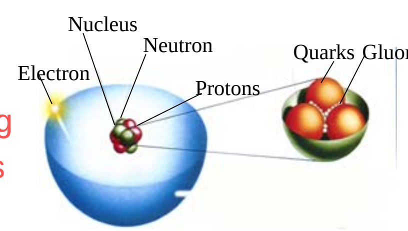
Chapter 2: Atomic structure and interatomic bonding

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

Chapter 2: Atomic structure and interatomic bonding

- Fundamental concepts
  - Proton and electron, charged 1.60 x10^{-19} C
  - Mass of electron 9.11x10^{-31} kg
  - Mass of protons and neutrons
    1.67 x 10^{-27} kg



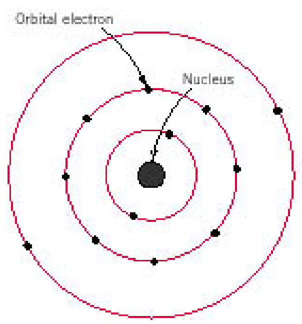
  - Atomic number: the number of protons
  - Atomic mass =protons+neutrons
  - Isotope
  - Atomic mass unit(amu): 1amu=1/12 C
  - One mole = 6.023x10^{23} atoms(Avogadro's)

Electrons in atoms

- Atomic models
  - Bohr atomic

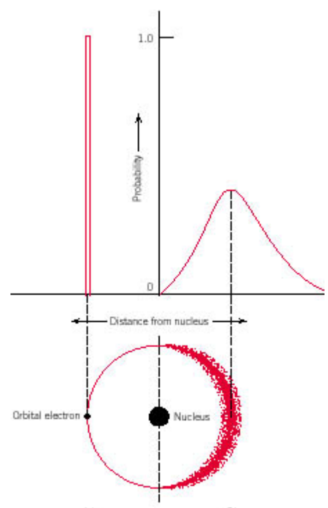
    electrons revolve around the atomic nucleus in discrete orbital and the energies of electrons are quantized
  - Wave-mechanical

    Electron exhibits both wavelike and particle-like characteristics, its position is considered to be a probability distribution



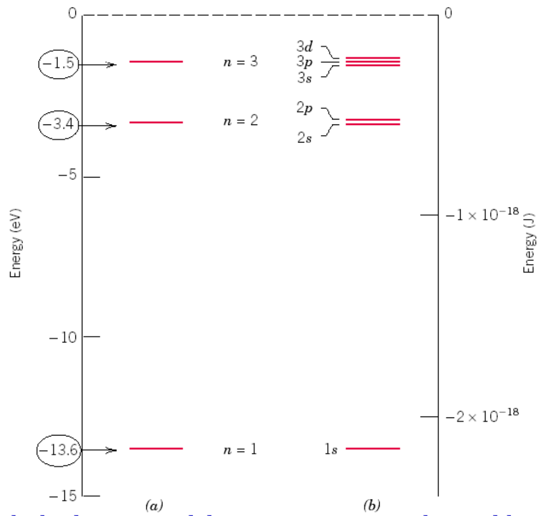
Electrons in atoms (*continue*)

- **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

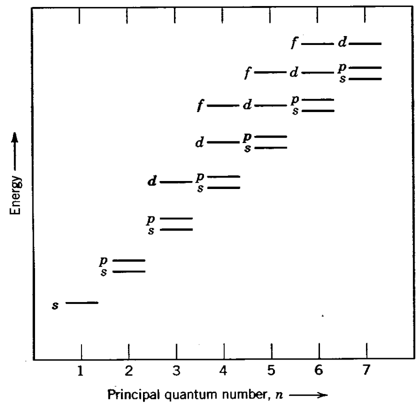
- Principle quantum number n=1, 2 ..; K, L, M, N, O
- Orbital quantum number l=0, ..n-1; subshell, s, p, d, or f; the shape of the electron subshell
- Spin moment ms 1/2 or -1/2

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	

Quantum numbers

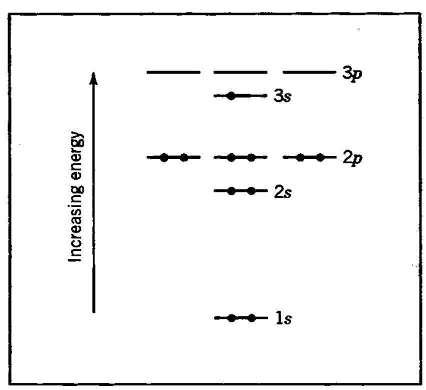
- The smaller n, the lower energy
- The smaller l, the lower energy
- There are some overlaps in energy, especially for d and f states



