Materials Science & Engineering

- Development and advancement of societies are tied to production and use of materials
  - From naturally occurring → processed → alteration of existing ones
  - Material selection: from a limited set → wide range for use from simple to complex designs
- Discovery of relationship between *structural* elements and properties is recent (60 yrs)
- All stepwise modern technological development driven by advent of suitable materials with the right combination of properties
  - Automobiles, aircraft, electronics
- Matls Science = study of relationships between *structure* and *properties*
- Matls Engineering = *designing structure* that will produce the *desired properties*

Structure - Properties

- *Structure* = arrangement of constituent elements of material
  - Sub-atomic – electronic structure,
  - Atomic – crystal structure
  - Microscopic – observable under microscope
  - Macroscopic – observable under unaided eyes
- *Properties* = response to various stimuli
  - Mechanical – response to mechanical stress
  - Electrical – response to electrical field (current)
  - Thermal – response to heat
  - Chemical – response to corrosion or other chemical degradation
  - Magnetic – response to magnetic field
  - Optical – response to light or electromagnetic radiation

Material Classification

- Metals
  - Elemental, Non-localized electrons, good electrical and thermal conductivity, lustrous, strong but deformable
- Ceramics
  - Compounds (oxides, nitrides, carbides) and elemental, heat resistant, hard but also brittle, poor electrical conductors
- Polymers
  - Organic, large molecules, low densities and flexible: plastics, rubbers
- Composites
  - Combining more than one material class, concrete, fiberglass, carbon fiber reinforced plastics, honeycomb
- Semi-conductors
  - Electrical properties intermediate between metals and ceramics; may be precisely controlled through doping with other elements
- Bio-materials
  - Materials selected for compatibility with human body
- Smart materials
  - May sense changes in the environment and respond to them: shape memory, piezoelectric, magnetorestrictive, electro/magneto-rheological

CHAPTER 2:
BONDING AND PROPERTIES

ISSUES TO ADDRESS...

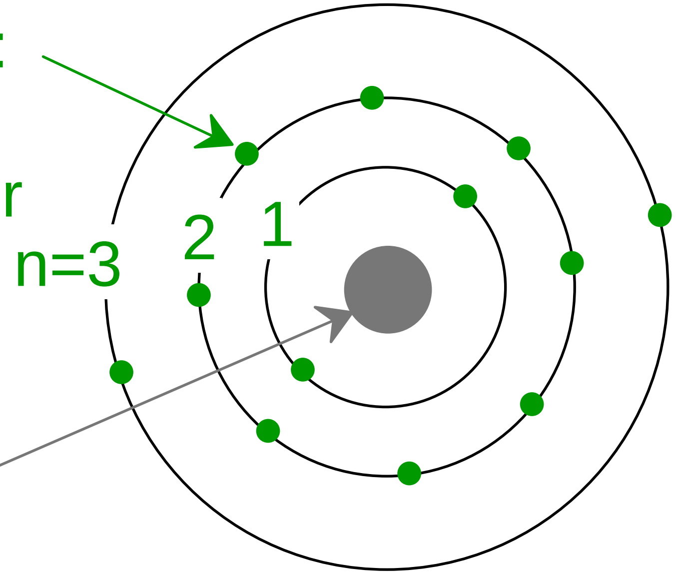
- What promotes bonding?
- What types of bonds are there?
- What properties are inferred from bonding?

Atomic Models

- *Quantum mechanic model*
  - BOHR Atomic model: electrons revolve around the nucleus in discrete orbitals (i.e. *trajectory of the electron is well defined*)
    - Established that ***Energy is quantized***: Only specific amount of energies, described by *quantum numbers*, can be absorbed or lost so only specific trajectories are allowed (i.e upon absorbing or loosing energy, trajectory does not immediately change to account for change in energy.
- *Wave-Mechanic Model*
  - Electron does not move along a specific trajectory BUT
    - (1) Probability of electron being found at given location around the nucleus (**A cloud of possible locations around nucleus.)**
    - (2) ***Energy is quantized*** into *shells* and *sub-shells* – size, shape, spatial orientation described by quantum numbers

