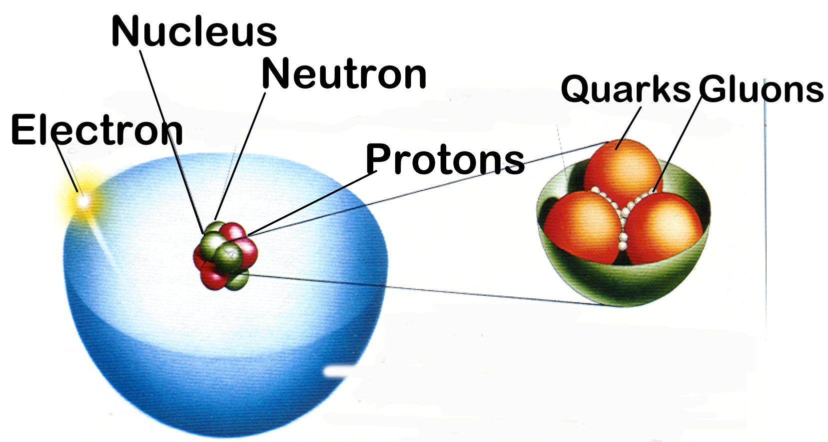
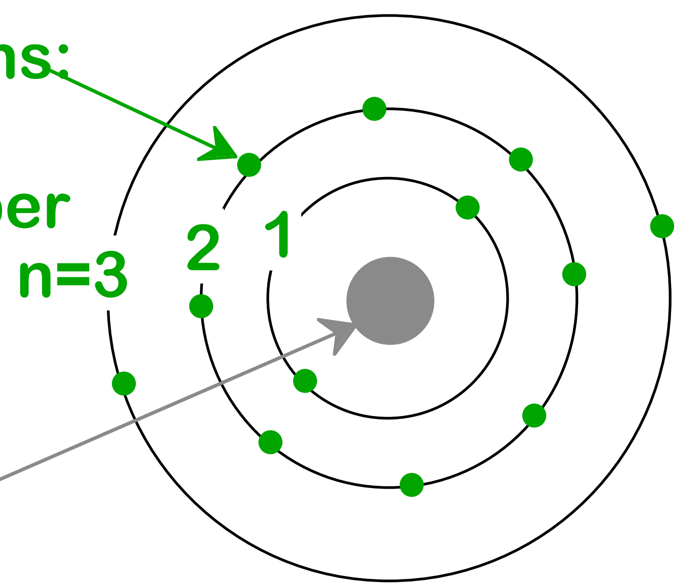
Atomic structure



BOHR ATOM

orbital electrons:
n = principal
quantum number



Nucleus: Z =

Atomic mass A ≈ N =

Electronic structure

Valence electrons determine all of the following properties:

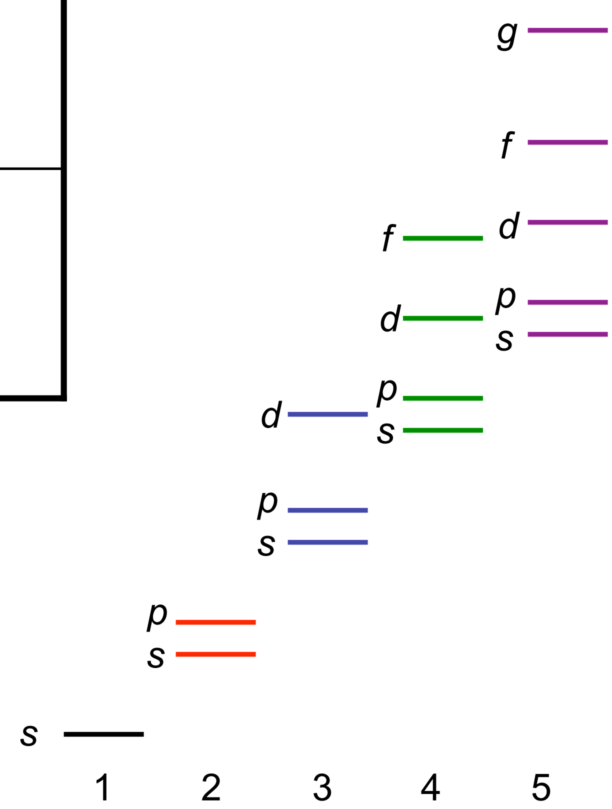
Electrons have wavelike and particulate properties.

- This means that electrons are in orbitals defined by a probability.
- Each orbital at discrete energy level determined by quantum numbers.

