Reminder of Fundamental Concepts

- **Example of Isotopes:**



- The three naturally-occurring isotopes of hydrogen.
- The fact that each isotope has one proton makes them all variants of hydrogen: the identity of the isotope is given by the number of neutrons. From left to right, the isotopes are protium with zero neutrons, deuterium with one neutron, and tritium with two neutrons.

2.1. Atomic Structure

Reminder of Fundamental Concepts

- The **atomic weight** of an element corresponds to the **weighted average of the atomic masses of the atom's naturally occurring isotopes**.
- The **atomic mass unit (amu) or Dalton (Da)** may be used to compute atomic weight.
- A scale has been established whereby **1 amu is defined as 1/12** of the atomic mass of the most common isotope of carbon, carbon 12 (**^{12}C**) because it's atomic mass is exactly **A = 12 amu**.
- Within this scheme, the masses of protons and neutrons are slightly greater than unity, and:

$$\boxed{A \cong Z + N}$$

2.1. Atomic Structure

Reminder of Fundamental Concepts

- In **one mole of a substance**, there are **6.022 x 10^{23} (Avogadro's number) atoms or molecules.**

- The atomic weight of an element or the molecular weight of a compound may be specified on the basis of **amu per atom (molecule)** **or** **mass per mole of material**.

- These two atomic weight schemes are related through the following equation:

$$\boxed{1 \text{ amu/atom (or molecule)} = 1 \text{ g/mol}}$$

- **Example 1:** the atomic weight of iron is 55.85 amu/atom, or 55.85 g/mol.

- **Example2:** one mole of NaCl contains Avogadro's number of Na atoms and Avogadro's number of Cl atoms.

2.1. Atomic Structure

Reminder of Fundamental Concepts: Atomic Models

- **During the latter part of the nineteent**h century, it was realized that many **phenomena involving electrons in solids could not be explained in terms of classical mechanics.**

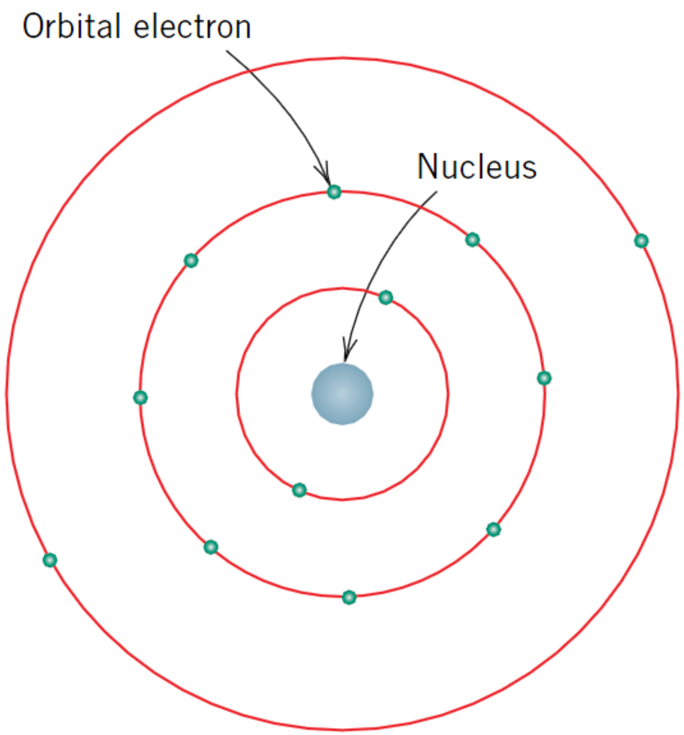
- What followed was the establishment of a **set of principles and laws that govern systems of atomic and subatomic entities** that came to be known as **quantum mechanics**.

- **An understanding of the behavior of electrons in atoms and crystalline solids necessarily** involves the discussion of quantum-mechanical concepts.

2.1. Atomic Structure

Reminder of Fundamental Concepts: Atomic Models

- One early outgrowth of quantum mechanics was the simplified **Bohr atomic model**, in which electrons are assumed to revolve around the atomic nucleus in **discrete orbitals**, and the position of any particular electron is more or less well defined in terms of its orbital.



Schematic representation of the Bohr atom.

2.1. Atomic Structure

Reminder of Fundamental Concepts: Atomic Models

- Another important quantum-mechanical principle stipulates that the energies of electrons are **quantized**—that is, **electrons are permitted to have only specific values of energy.**

- An **electron may change energy**, but in doing so, it must make a **quantum jump** either to an allowed higher energy (with absorption of energy) or to a lower energy (with emission of energy).

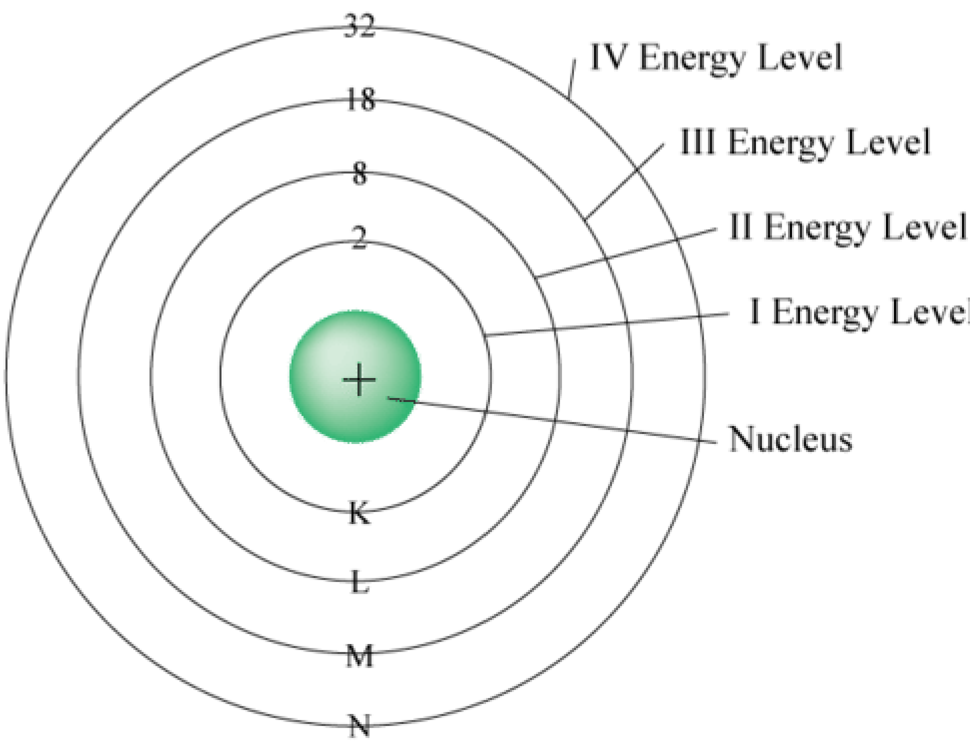
- Often, it is convenient to think of these allowed electron energies as being associated with **energy levels or states**.

- These states **do not vary continuously** with energy— that is, adjacent states are separated by finite energies.
- **Energy levels (also called electron shells)** are **fixed distances from the nucleus** of an atom where electrons may be found.
- Electrons are **tiny, negatively charged particles in an atom that move around the positive nucleus at the center.**

2.1. Atomic Structure

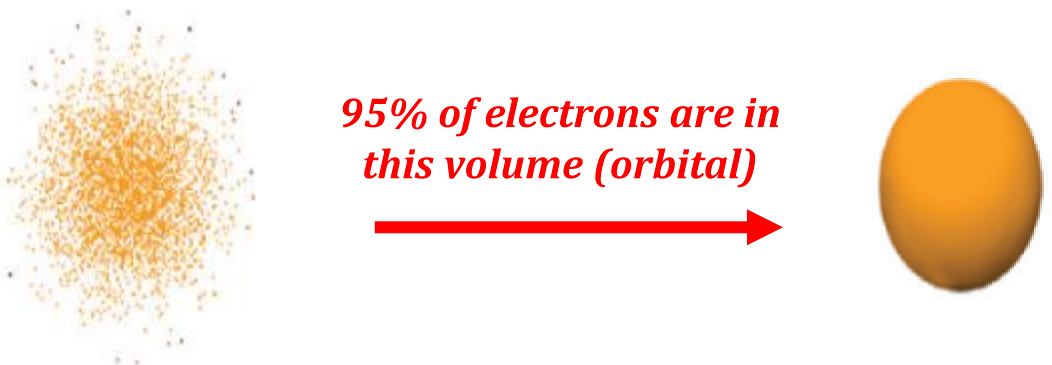
Reminder of Fundamental Concepts: Atomic Models

- **Energy levels** are a little **like the steps of a staircase**. You can stand on one step or another but not in between the steps.
- The same goes for electrons. They can occupy one energy level or another but not the space between energy levels.



Reminder of Fundamental Concepts: Atomic Models

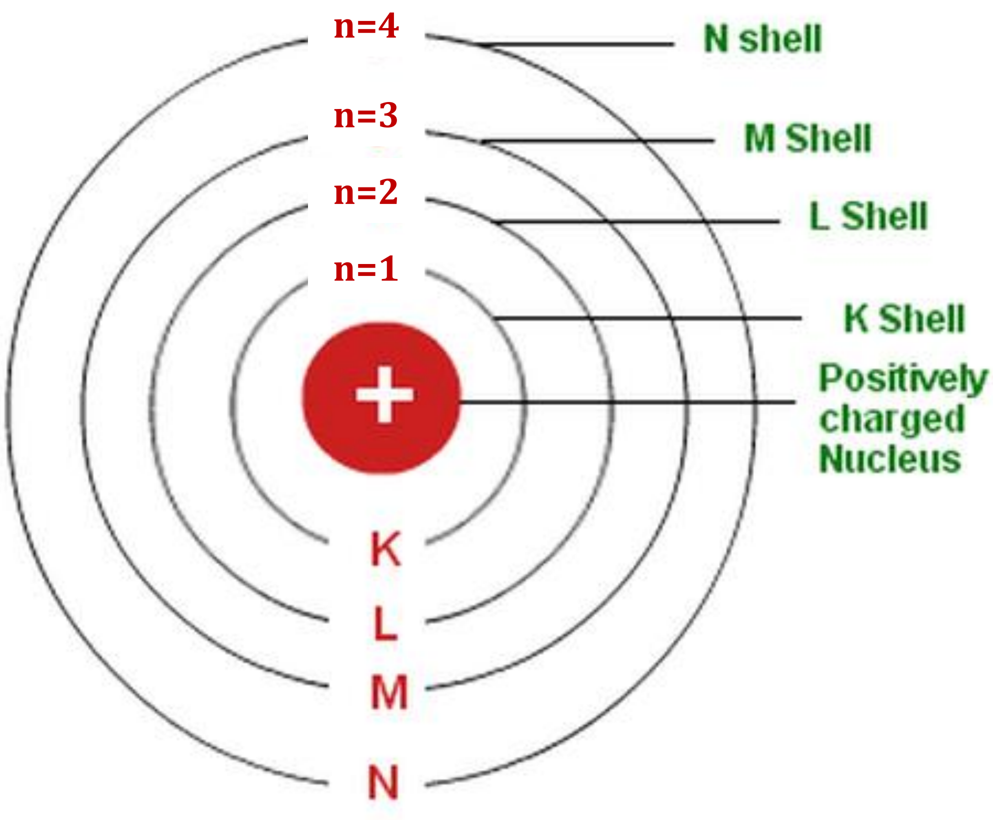
- Bohr model was eventually found to have **some significant limitations** because of its **inability to explain several phenomena involving electrons**.
- A resolution was reached with a **wave-mechanical model (Quantum Mechanics model)**, in which the electron is considered to exhibit **both wavelike and particle-like characteristics**.
- With this model, an electron **is no longer treated as a particle moving in a discrete orbital**; rather, position is considered to be the **probability** of an electron's **being at various locations around the nucleus**.
- In other words, **position is described by a probability distribution or electron cloud**.