BOHR ATOM

orbital electrons:
n = principal
quantum number



Adapted from Fig. 2.1, *Callister 6e.*

Nucleus: Z = # protons

= 1 for hydrogen to 94 for plutonium

N = # neutrons

Atomic mass A ≈ Z + N

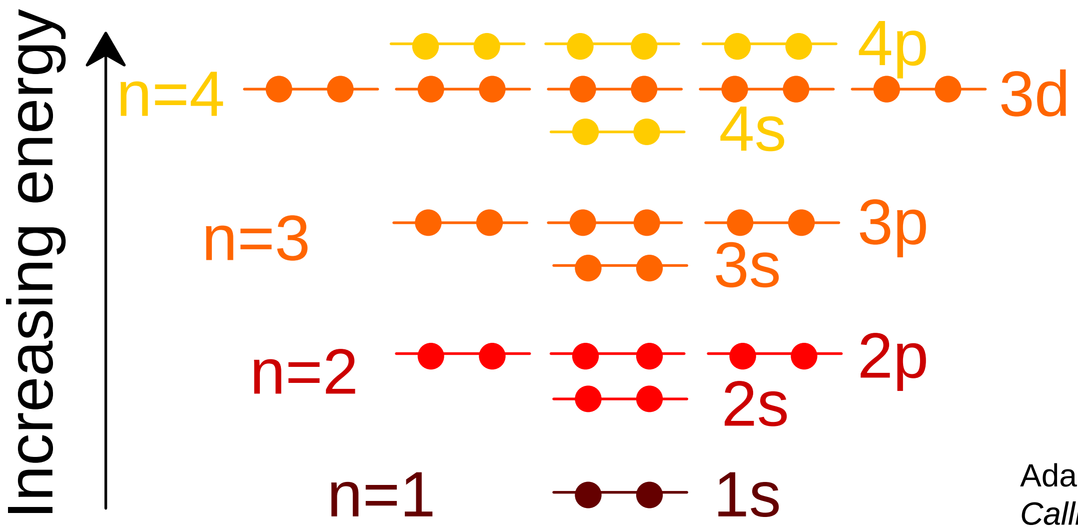
Quantum numbers

- *Principal* quantum n=1, 2, 3, 4, 5 etc. or K, L, M, N, O **shell** refers to *size*
- Second (*azimuthal*) quantum number: l = 0, 1, 2, 3…n-1 or corresponding to s, p, d, f … **sub-shell** (orbital) refers to shape (# of elecrons in each shell)
- Third (*magnetic*) quantum number: number of electrons states in each subshell (orbital), m = integers from -l to +l
- Number of possible energy levels determined by Principal azimuthal and magnetic quantum numbers
- Fourth (*spin*) quantum number: 2 possible values -½ and +½
- Pauli exclusion principle No more than two electrons with opposing spins may be present in each orbitals
- **Electron states** = value of energies electrons are allowed to possess.

ELECTRON ENERGY STATES

Electrons...

- have discrete energy states
- tend to occupy lowest available energy state.



Adapted from Fig. 2.5, *Callister 6e.*

Electronic structure of Sodium =$1s^2 2s^2 2p^6 3s^1$;

Germanium $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$

STABLE ELECTRON CONFIGURATIONS

Stable electron configurations...

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

Z	Element	Configuration
2	He	$1s^2$
10	Ne	$1s^2 2s^2 2p^6$
18	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$
36	Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

Adapted from Table 2.2, *Callister 6e.*

SURVEY OF ELEMENTS

- Most elements: Electron configuration not stable.

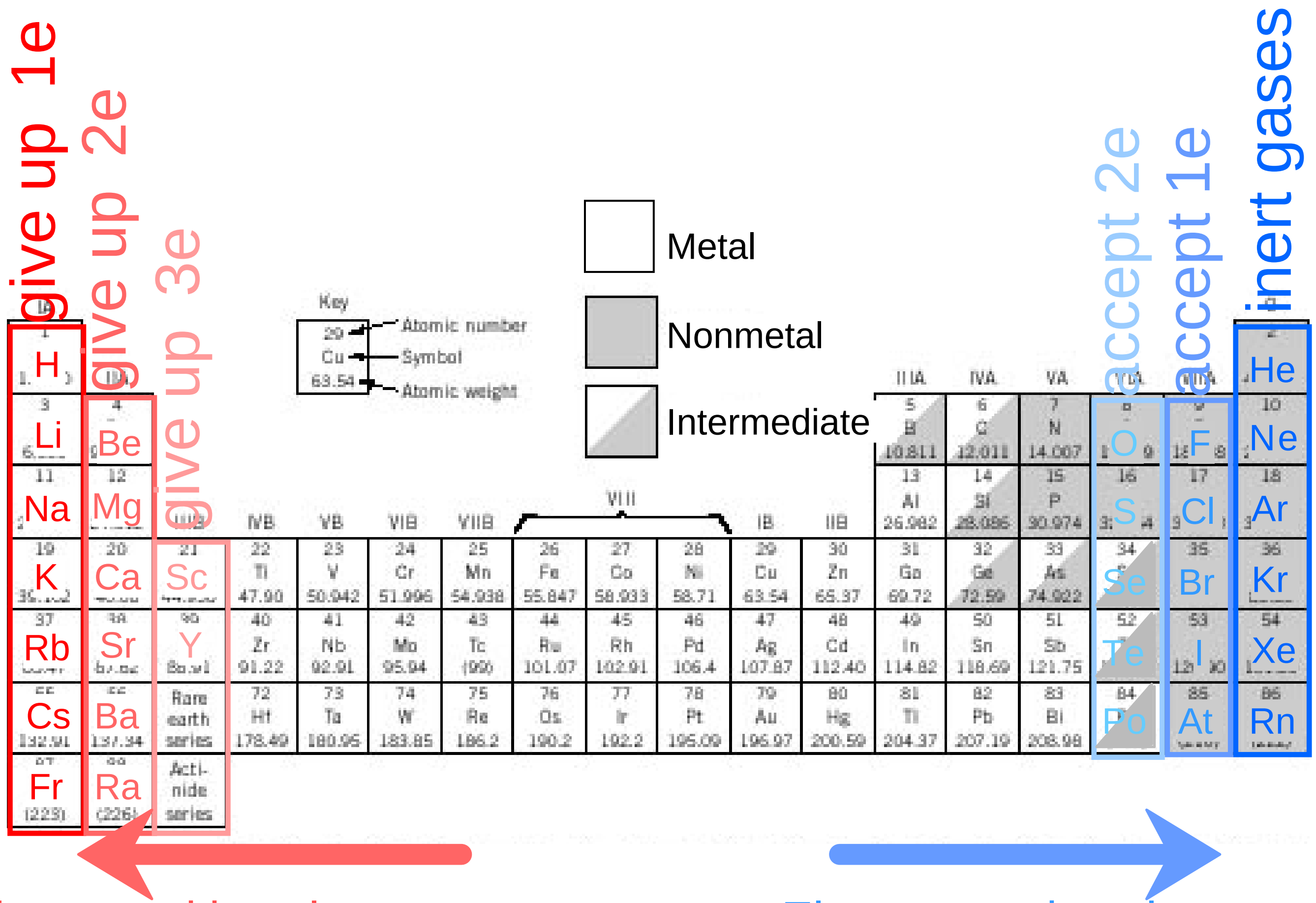
Element	Atomic #	Electron configuration	
Hydrogen	1	$1s^1$	
Helium	2	$1s^2$	(stable)
Lithium	3	$1s^2 2s^1$	
Beryllium	4	$1s^2 2s^2$	
Boron	5	$1s^2 2s^2 2p^1$	
Carbon	6	$1s^2 2s^2 2p^2$	
...		...	
Neon	10	$1s^2 2s^2 2p^6$	(stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$	
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$	
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$	
...		...	
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$	(stable)
...	...	...	
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4^6$	(stable)