Quantum #	Designation

Electronic structure

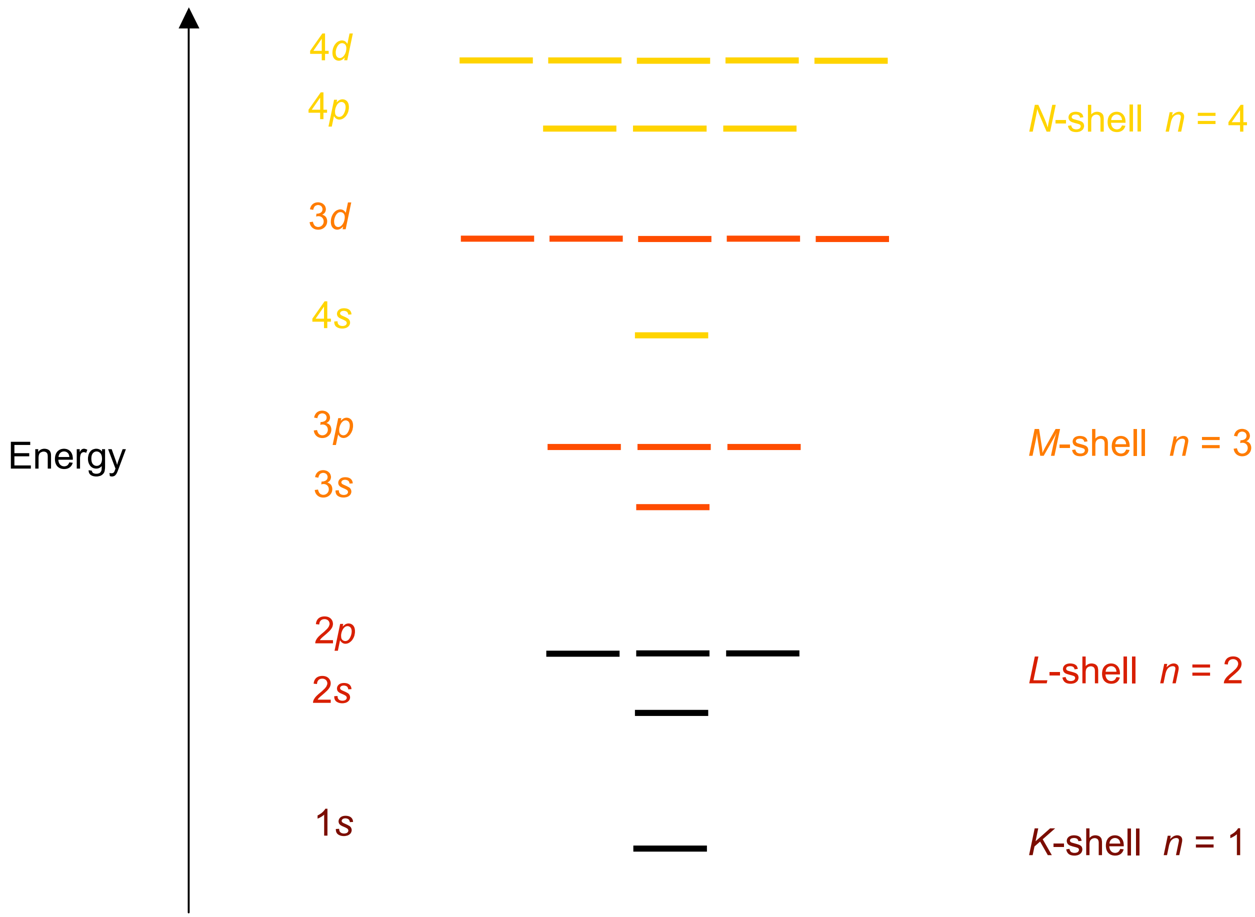
Principal quantum no.	Shell designation	Subshells	No. of states	Number of electrons	
				Per subshell	Per shell
1	*K*	*s*	1	2	2
2	*L*	*s*	1	2	8
		p	3	6	
3	*M*	*s*	1	2	18
		p	3	6	
		d	5	10	
4	*N*	*s*	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	



Electron energy states

Electrons...

