Material Science
ME 221

Fall 2020

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Chapter 2: Atomic Structure and Interatomic Bonding

- Fundamental Concepts
- Electrons in Atoms
- Atomic Models
- Electron Configuration
- Atomic Bonding in Solids

Materials Contents in this Slides adapted from : Materials science and engineering: an introduction / William D. Callister, Jr., David G. Rethwisch.–8th ed.

Fundamental Concepts

- Atom = nucleus (protons + neutron) + moving electrons
- Charge magnitude =1.602 10^{-19}C
  - negative in sign for electrons
  - positive for protons;
  - neutrons are electrically neutral.
- **Atomic number (*Z*):** number of protons in the nucleus
- Electrically neutral or complete atom => atomic number = number of electrons.

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Fundamental Concepts

- The ***atomic mass*** (*A*) = masses of protons + neutrons within the nucleus
- **Isotopes** : atoms of some elements have two or more different atomic masses at fixed number of proton.
- The **atomic weight:** average weight of the atomic masses

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

- The **atomic mass unit (amu)**.

1 amu/atom or (molecule) = 1 g/mol

- For example, the atomic weight of iron is 55.85 amu/atom, or 55.85 g/mol.

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Electrons in Atoms

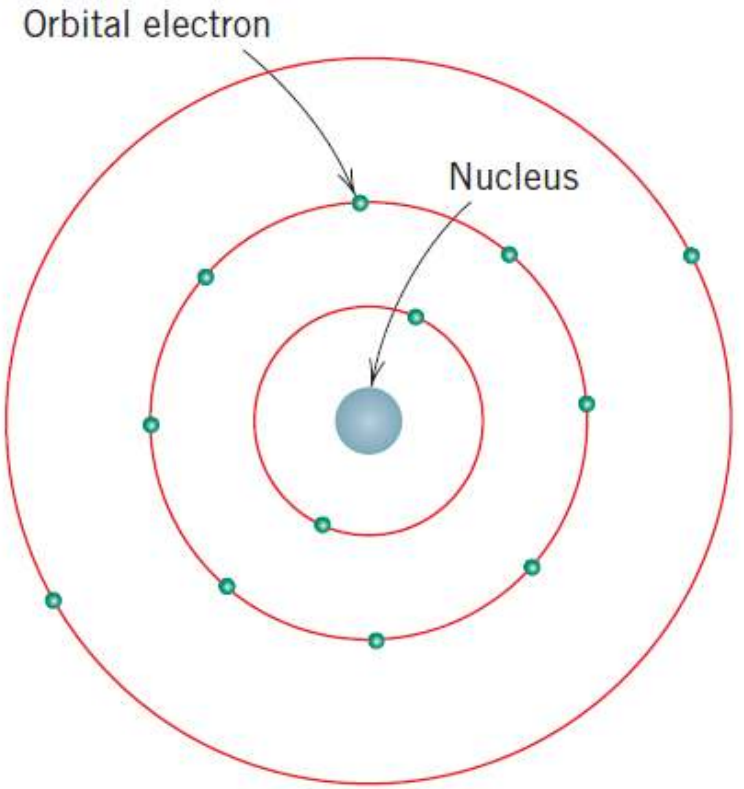
- **Quantum mechanics:** principles and laws that govern systems of atomic and subatomic entities.
- Quantum-mechanical concepts is important to understand the behavior of electrons in atoms.