Adapted from Table 2.2, *Callister 6e.*

- Why? Valence (outer) shell usually not filled completely.

THE PERIODIC TABLE

- Columns: Similar Valence Structure



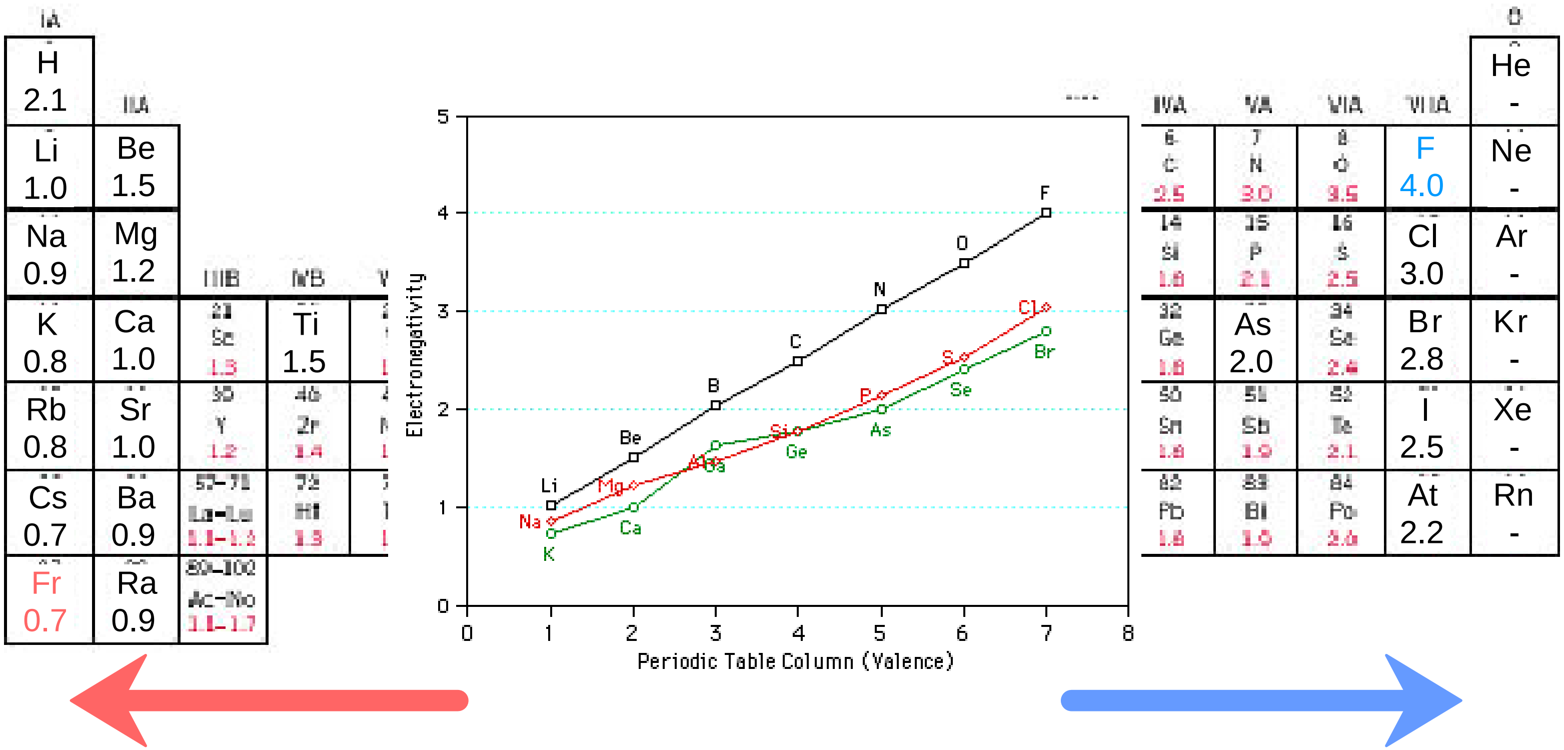
Adapted from Fig. 2.6, *Callister 6e.*

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

Electronegative elements:
Readily acquire electrons
to become - ions.