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

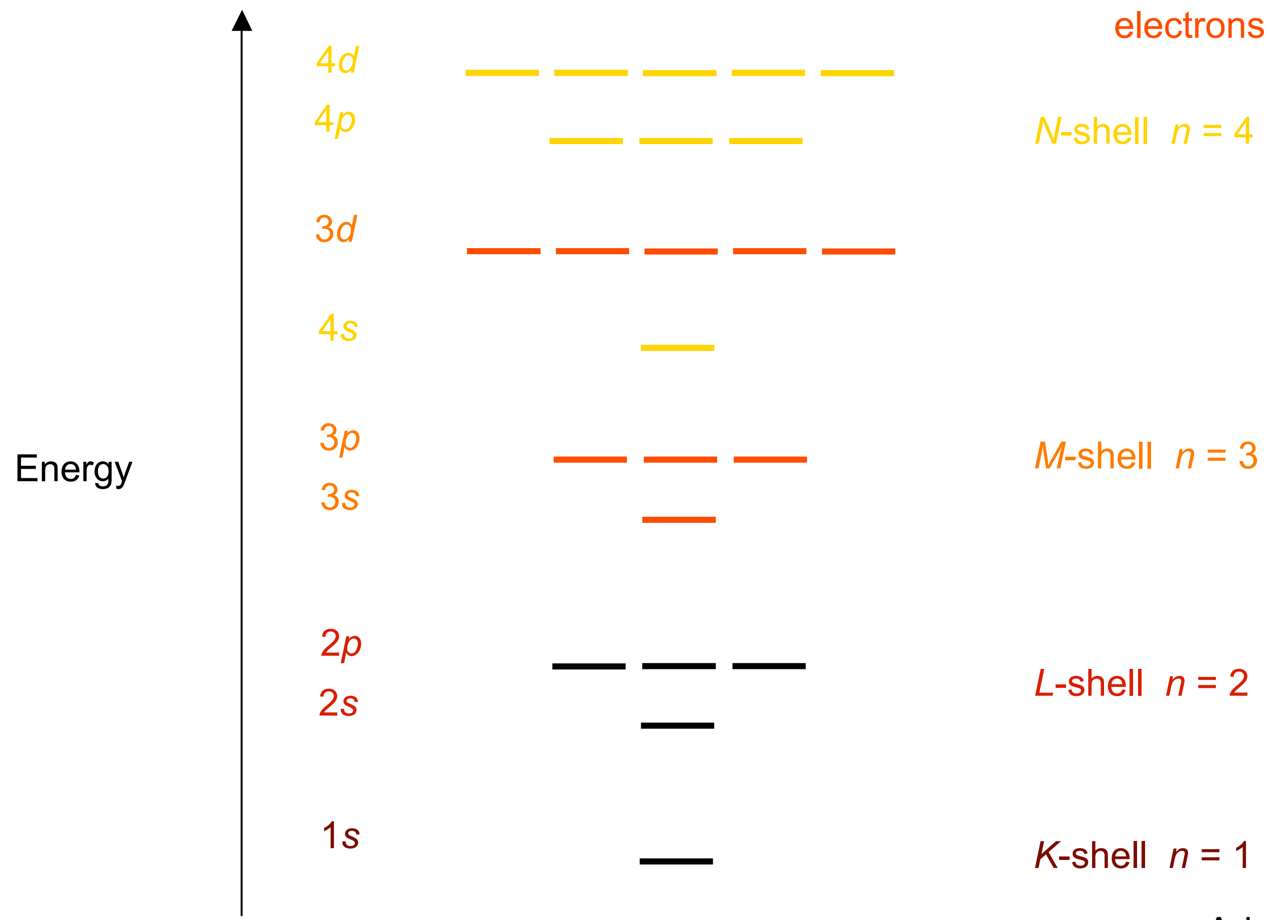


Adapted from Fig. 2.4, *Callister 7e.*

Electronic configuration

ex: Fe - atomic # = $1s^2 \ 2s^2 2p^6 \ 3s^2 3p^6 \ \boxed{3d^6 \ 4s^2}$

valence electrons



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

Survey of elements

- Most elements: Electron configuration not stable.