2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

- Bohr energy levels (shells) are separated into electron subshells



Reminder of Fundamental Concepts: Quantum Numbers

- Bohr energy levels (shells) are separated into electron subshells

n = Shell:	1	2	3	4	5	6	7
SubShells:	*s*	*s, p*	*s, p, d*	*s, p, d, f*	*s, p, d, f*	*s, p, d, f*	*s, p, d, f*

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

- In wave mechanics, every electron in an atom is characterized by **four** parameters called **quantum numbers (n, l, m_l and m_s).**

- The **size, shape, and spatial orientation** of an electron's probability density (or orbital) are specified by **three** of these quantum numbers (n, l, m_l).

1. **n:** Shells are specified by a **principal quantum number n**, which may take on integral values beginning with unity; sometimes these shells are designated by the **letters K, L, M, N, O**, and so on, which correspond, respectively, to **n =1, 2, 3, 4, 5, . .**

- This quantum number is **related to the size** of an electron's orbital (or its average distance from the nucleus).

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

2. l: The second (or azimuthal) quantum number.

- Specifies the **shape of an orbital** with a particular principal quantum number. The secondary quantum number divides the shells into smaller groups of orbitals called **subshells (sublevels).**
- Values of l are restricted by the magnitude of **n** and can take on integer values that range from **l = 0 to l = (n - 1).**
- Each subshell is denoted by a **lowercase letter**—an **s, p, d, or f**—related to l values as follows:

Value of l	*Letter Designation*
0	*s*
1	*p*
2	*d*
3	*f*

- Subshells for $\ell > 3$ continue alphabetically, **omitting j** (g, h, i, k, ...) because some languages do not distinguish between the letters "i" and "j".

Reminder of Fundamental Concepts: Quantum Numbers

3. m_l: Third (or magnetic) quantum number.

- It refers to the **electron orbitals**.
- It Specifies the **orientation** in space of an orbital of a given energy (n) and shape (l).
- This number **divides the subshell into individual orbitals** which hold the electrons; there are **2l+1 orbitals in each subshell.**
- It can take on integer values **between –l and +l,** including 0.

- **Example1:** When l = 0, m_l can only have a value of 0 because -0 and +0 are the same. This corresponds to an s subshell, which can have only one orbital.
- **Example2:** Furthermore, for l = 1, m_l can take on values of **-1, 0, and +1**, and **three** p orbitals are possible.

Orbital	s	p	d	f
No. of states	1	3	5	7

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

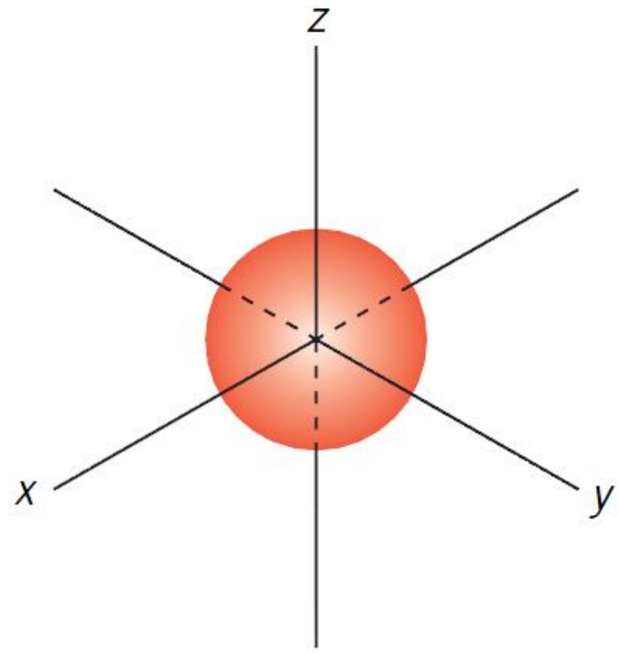
Value of n	*Value of l*	*Values of m_l*	*Subshell*	*Number of Orbitals*	*Number of Electrons*
1	0	0	1*s*	1	2
2	0	0	2*s*	1	2
	1	−1, 0, +1	2*p*	3	6
3	0	0	3*s*	1	2
	1	−1, 0, +1	3*p*	3	6
	2	−2, −1, 0, +1, +2	3*d*	5	10
4	0	0	4*s*	1	2
	1	−1, 0, +1	4*p*	3	6
	2	−2, −1, 0, +1, +2	4*d*	5	10
	3	−3, −2, −1, 0, +1, +2, +3	4*f*	7	14

Summary of the Relationships among the Quantum Numbers n, l, m_l and Numbers of Orbitals and Electrons

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

- s orbitals are spherical and centered on the nucleus. For a sphere, the orientation is the same to the nucleus (the angles between x, y and z).

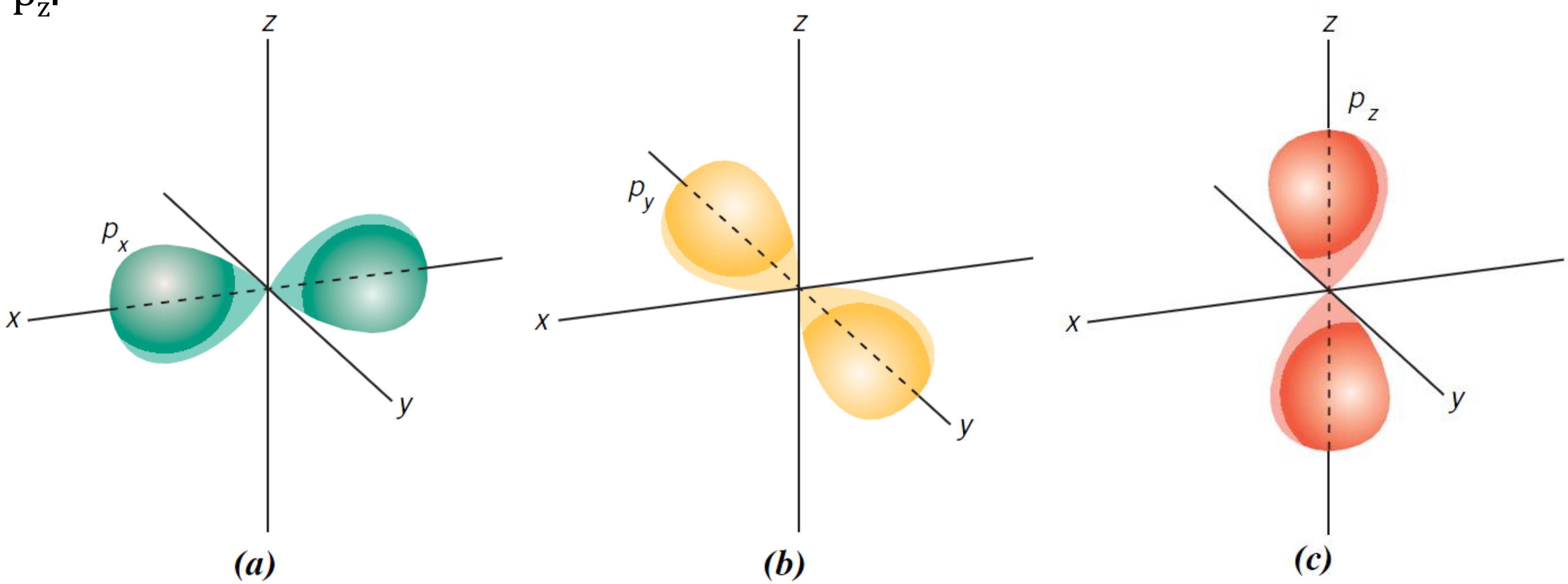


Spherical shape of an s electron orbital

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

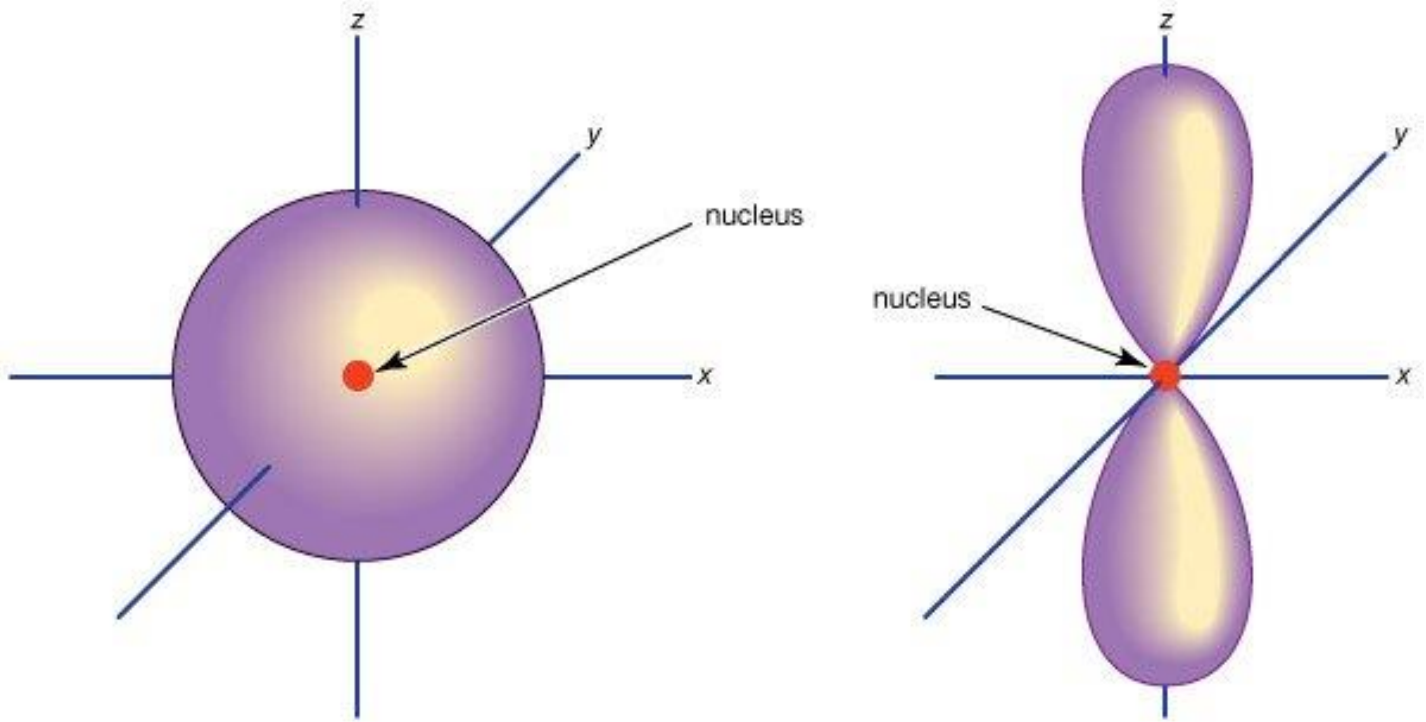
- For a **p subshell**, There are **three orbitals** each has a nodal surface in the shape of a **dumbbell** (or polar shape).
- Axes for these three orbitals are mutually **perpendicular** to one another like those of an x-y-z coordinate system; thus, it is convenient to label these orbitals p_x, p_y, and p_z.