- Atomic models
  - Bohr Model
  - Wave Mechanical Model

Atomic Models

- **Bohr atomic model**
  - **Represent electron** position (electron orbitals) and energy (quantized energy levels)

- An electron may change energy (higher, Absorption or lower, emission) through energy level or states



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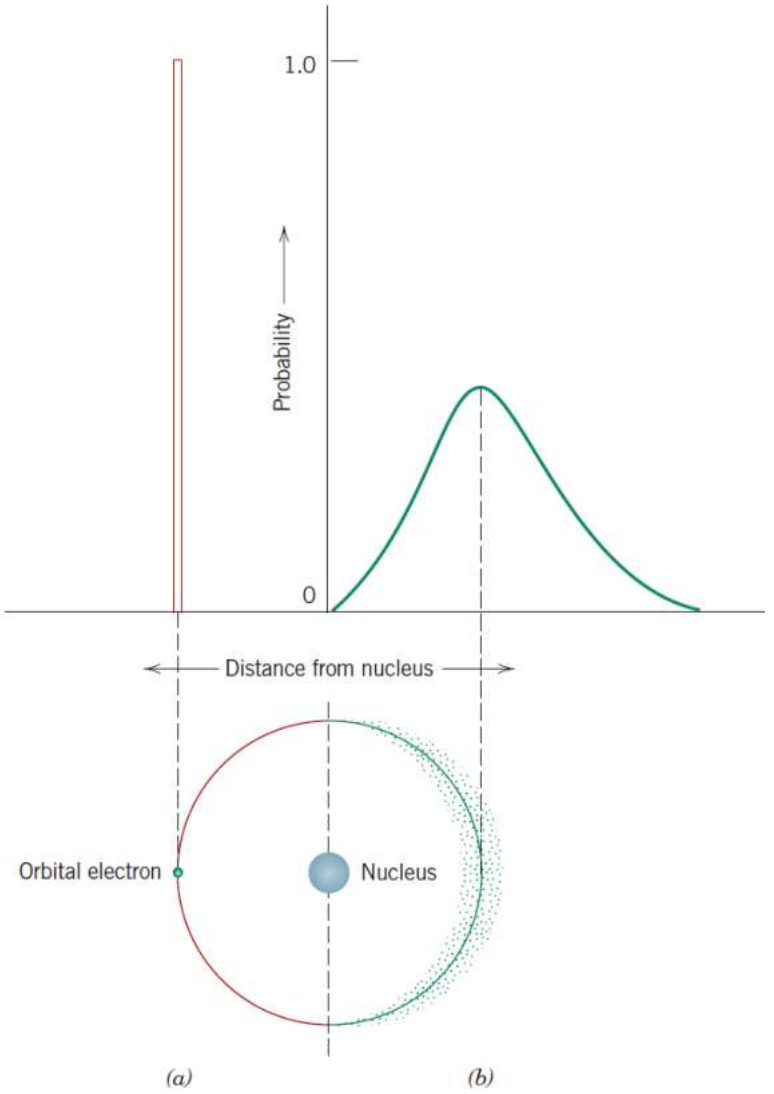
Atomic Models

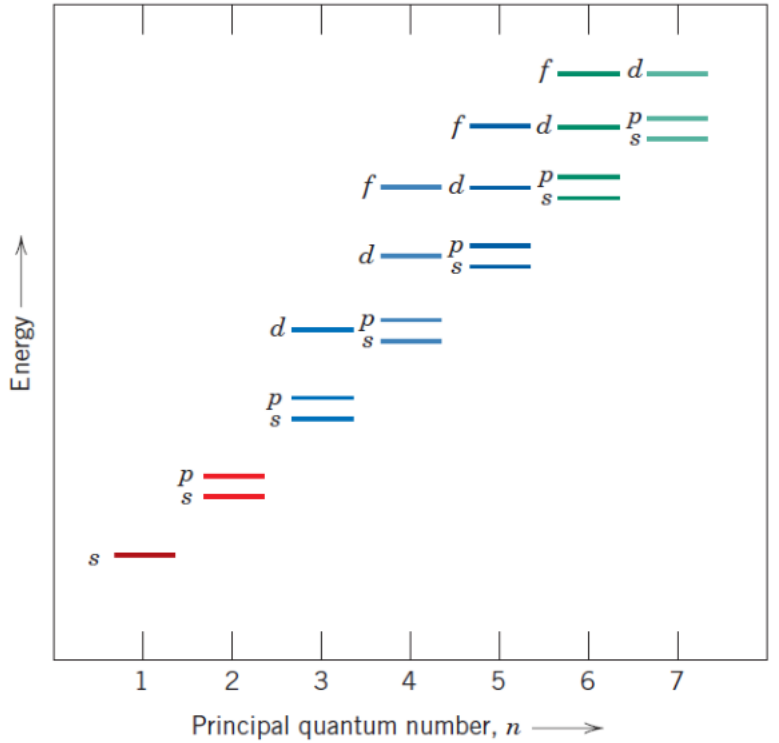
- **Wave-mechanical model**
  - the electron is considered to exhibit both
  - wavelike and particle-like characteristics.