ELECTRONEGATIVITY

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



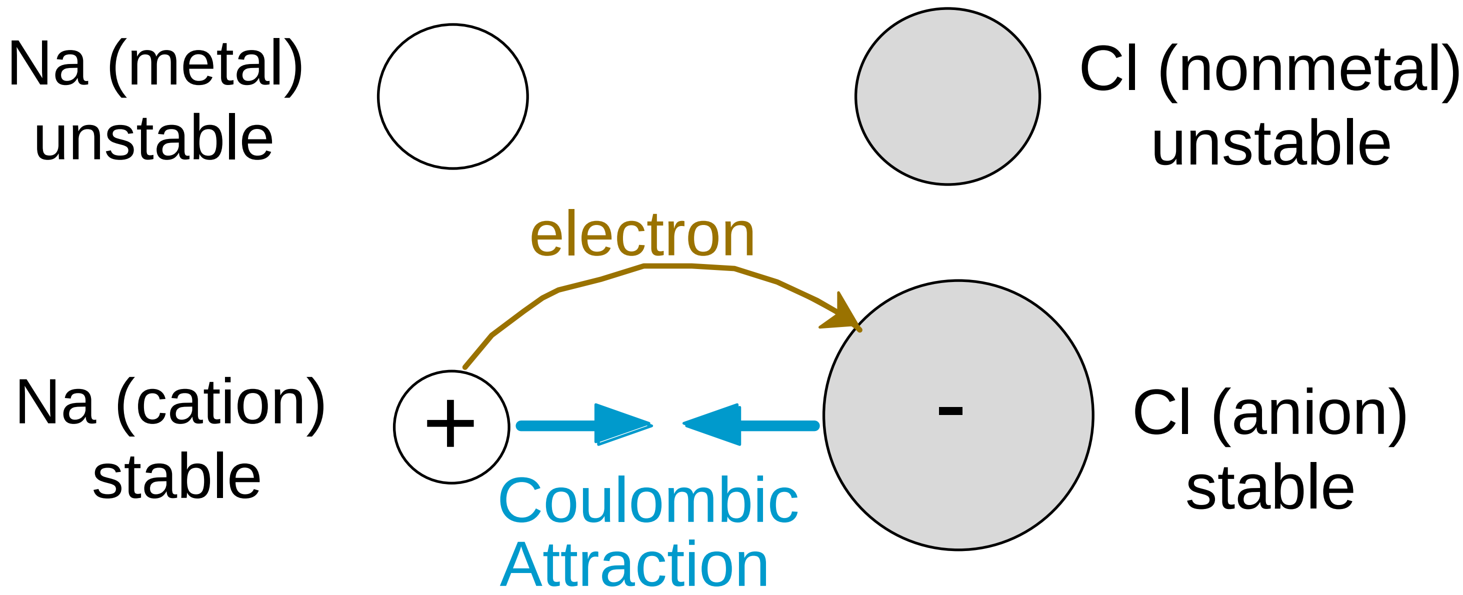
Smaller electronegativity

Larger electronegativity

Adapted from Fig. 2.7, *Callister 6e.* (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.

