CH203 Lecture 2
September 7, 2010

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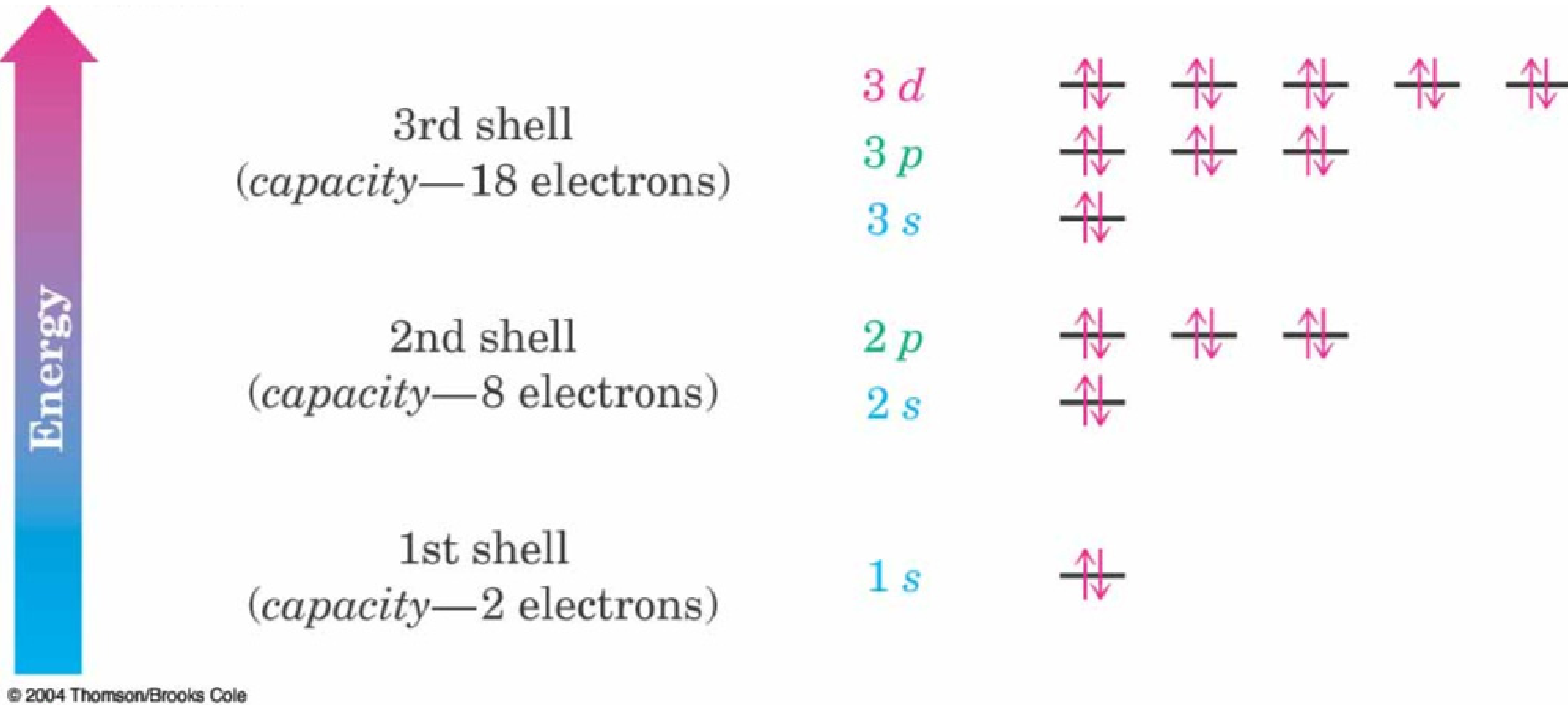
Meet the CH203 AA AA Class !



This is incorrect (Figure 1.4 in text)

Review of Lecture 1: Atomic Structure: Electron Configurations

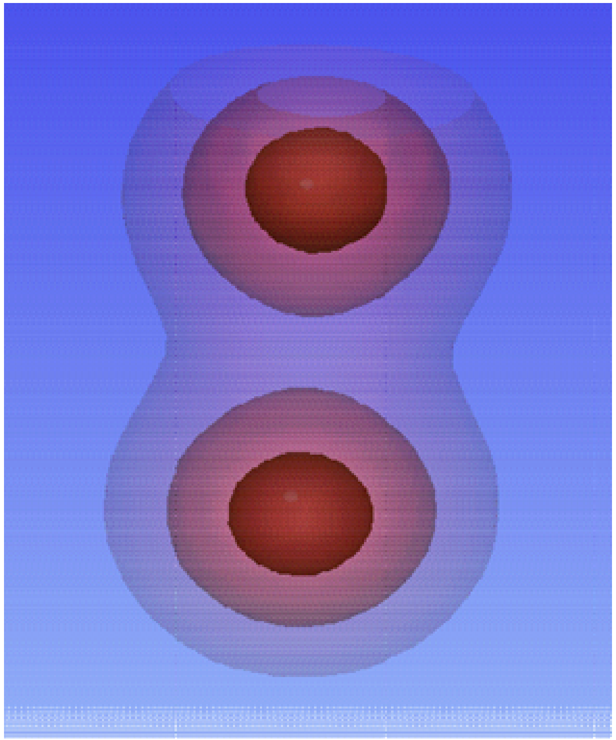
- **Ground-state electron configuration** of an atom lists orbitals occupied by its electrons. Rules:
- 1. Lowest-energy orbitals fill first: 1*s* → 2*s* → 2*p* → 3*s* → 3*p* → 4*s* → 3*d* (*Aufbau (*"build-up") principle)
- 2. Electron spin can have only two orientations, up ↑ and down ↓. Only two electrons can occupy an orbital, and they must be of opposite spin (*Pauli exclusion principle*)
- 3. If two or more empty orbitals of equal energy are available, electrons occupy each with spins parallel until all orbitals have one electron (*Hund's rule*).