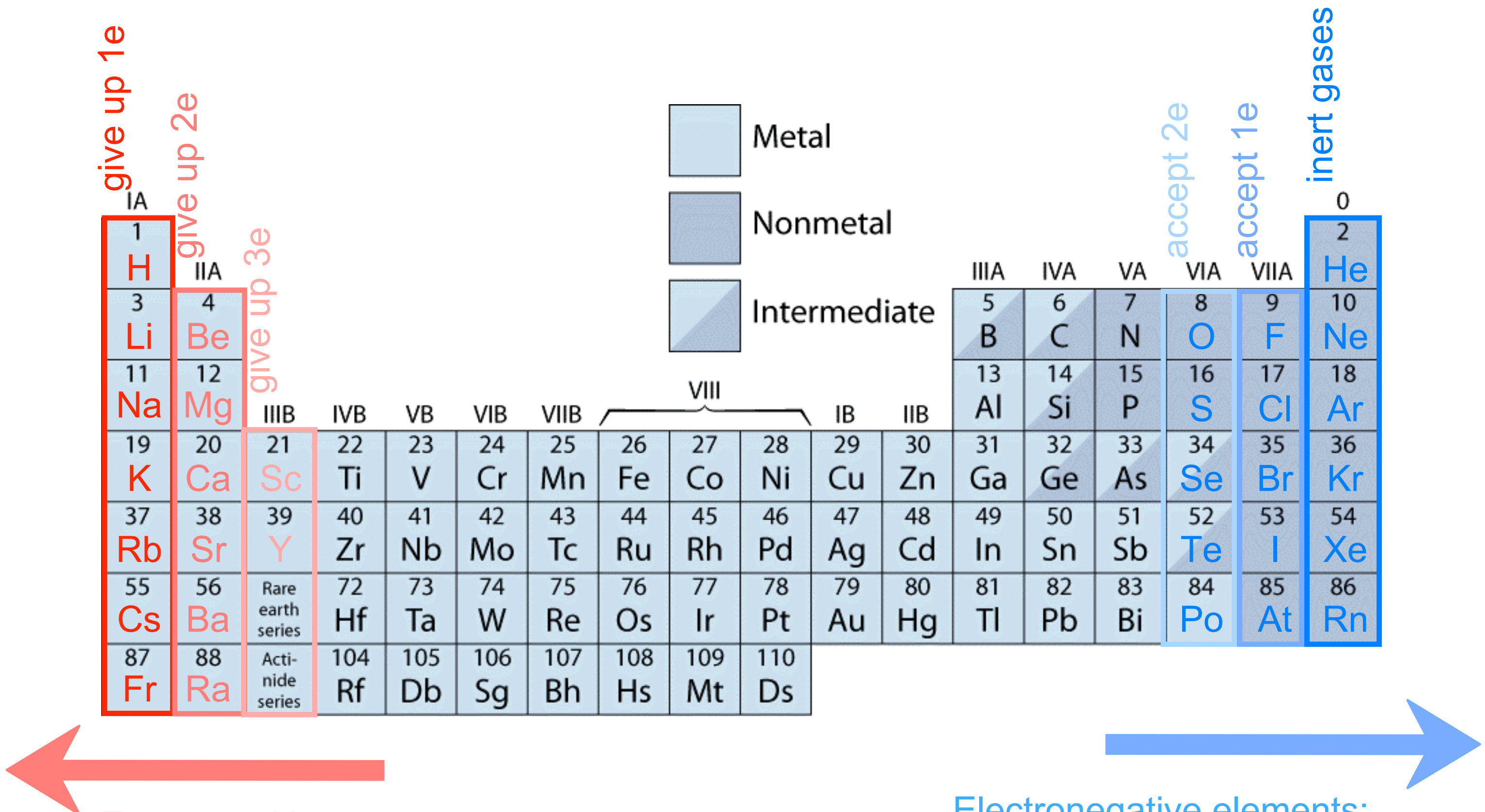
Element	Atomic #	Electron configuration	
Hydrogen	1	$1s^1$	
Helium	2	$1s^2$	(stable)
Lithium	3	$1s^2 2s^1$	
Beryllium	4	$1s^2 2s^2$	
Boron	5	$1s^2 2s^2 2p^1$	
Carbon	6	$1s^2 2s^2 2p^2$	
...		...	
Neon	10	$1s^2 2s^2 2p^6$	(stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$	
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$	
Aluminum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

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

Adapted from Table 2.2, *Callister 7e.*

The periodic table

- Columns: Similar Valence Structure



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

Electronegative elements:
Readily acquire electrons
to become - ions.

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

Electronegativity

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

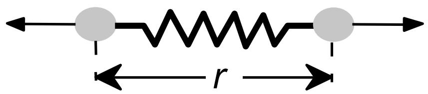
IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	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

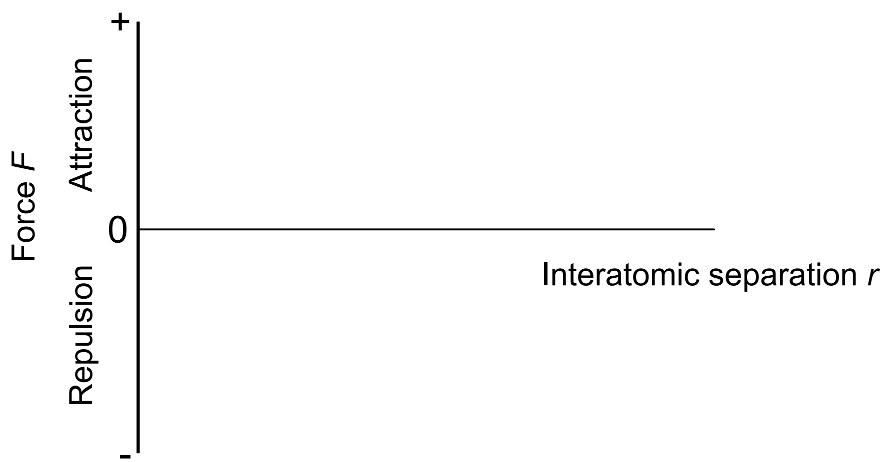
Larger electronegativity

Adapted from Fig. 2.7, *Callister 7e.* (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.