Orientations and shapes of (a) p_x, (b) p_y, and (c) p_z electron orbitals.

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

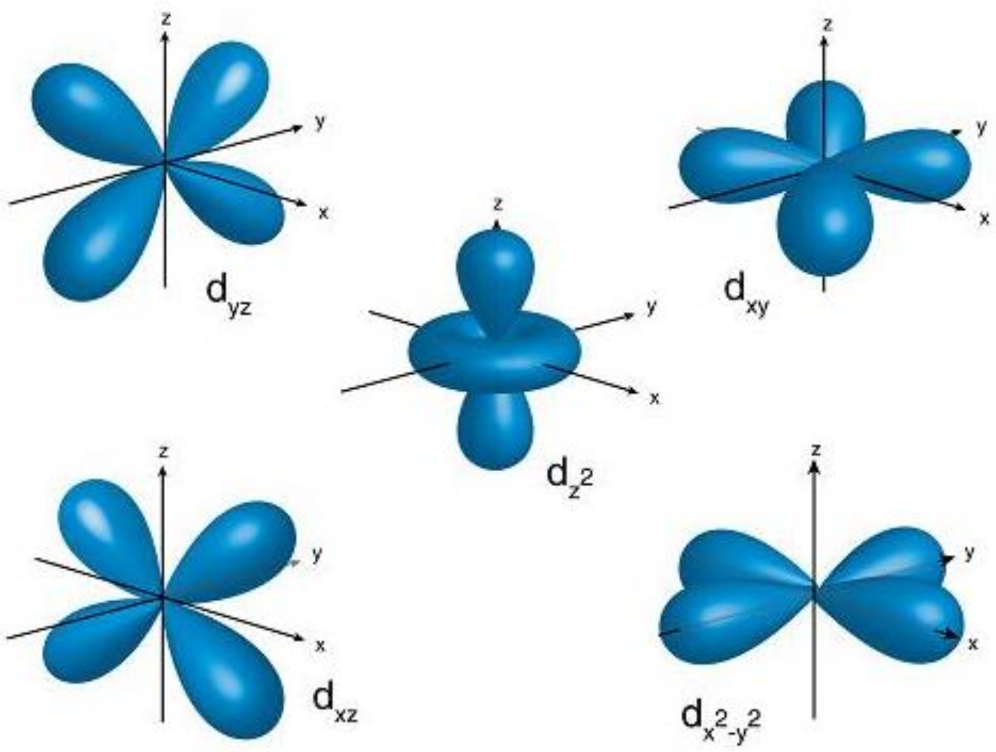


Example of the position of the nucleus for "s" and "p_z" orbitales

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

- Orbital configurations for d and f subshells are **more complex and are not discussed here.**

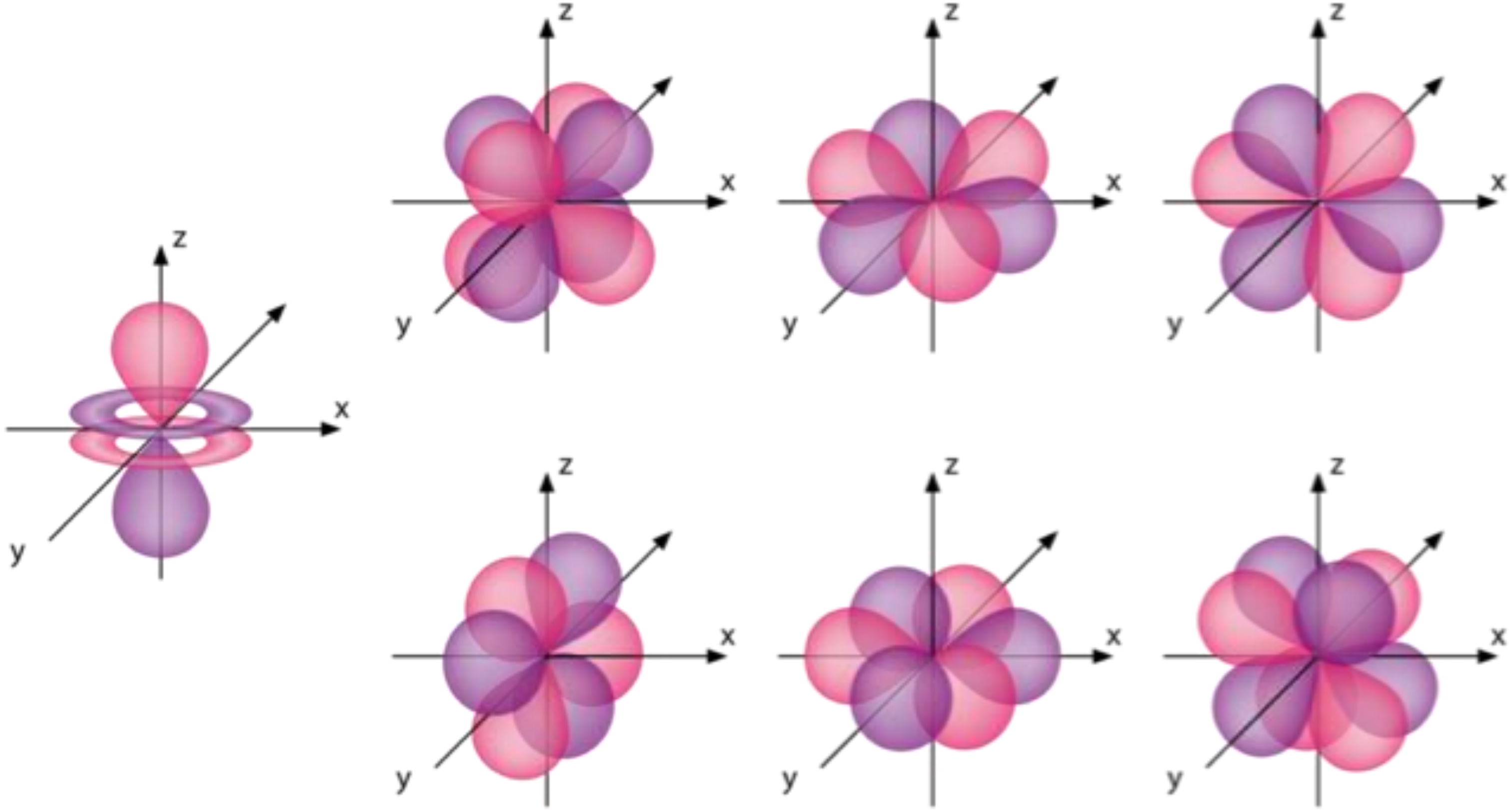


Orientations and shapes of "d" orbitals

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

- Orbital configurations for d and f subshells are more complex and are not discussed here.



Orientations and shapes of "f" orbitals

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

4. m_s: The "**electron spin" or "spin quantum number**" is the **forth** quantum number. It parameterizes the intrinsic **angular momentum** of a given electron.

- **The electron spin describe the magnetic field of the electron.**

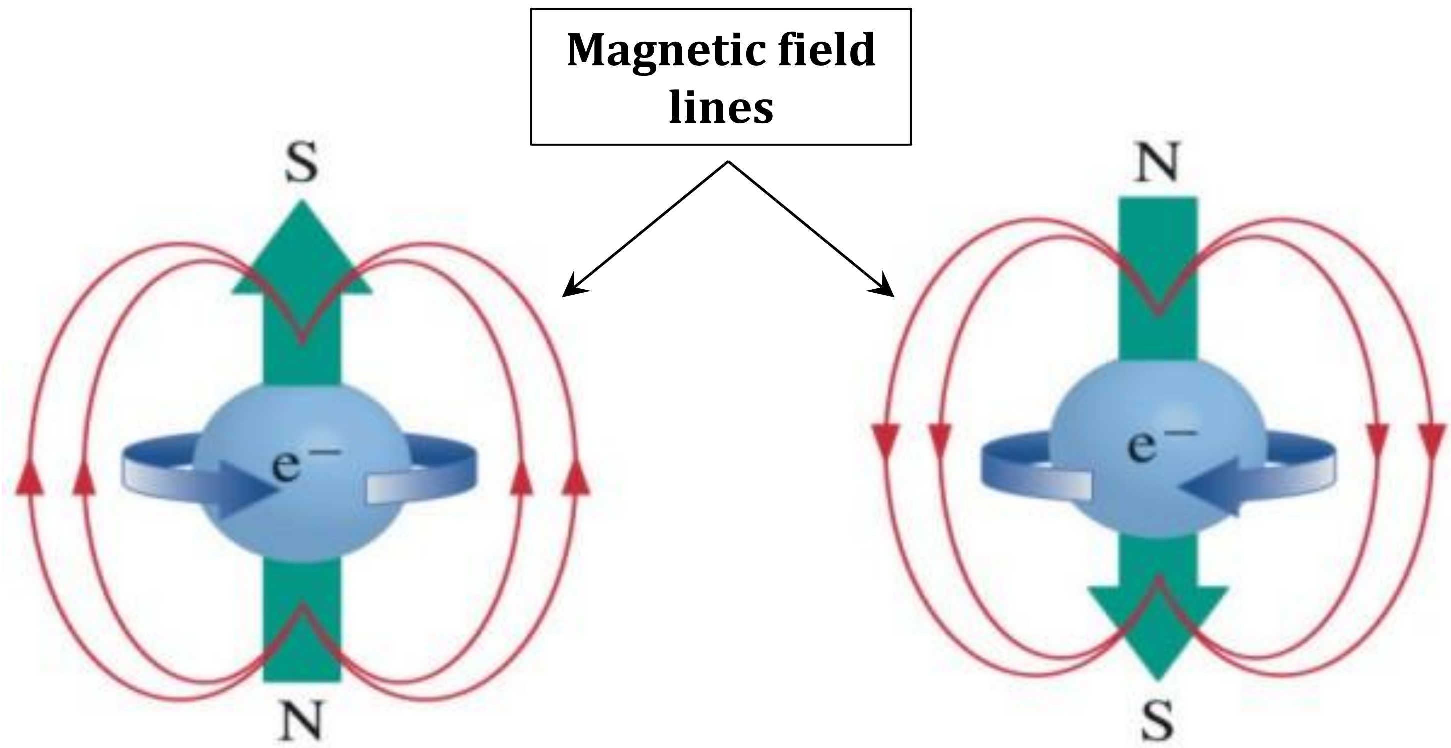
- An electron spins around an axis and has both angular momentum and orbital angular momentum. **Because angular momentum is a vector**, the **Spin Quantum Number has both a magnitude (1/2) and 2 directions (+ or -)**.