TABLE 1.1 Ground-State Electron Configurations of Some Elements

Element	Atomic number	Configuration				Element	Atomic number	Configuration			
Hydrogen	1	1*s*	↑			Lithium	3	2*s*	↑		
								1*s*	↑↓		
Carbon	6	2*p*	↑	↑	—	Neon	10	2*p*	↑↓	↑↓	↑↓
		2*s*	↑↓					2*s*	↑↓		
		1*s*	↑↓					1*s*	↑↓		
Sodium	11	3*s*	↑			Argon	18	3*p*	↑↓	↑↓	↑↓
		2*p*	↑↓	↑↓	↑↓			3*s*	↑↓		
		2*s*	↑↓					2*p*	↑↓	↑↓	↑↓
		1*s*	↑↓					2*s*	↑↓		
								1*s*	↑↓		

What do ``shared'' electrons actually look like?

1)



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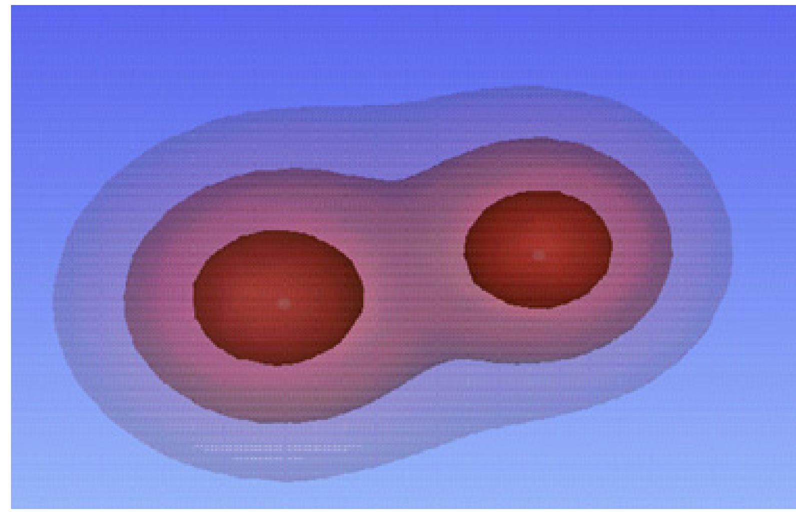

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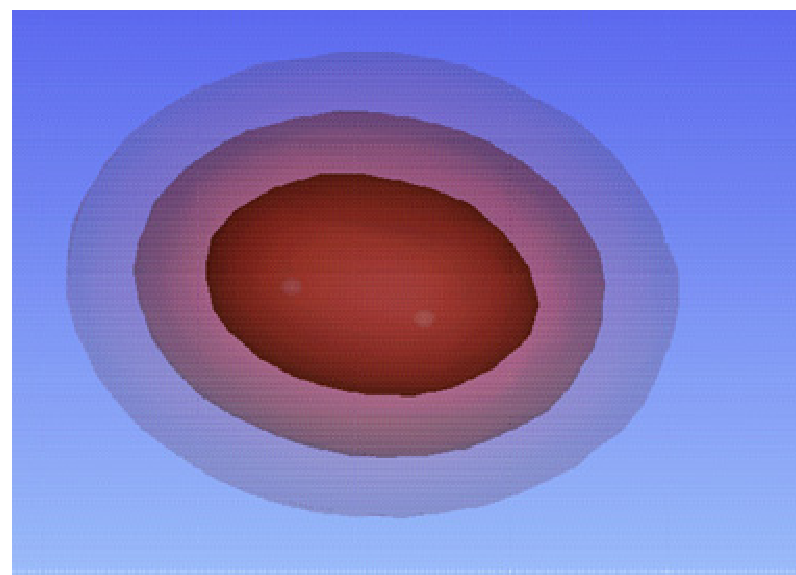
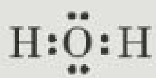
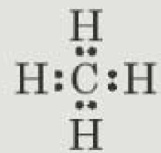
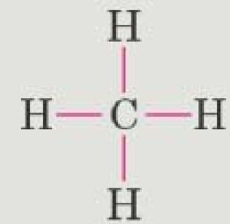
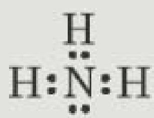
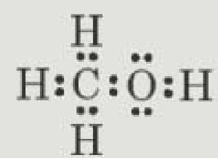
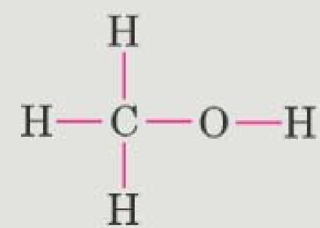