Bonding forces and energies

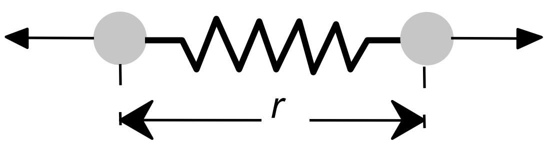


- Attractive force, F_A
- Repulsive force, F_R

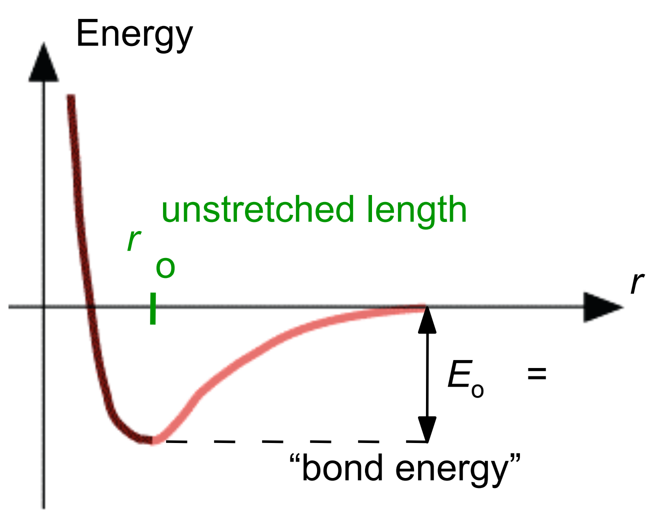


Properties from bonding

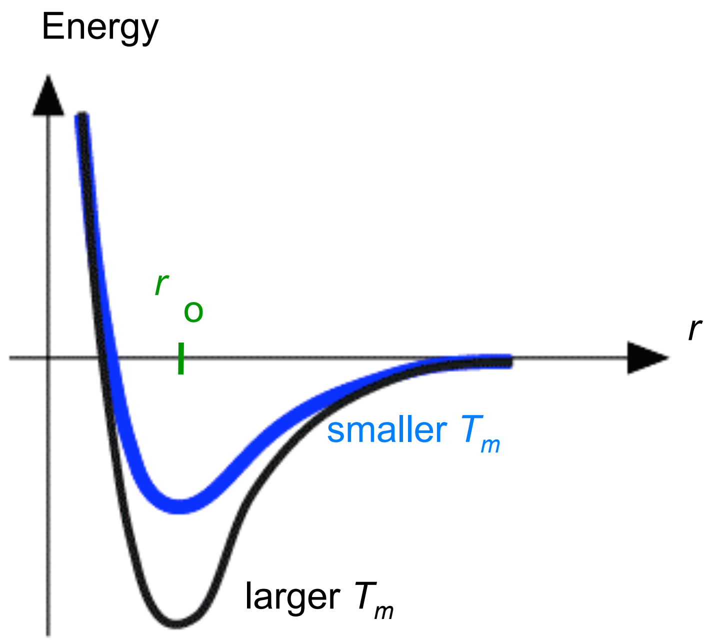
- Bond length, *r*



- Bond energy, E_o



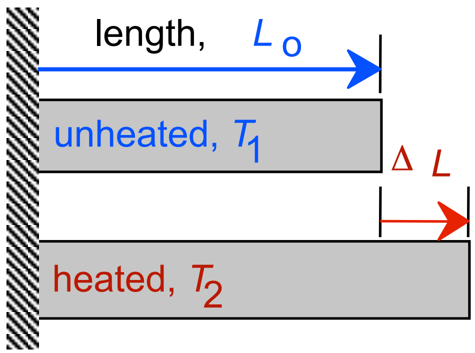
- Melting Temperature, T_m



T_m is larger if E_o is larger.

Properties from bonding: thermal expansion coefficient

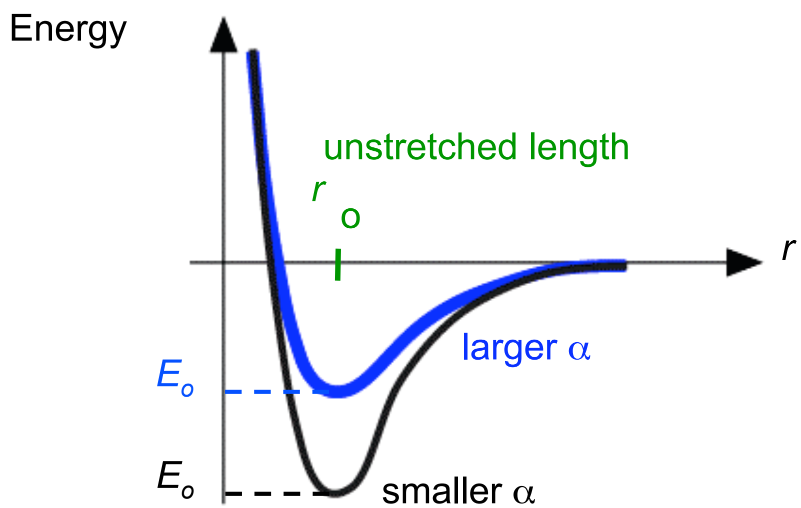
- Coefficient of thermal expansion, α



coeff. thermal expansion

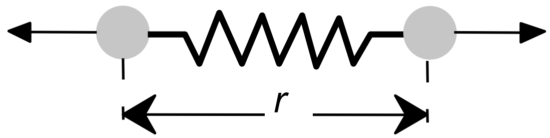
$$\frac{\Delta L}{L_o} = \alpha (T_2 - T_1)$$

