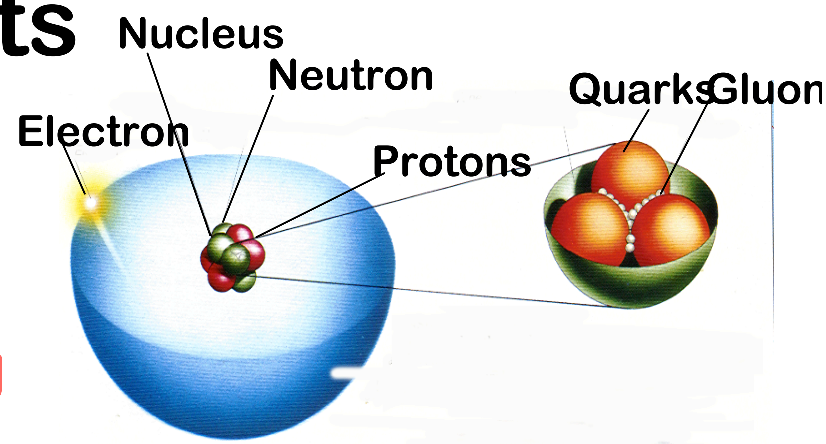
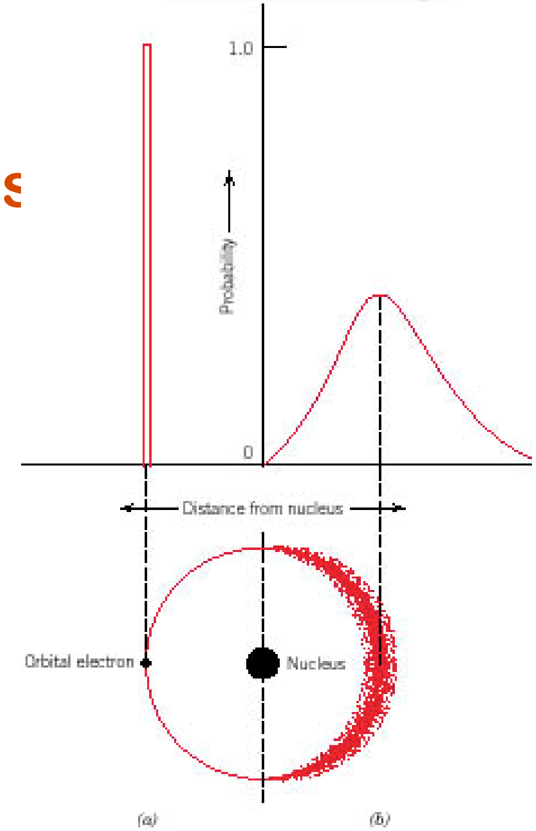
CHAPTER 2:
BONDING AND PROPERTIES

ISSUES TO ADDRESS...

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

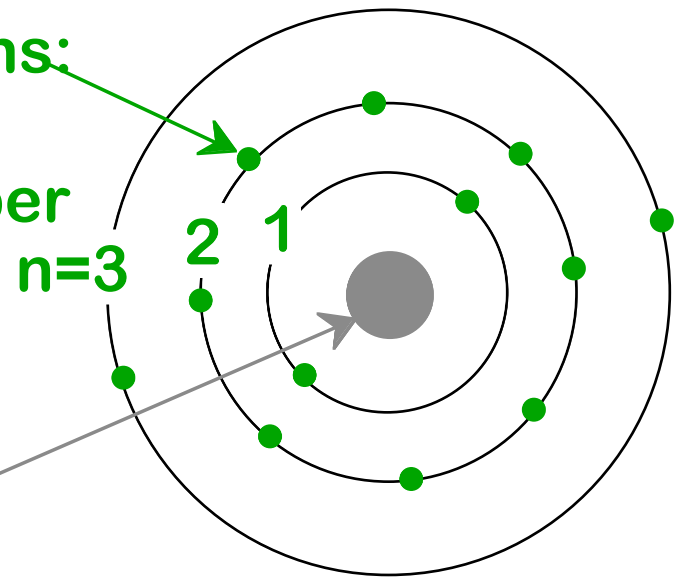
- **Fundamental concepts**
  - Proton and electron, charged 1.60×10^{-19} C
  - Mass of electron 9.11×10^{-31} kg
  - Mass of protons and neutrons
    - 1.67×10^{-27} kg
  - Atomic number: the number of protons
  - Atomic mass =protons+neutrons
  - Isotope
  - Atomic mass unit(amu): 1amu=1/12 C
  - One mole = 6.023×10^{23} atoms(Avogadro's)