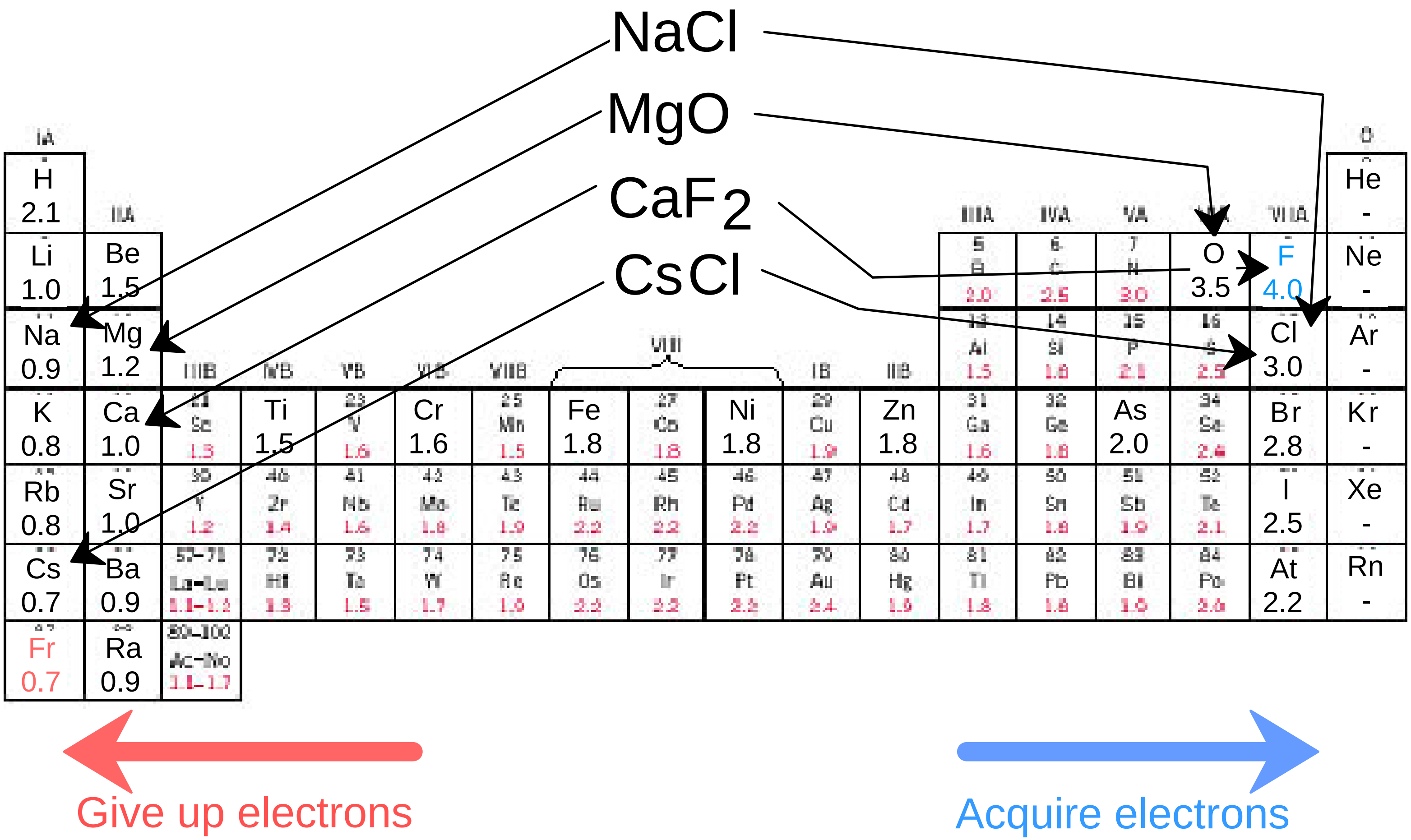
IONIC BONDING

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



EXAMPLES: IONIC BONDING

- Predominant bonding in Ceramics



Adapted from Fig. 2.7, *Callister 6e.* (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.

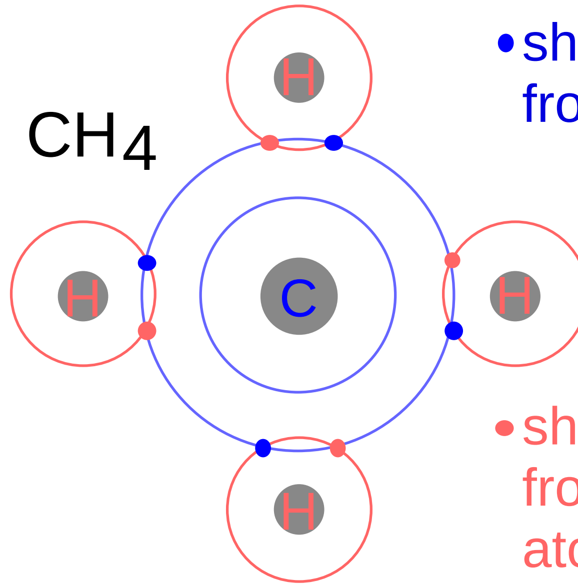
COVALENT BONDING

- Requires shared electrons
- Example: CH_4

C: has 4 valence e,
needs 4 more

H: has 1 valence e,
needs 1 more

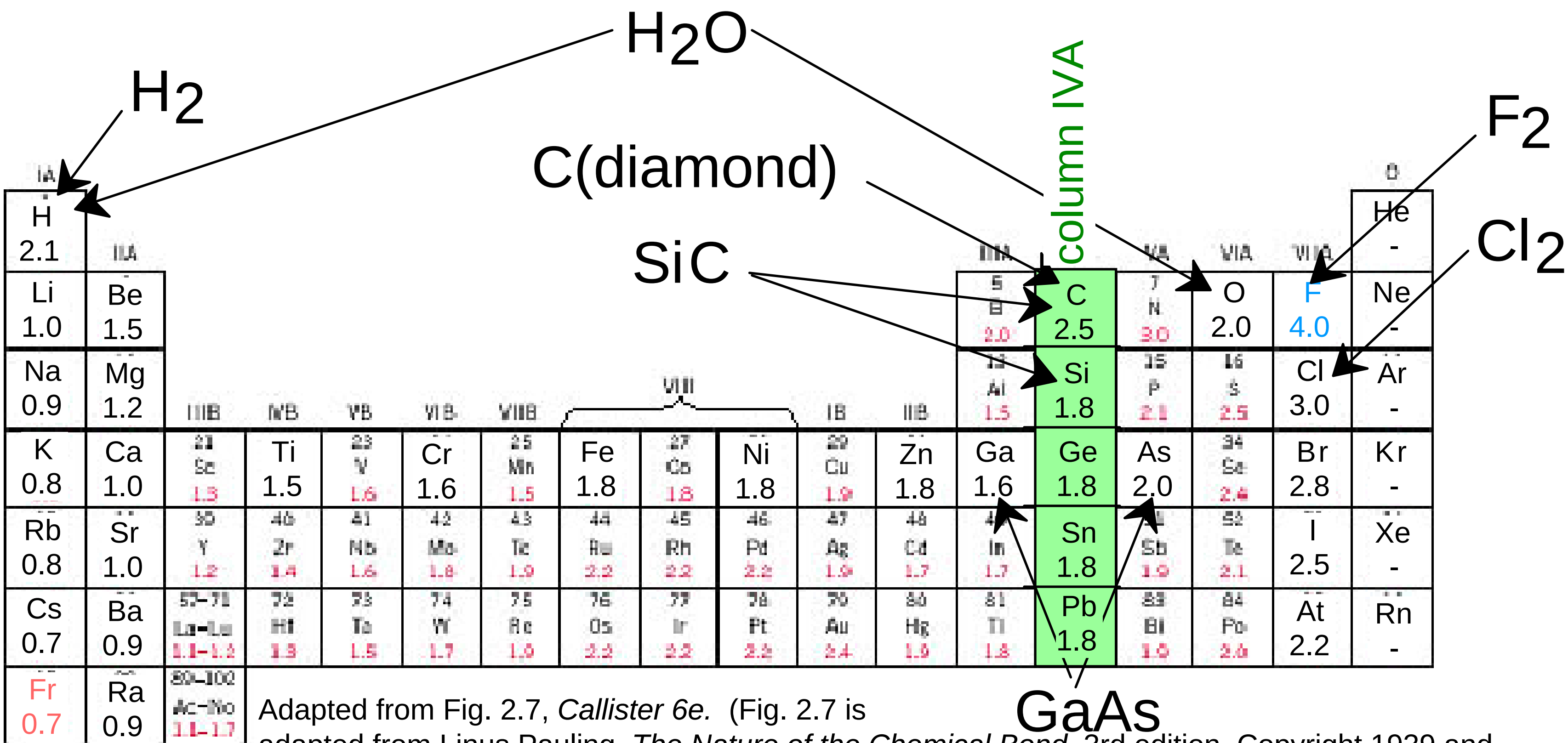
Electronegativities
are comparable.