- **"Pauli exclusion principle"**, another quantum-mechanical concept, stipulates that **each electron state can hold no more than two electrons** that must have opposite spins. In other words, each orbital can only hold two electrons. One electron will have a +1/2 spin and the other will have a -1/2 spin. So, they are rotating in opposite directions.

- Electrons **like to fill orbitals before they start to pair up**. **Therefore the first electron in an orbital will have a spin of +1/2**. The second electron in the orbital will have a spin of -1/2.

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers



$m_s = +\frac{1}{2}$ $\qquad$ $m_s = -\frac{1}{2}$

2.1. Atomic Structure

Reminder of Fundamental Concepts: Quantum Numbers

- **Example 1:** The s-subshell only contains 1 circular orbital that can house a total of two electrons.
- **Example 2:** The p-subshell contains a total of 3 dumbbell-shaped orbitals that can house a total of 6 electrons.
- **Example 3:** The d-subshell contains 5 uniquely shaped orbitals that can house a total of 10 electrons.

2.1. Atomic Structure

Reminder of Fundamental Concepts: Energy

- The energy of electrons **increases** with the shells and subshells. **The bigger the shell number, the higher the amount of energy.**

- The first principal shell **"s"** is also called the **ground state**, or **lowest energy state.**

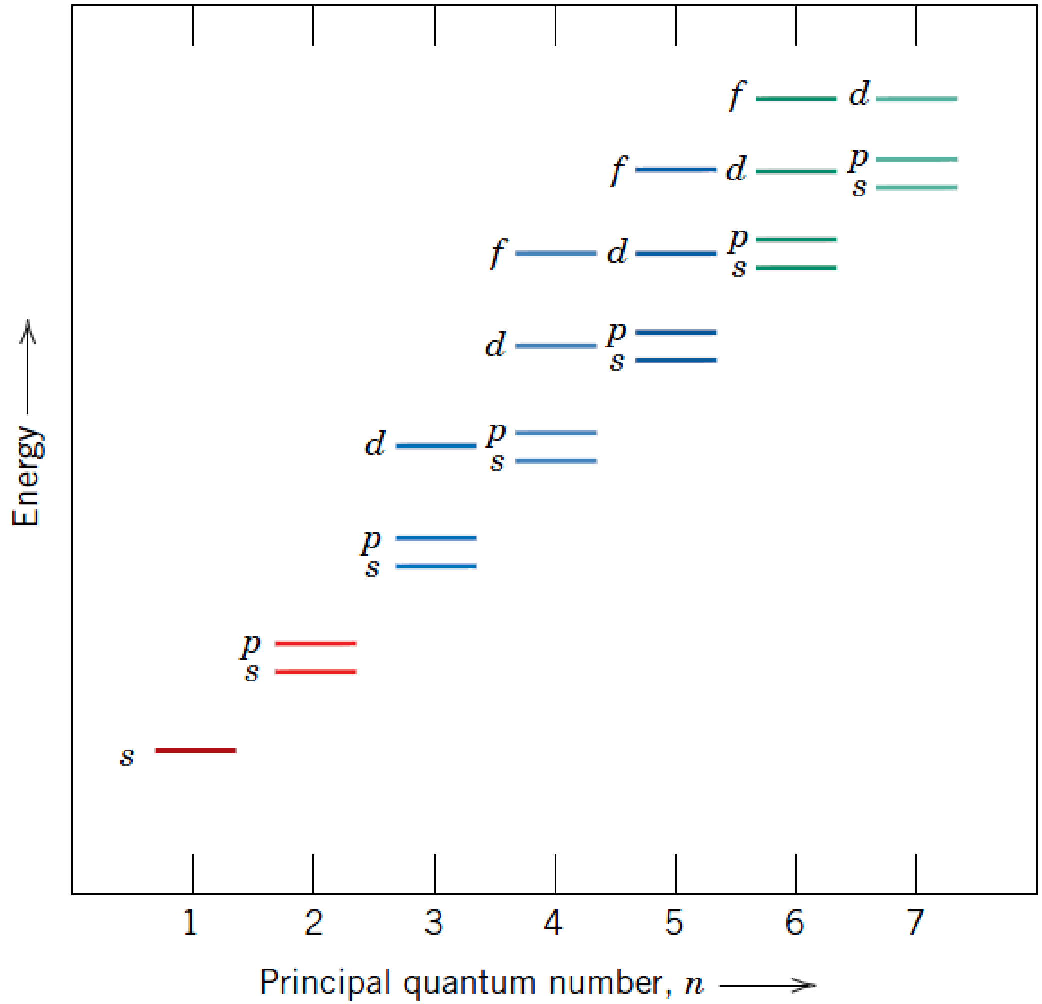
- When an electron is in an **excited state** or gains energy, it may **jump to the second principle shell, where n=2**. This process is called **absorption** because the electron is "**absorbing" photons, or gaining energy**.

- Thus, as the energy of the electron **increases during absorption**, so does the principal quantum number, e.g., if an electron in the n = 3 shell absorbs energy, it will jump to the fourth principal shell, n = 4.

- The opposite process is emission, where **electrons "emit" or release energy as they fall from higher to lower principle shells**. In this case, n decreases.

2.1. Atomic Structure

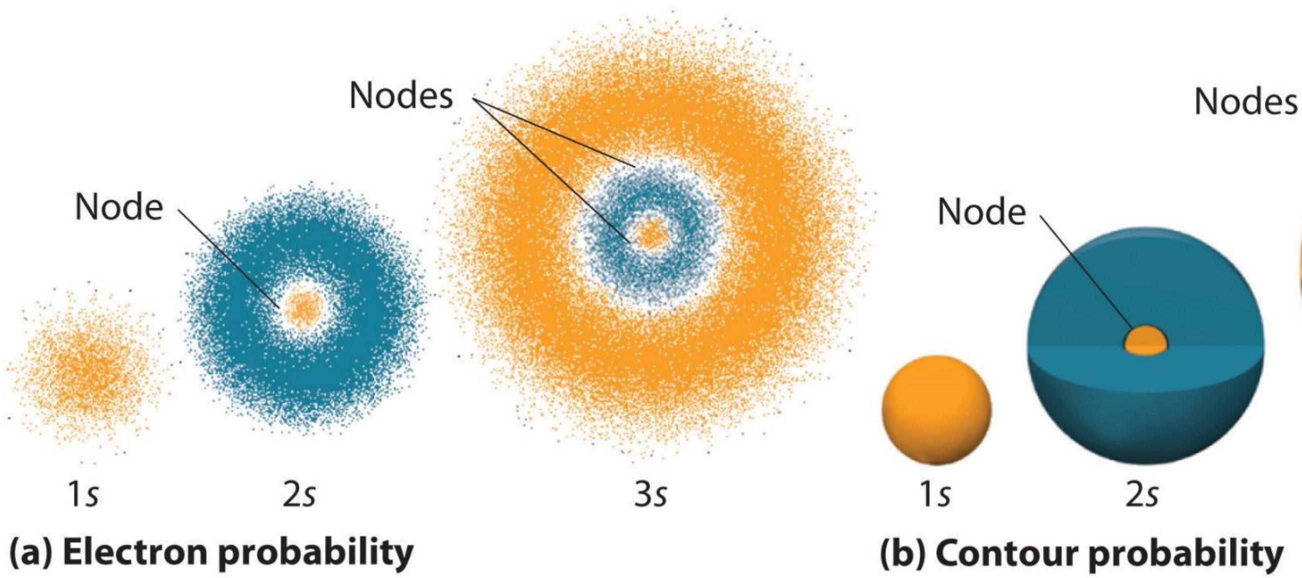
Reminder of Fundamental Concepts: Energy



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

2.1. Atomic Structure

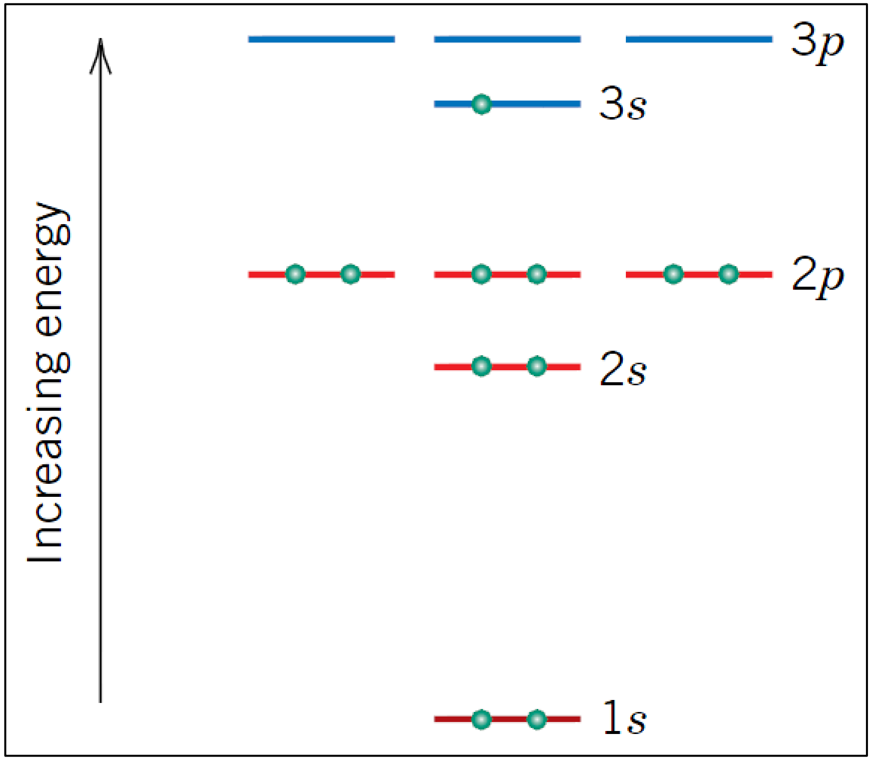
Reminder of Fundamental Concepts: Energy



Nodes: Regions of zero electron probability.

2.1. Atomic Structure

Reminder of Fundamental Concepts: Energy



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

- Within each shell, the energy of a subshell level increases with the value of the l quantum number. For example, the energy of a **3d state is greater than that of a 3p, which is larger than 3s.**

- Finally, there may be **overlap in energy** of a state in one shell with states in an adjacent shell, which is especially true of d and f states**; for example, the energy of a 3d state is generally greater than that of a 4s** **(will be explained later in this chapter).**

2.1. Atomic Structure

Reminder of Fundamental Concepts:

- **Example:**

n	l	m_l	Nb of Orbitals	Nb of electrons
3	0	0	1 orbital of s	2
	1	-1, 0, +1	3 orbitals of p	2x3=6
	2	-2, -1, 0, +1, +2	5 orbitals of d	2x5=10
		Total	9 orbitals	18 electrons

- A simple method to find the number of orbitals and number of electrons per shell:

Nb of orbitals = n^2

Nb of electrons = $2n^2$

- For this example (n=3), $3^2 = 9$ (nb of orbitals), and $2(3^2) = 18$ (nb of electrons).