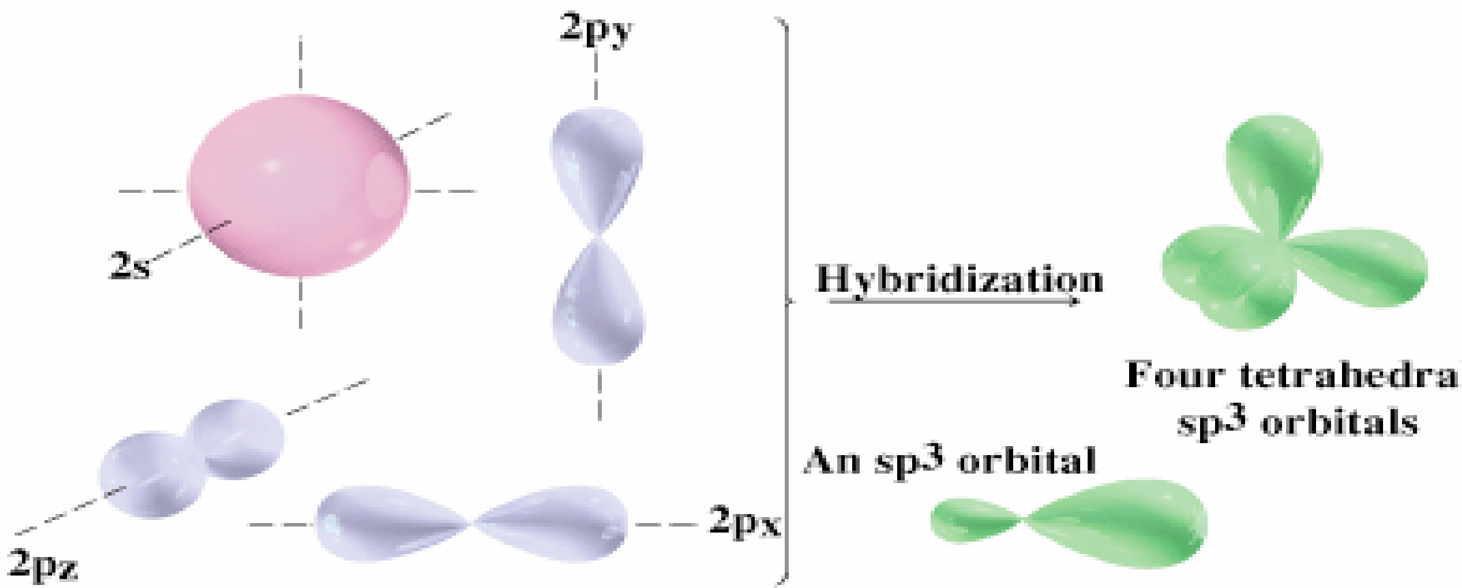
The sequence shows how electron density changes as two H atoms are brought closer together until they reach their true bond length

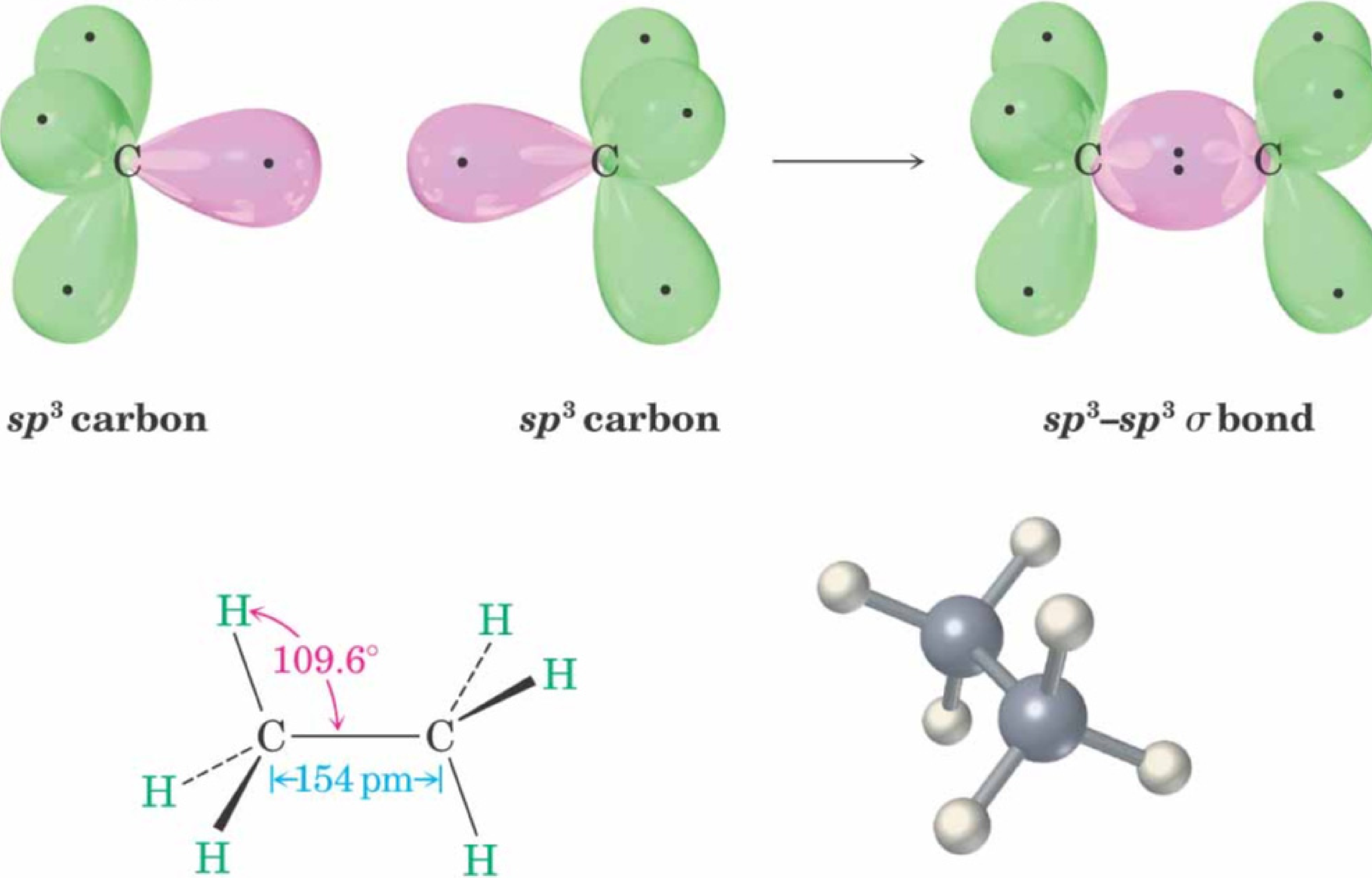
TABLE 1.2 Lewis and Kekulé Structures of Some Simple Molecules