Relative energies of the electrons for various shells and subshells

Electron configurations

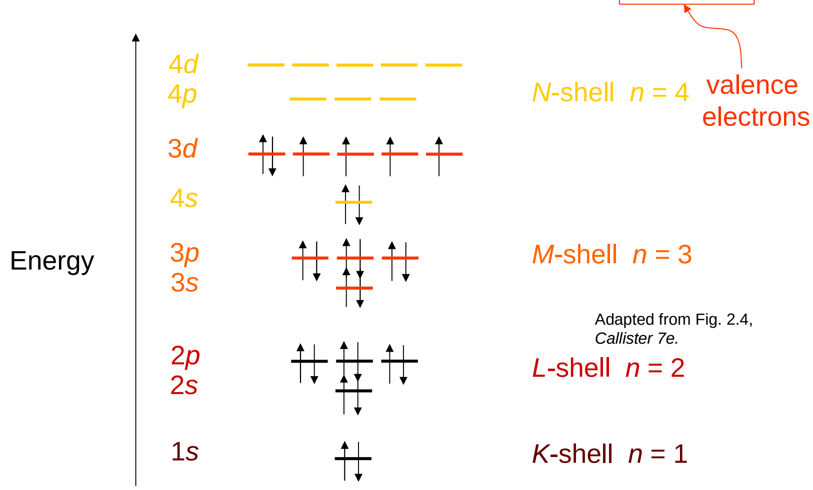
- Energy minimum rule
- Pauli exclusion
- Hund's rule: as many unpaired electrons as possible
- Ground state
- Valence electrons



Filled energy states for a sodium atom

Electronic configurations

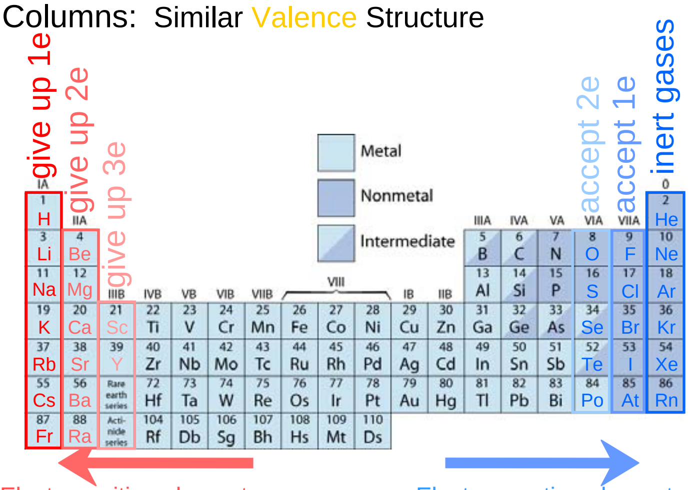
ex: Fe - atomic # = 26 $1s^2$ $2s^2 2p^6$ $3s^2 3p^6$ $3d^6$ $4s^2$



Adapted from Fig. 2.4, *Callister 7e.*

The periodic table

- Columns: Similar Valence Structure



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

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

Electronegative elements:
Readily acquire electrons
to become - ions.

The periodic table

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

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La-Lu 1.1-1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac-No 1.1-1.7															