2.1. Atomic Structure

Electron Configurations

- The **electron configuration or structure of an atom** represents the **manner in which these states are occupied.**
- In the conventional notation, the number of electrons in each subshell is indicated by a superscript after the shell–subshell designation.
- **Example 1**: the electron configurations for hydrogen (having 1 electron) is $1s^1$.
- **Example 2**: the electron configurations for sodium Na (having 11 electrons) is $\mathbf{1s^2 2s^2 2p^6 3s^1}$.

$$\boxed{1s^2}$$

Nb of electrons on the subshell

Shell (n=1, 2, 3, …)

2.1. Atomic Structure

Electron Configurations

- **Example:** Carbone C having 6 electrons

$$1s^2 2s^2 2p^2$$

- **Example:** Silicon Si having 14 electrons

$$1s^2 2s^2 2p^6 3s^2 3p^2$$

2.1. Atomic Structure

Electron Configurations

- **Example:** Iron Fe having 26 electrons

$$1s^2 2s^2 2p^6 3s^2 3p^6 \underline{4s^2} 3d^6$$

Why 4s is before 3d ???

Klechkowsky Rule

- According to the **energy increasing principle** *(see the figure in slide 30)*, the Russian chemist "Klechkowsky" finds a simple method to find the next subshell. It is called **"Klechkowsky Rule" or "Madelung Rule".**

- In neutral atoms, the **order in which subshells are filled** is given by the "**$n + \ell$**".
- Orbitals with a **lower** "**$n + \ell$**" value are filled **before** those with **higher** "**$n + \ell$**" values.
- In the case of equal "**$n + \ell$**" values, the orbital with a **lower n** value is **filled first**.

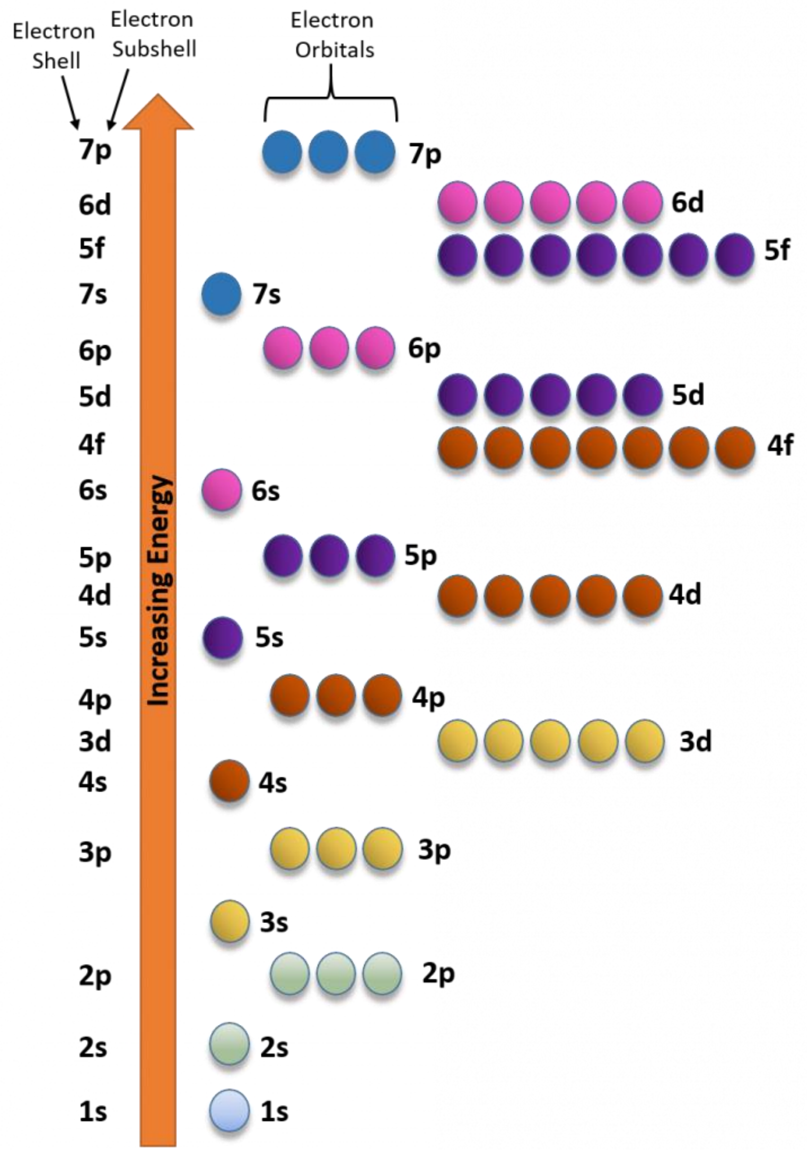
2.1. Atomic Structure

Klechkowsky Rule

Sum $n+\ell$	Principal quantum number n	Azimuthal number ℓ	Subshell
$n+\ell = 1$	1	0	1s
$n+\ell = 2$	2	0	2s
$n+\ell = 3$	2	1	2p
	3	0	3s
$n+\ell = 4$	3	1	3p
	4	0	4s
$n+\ell = 5$	3	2	3d
	4	1	4p
	5	0	5s
$n+\ell = 6$	4	2	4d
	5	1	5p
	6	0	6s

2.1. Atomic Structure

Klechkowsky Rule



Electron Energy Filling Diagram

Orbitals with the lowest energy are filled with electrons before orbitals at higher energy levels.

2.1. Atomic Structure

Klechkowsky Rule

- **Example:** Nickel Ni having 28 electrons

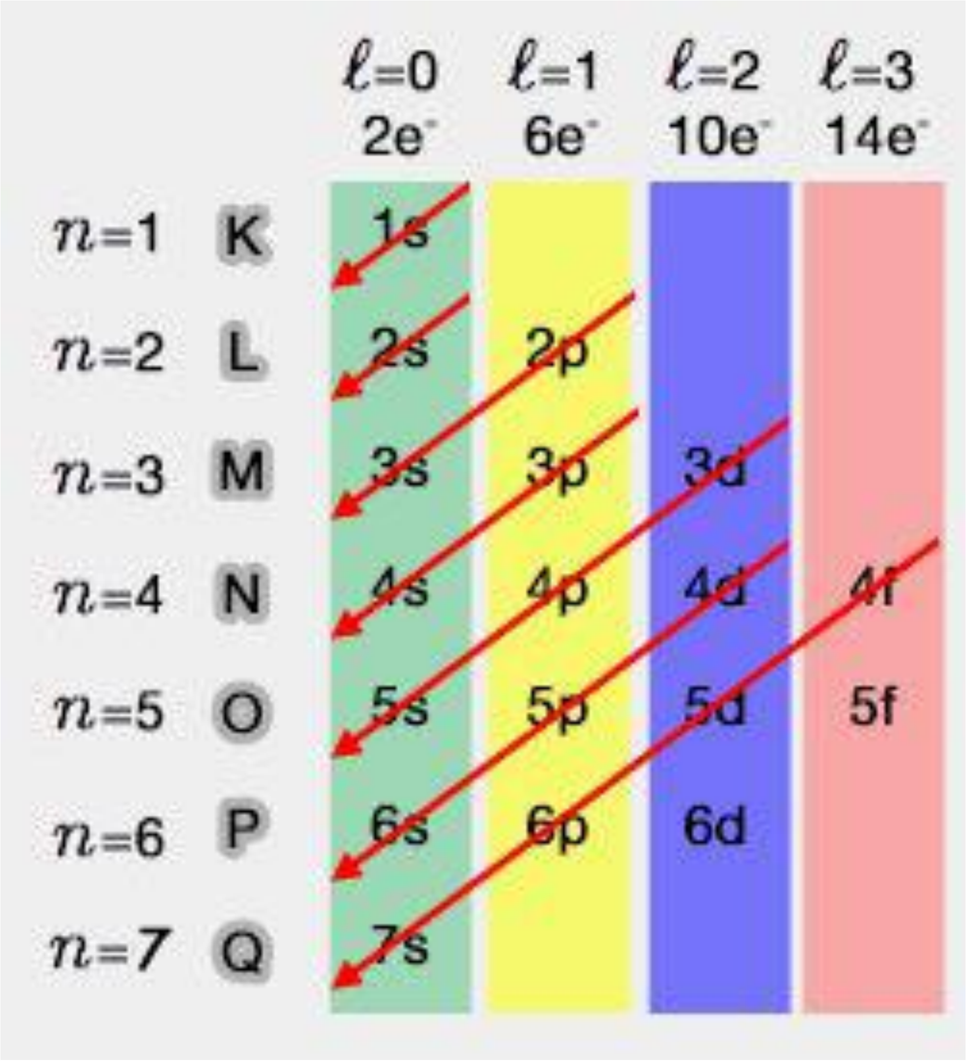
$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$$

- To replace this complex rule of Klechkowsky, **two simple methods** can be used:

1. **Aufbau principle**
2. **The periodic table**

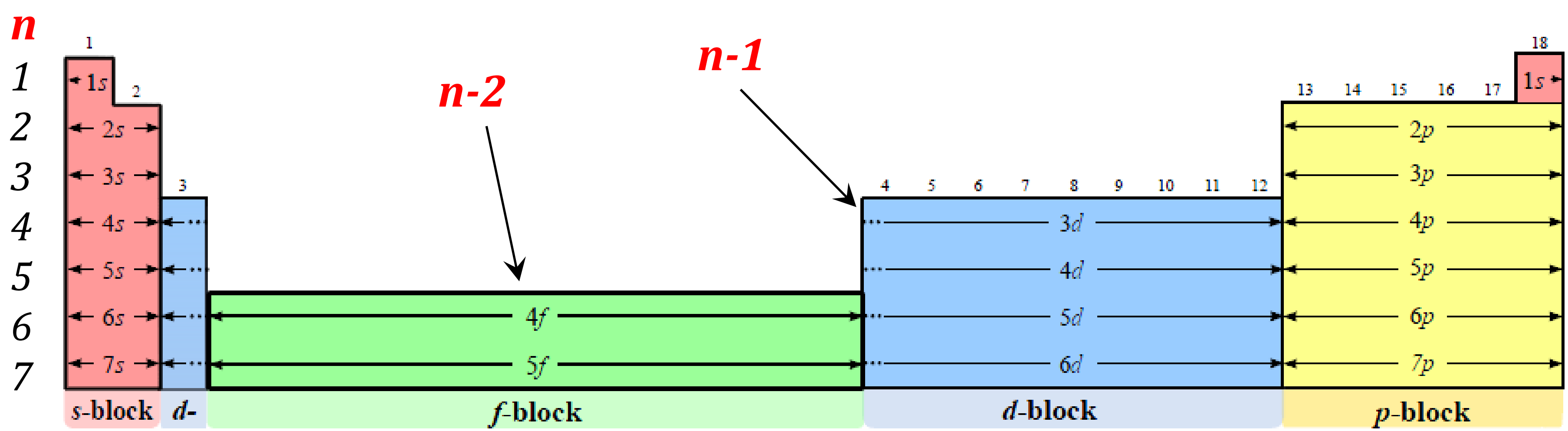
1. Aufbau principle

- Using the **downward diagonals** (from right to left), we obtain the right order of subshells.