Name	Lewis structure	Kekulé structure	Name	Lewis structure	Kekulé structure
Water (H_2O)			Methane (CH_4)		
Ammonia (NH_3)			Methanol (CH_3OH)		

Hybridization: sp^3 Orbitals and the Structure of Methane

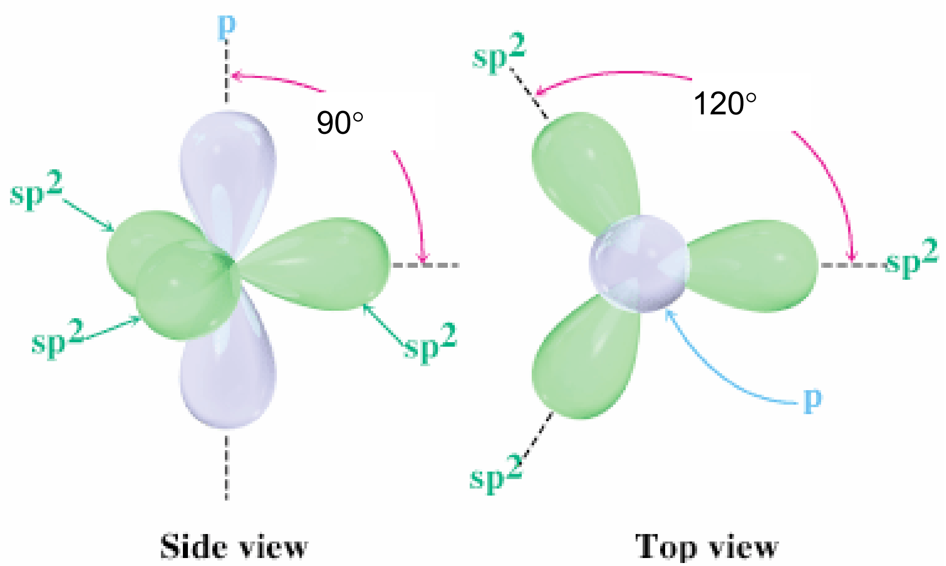
- Carbon has 4 valence electrons ($2s^2\ 2p^2$)
- In CH_4, all C–H bonds are identical (tetrahedral)
- ***sp^3* hybrid orbitals**: *s* orbital and three *p* orbitals combine to form four equivalent, unsymmetrical, tetrahedral orbitals (sppp = sp^3), Pauling (1931)