Atomic Models

- **Wave-mechanical model**

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	



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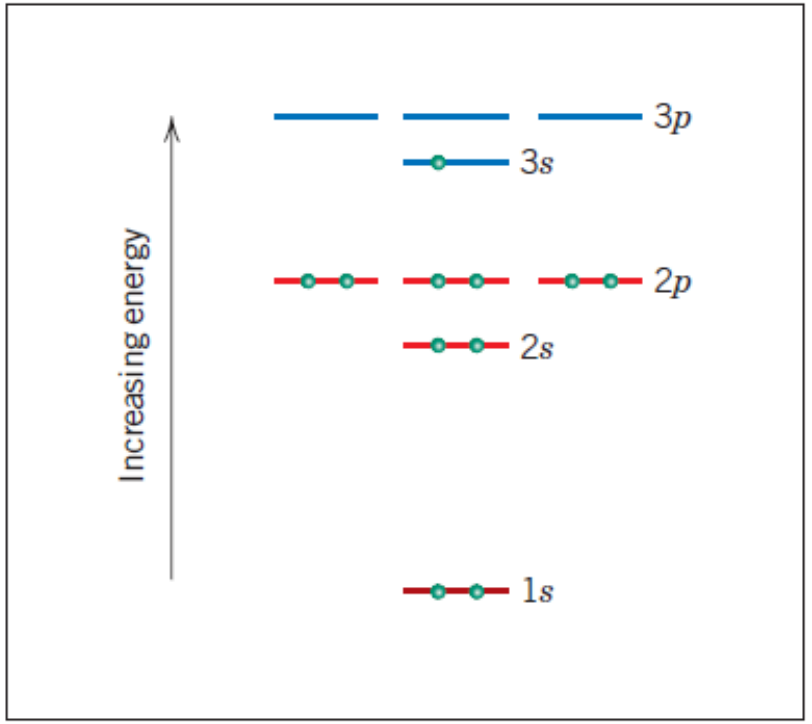
Electron Configuration

- **Electron configuration of an atom:**
  - represents the manner in which these states are occupied

- **Pauli exclusion principle,**
  - each electron state can hold no more than two electrons, which must have
  - Electrons must have opposite spins
  - electrons fill up the lowest possible

  energy states in the electron shells and

- **Ground state:** all the electrons occupy
- the lowest possible energies



Electron Configuration

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

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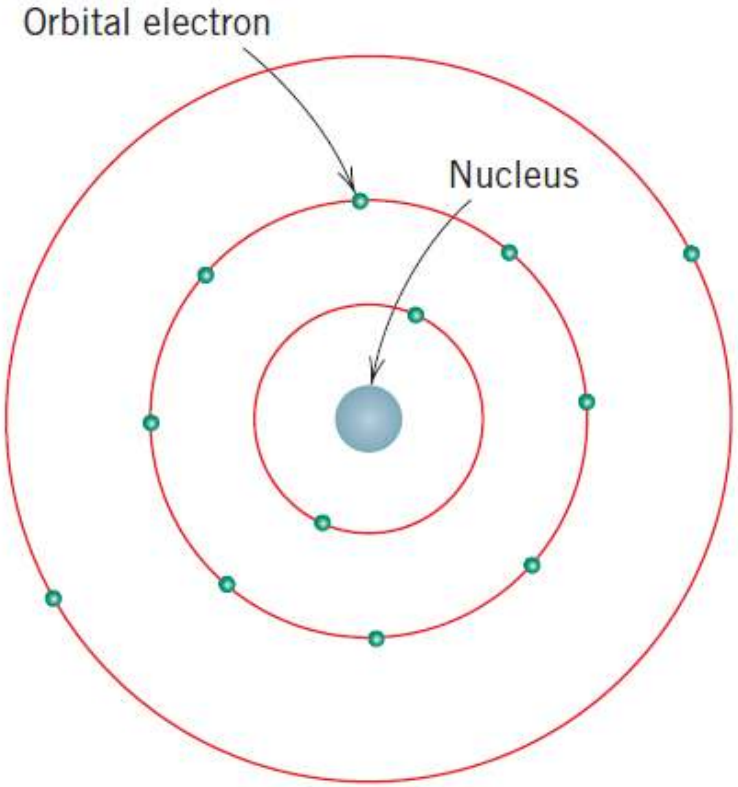
Valence electrons

- Electrons occupy the outermost shell.
- Participate in Atomic bonding
- Physical and chemical properties of solids

 are based on these valence electrons
- *Stable electron configurations;*
  - outermost or valence electron shell are completely
    - For example: He gas, it is inert gas, unreactive.



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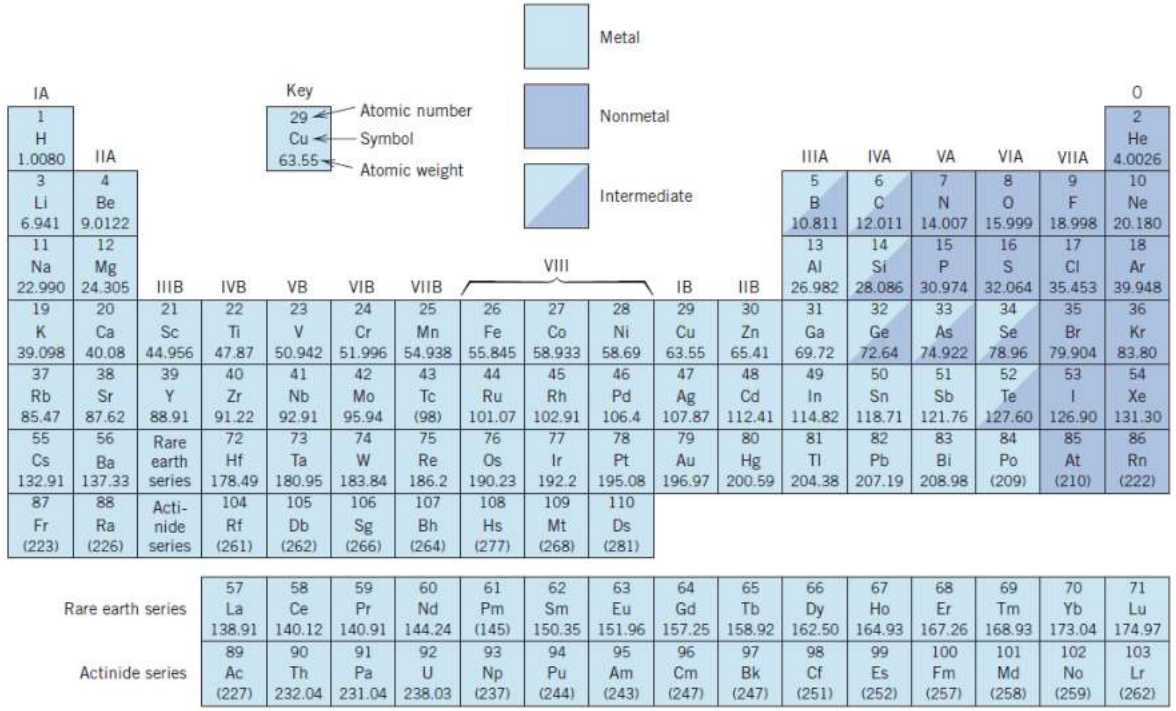
The Periodic Table

- Each row based on atomic number
- Each column same valence electron
- **Electropositive:** give up electron
  - Form positively charged ions
- **Electronegative**; accept electrons
  - Form negatively charged ions



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Atomic Bonding in Solids

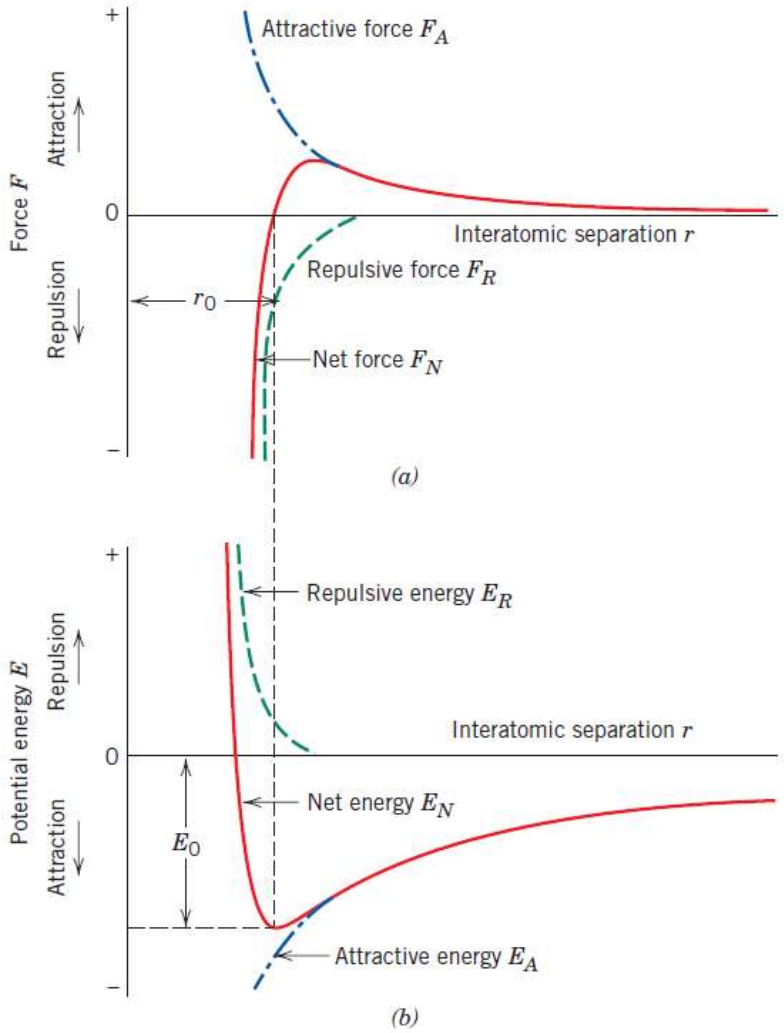
- **Bonding Forces and Energy**
  - Interatomic forces that bind the atoms

$$F_N = F_A + F_R$$

$$E_N = \int_{\infty}^{r} F_N dr$$

$$= \int_{\infty}^{r} F_A dr + \int_{\infty}^{r} F_R dr$$

$$= E_A + E_R$$



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Primary and secondary interatomic bonds

- **Primary Bonds**
  - **Ionic**
  - **Covalent**
  - **Metallic**

- **Secondary Bonds**
  - **van der Waals**
  - **Fluctuating Induced Dipole Bonds**
  - **Polar Molecule-Induced Dipole Bonds**
  - **Permanent Dipole Bonds**

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Ionic Bonding

- Found in compounds that are composed of both metallic and nonmetallic elements

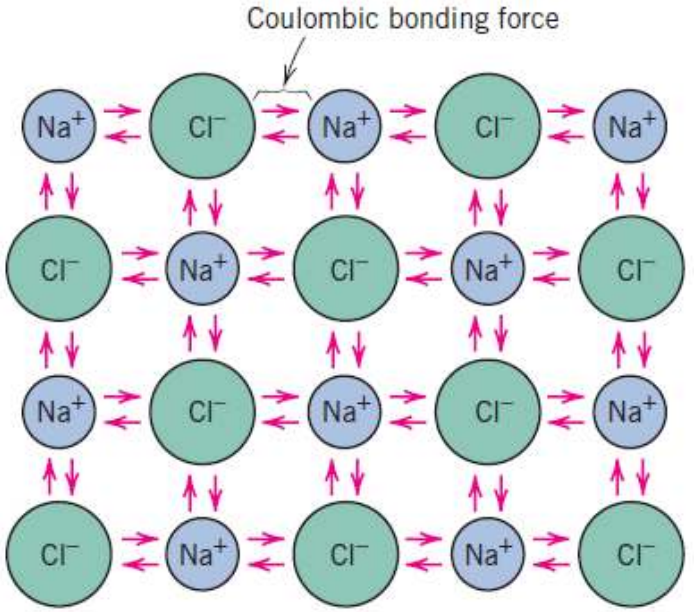
  e.g. NACL : all atoms here are ions (one give and one accept)

- The attractive bonding forces are **coulombic**

$$E_A = -\frac{A}{r} \qquad E_R = \frac{B}{r^n}$$

- *A*, *B*, and *n* are constants
- *Nondirectional =>* magnitude of the bond

is equal in all directions around an ion.



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Classification of Materials

- Ionic materials: hard, brittle and electrically and thermally insulative

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

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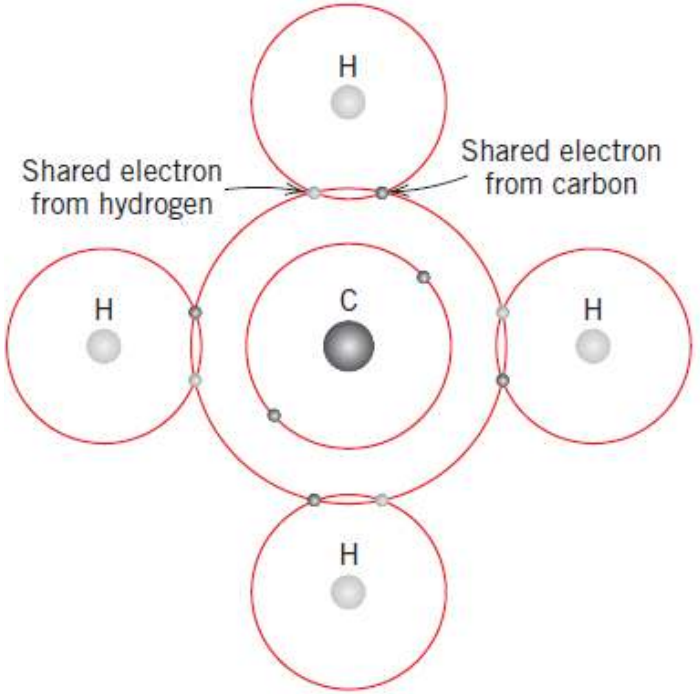
Covalent Bonding

- **Covalent bonding:** sharing of electrons between adjacent atoms.

- Directional bond: it is between specific atoms
  - Nonmetallic elemental molecules (H2, Cl2, F2, etc.)
  - Dissimilar atoms, such as CH4, H2O, HNO3, and HF,



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Covalent Bonding

- Number of covalent bonds ($8 - N$)
- carbon, $N = 4$, and each carbon atom has 8 – 4, or four, electrons to share.
- Found in Polymer: carbon chain

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

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Ionic + Covalent Bond

- Very few compounds exhibit pure ionic or covalent bonding.

$$\%\ \text{ionic character} = \{1 - \exp[-(0.25)(X_A - X_B)^2]\} \times 100$$

where X_A and X_B are the electronegativities for the respective elements

IA							VIII					IIIA	IVA	VA	VIA	VIIA	0
1 H 2.1	IIA									IB	IIB						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	IIIB	IVB	VB	VIB	VIIB						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															

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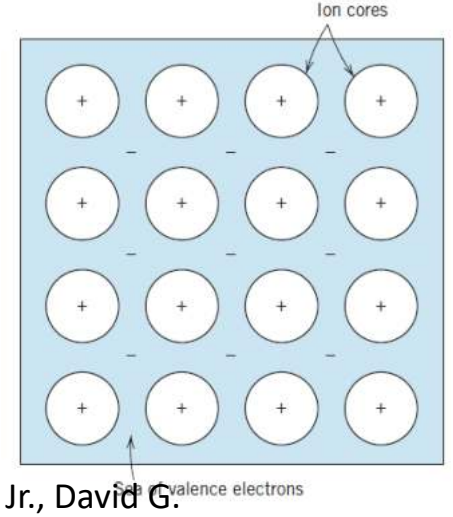
Metallic Bonding

- Found in metals and their alloys.
- Metallic materials have one, two, or at most, three valence electrons.
- Valence electrons are not bound to any particular atom and are more or less free to drift throughout the entire metal forming a “sea of electrons” or an “electron cloud.”
- Non-valence electrons and atomic nuclei form what are called ***ion cores***
- The free electrons shield the positively charged ion cores from mutually repulsive electrostatic forces => act as a “glue” to hold the ion cores together.
- Nondirectional Bond.

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



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Atomic bonds and Material Property

- Metals have free electrons => good conductors of both electricity and heat
- Ionically and covalently bonded materials are typically electrical and thermal insulators **because** of free electrons.

- Metallic bonds…Ductile

- Ionic and Covalent bond….. brittle

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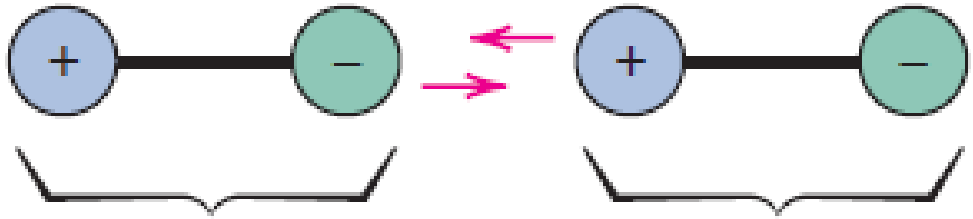
Secondary, van der Waals Bonding

- Or physical **bonds:** Secondary bonding forces arise from atomic or molecular **dipoles.**
- Weak and may be obscured in the presence of primary bonding types
- Bonding results from the coulombic attraction between the positive end of one dipole and the negative region of an adjacent one.



Atomic or molecular dipoles

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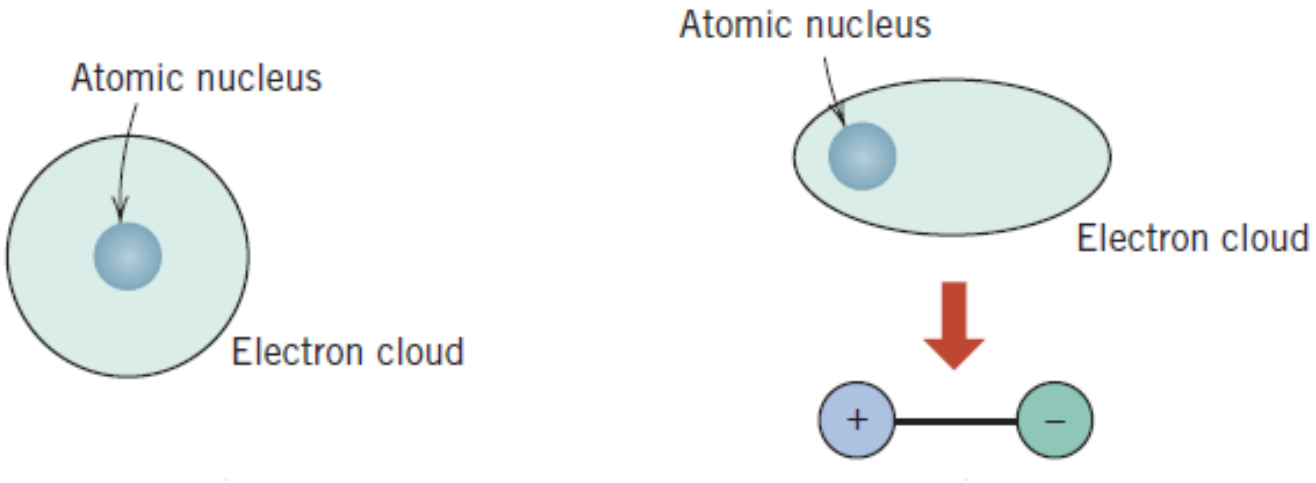
Fluctuating Induced Dipole Bonds

- A dipole may be created or induced in an atom or molecule that is normally electrically symmetric



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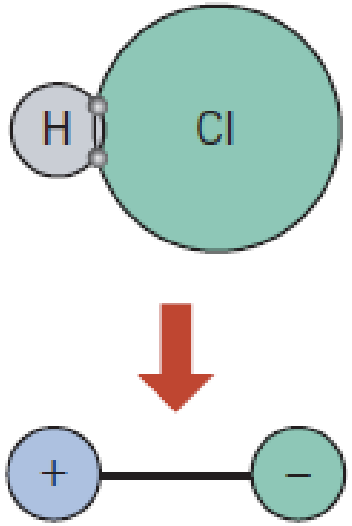
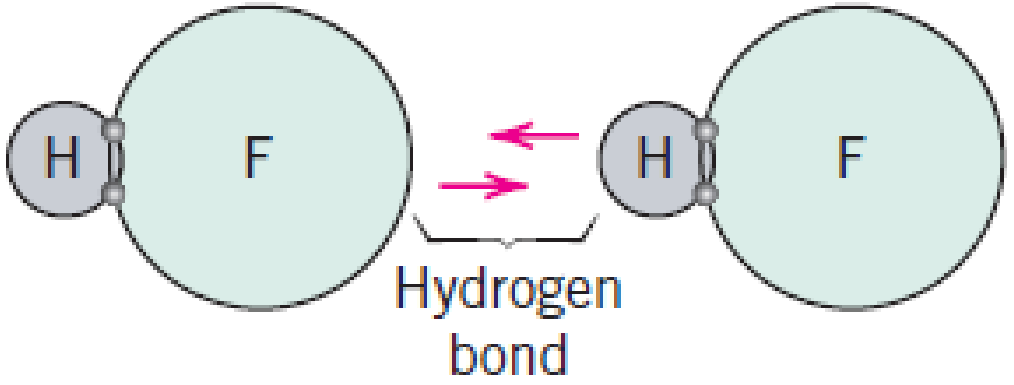
Polar Molecule-Induced Dipole Bonds

Permanent dipole moments exist due to asymmetrical arrangement of positively and negatively charged regions; such molecules are termed **polar molecules.**



Permanent Dipole Bonds

Van der Waals forces will also exist between adjacent polar molecules.



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