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

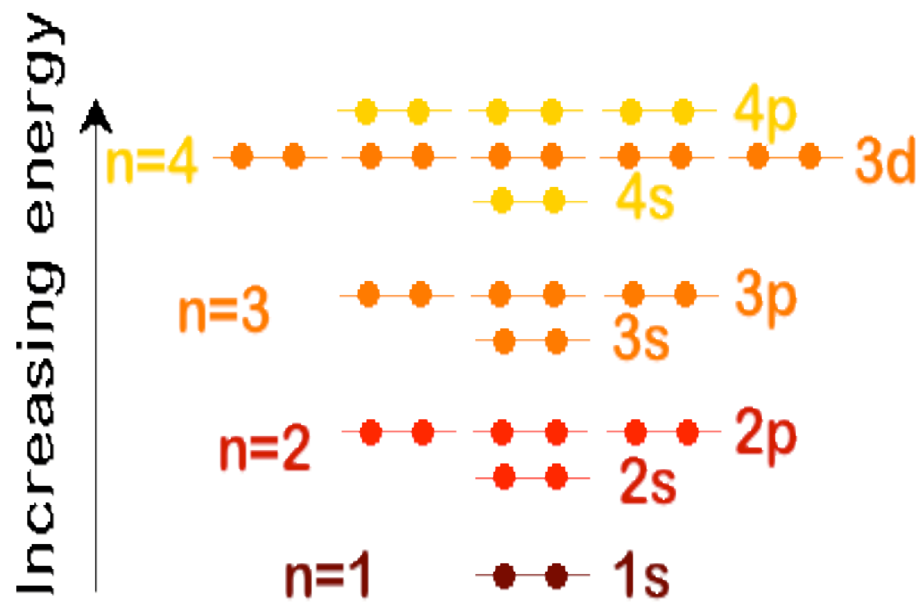
N = # neutrons

Atomic mass A ≈ Z + N

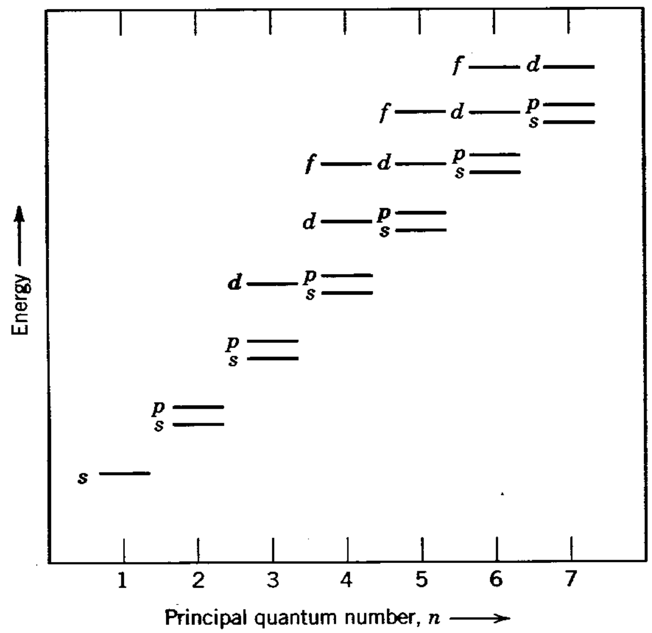
ELECTRON ENERGY STATES

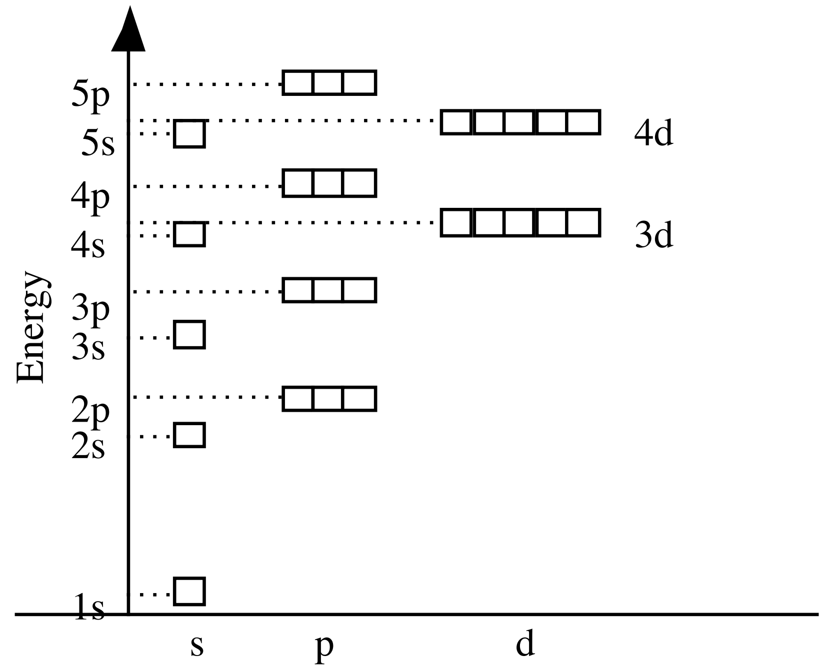
Electrons...
- **have discrete energy states**
- **tend to occupy lowest available energy state.**

n	l	m_l	Orbital	# of orbitals
1	0	0	1s	1
2	0	0	2s	4
	1	1	$2p_1$	
		0	$2p_0$	
		-1	$2p_{-1}$	
3	0	0	3s	9
	1	1	$3p_1$	
		0	$3p_0$	
		-1	$3p_{-1}$	
	2	2	$3d_2$	
		1	$3d_1$	
		0	$3d_0$	
		-1	$3d_{-1}$	
		-2	$3d_{-2}$	