- shared electrons from carbon atom
- shared electrons from hydrogen atoms

Adapted from Fig. 2.10, *Callister 6e.*

EXAMPLES: COVALENT BONDING

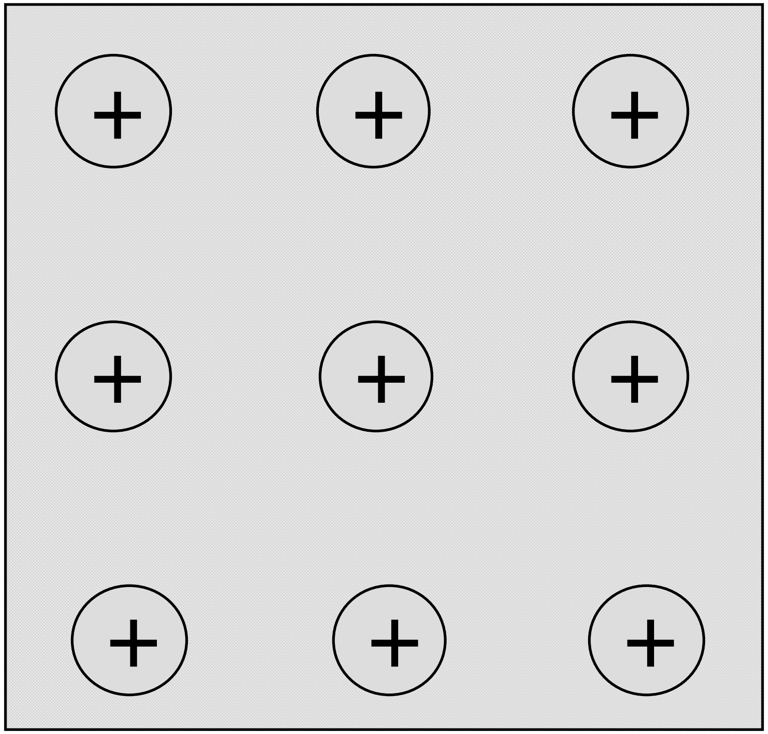


Adapted from Fig. 2.7, *Callister 6e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

- Molecules with nonmetals
- Molecules with metals and nonmetals
- Elemental solids (RHS of Periodic Table)
- Compound solids (about column IVA)

METALLIC BONDING

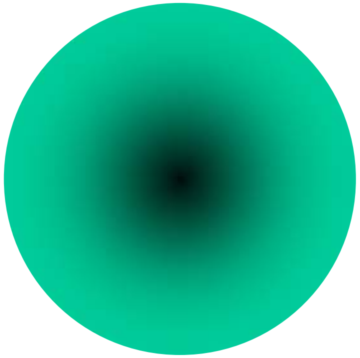
- Arises from a sea of donated valence electrons (1, 2, or 3 from each atom).