2.1. Atomic Structure

2. Using the periodic table



2. Using the periodic table

Example: Find the Electron Configuration of **Zirconium Zr** having 40 electrons.

1. Using Aufbau principle
2. Using the periodic table

Solution: $\mathbf{1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^2}$

- **Note:** to simplify, we can write the **previous Nobel gas** and add the last line (in the periodic table).
- In this example (Zr), the above configuration can be written as:

$$\mathbf{[Kr]\ 5s^2 4d^2}$$

2.1. Atomic Structure

Valence electrons

- The **most reactive** electrons of the element.

- They have **the highest energy** => they are **the farthest from the nucleus** => occupy **the outermost shell** (this definition if true for the principal subshells “s & p”, a more detailed definition will be explained later).

- They are **on the origin of ionic transformation** (anion & cation), therefore, the **reactivity and the bonding** (creation of bond, breaking of bond …).

- 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.

- In addition, some atoms have what are termed **stable electron** configurations— that is, the states within the outermost or valence electron **shell are completely filled**.

2.1. Atomic Structure

Valence electrons

- 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**.

- **Some atoms** of the elements that have **unfilled valence shells** assume **stable electron configurations by** gaining or losing electrons to **form charged ions** or by **sharing electrons** with other atoms.

- This is the basis for some chemical reactions and also for atomic bonding in solids, as explained later in this chapter.

2.1. Atomic Structure

Valence electrons

Example 1: for Hydrogen H ?

- Electrons configuration: $1s^1$ => 1 valence electron
- The Lewis structure: H•

Example 2: Sodium Na? **$1s^2 2s^2 2p^6 3s^1$ or [Ne] $3s^1$** => 1 valence electron

- The Lewis structure: Na•

Example 3: Helium He?

- **$1s^2$** => 2 valence electrons. The shell 1 is completely filled => High stability => He is a noble gas (last column of the periodic table).
- The Lewis structure: **He:** or **He|**

2.1. Atomic Structure

The periodic table

- All the elements have been classified **according to electron configuration** in the periodic table.
- Here, 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, as well as **chemical and physical properties**.
- These properties change gradually, moving horizontally across each period and vertically down each column.
- The **columns are numbered from 1 to 18** (without any signification). They are also **numbered by groups**.
- **Columns 1-2 (without H):** The **alkali metals (column 1) and the alkaline earth metals (column 2)** (Li, Na, K, Be, Mg, Ca, etc.) are labeled as **Groups IA and IIA**, having, respectively, **one and two electrons in excess** of stable structures. **Bright, Soft, very reactive, react very well with water, don't exist alone in the nature but in ionic form (in molecule with other elements).**

2.1. Atomic Structure

The periodic table

- **Columns 3-12:** The elements in the three long periods, **Groups IIIB through IIB**, are termed the **transition metals**, which have **partially filled d** electron states and in some cases one or two electrons in the next higher energy shell. **Solid at room temperature (except Mercury Hg), good ductility (ability to be deformed without fracture), good thermal and electrical conductor.** The Group VB metals (V, Nb, and Ta) have very high melting temperatures, which increase in going down this column.

- **Columns 13-15:** **Groups IIIA, IVA, and VA** (B, Si, Ge, As, etc.) display **characteristics** that are **intermediate between the metals and nonmetals** by virtue of their valence electron structures. **For the Group IVA elements** [C (diamond), Si, Ge, Sn, and Pb], **electrical conductivity increases as we move down this column.**

- **Columns 16-17:** **Group VIIA and VIA elements** are one and two electrons deficient, respectively, from having stable structures.

- The **Group VIIA elements** (F, Cl, Br, I, and At) are sometimes termed the **halogens**.

- **Column 18:** The elements positioned in **Group 0,** the rightmost group, are the **inert gases,** which have **filled electron shells and stable electron configurations**.

2.1. Atomic Structure

The periodic table

- As may be noted from the periodic table, **most of the elements really come under the metal classification.**

- These are sometimes termed **electropositive elements**, indicating that **they are capable of giving up their few valence electrons to become positively charged ions.**

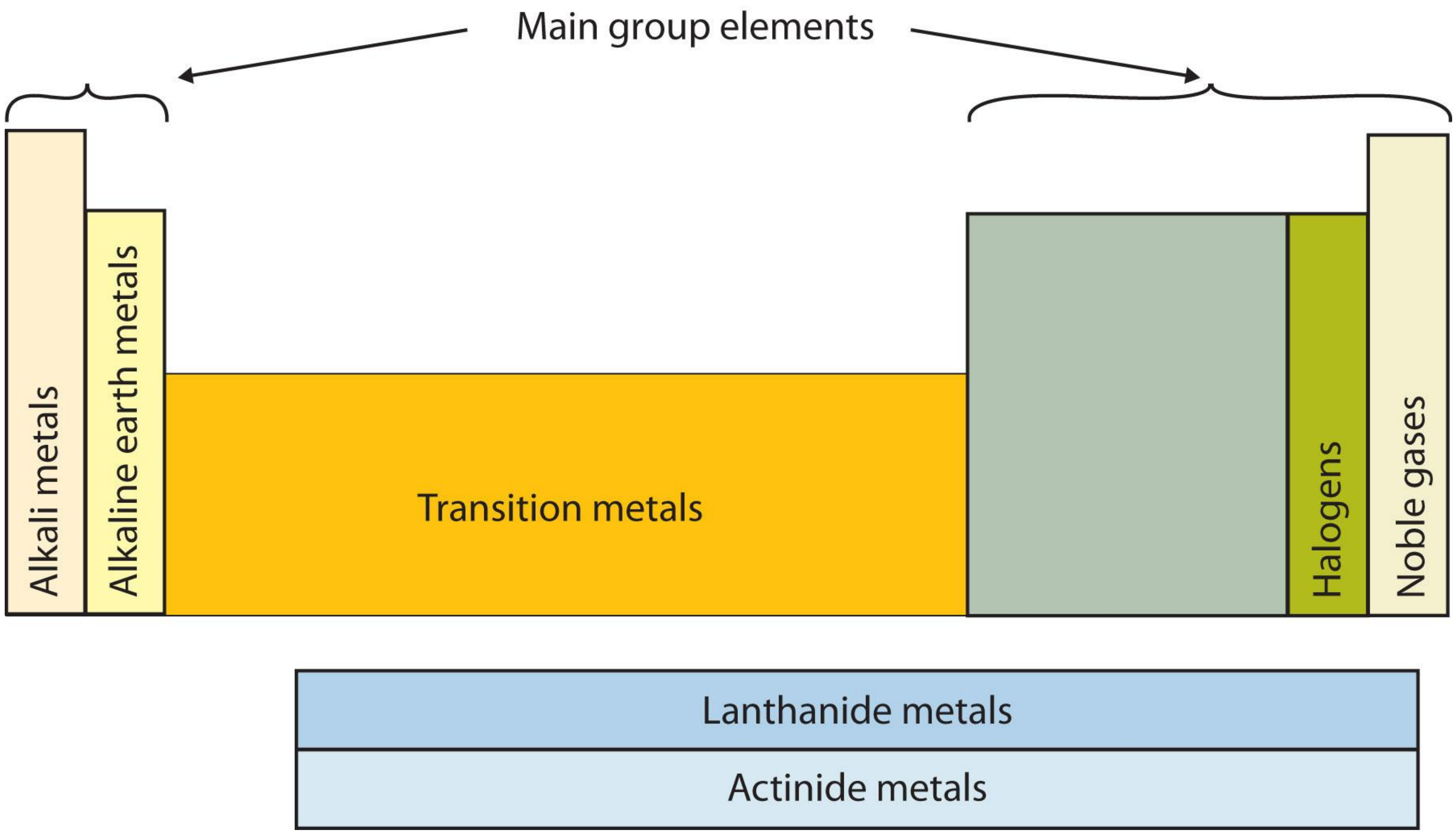
- Furthermore, the elements situated on **the right side of the table are electronegative**—that is, they readily **accept electrons to form negatively charged ions,** or sometimes they **share electrons** with other atoms.

- As a general rule, ele**ctronegativity increases in moving from left to right and from bottom to top.**

- **Atoms are more likely to accept electrons if their outer shells are almost full and if they are less "shielded" from (i.e., closer to) the nucleus.**