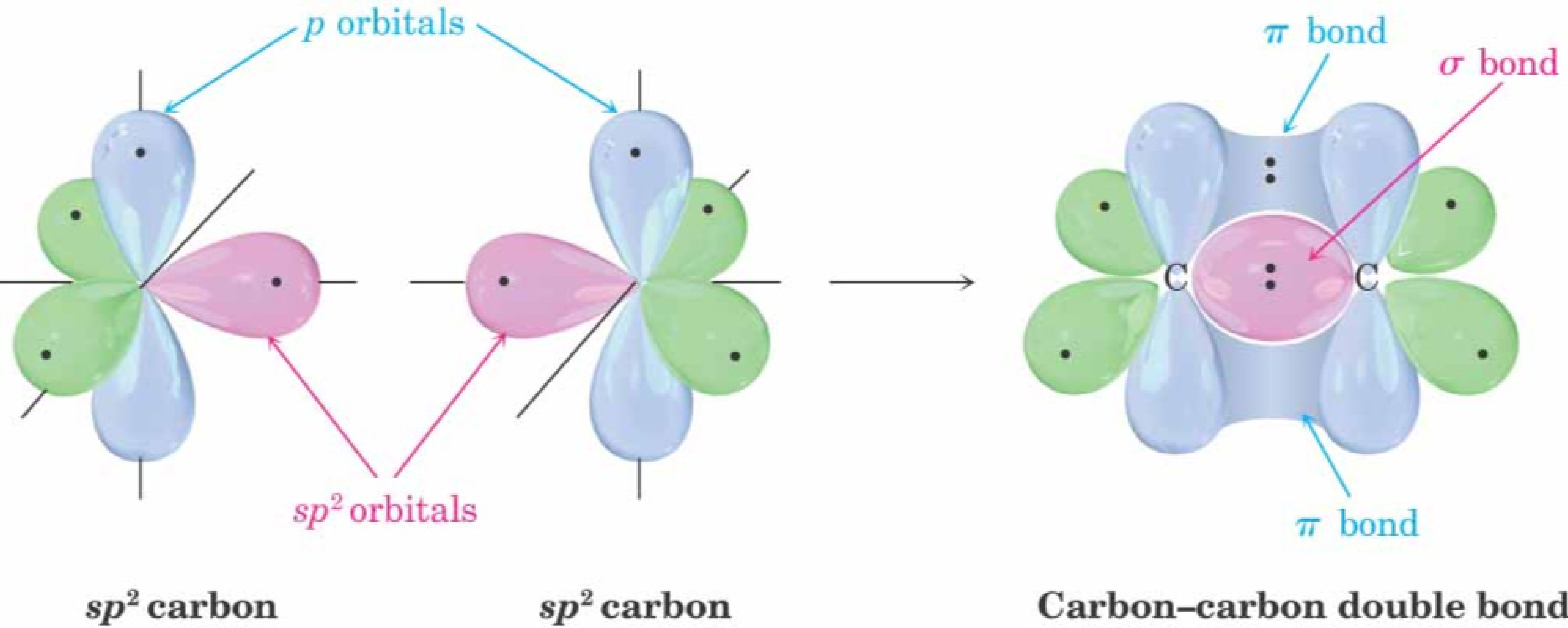



C
C
C
C
sp^3 carbon
sp^3 carbon
sp^3–sp^3 σ bond
H
H
H
H
H
H
C
C
109.6°
154 pm

Hybridization: sp^2 Orbitals and the Structure of Ethylene

- ***sp*^{2} hybrid orbitals:** 2*s* orbital combines with *two* 2*p* orbitals, giving 3 orbitals (spp = sp^2)
- *sp*^{2} orbitals are in a plane with 120° angles
- Remaining *p* orbital is perpendicular to the plane

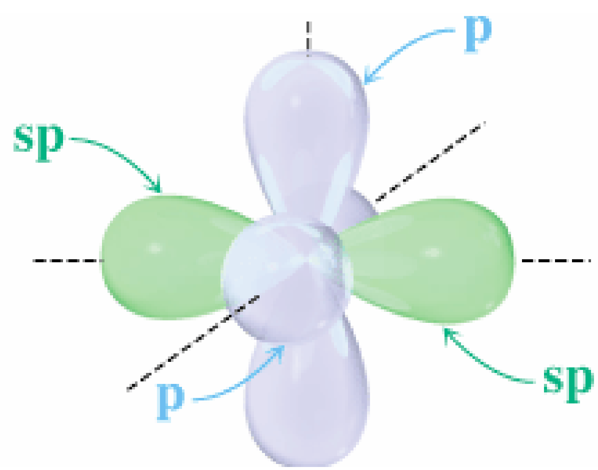




p orbitals
π bond
σ bond
C
C
sp² orbitals
π bond
sp² carbon
sp² carbon
Carbon–carbon double bond

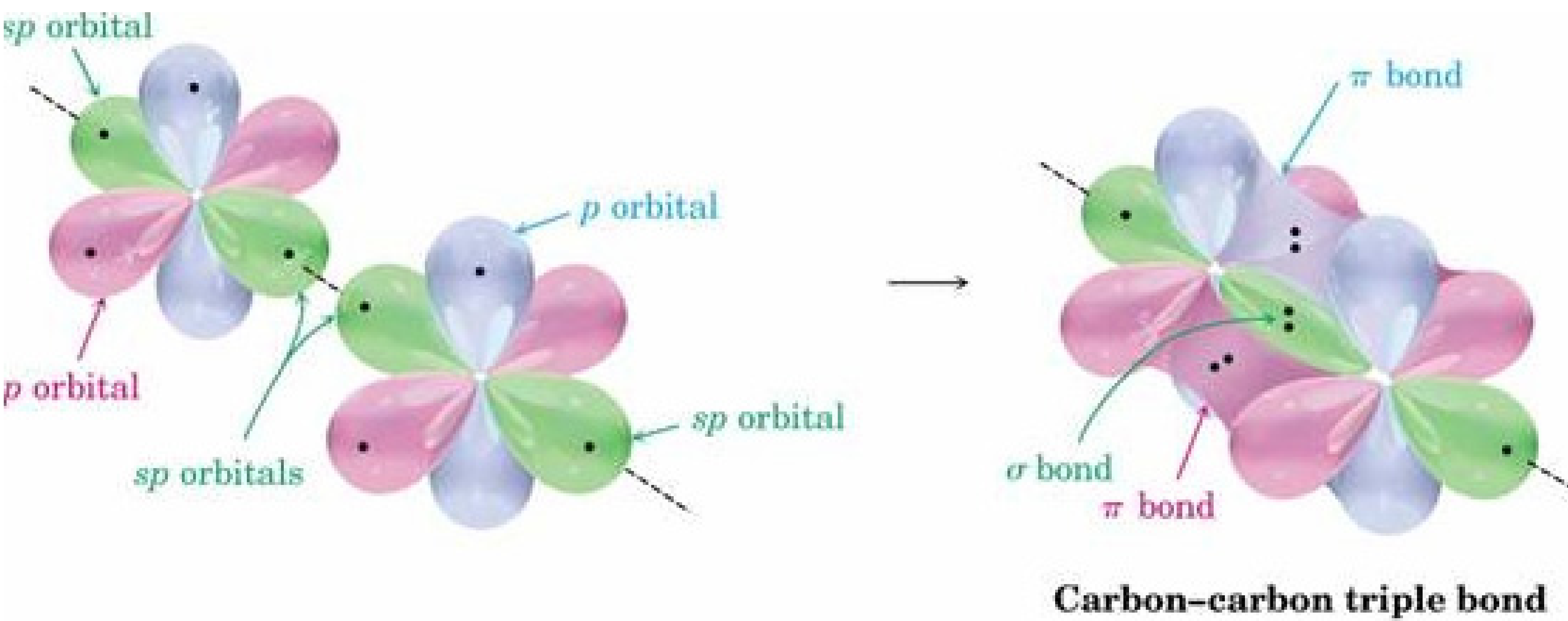
Hybridization: sp Orbitals and the Structure of Acetylene