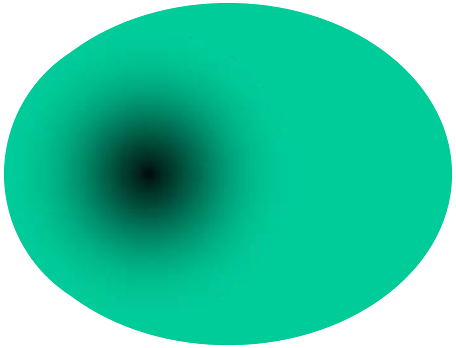
Adapted from Fig. 2.11, *Callister 6e.*

- Primary bond for metals and their alloys

Polarization



Atom

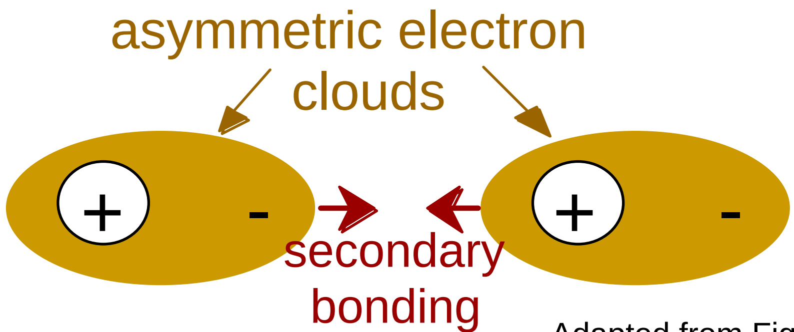


Polarized atom

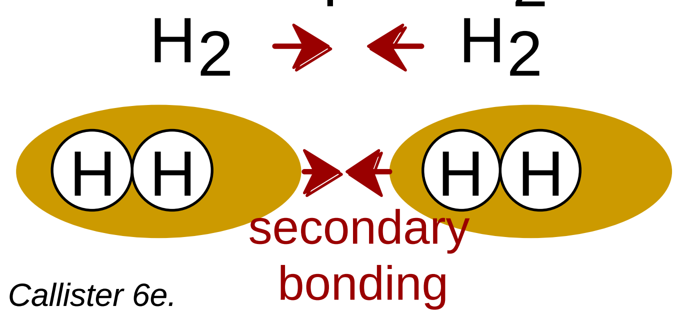
SECONDARY BONDING

Arises from interaction between dipoles

- Fluctuating dipoles



ex: liquid H_2



Adapted from Fig. 2.13, *Callister 6e.*

- Permanent dipoles-molecule induced

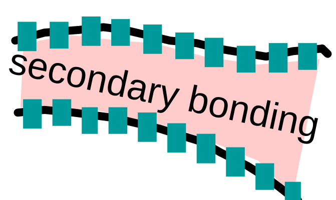
-general case:

Adapted from Fig. 2.14, *Callister 6e.*

-ex: liquid HCl

Adapted from Fig. 2.14, *Callister 6e.*

-ex: polymer

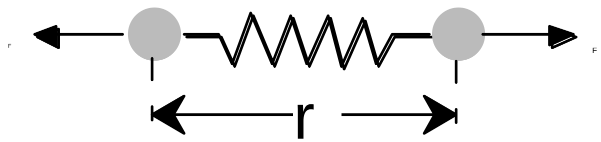


SUMMARY: BONDING

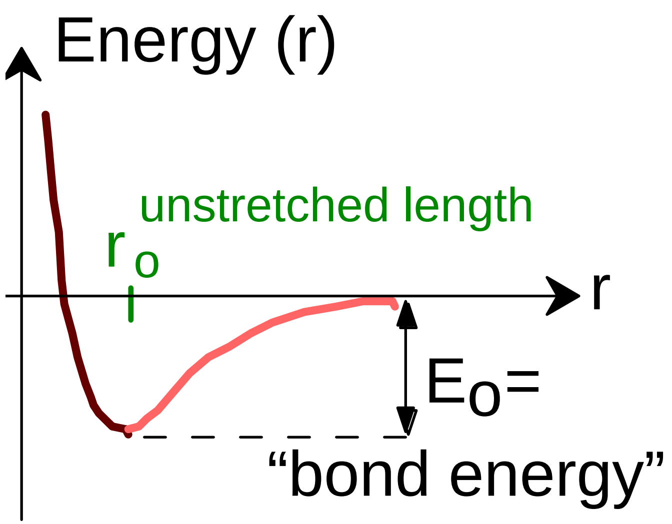
Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional semiconductors, ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular

PROPERTIES FROM BONDING: T_M

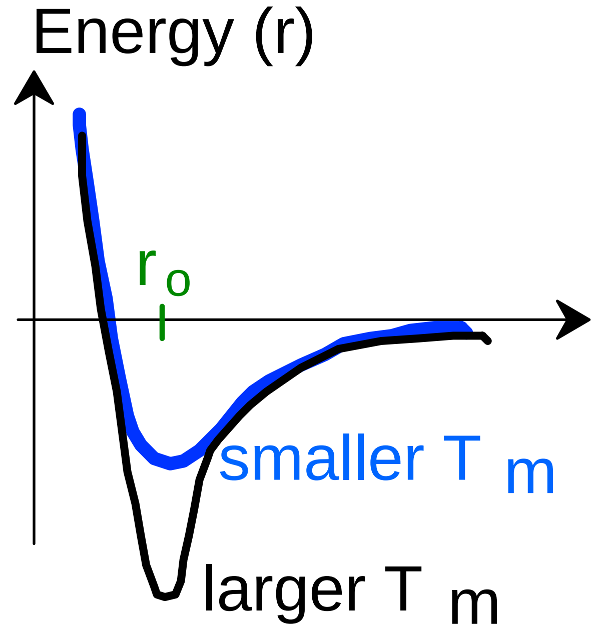
- Bond length, r



- Bond energy, E_o



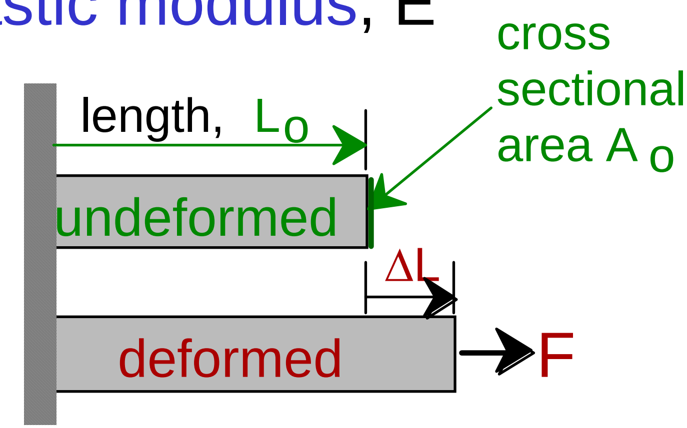
- Melting Temperature, T_m



T_m is larger if E_o is larger.