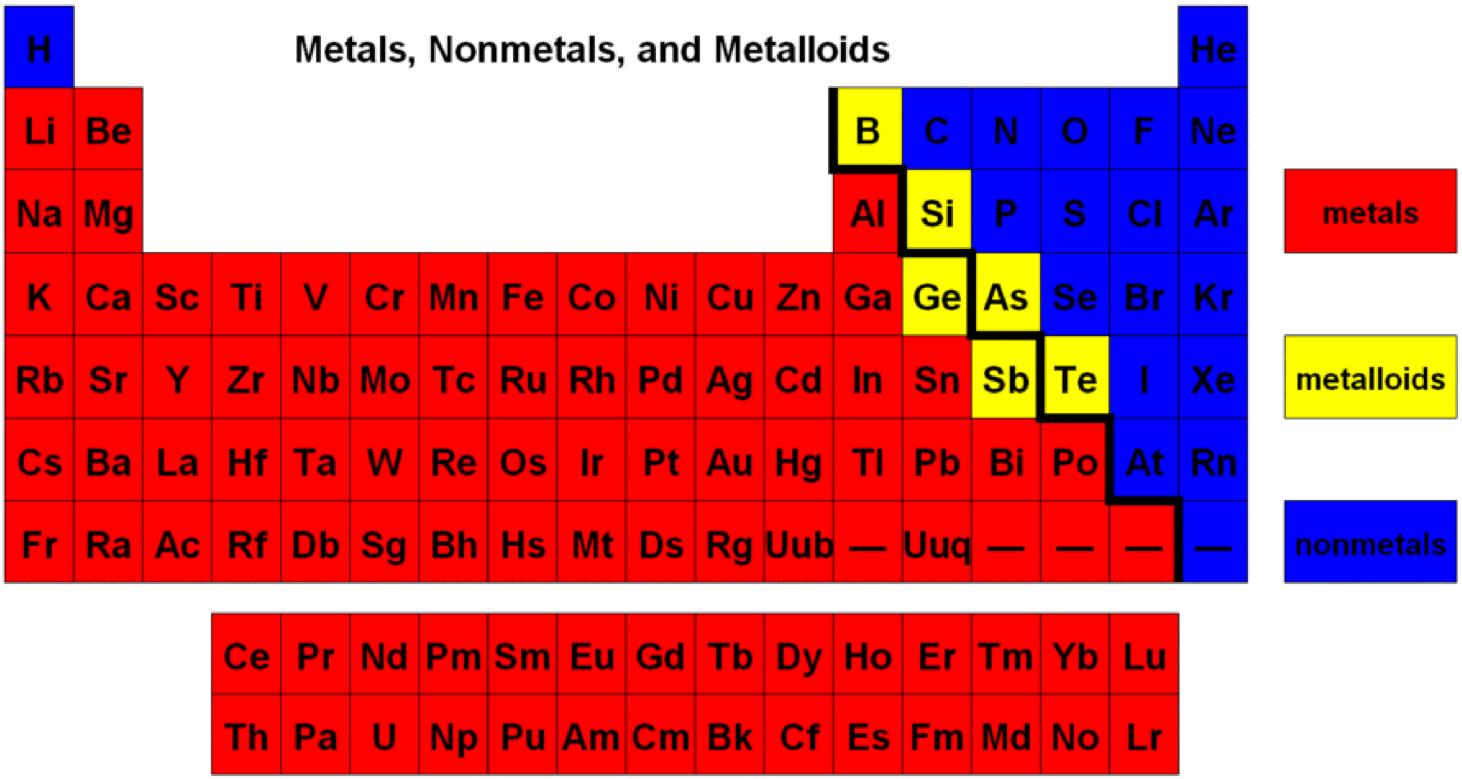
2.1. Atomic Structure

The periodic table



2.1. Atomic Structure

The periodic table



- **Metalloids:** separate metals and nonmetals. Their properties are between the two groups (semi-conductor ...).
- **Nonmetals:** are typically electrical and thermal insulators. Most of the nonmetals are either gases or liquids, or in the solid state are brittle in nature.

Contents

Lecture 3:

Chap2: Atomic Structure & Bonding

2.2. The Ionic Bond

Atomic Bonding in Solids: Bonding Forces And Energies

- An understanding of many of the **physical properties** of materials is enhanced by a knowledge of the **interatomic forces** that bind the atoms together.

- Perhaps the principles of atomic bonding are best **illustrated** by considering how **two isolated atoms interact** as they are brought close together from an infinite separation.

- At **large distances**, interactions are **negligible** because the atoms are **too far** apart to have an influence on each other; however, at **small separation distances**, **each atom exerts forces on the others**.

- These forces are of **two types**, **attractive (F_A)** and **repulsive (F_R)**, and the magnitude of each depends on the separation or interatomic distance (**r**).

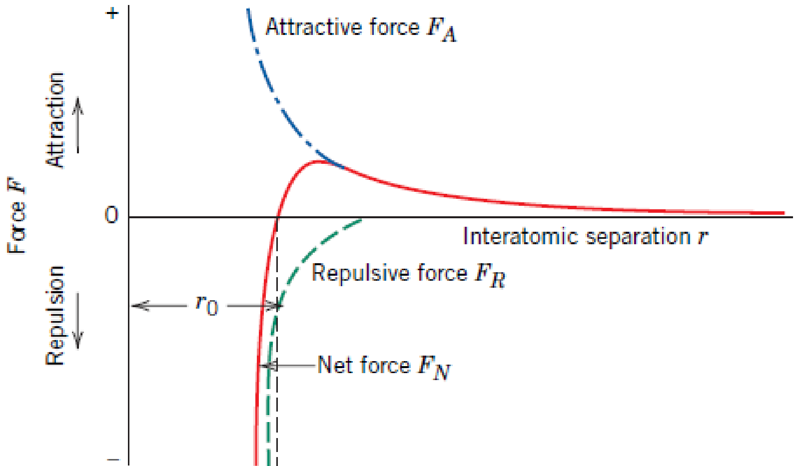
- The origin of an attractive force F_A depends on a **particular type of bonding** that exists **between the two atoms**.

2.2. The Ionic Bond

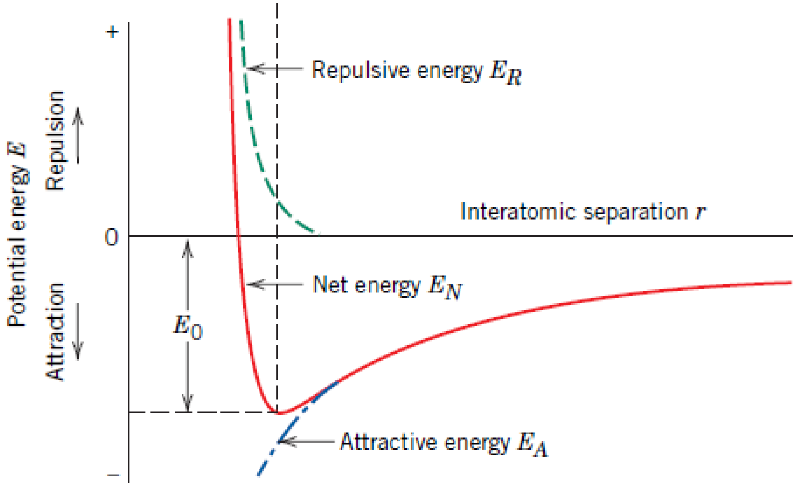
Atomic Bonding in Solids: Bonding Forces And Energies

(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 fortwo isolated atoms.



(a)



(b)

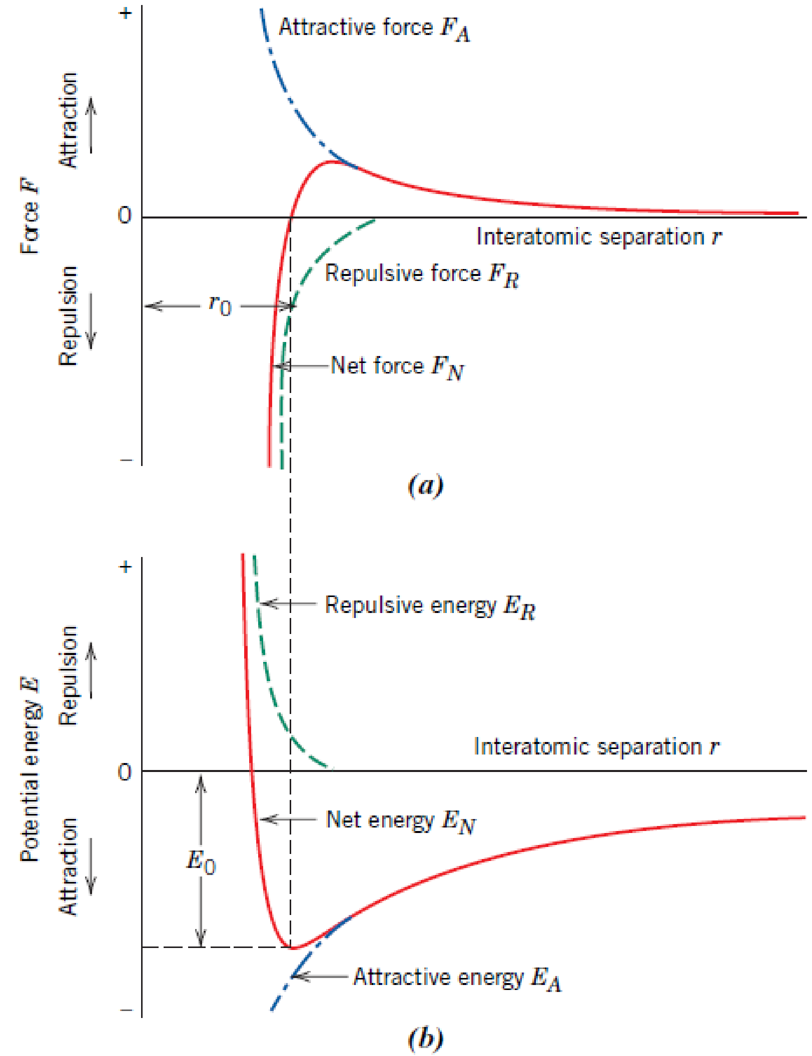
2.2. The Ionic Bond

Atomic Bonding in Solids: Bonding Forces And Energies

- **Repulsive** forces arise from **interactions between the negatively charged electron clouds** for the two atoms and are important only at **small values of r** as the outer electron shells of the two atoms begin to overlap.

- The **net force F_N** between the two atoms is just the **sum** of both attractive and repulsive components; that is,

$$\boxed{F_N = F_A + F_R}$$



2.2. The Ionic Bond

Atomic Bonding in Solids: Bonding Forces And Energies

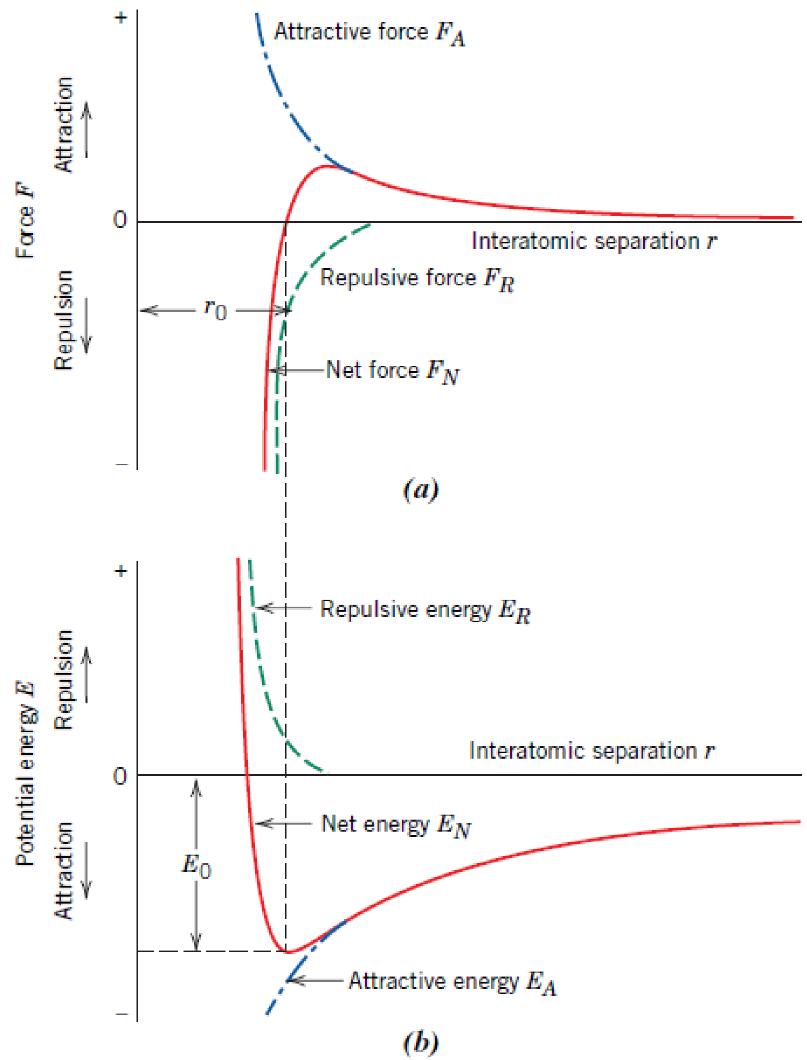
- When F_A and F_R are **equal** in **magnitude** but **opposite** in **sign**, there is no net force and a state of equilibrium exists.

$$\boxed{F_A + F_R = 0}$$

- The centers of the two atoms remain separated by the **equilibrium spacing r_0**.