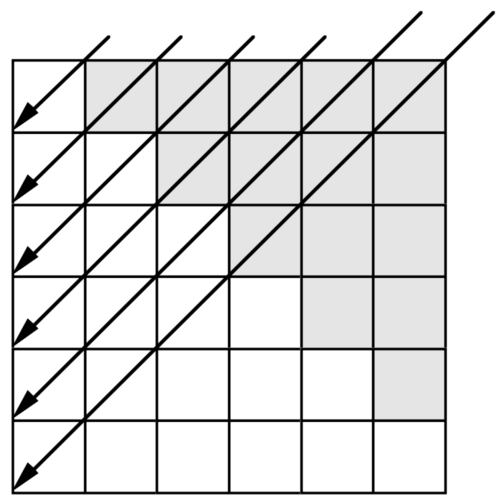


Relative energies of the electrons for various shells and subshells





1s					
2s	2p				
3s	3p	3d			
4s	4p	4d	4f		
5s	5p	5d	5f	5g	
6s	6p	6d	6f	6g	



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.**

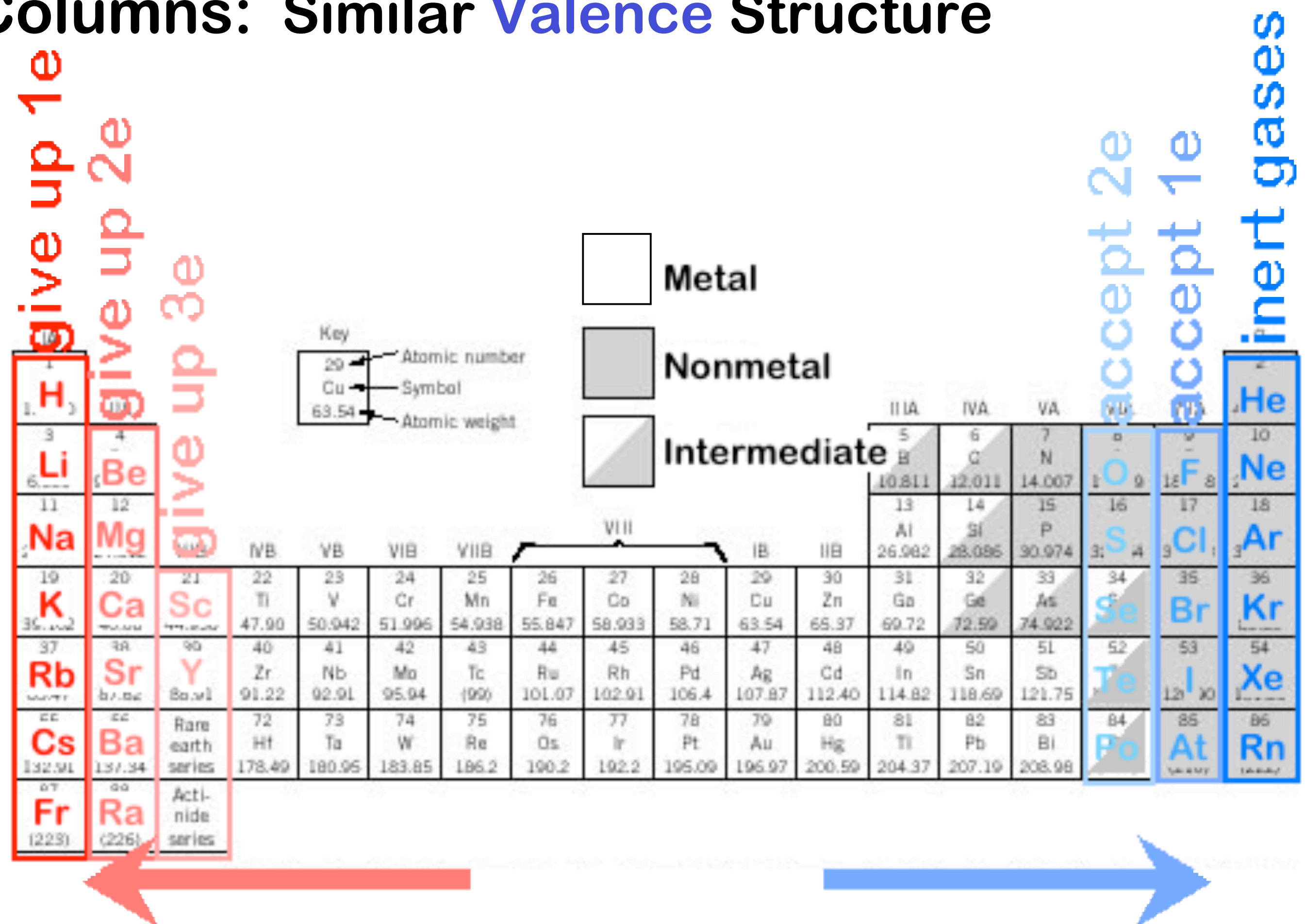
Element	Atomic #	Electron configuration
Hydrogen	1	$1s^1$
Helium	2	$1s^2$ (stable)
Lithium	3	$1s^2 2s^1$
Beryllium	4	$1s^2 2s^2$
Boron	5	$1s^2 2s^2 2p^1$
Carbon	6	$1s^2 2s^2 2p^2$
...		...
Neon	10	$1s^2 2s^2 2p^6$ (stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	13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

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											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	F 4.0	Ne -
Na 0.9	Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	Cl 3.0	Ar -
K 0.8	Ca 1.0	21 Sc 1.3	Ti 1.5	23 V 1.6	Cr 1.6	25 Mn 1.5	Fe 1.8	27 Co 1.8	Ni 1.8	29 Cu 1.9	Zn 1.8	31 Ga 1.6	32 Ge 1.8	As 2.0	34 Se 2.4	Br 2.8	Kr -
Rb 0.8	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	I 2.5	Xe -
Cs 0.7	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	At 2.2	Rn -
Fr 0.7	Ra 0.9	89–102 Ac–No 1.1–1.7															

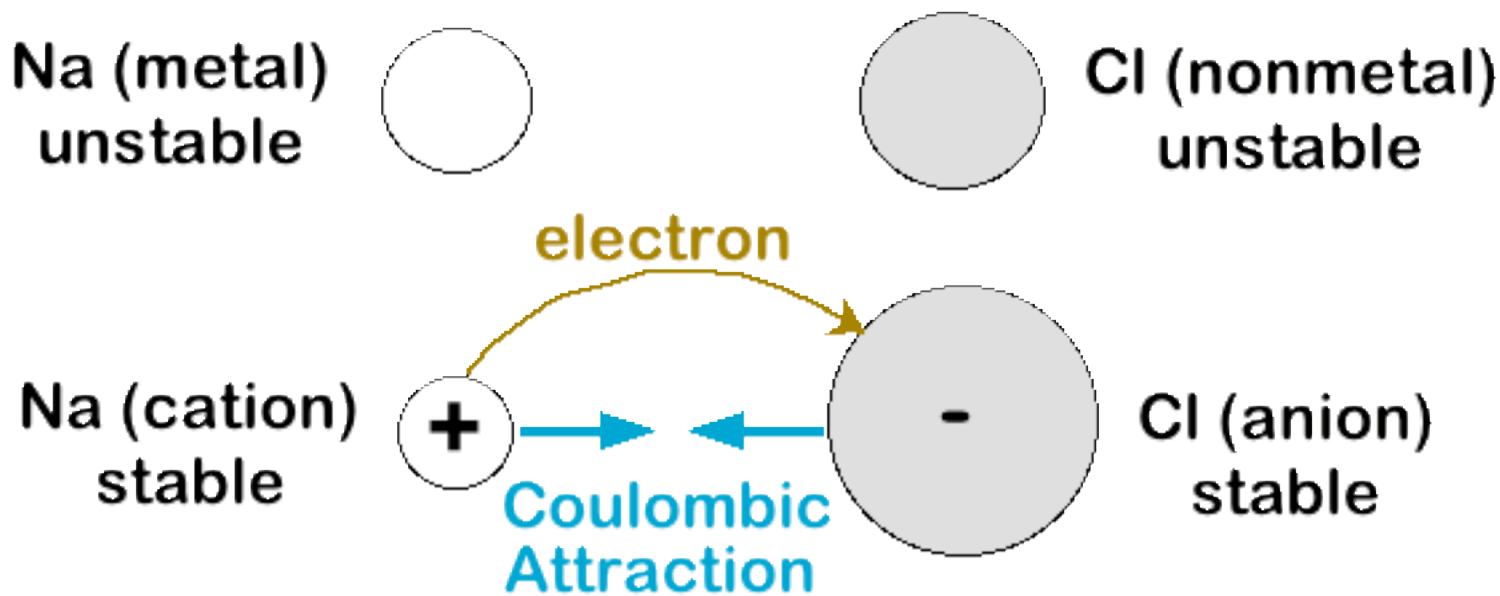
Smaller electronegativity ← → Larger electronegativity

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.

Group	Ia	IIa	IIIa	IVa	Va	VIa	VIIa	0
Elements	Na	Mg	Al	Si	P	S	Cl	Ar
Atomic #	11	12	13	14	15	16	17	18
Outer shell e-	$3s^1$	$3s^2$	$3s^2 3p^1$	$3s^2 3p^2$	$3s^2 3p^3$	$3s^2 3p^4$	$3s^2 3p^5$	$3s^2 3p^6$
Crystal structure	bcc	hcp	fcc	diamond		complex		fcc
Electrical resistivity at RT (10^{-4} ohmm)	5.2	4.45 metal	2.65	2.5×10^5 semicon	1×10^{17} insulator	2×10^{23} insulator	-- gas	-- gas
Bond strength (in eV)	1.13	1.53	3.34	4.62	?	2.86	?	0.08
Melting point ˚C	98	650	660	1400	44	120	-100	-189
Boiling point ˚C	890	1100	2500	2400	280	440	-35	-186

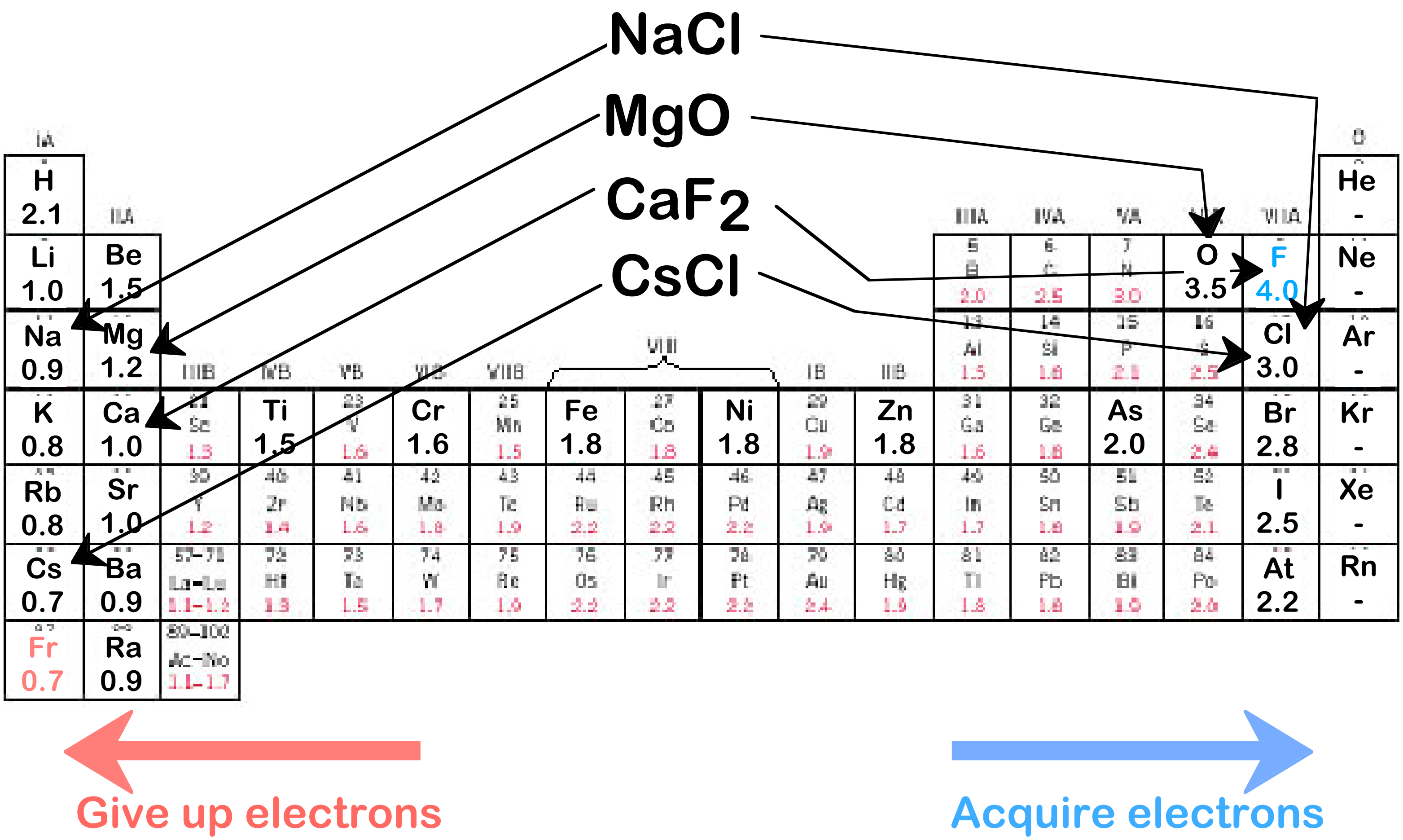
IONIC BONDING

- 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.

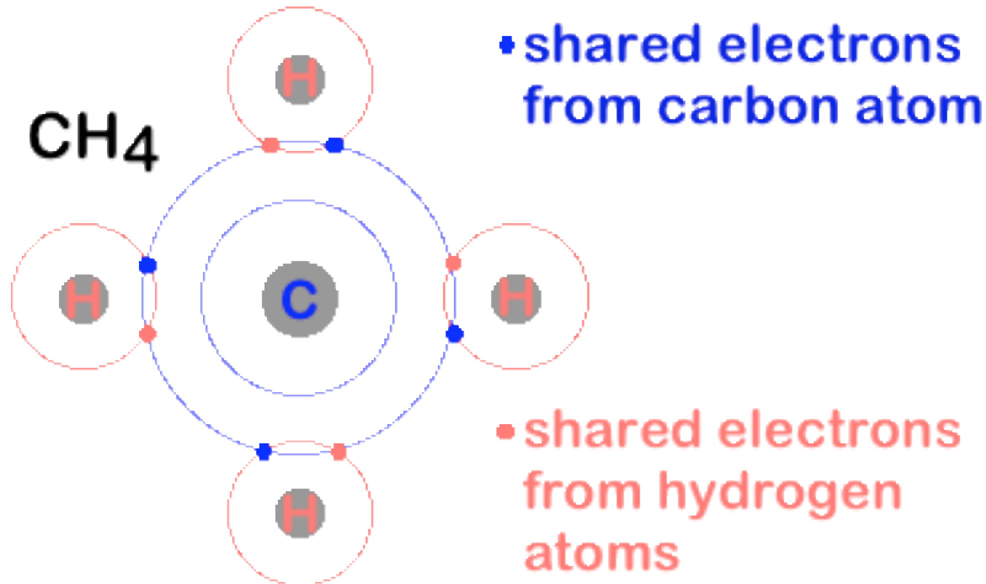
COVALENT BONDING

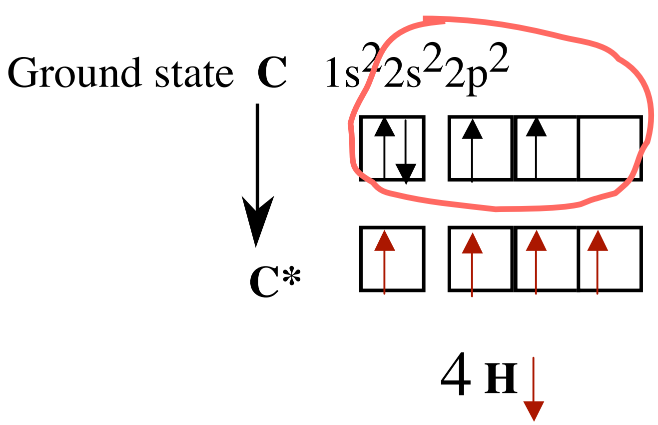
- Requires shared electrons
- Example: CH_4

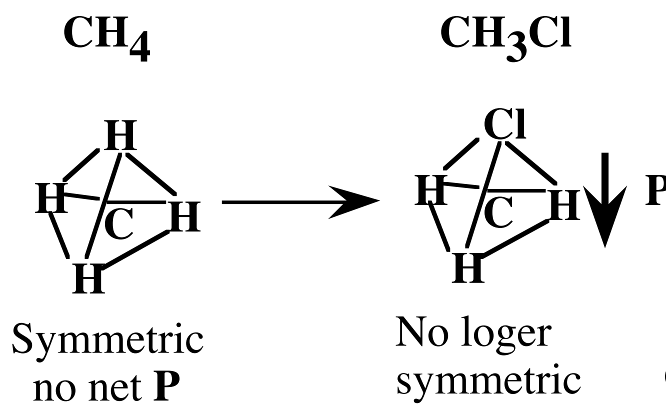
C: has 4 valence e, needs 4 more

H: has 1 valence e, needs 1 more

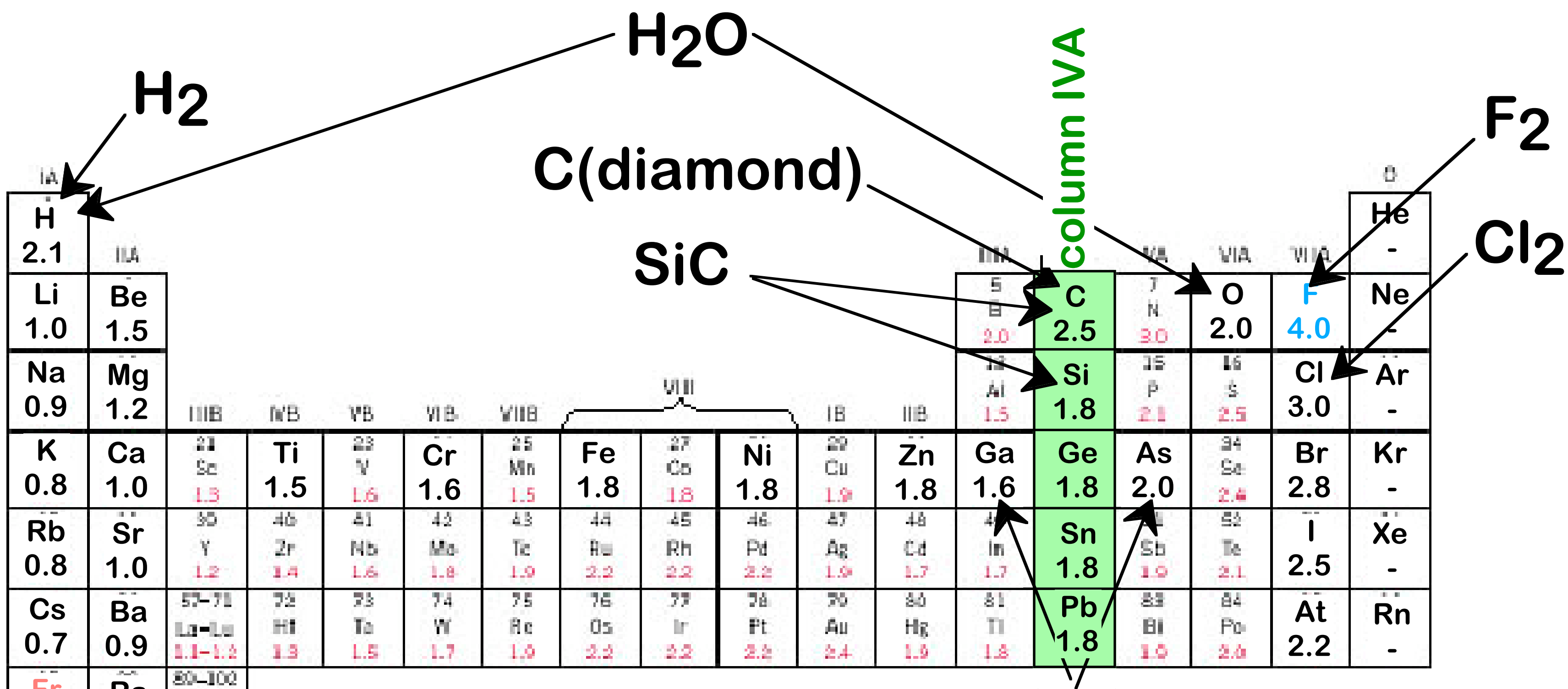
Electronegativities are comparable.







EXAMPLES: COVALENT BONDING

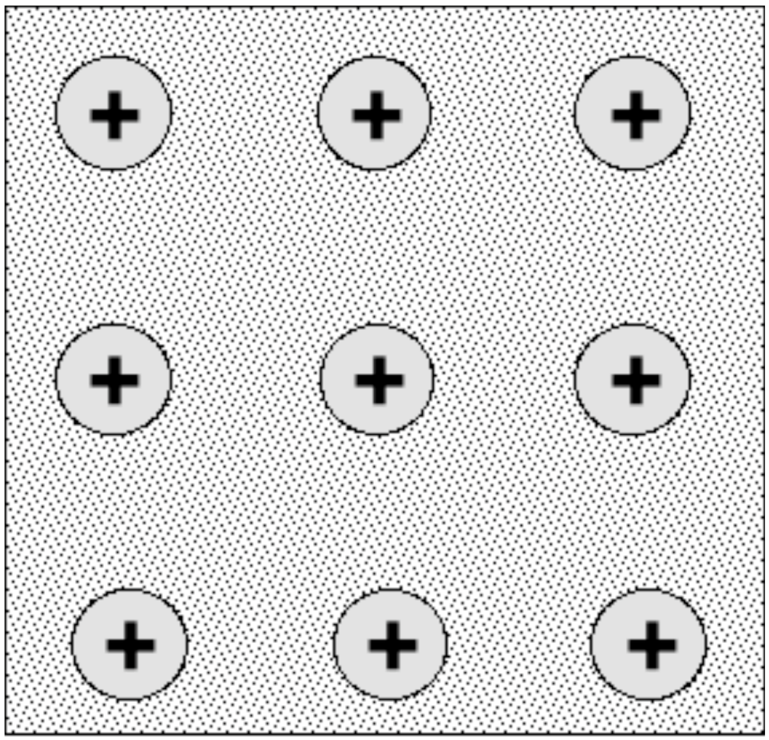


Adapted from Fig. 2.7, *Callister 6e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

- 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).