- α ~ symmetry at r_o

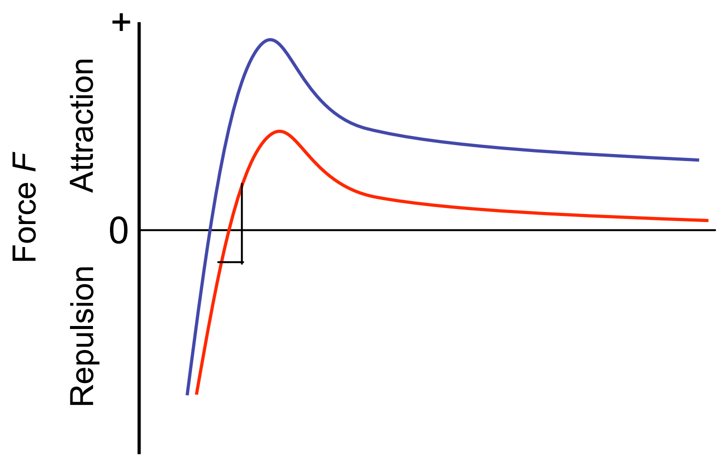


α is larger if E_o is smaller.

Properties from bonding: modulus *E*

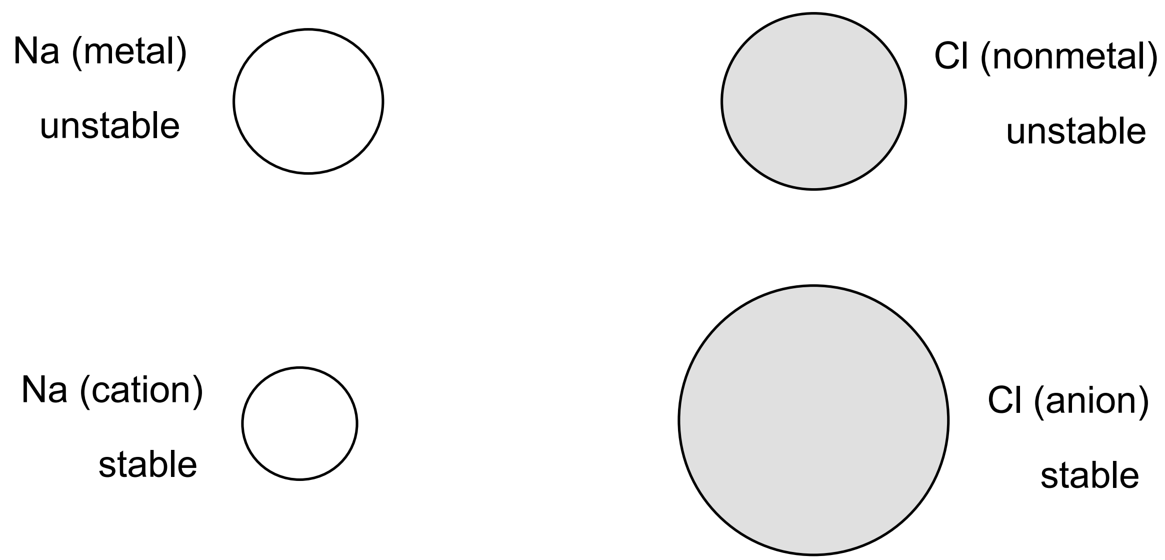


$F = kx$



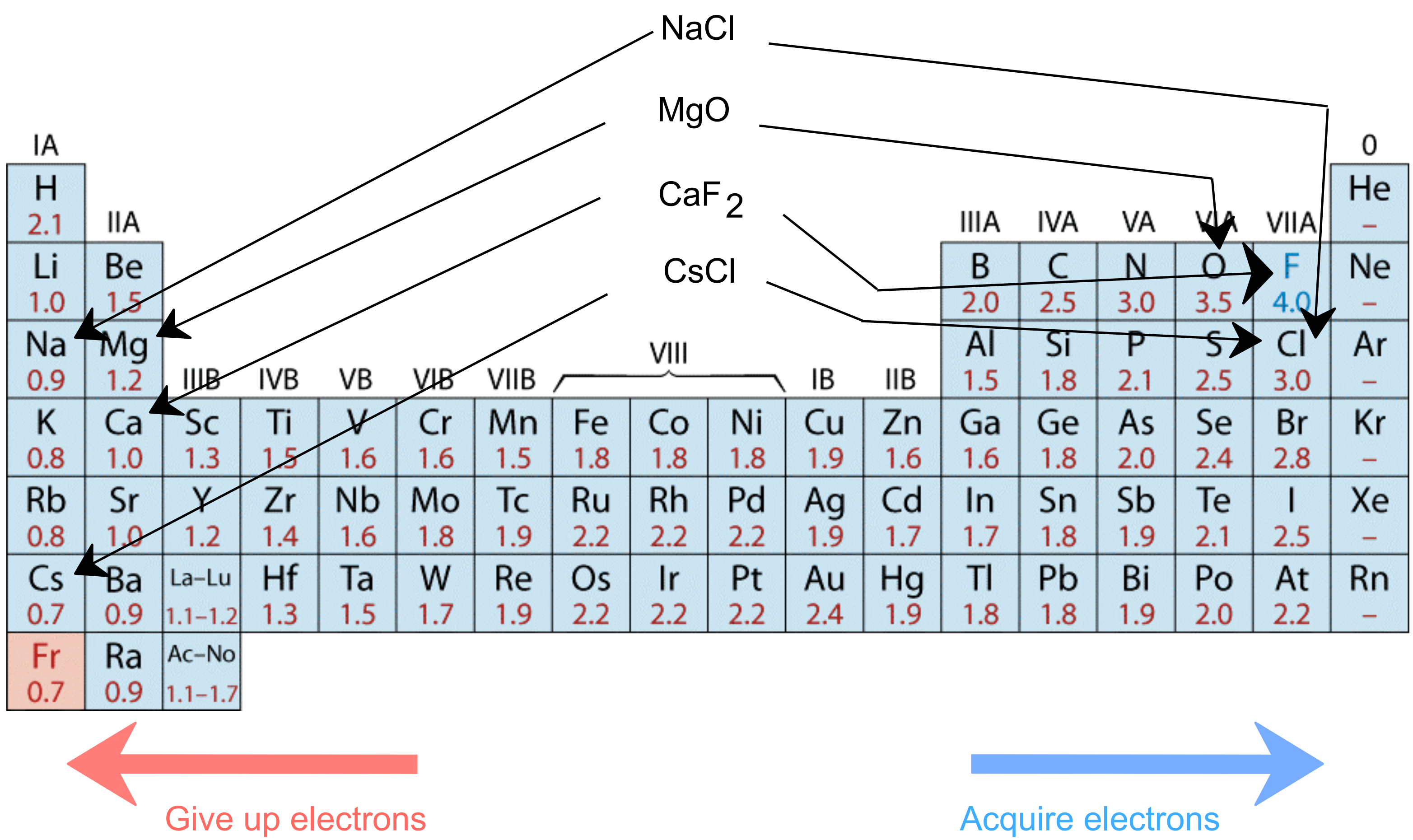
Types of bonding: ionic

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