- For **many** atoms, **r_0 is approximately 0.3 nm.**

- Once **in this position**, any attempt to move the two atoms farther apart is **counteracted** by the **attractive force**, while **pushing** them closer together **is resisted** by the **increasing repulsive force**.

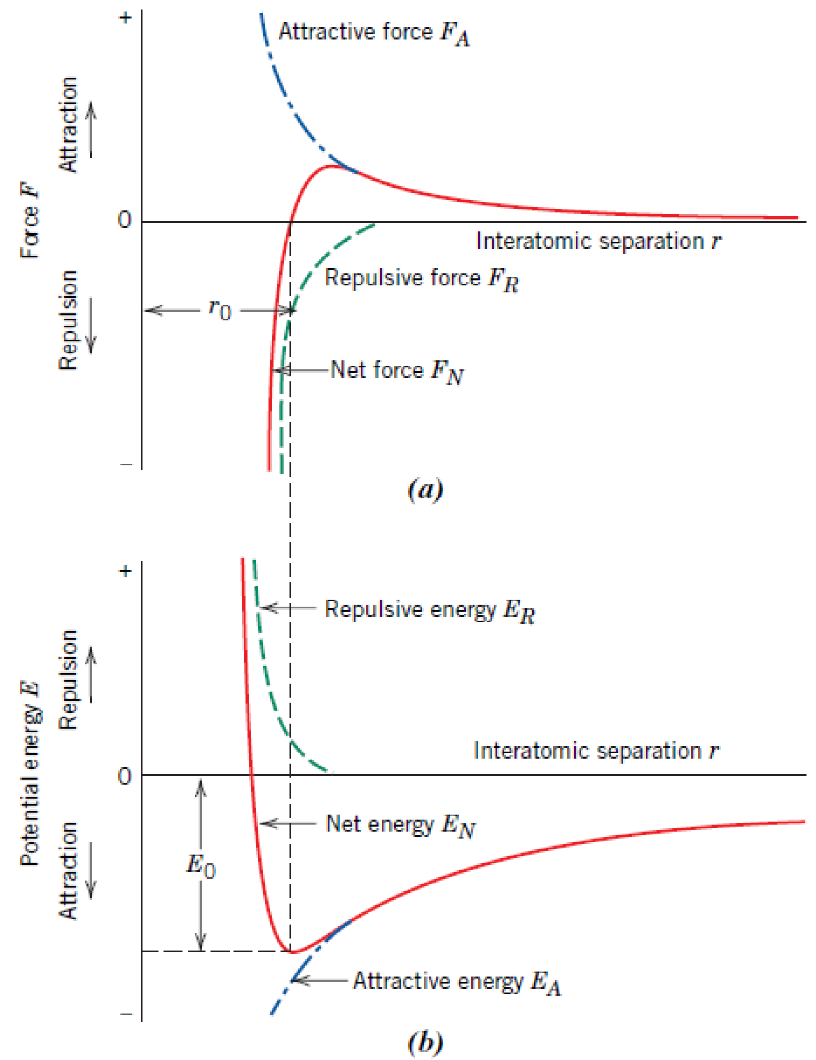


Atomic Bonding in Solids: Bonding Forces And Energies

- **Sometimes** it is more convenient to work with the **potential energies** between two atoms instead of forces.

- Mathematically, energy (E) and force (F) are related as:

$$E = \int F\, dr$$



2.2. The Ionic Bond

Atomic Bonding in Solids: Bonding Forces And Energies

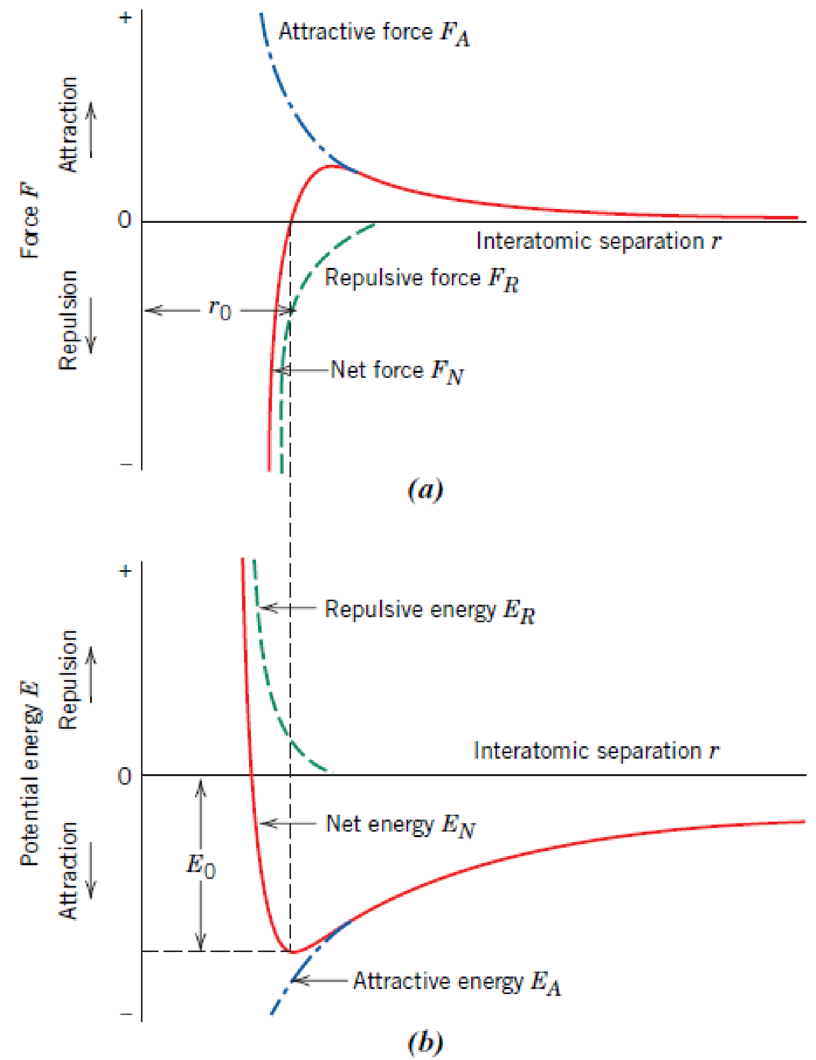
- And, for atomic systems:

$$E_N = \int_r^\infty F_N\,dr$$

$$= \int_r^\infty F_A\,dr + \int_r^\infty F_R\,dr$$

$$= E_A + E_R$$

in which **E_N, E_A, and E_R are, respectively, the net, attractive, and repulsive energies for two isolated and adjacent atoms.**



2.2. The Ionic Bond

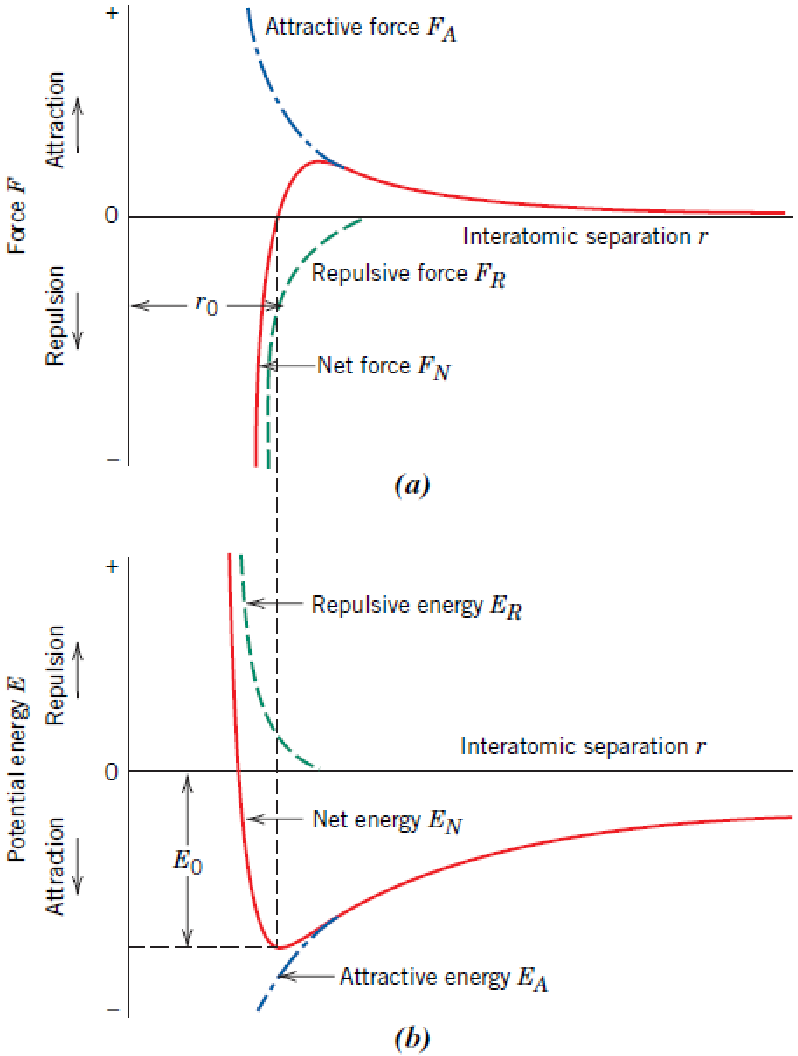
Atomic Bonding in Solids: Bonding Forces And Energies

- The net curve is the sum of the attractive and repulsive curves.

- The **minimum** in the net energy curve corresponds to the equilibrium spacing, $\mathbf{r_0}$.

- Furthermore, the **bonding energy** for these two atoms, $\mathbf{E_0}$, corresponds to the **energy** at this minimum point.

- It represents the **energy required** to **separate** these **two atoms** to an infinite separation.



2.2. The Ionic Bond

Atomic Bonding in Solids: Bonding Forces And Energies

- Although the preceding treatment deals with an ideal situation involving **only two atoms**, a similar yet **more complex condition exists for solid materials** because force and energy interactions among atoms must be considered. Nevertheless, a bonding **energy, analogous to E_0 above**, may be **associated with each atom**.

- The **magnitude of this bonding energy and the shape of the energy–versus–interatomic separation** curve **vary from material to material**, and they both depend on the type of atomic bonding.

- Furthermore, a **number of material properties depend on E_0**, the **curve shape**, and **bonding type**.

- **For example**, materials having **large bonding energies** typically also have **high melting temperatures**.

- At room temperature, **solid substances** are formed for **large bonding energies**, whereas for **small energies**, the **gaseous state** is favored; **liquids** prevail when the energies are of **intermediate magnitude**.