PROPERTIES FROM BONDING: E

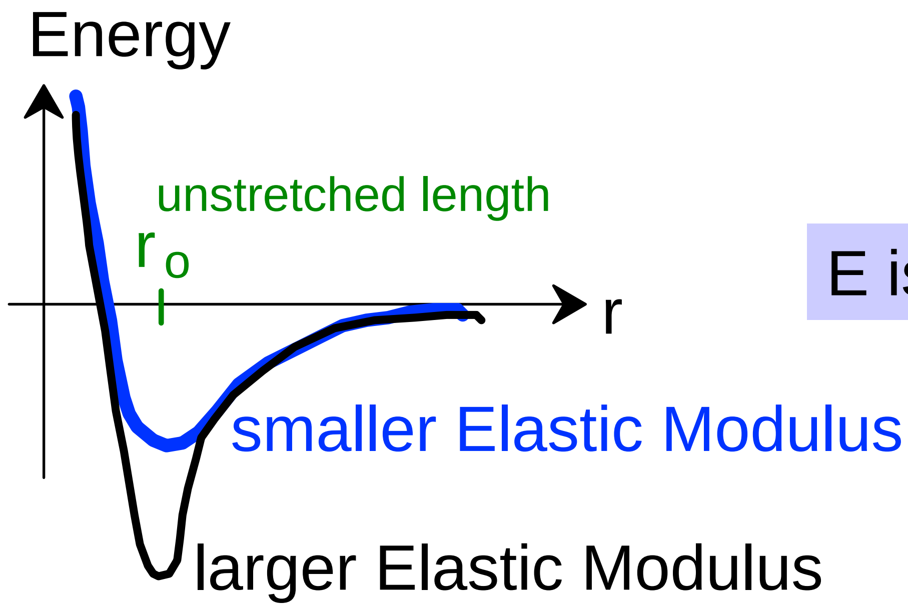
- Elastic modulus, E



Elastic modulus

$$\frac{F}{A_o} = E\,\frac{\Delta L}{L_o}$$

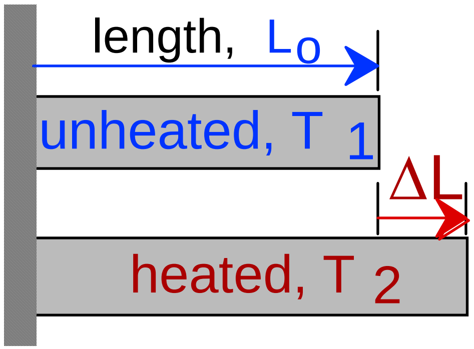
- E ~ curvature at r_o



E is larger if E_o is larger.

PROPERTIES FROM BONDING: α

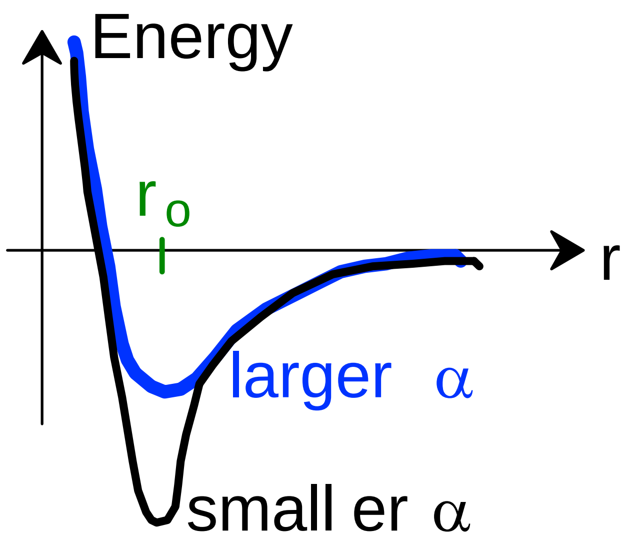
- Coefficient of thermal expansion, α



coeff. thermal expansion

$$\frac{\Delta L}{L_o} = \alpha\,(T_2 - T_1)$$

- α ~ symmetry at r_o



α is larger if E_o is smaller.

SUMMARY: PRIMARY BONDS

Ceramics

(Ionic & covalent bonding):

Large bond energy

large T_m

large E

small α

Metals

(Metallic bonding):

Variable bond energy

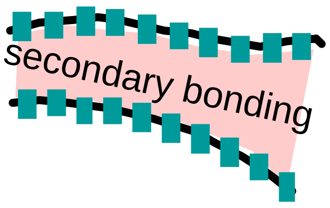
moderate T_m

moderate E

moderate α

Polymers

(Covalent & Secondary):



Directional Properties

Secondary bonding dominates

small T

small E

large α

ANNOUNCEMENTS

Reading:

Core Problems:

Self-help Problems: