

# CHAPTER 2: BONDING AND PROPERTIES

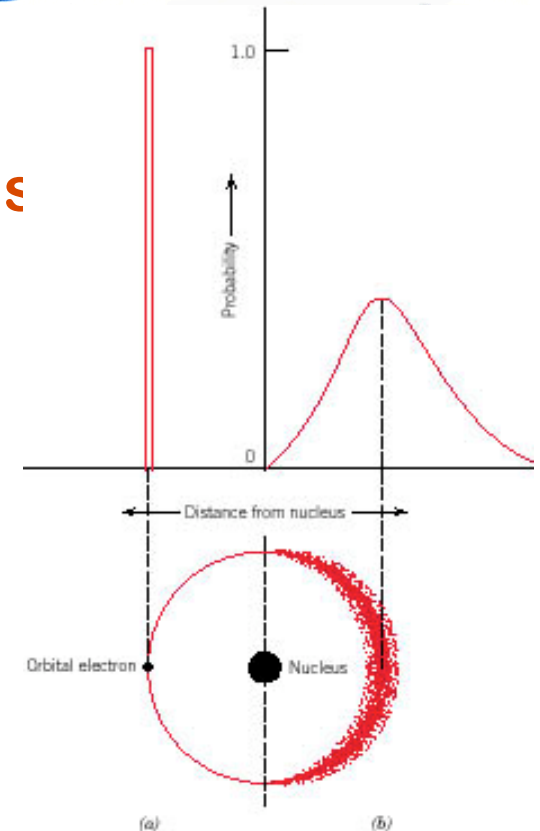
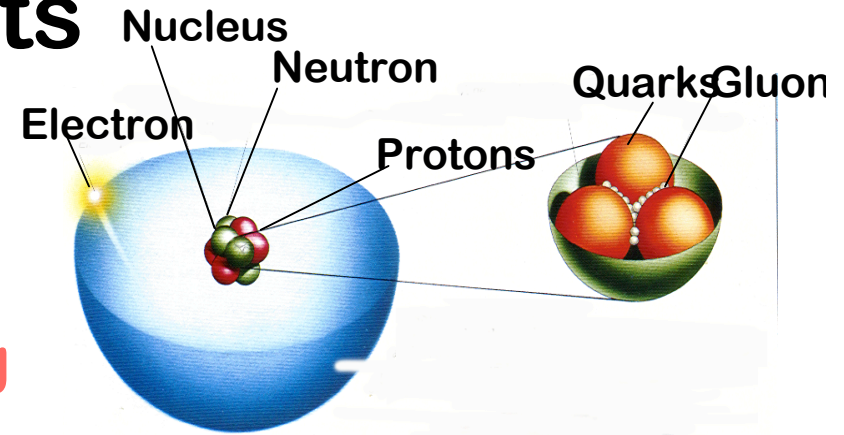
## ISSUES TO ADDRESS...

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



# • Fundamental concepts

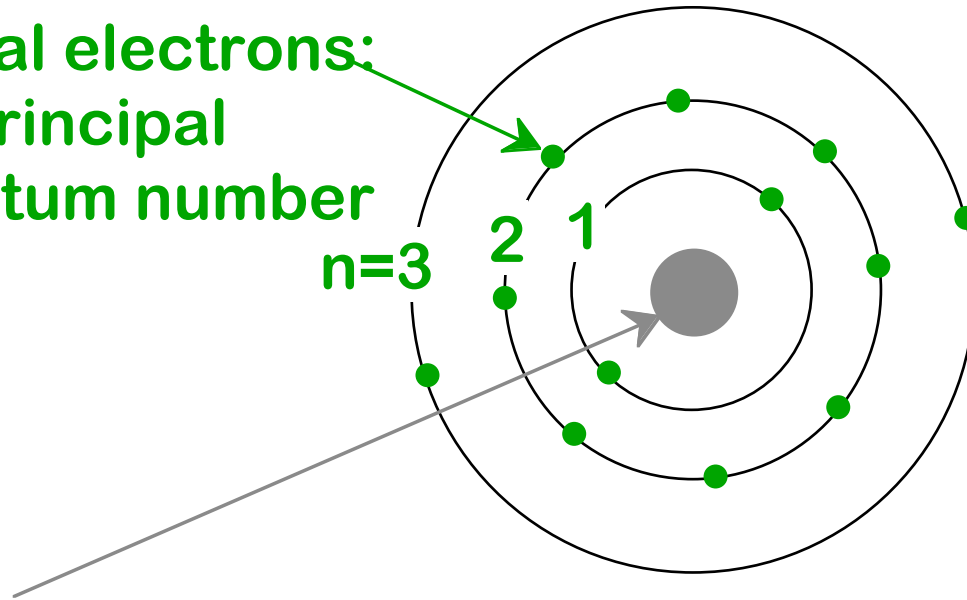
- Proton and electron, charged  
 $1.60 \times 10^{-19} \text{ C}$
- Mass of electron  $9.11 \times 10^{-31} \text{ kg}$
- Mass of protons and neutrons
  - $1.67 \times 10^{-27} \text{ kg}$
- Atomic number: the number of protons
- Atomic mass = protons + neutrons
- Isotope
- Atomic mass unit (amu): 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



# BOHR ATOM

orbital electrons:  
 $n$  = principal  
quantum number

$n=3$



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

Nucleus:  $Z$  = # protons

= 1 for hydrogen to 94 for plutonium

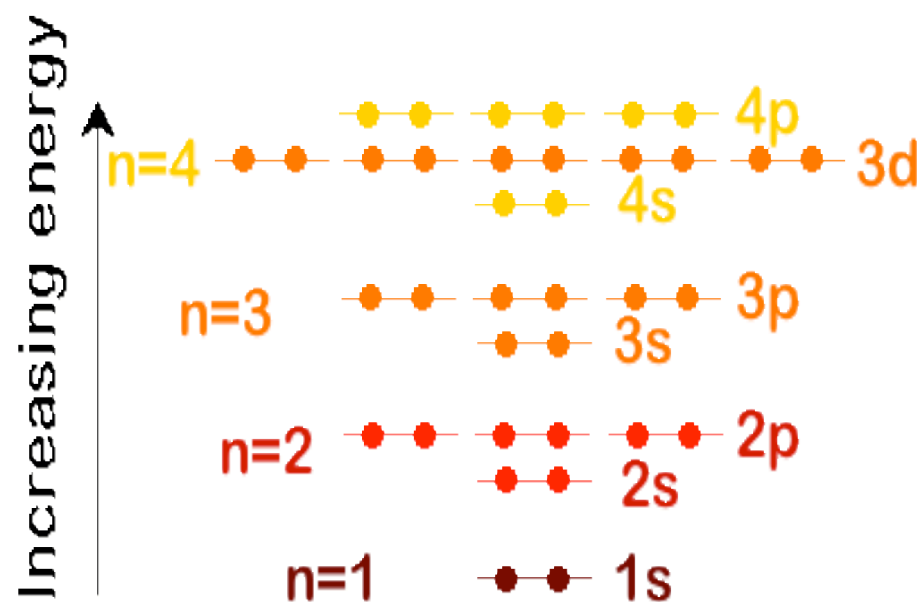
$N$  = # neutrons

Atomic mass  $A \approx Z + N$

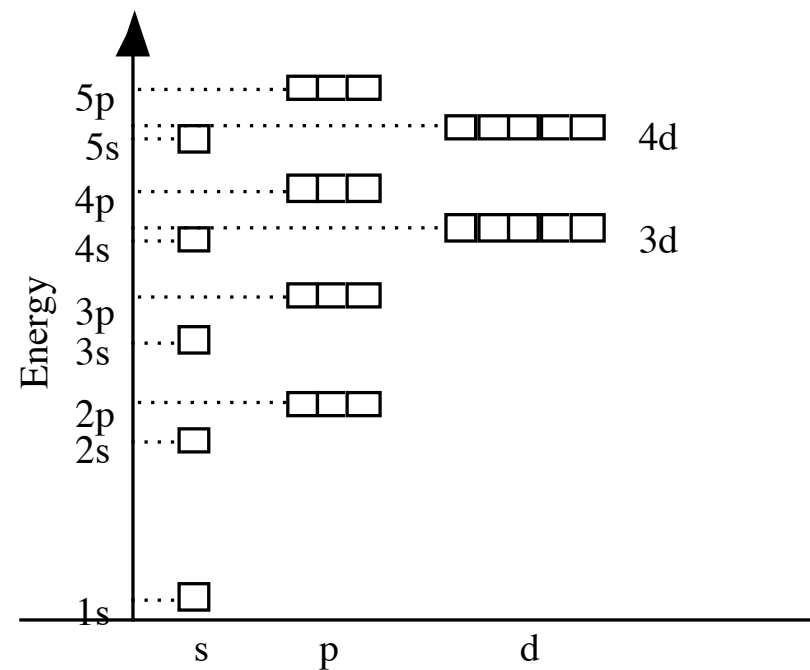
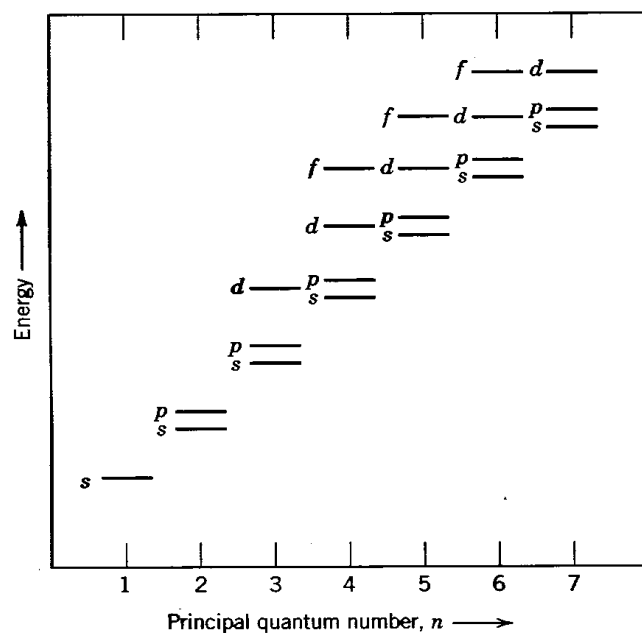
# ELECTRON ENERGY STATES

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

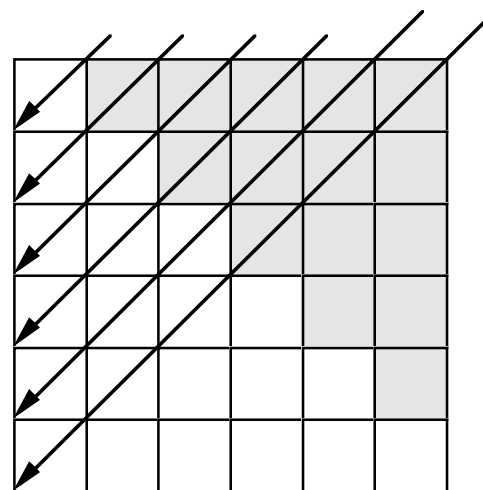
n	l	m <sub>l</sub>	Orbital	# of orbitals
1	0	0	1s	1
2	1	0	2s	4
		1	2p <sub>1</sub>	
		0	2p <sub>0</sub>	
		-1	2p <sub>-1</sub>	
3	0	0	3s	9
		1	3p <sub>1</sub>	
		0	3p <sub>0</sub>	
		-1	3p <sub>-1</sub>	
	2	2	3d <sub>2</sub>	
		1	3d <sub>1</sub>	
		0	3d <sub>0</sub>	
		-1	3d <sub>-1</sub>	
		-2	3d <sub>-2</sub>	



## 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	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ (stable)

Adapted from Table 2.2,  
Callister 6e.

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



# THE PERIODIC TABLE

- Columns: Similar **Valence** Structure

# Columns: Similar Valence Structure

give up 1e

give up 2e

give up 3e

Metal

Nonmetal

Intermediate

Key

29

Cu

63.54

Atomic number

Symbol

Atomic weight

										IIA	IVA	VA																	
1 H 1.008	2 He 4.003											3 Li 6.941	4 Be 9.012											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.06	17 Cl 35.45	18 Ar 39.948												
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.88	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.69	29 Cu 63.546	30 Zn 65.38	31 Ga 69.723	32 Ge 72.64	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80												
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.6	53 I 126.905	54 Xe 131.29												
55 Cs 132.91	56 Ba 137.33	Rare earth series		72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.19	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)											
87 Fr (223)	88 Ra (226)	Actinide series																											

accept 2e

accept 1e

inert gases

Adapted from Fig. 2.6, Callister 6e.

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

Electronegative elements:  
Readily acquire electrons  
to become - ions.





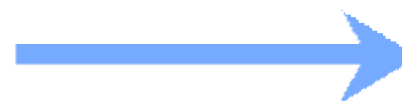
# ELECTRONEGATIVITY

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

IA H 2.1	IIA																0 He -
Li 1.0	Be 1.5											IIIA B 2.0	IVA C 2.5	VA N 3.0	VIA O 3.5	VIIA 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 -
		IIIB	IVB	VB	VIB	VIIA	VIII			IB	IIB						
K 0.8	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 1.8	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 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	53 I 2.5	54 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	85 At 2.2	86 Rn -
Fr 0.7	Ra 0.9	87-103 Ac-Lr 1.1-1.7															



Smaller electronegativity



Larger electronegativity

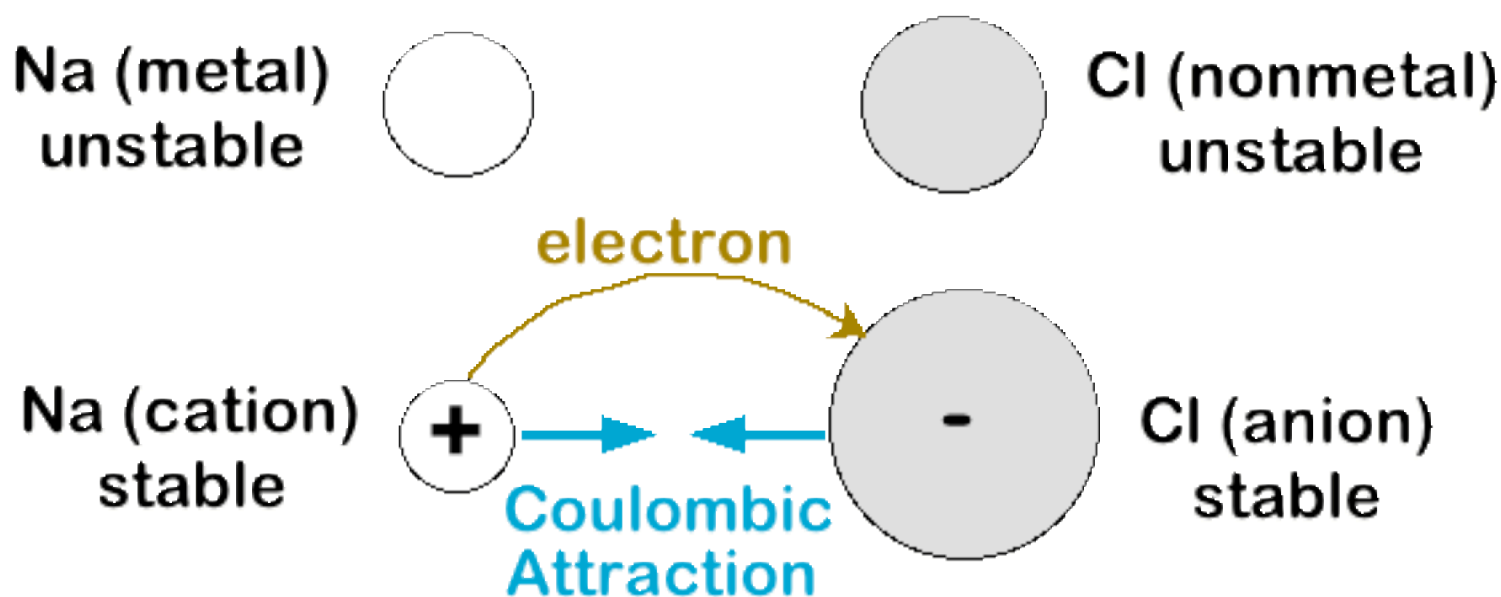
Adapted from Fig. 2.7, *Callister 6e*. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.



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 <sup>1</sup>	3s <sup>2</sup>	3s <sup>2</sup> 3p <sup>1</sup>	3s <sup>2</sup> 3p <sup>2</sup>	3s <sup>2</sup> 3p <sup>3</sup>	3s <sup>2</sup> 3p <sup>4</sup>	3s <sup>2</sup> 3p <sup>5</sup>	3s <sup>2</sup> 3p <sup>6</sup>
Crystal structure	bcc	hcp	fcc	diamond		complex		fcc
Electrical resistivity at RT (10 <sup>-4</sup> ohmm)	5.2	4.45 metal	2.65	2.5x10 <sup>5</sup> semicon	1x10 <sup>17</sup> insulator	2x10 <sup>23</sup> 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**

NaCl

MgO

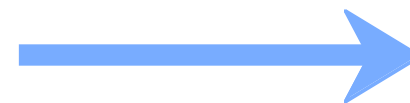
CaF<sub>2</sub>

CsCl

IA																	0
H 2.1																	He -
Li 1.0	Be 1.5															Ne -	
Na 0.9	Mg 1.2	IIIA B 2.0	IIIA Al 1.5	IVA C 2.5	IVA Si 1.8	VA N 3.0	VA P 2.1	VIA O 3.5	VIA S 2.5	VIIA F 4.0	VIIA Cl 3.0	VIIA Br 2.8	VIIA I 2.5	VIIA At 2.2	0 Xe -		
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 1.8	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	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	89-103 Ac-No 1.1-1.7															



Give up electrons



Acquire electrons

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.



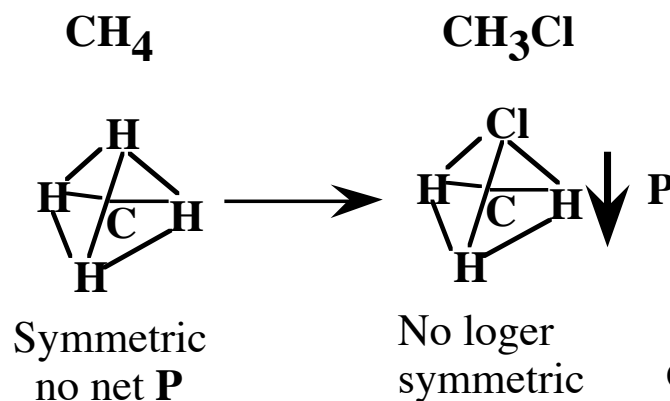
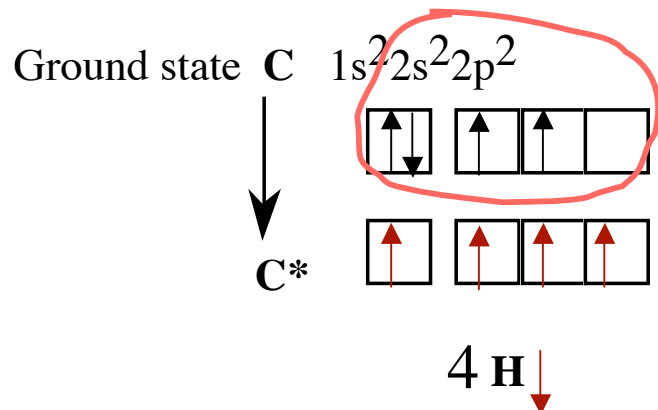
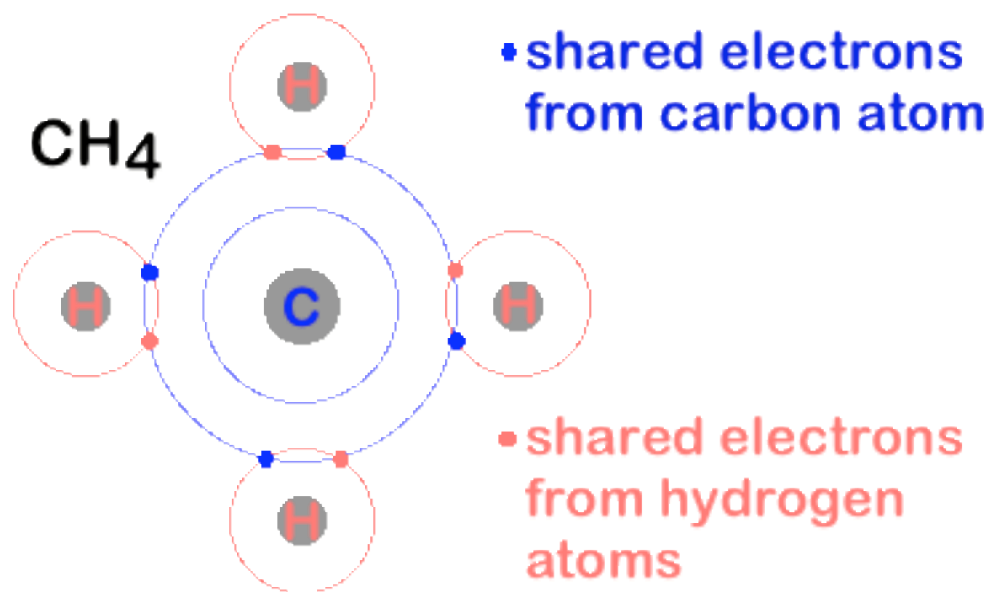
# COVALENT BONDING

- Requires **shared electrons**
- Example:  $\text{CH}_4$

C: has 4 valence e,  
needs 4 more

H: has 1 valence e,  
needs 1 more

Electronegativities  
are comparable.



## EXAMPLES: COVALENT BONDING

The image shows a periodic table with electronegativity values. Arrows point from material names to specific elements or groups:

- H<sub>2</sub>** points to H (2.1).
- H<sub>2</sub>O** points to O (2.0).
- C(diamond)** points to C (2.5).
- SiC** points to Si (1.8) and C (2.5).
- column IVA** points to the column containing C, Si, Ge, and Sn.
- F<sub>2</sub>** points to F (4.0).
- Cl<sub>2</sub>** points to Cl (3.0).
- GaAs** points to Ga (1.6) and As (2.0).

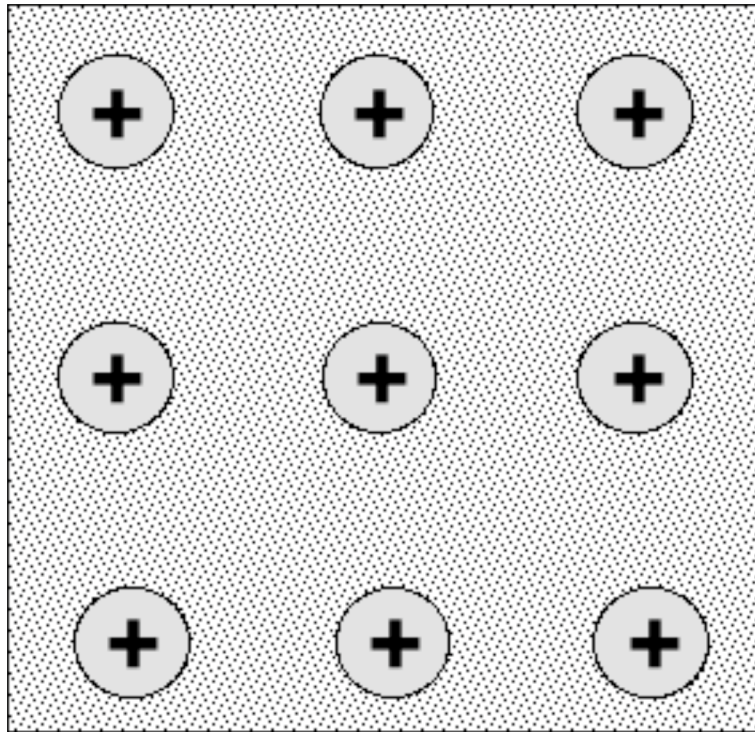
Adapted from Fig. 2.7, *Callister 6e*. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition. Copyright

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).



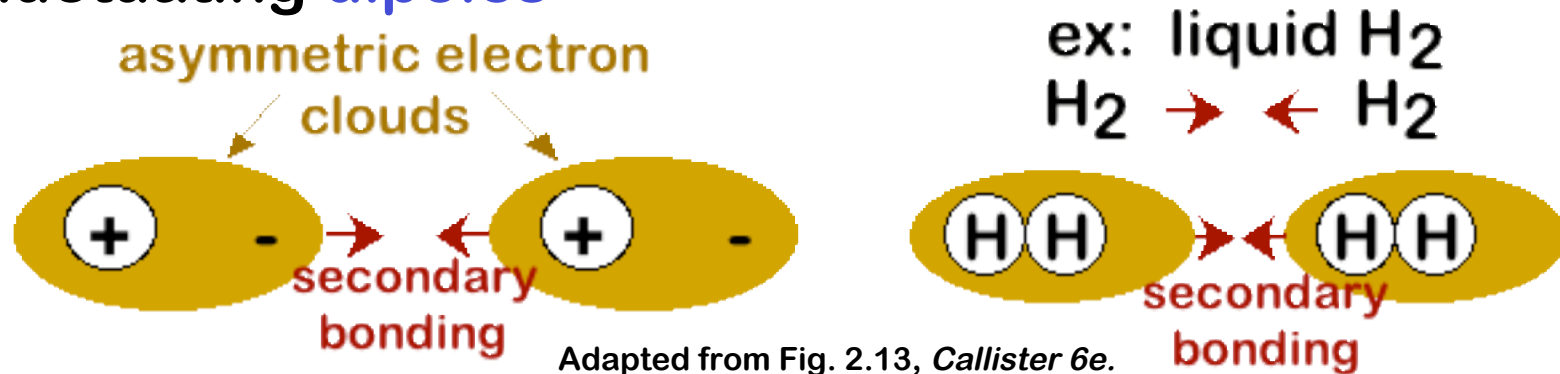
Adapted from Fig. 2.11, *Callister 6e*.

- Primary bond for **metals** and their **alloys**

# SECONDARY BONDING

Arises from interaction between **dipoles**

- Fluctuating **dipoles**



- Permanent **dipoles**-molecule induced



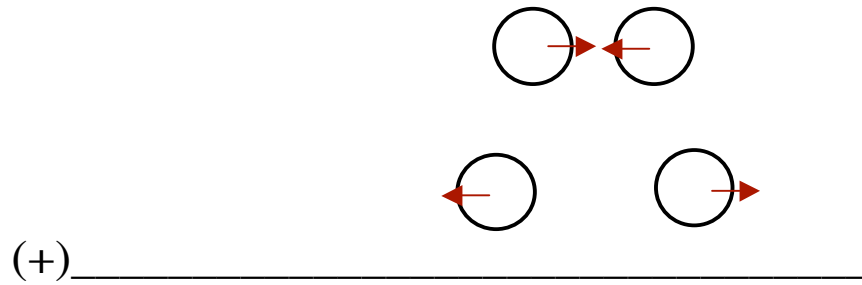


# SUMMARY: BONDING

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

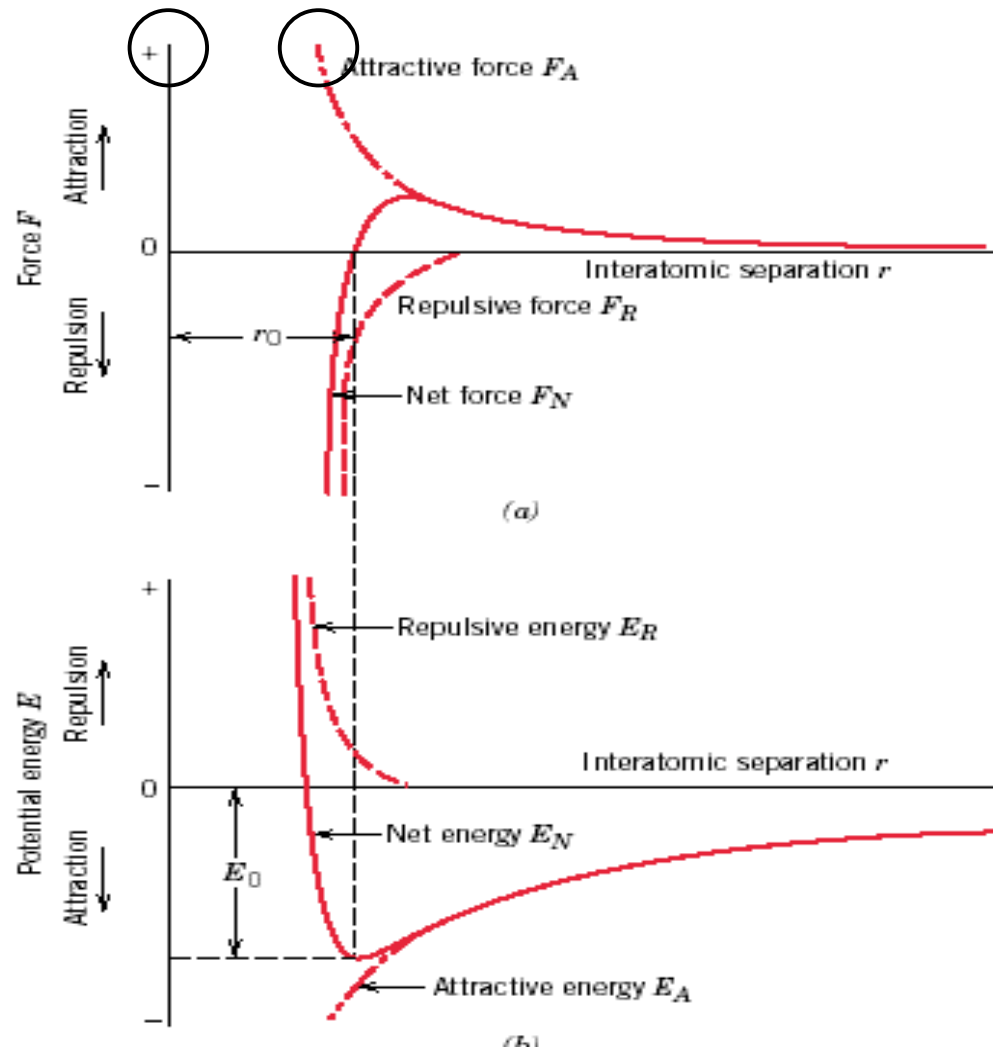


## Force between atoms



- 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



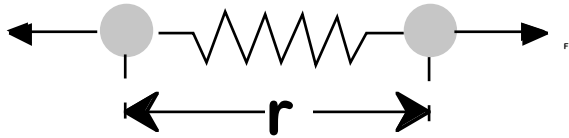
**HW assignment change:**

**Please do 2.14 instead of 2.13**

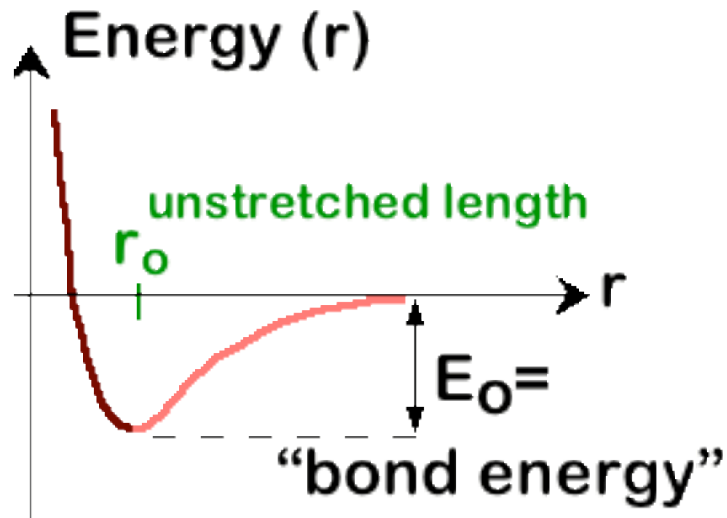


# PROPERTIES FROM BONDING: $T_M$

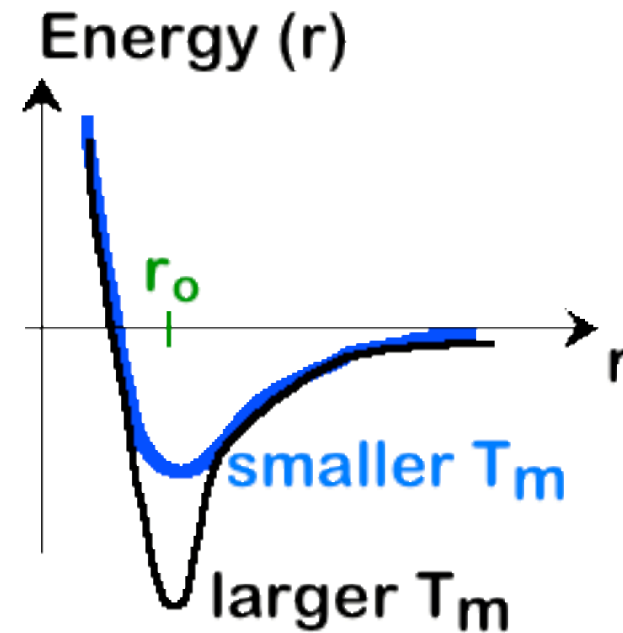
- Bond length,  $r$



- Bond energy,  $E_o$



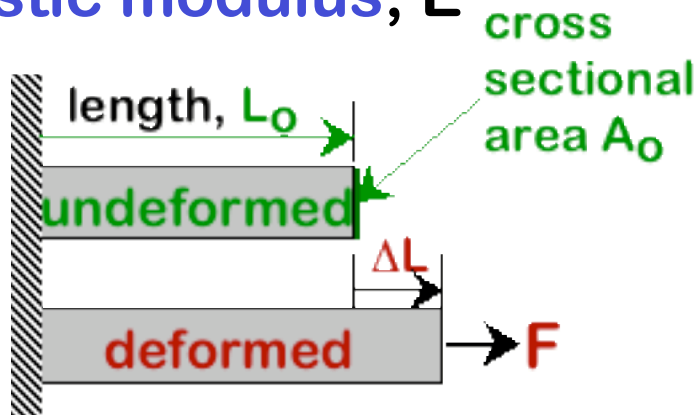
- Melting Temperature,  $T_m$



$T_m$  is larger if  $E_o$  is larger.

# PROPERTIES FROM BONDING: E

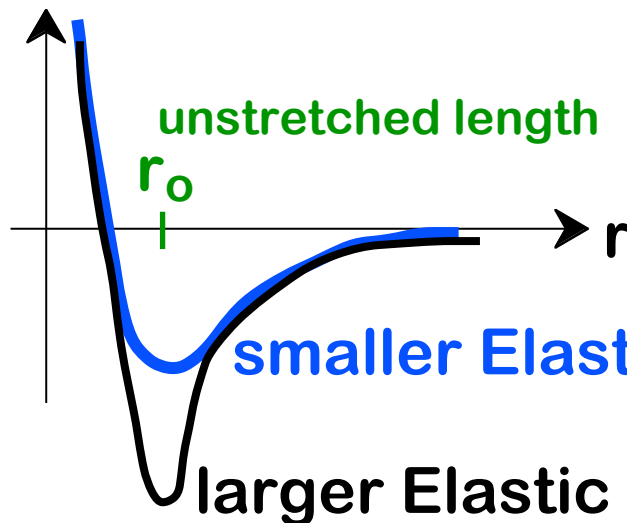
- Elastic modulus, E



Elastic modulus

$$\frac{F}{A_0} = E \frac{\Delta L}{L_0}$$

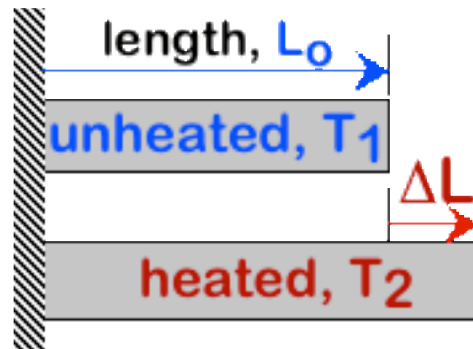
- $E \sim$  curvature at  $r_0$   
Energy



E is larger if  $E_0$  is larger.

# PROPERTIES FROM BONDING: $\alpha$

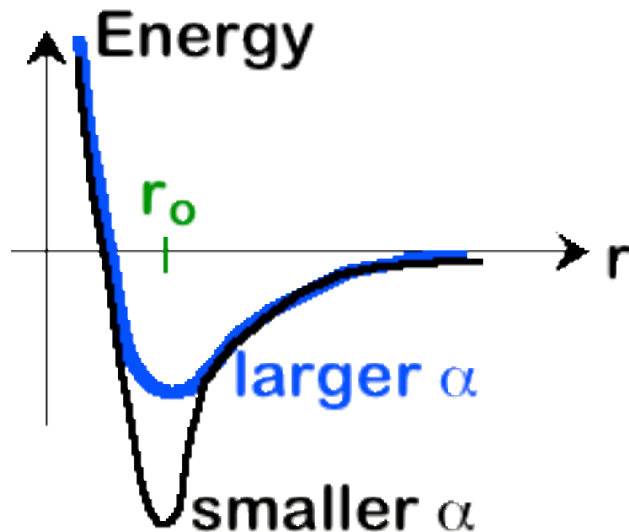
- Coefficient of thermal expansion,  $\alpha$



coeff. thermal expansion

$$\frac{\Delta L}{L_0} = \alpha (T_2 - T_1)$$

- $\alpha \sim$  symmetry at  $r_0$



$\alpha$  is larger if  $E_0$  is smaller.

# SUMMARY: PRIMARY BONDS

## Ceramics

(Ionic & covalent bonding):

Large bond energy

large  $T_m$

large  $E$

small  $\alpha$

## Metals

(Metallic bonding):

Variable bond energy

moderate  $T_m$

moderate  $E$

moderate  $\alpha$

## Polymers

(Covalent & Secondary):



Directional Properties

Secondary bonding dominates

small  $T$

small  $E$

large  $\alpha$