- C-C a *triple* bond sharing six electrons
- Carbon 2*s* orbital hybridizes with a single *p* orbital giving two *sp* hybrids
  - two *p* orbitals remain unchanged
- *sp* orbitals are linear, 180° apart on *x*-axis
- Two *p* orbitals are perpendicular on the *y*-axis and the *z*-axis

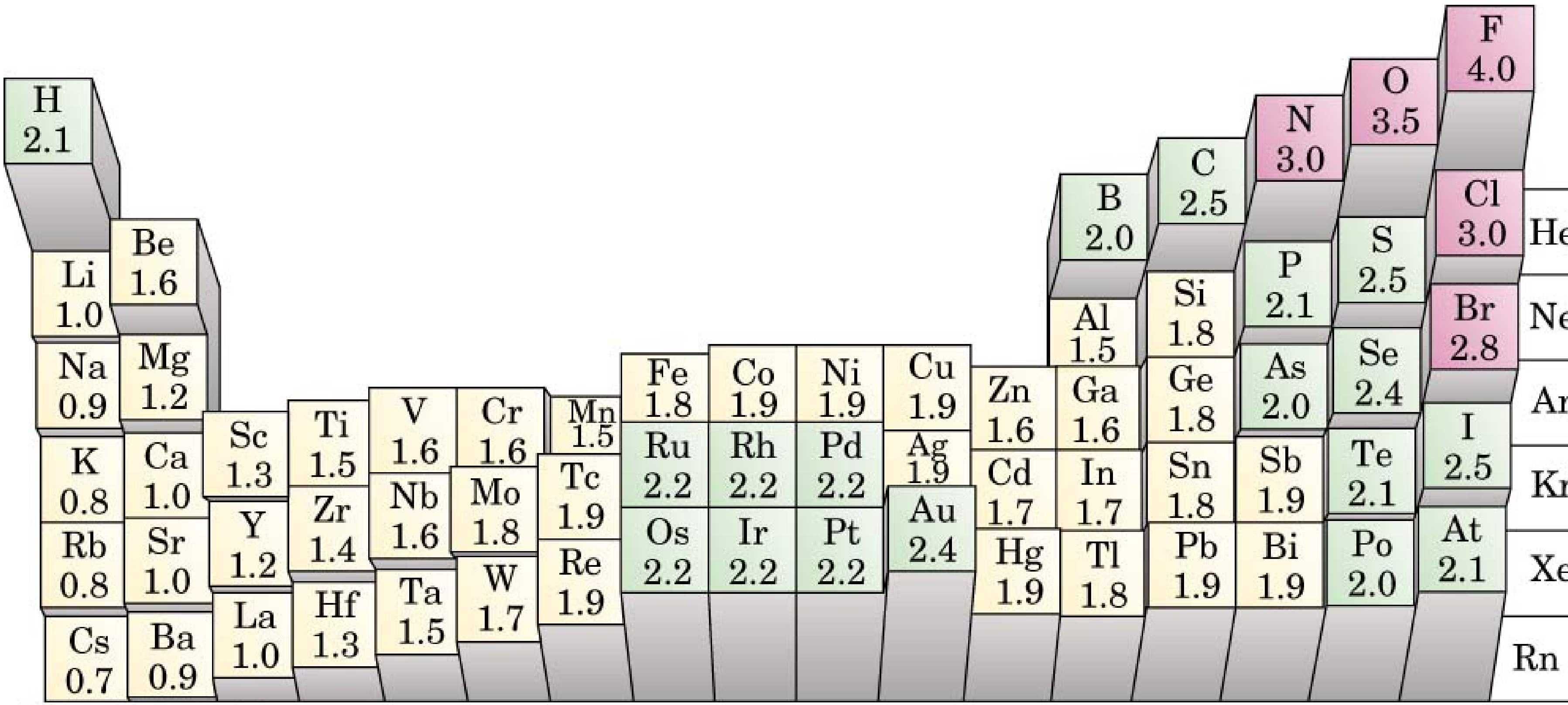


Orbitals of Acetylene

- Two *sp* hybrid orbitals from each C form *sp*–*sp* σ bond
- *pz* orbitals from each C form a p_z–p_z π bond by sideways overlap and p_y orbitals overlap similarly



The Periodic Table and Electronegativity



Bond Polarities

Bond	**Diff in EN**	**Negative atom**	**Type of Bond**
H - H	0.0	N/A	pure covalent
C - H	0.4	C	(weakly) polar covalent
O - H	1.4	O	polar covalent
H - F	1.9	F	polar covalent
S - O	1.0	O	polar covalent
C - O	1.0	O	polar covalent
Al - C	1.0	C	polar covalent
Na - Cl	2.1	Cl	ionic
Li - F	3.0	F	ionic
Mg - O	2.3	O	ionic
Mg - C	1.3	C	polar covalent

Less than 0.5 difference in EN : *Nonpolar covalent*

0.5 to 2 EN units – *Polar covalent*

Greater than 2 EN units - *Ionic*

CH 203 Lecture # 2 (1)

9/07/10

Clarification / Correction from last lecture (Figure 1.4 incorrect)

Ni atomic # 28

3d ↑↓ ↑↓ ↑↓ ↑ ↑

4s ↑↓

3p ↑↓ ↑↓ ↑↓

3s ↑↓

$\therefore 1s^2 2s^2 2p^6$
$3s^2 3p^6$
$4s^2 3d^8$

not $3d^{10}$

Chemical Bonds

– An e^- octet in the outermost shell imparts special stability to nobel gas elements

e.g. Neon group 8A $1s^2 2s^2 2p^6$

- Atoms closer to middle of periodic table achieve this by sharing e^-s.

shared e^- bond

- Covalent bonds involve sharing of e^-s between atoms to form "molecules" $\longrightarrow$ collection of atoms held together by covalent bonds.

(eg., H_2 molecule)

~~Note that~~
~~Noble gas~~

H_2 molecule

$$H\cdot \;+\; H\cdot \;\longrightarrow\; H:H \quad \text{or } H-H$$

Lewis dot structure* — Kekule structure (line bond structure)

Shows e^-s of valence shell

CH_4 molecule

$$\cdot\dot{\underset{\cdot}{C}}\cdot \;+\; 4\,H\cdot \;\longrightarrow\; \begin{array}{c} H \\ \cdot\cdot \\ H:C:H \\ \cdot\cdot \\ H \end{array} \quad \text{or} \quad \begin{array}{c} H \\ | \\ H-C-H \\ | \\ H \end{array}$$

C: Four valence e^-s

- $2s^2, 2p^2$
- used to form 4 bonds

$2e^-$ covalent bond = line

Noble gas config

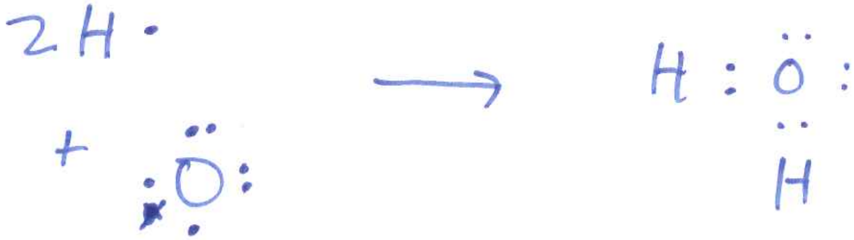
$8\ e^-$s or octet achieved

Valences of O

- O has six valence e^-s $2s^2 2p^4$

~~two~~ and forms two bonds $H-O-H$

(needs 2 more e^-s)



Valences of N

- N has five valence e^-s $(2s^2 2p^3)$

and forms 3 bonds. e.g. NH_3

ammonia

non-bonding or

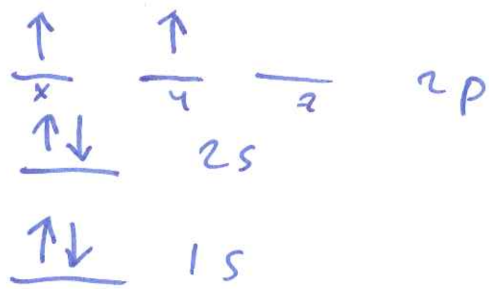
lone-pair e^-s

not used in bonding

Hybridization of atomic orbitals

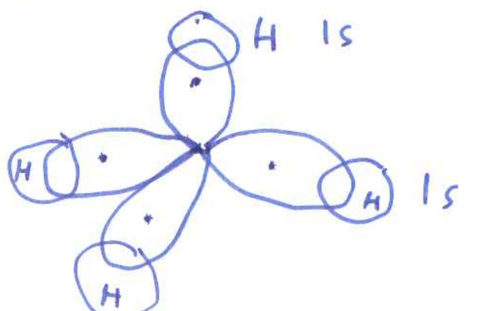
in C

- orbitals are diff. energy levels



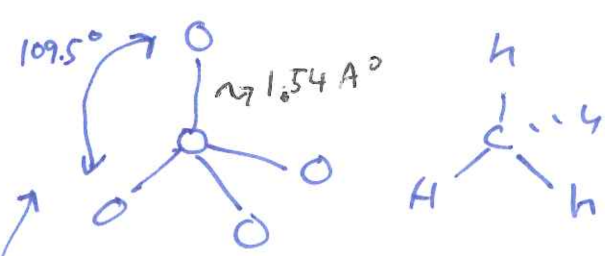
- However for CH_4, all C-H bonds are equivalent (1.54 A°). How is that?

- orbitals mix to form new orbitals
- orbital "hybridization" : combine s & p orbitals to obtain hybrid atomic orbitals



sp3 hybrids

sp3 orbs. on C overlap with 1s orbitals on H



sp 3 orbitals

tetrahedral angle

4 identical CH bonds

sp3 orbital

– sp^3 orbital – 1s orbital bond

example of a σ bond (sigma) → bond in which the overlap region lies directly between the nuclei

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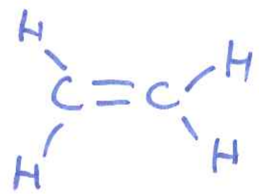
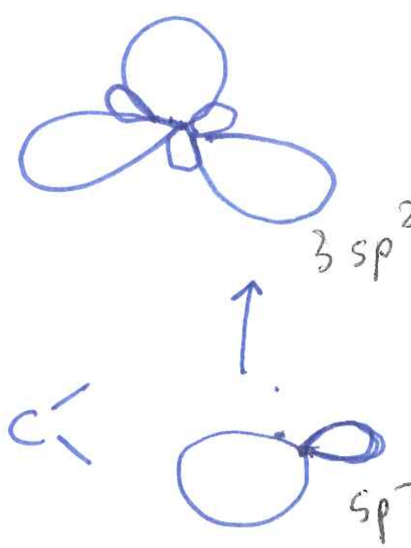
sp^2 hybridization

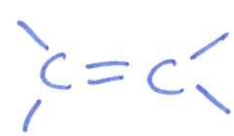
Many important organic molecules exist in which C atoms share more than $2e^-$'s with another atom

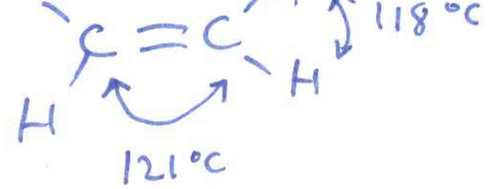


ethylene



or





In this case 2s orbital combines with 2 2p orbitals

→ 3 sp^2 hybrids + one unchanged p

(Slide)

A σ bond forms by sp^2-sp^2 overlap

7

– unhybridized p orbitals form a pi (π) bond. 2p

– overall π bond shares $4e^-$s and ~~share~~ forms C–C double bond

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sp hybridization · 3rd kind of hybrid orbital

carbon can also form a triple bond by sharing $6e^-$s

H:C:::C:H

H–C≡C–H

180°

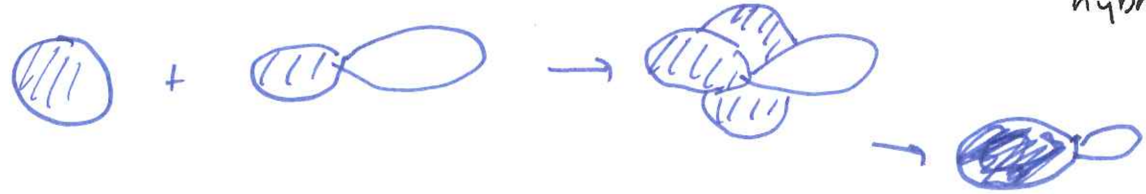
linear molecule

to account for triple bond need 3rd kind of hybrid orbital

Two sp-hybridized C atoms joined by sp-sp σ bond and 2π bonds

sp hybrid

Sum



	bond length (pm)
$C \equiv C$	120
$C = C$	133
$C - C$	154

$pm = 10^{-12} m$

8

section 1.11 MO theory, alt. approach involving mathematical combination of atomic orbitals to form molecular orbitals

~~valence~~

we will focus our approaches on

valence bond theory

(hybrid atomic orbitals account for geometry + e^- sharing)

Chapter 2: Polar Covalent Bonds – Acids & Bases

Skip sections 2.2, 2.13

Problems

24

8, 9, 10, 15, 25, 32, 33, 34,

37, 38, 39, 40, 41, 47, 54, 55, 56,

& 58

Chapter 2: Polar Covalent Bonds - Acids & Bases

electronegativity

$X : X$

Symm. covalent bond

$\delta^+ \quad \delta^-$

$X : Y$

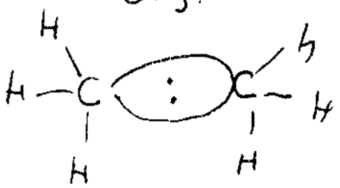
Polar covalent bond

$\xrightarrow{\text{ionic character}}$

$X^+ \quad Y^-$

ionic bond

e.g.

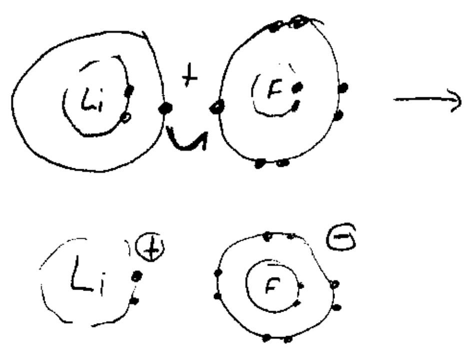


2 bonding e^-s shared equally by equiv C atoms

ionic bond:

Li
$1s^2\, 2s$

F
$1s^2\, 2s^2\, 2p^5$



- Electroneg. (EN) measures ability of an atom to attract e^-s (arbitrary scale)
- Increases as we go across a hor. row of the periodic table from left to right:

1.0			2.5			4.0
Li	Be	B	C	N	O	F

$\xrightarrow{\hspace{6cm}}$

increasing EN (number of charges (protons) on the nucleus increases)

and increases going up a vertical column

F
Cl
Br
I
$\uparrow$

F
$\downarrow$
I

} en decr. because bonding pair of e^-s is incr. distant from attrac. of the nucleus