Examples of ionic bonding

- Predominant bonding in Ceramics



Adapted from Fig. 2.7, *Callister 7e.* (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

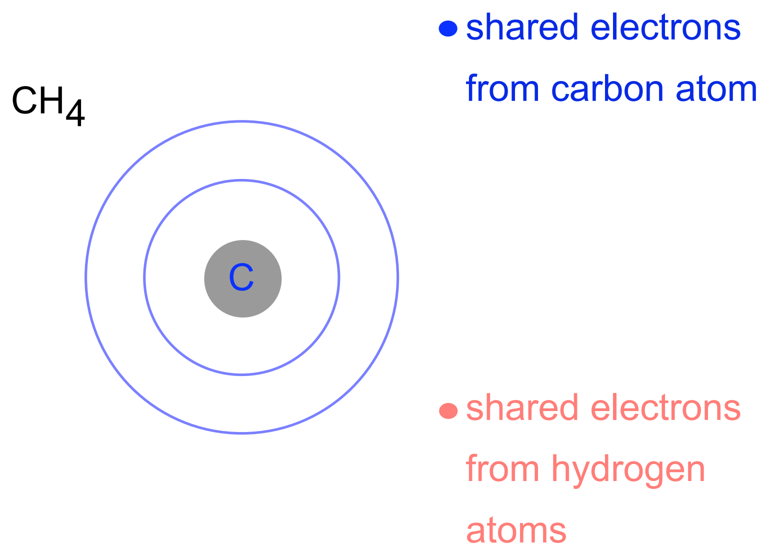
•similar electronegativity ∴ share electrons
•bonds determined by valence – *s* & *p* orbitals dominate bonding

•Example: CH_4

C: has 4 valence e^-,
needs 4 more

H: has 1 valence e^-,
needs 1 more

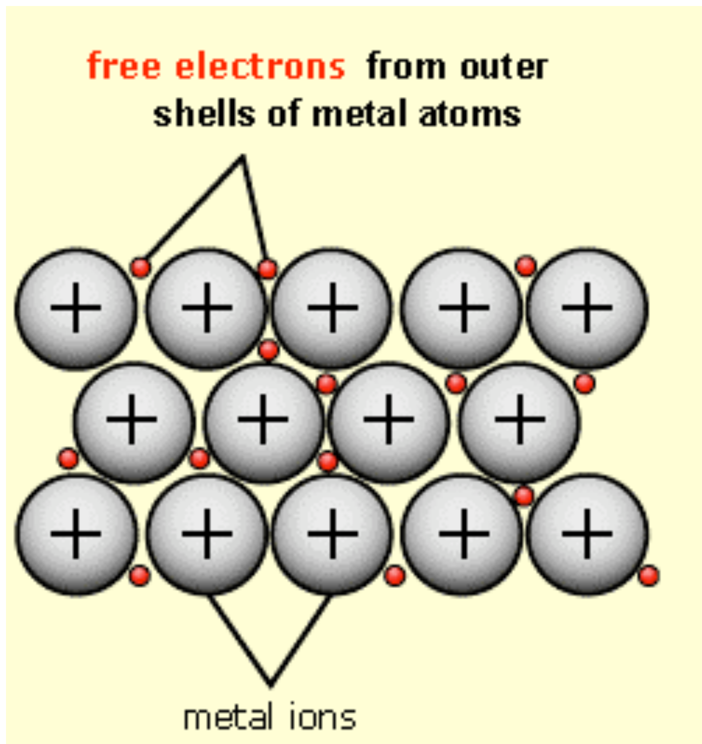
Electronegativities
are comparable.



Adapted from Fig. 2.10, *Callister 7e.*

Metallic bonding

- Ions in a sea of electrons
- Attraction between free electrons and metal ions



Ionic-covalent mixed bonding

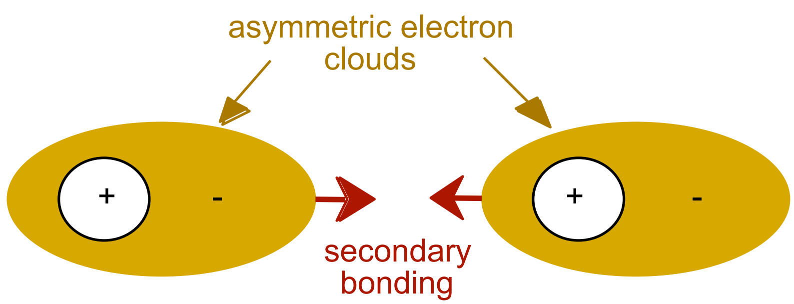
$$\text{\% ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \text{x} \ (100\ \%)$$

where X_A & X_B are Pauling electronegativities

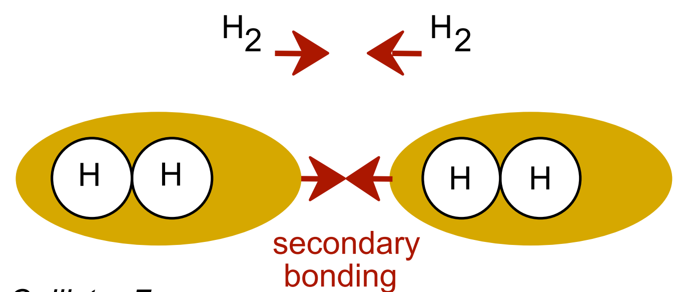
Secondary bonding

Arises from interaction between dipoles

- Fluctuating dipoles



example: liquid H_2

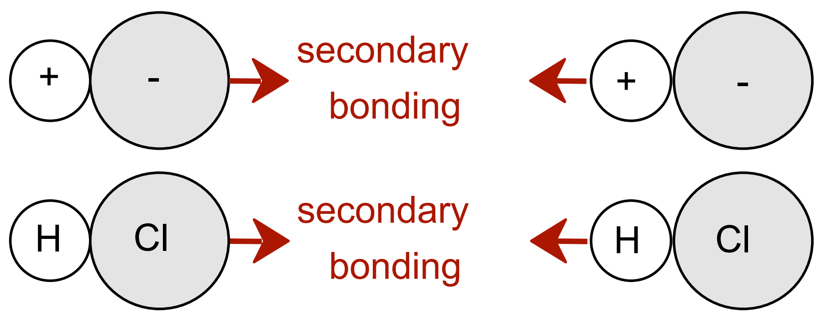


Adapted from Fig. 2.13, *Callister 7e.*

- Permanent dipoles-molecule induced

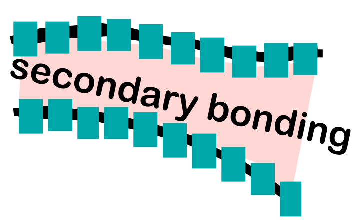
-general case:

-example: liquid HCl



Adapted from Fig. 2.14, *Callister 7e.*

-example: polymer



secondary bonding

Summary

Type	Bond Energy	Comments
Ionic	Large!	Non-directional (ceramics)
Covalent	Variable Diamond (large) Bismuth (small)	Directional (semiconductors, ceramics, polymer chains)
Metallic	Variable Tungsten (large) Mercury (small)	Non-directional (metals)
Secondary	Smallest	Directional Interchain (polymer) Intermolecular

Ceramics (Ionic & covalent bonding)	Large bond energy Large T_m and E, small α
Metals (Metallic bonding)	Variable bond energy Moderate T_m, E, and α
Polymers (Covalent & secondary)	Directional properties, Secondary bonding dominates Small T_m and E, large α