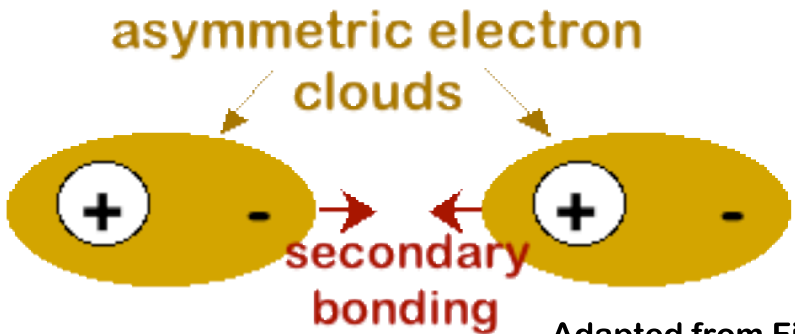
Adapted from Fig. 2.11, *Callister 6e.*

- Primary bond for metals and their alloys

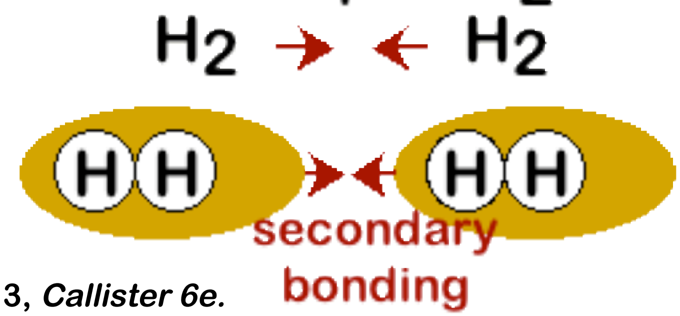
SECONDARY BONDING

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

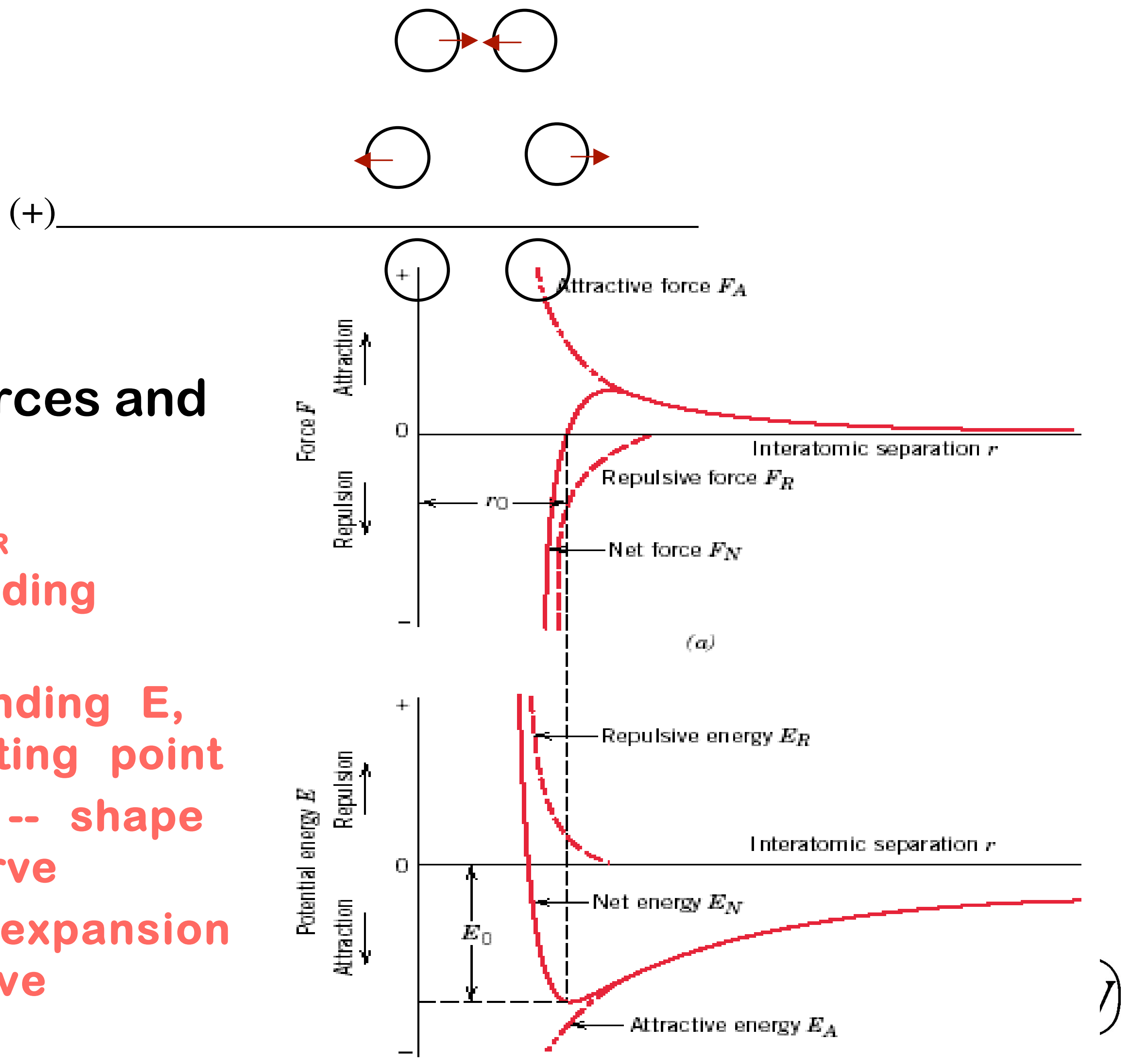
Adapted from Fig. 2.14, *Callister 6e.*

-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

Force between atoms



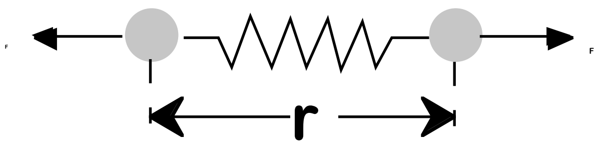
- **Bonding forces and energies**
  - $F_n = F_A + F_R$
  - E_0 -- bonding energy
  - large bonding E, high melting point
  - stiffness -- shape of f-r curve
  - thermal expansion --E-r curve

HW assignment change:

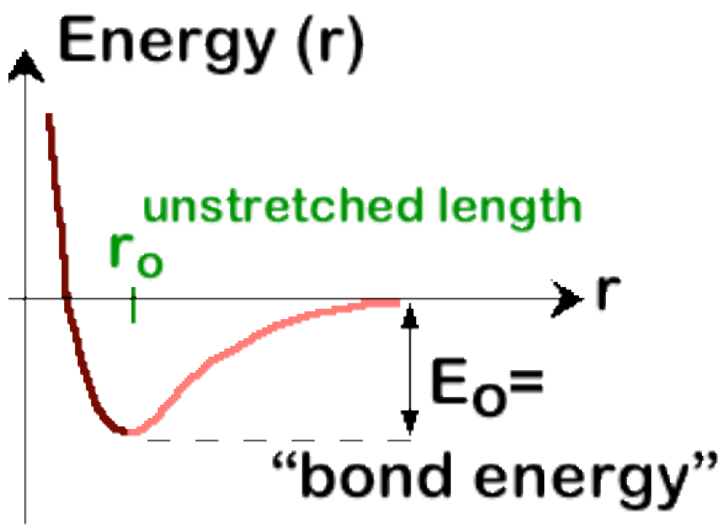
Please do 2.14 instead of 2.13

PROPERTIES FROM BONDING: T_M

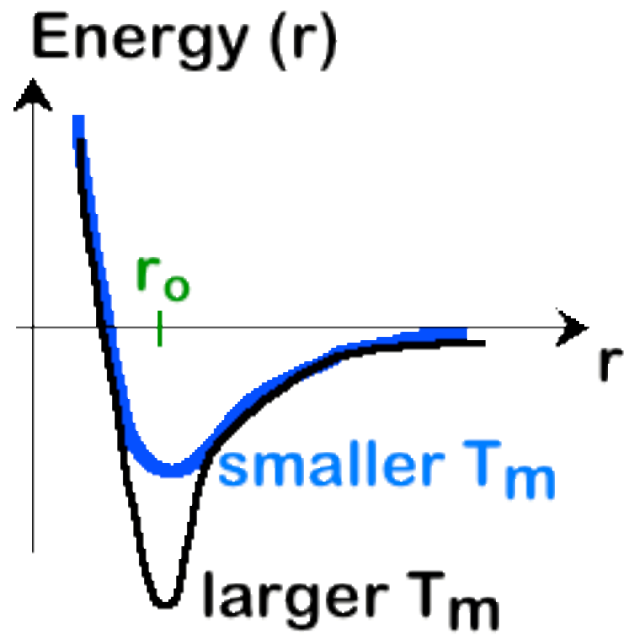
- **Bond length**, r



- **Bond energy**, E_o



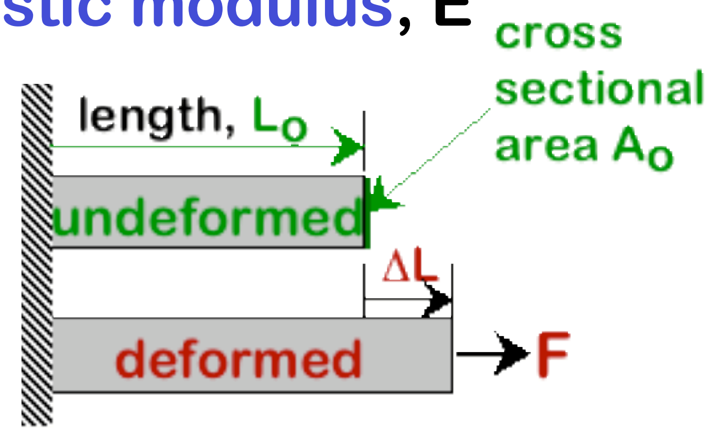
- **Melting Temperature**, T_m



T_m is larger if E_o is larger.

PROPERTIES FROM BONDING: E

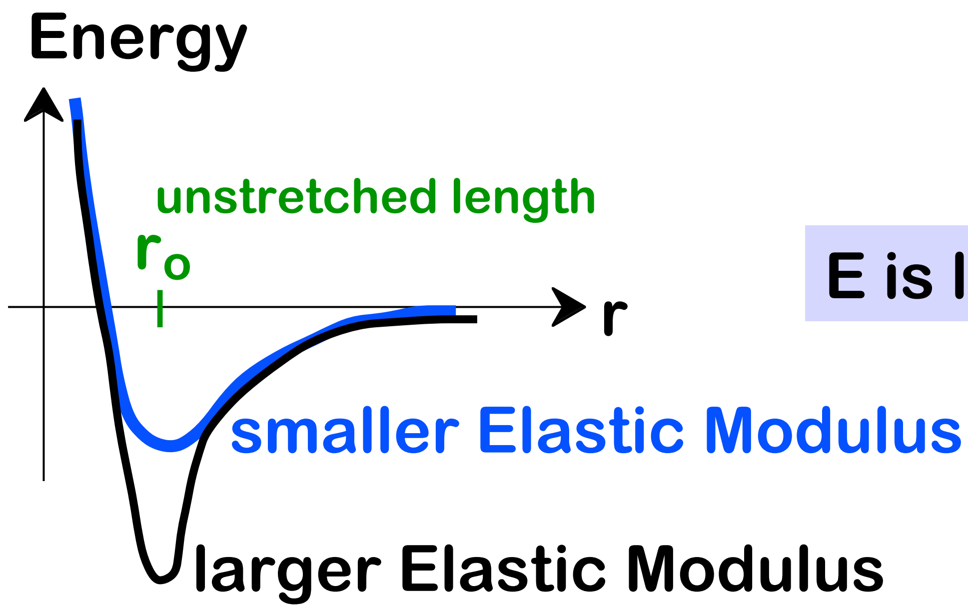
- Elastic modulus, E



Elastic modulus

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

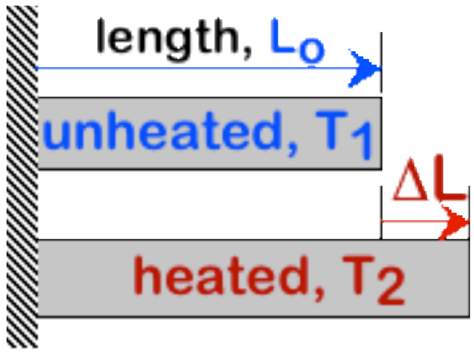
- E ~ curvature at r_o



E is larger if E_o is larger.

PROPERTIES FROM BONDING: α

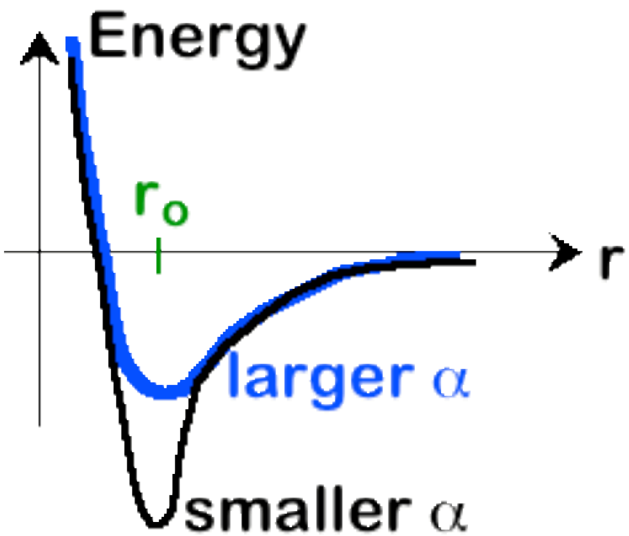
- Coefficient of thermal expansion, α



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 | **Large bond energy**
(Ionic & covalent bonding):
large T_m
large E
small □

Metals | **Variable bond energy**
(Metallic bonding):
moderate T_m
moderate E
moderate □

Polymers | **Directional Properties**
(Covalent & Secondary):
Secondary bonding dominates
small T
small E
large □