← Smaller electronegativity

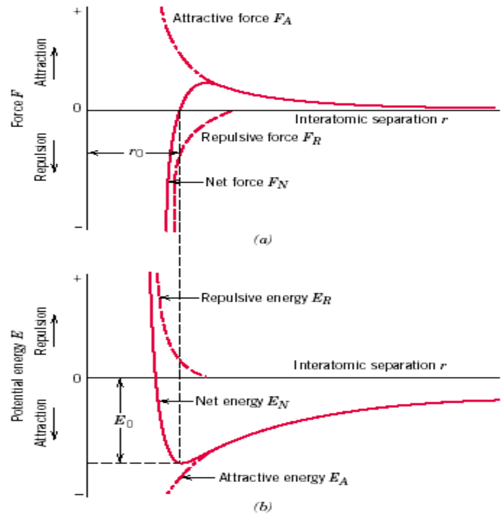
Larger electronegativity →

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

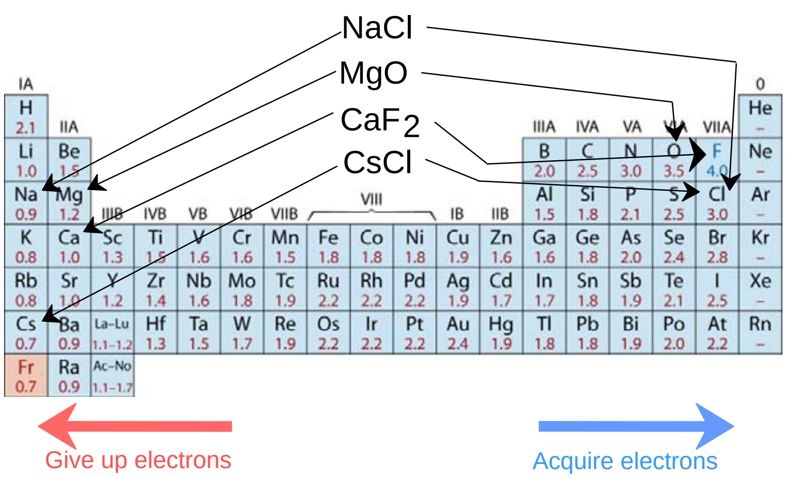
Atomic bonding in solids

- 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 bonding: Ionic Bonding

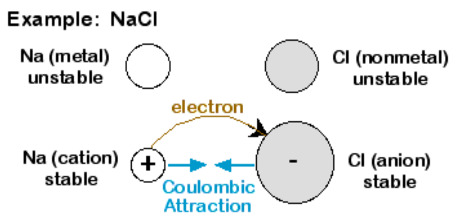
- Predominant bonding in Ceramics



Primary interatomic bonding (*continue*)

☐ Ironic bonding

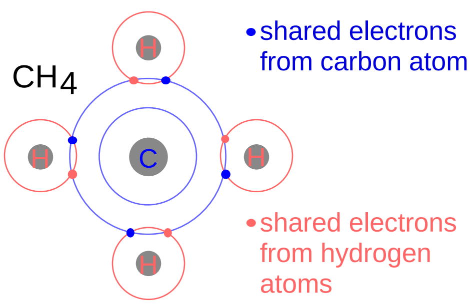
- An ionic bond is formed when an atom loses or gains one or more electrons from its outer shell
- Between metallic and nonmetallic
- Attractive bonding force--coulombic
- Non-directional
- E_A=-A/r, E_R=B/r^n , n~8



Primary interatomic bonds (*continue*)

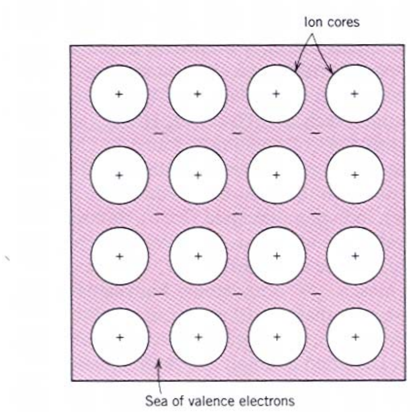
☐ Covalent bonding

- stable electron configurations are assumed by sharing electrons between adjacent atoms
- directional
- many non-metallic elements
- % ionic character={1-exp[-(0.25)$(X_A-X_B)^2$]}x100



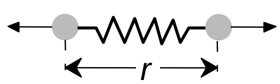
Primary interatomic bonds (*continue*)

- Metallic bonding
  - sea of valence electrons floating on ion cores
  - non-directional
  - metal and metal alloys
  - electrons are balanced with ion cores in charge

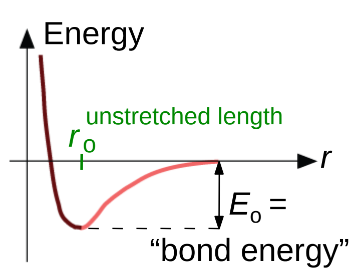


Properties From Bonding: T_m

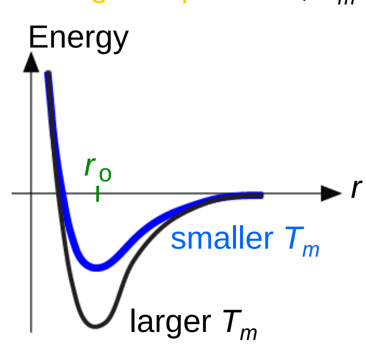
- Bond length, r



- Bond energy, E_o



- Melting Temperature, T_m



T_m is larger if E_o is larger.

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Summary: Bonding

Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional (semiconductors, ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular

Summary: Primary Bonds

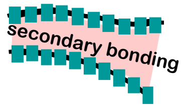
Ceramics
(Ionic & covalent bonding):

Large bond energy
large T_m
large E

Metals
(Metallic bonding):

Variable bond energy
moderate T_m
moderate E

Polymers
(Covalent & Secondary):



Directional Properties
Secondary bonding dominates
small T_m
small E

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