

10-1

### VSEPR Model

- The structure around a given atom is determined principally by minimizing electron pair repulsions.

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10-2

### Predicting a VSEPR Structure

- Draw Lewis structure.
- Put pairs as far apart as possible.
- Determine positions of atoms from the way electron pairs are shared.
- Determine the name of molecular structure from positions of the atoms.

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10-3

### Example Molecules in Two and Three Dimensions

- O<sub>2</sub> Linear
- H<sub>2</sub>O Bent, or angular
- NH<sub>3</sub> Pyramidal
- CH<sub>4</sub> Tetrahedral
- NH<sub>4</sub><sup>+</sup> Tetrahedral
- PCl<sub>5</sub> Trigonal bipyramidal
- SF<sub>6</sub> Octahedral
- Above list not all-inclusive: square pyramidal, e.g. ?What would cause this shape?
- Above list not all-inclusive: square pyramidal, trigonal planar, etc. ?What would cause these shapes?

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10-4

### Sample Test Questions

What is the molecular shape of the following compound, for which the correct Lewis dot structure is given?



- What is the molecular shape of  $\text{PF}_3$ ?
- What is the molecular shape of dinitrogen tetroxide?

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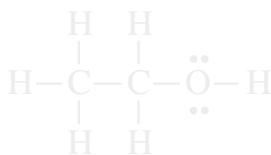
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10-5

### Shape of Molecule With More Than One "Central Atom"

- $\text{CH}_3\text{CH}_2\text{OH}$




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9-35

### Polarity of *Molecules*

- Using chart I, indicate whether the following *molecules* are polar or nonpolar

- $\text{CH}_4$
- $\text{CO}$
- $\text{CO}_2$
- $\text{CHCl}_3$
- $\text{H}_2\text{S}$
- $\text{BCl}_3$

Chart I. Electronegativities of Selected Elements

H 2.21								He —
Li 0.98	Be 1.57		B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne —
Na 0.93	Mg 1.31		Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar —
K 0.82	Ca 1.00		Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr —
Rb 0.82	Sr 0.95		In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe —
Cs 0.79	Ba 0.89		Tl 2.04	Pb 2.33	Bi 2.02	Po 2.0	At 2.2	Rn —

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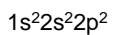
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10-6

## Atomic Orbitals

electron configuration of C



We might expect C to form two bonds ( the 2 unpaired p electrons)

We know that C forms 4 bonds

We might expect that  $\text{CH}_4$  would have 1 s-s bonds and 3 s-p bonds. These would have different lengths.

We know that all CH bonds are equivalent

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10-7

## Hybrid Atomic Orbitals

Fig. 9.5 Zumdahl and Zumdahl, 6<sup>th</sup> Ed.

- The mixing of atomic orbitals to form special orbitals for bonding.
- C has 4  $sp^3$  hybrid orbitals
  - called sigma bonds



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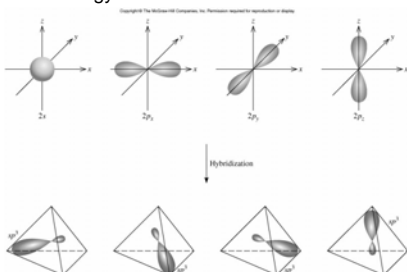
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10-8

## Hybrid Atomic Orbitals

Fig. 10.7 Chang, 9<sup>th</sup> Ed.

- The atoms are responding as needed to give the minimum energy for the molecule.



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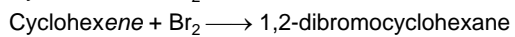
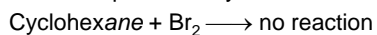
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10-9

## Not All Bonds Are Equally Reactive

We know experimentally:



And,

bond angles in *-ene* are  $120^\circ$ :

$sp^2$  hybridization occurs

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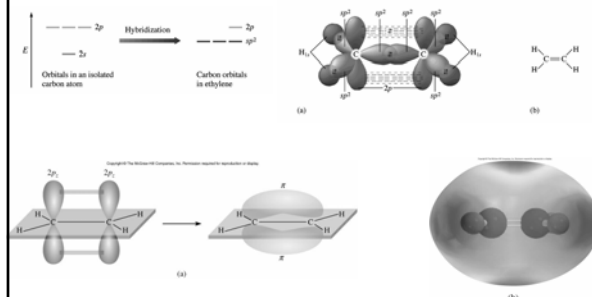
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10-10

## $sp^2$ Hybridization

Fig. 9.9 (top left) and 9.13 (top right) Zumdahl and Zumdahl, 6<sup>th</sup> Ed.  
Fig. 10.17a (bottom left) and 10.17 (bottom right) Chang, 9<sup>th</sup> Ed.



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10-11

## Not the End of the Story

Acetylene (ethyne) reacts very fast like ethene.

But, uses up twice as much bromine.

There must be two highly reactive bonds, and...

$sp$  hybridization occurs

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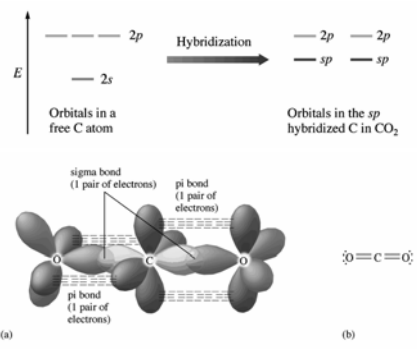
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10-12

### sp Hybridization

Fig. 9.16 (top) and 9.19 (bottom) Zumdahl and Zumdahl, 6<sup>th</sup> Ed.



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10-13

### How These Relate to Each Other

- A sigma ( $\sigma$ ) bond centers along the internuclear axis.
- A pi ( $\pi$ ) bond occupies the space above and below the internuclear axis.

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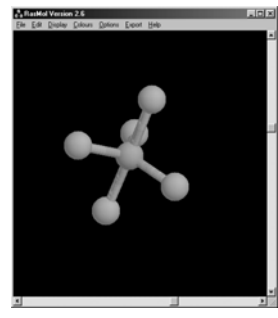
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10-14

### Question

- How many things need to be hybridized for PCl<sub>5</sub>?



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10-15

### The Localized Electron Model

- Draw the Lewis structure(s)
- Determine the arrangement of electron pairs (VSEPR model).
- Figure out what hybridization is required to get that shape

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10-16

### Sample Test Question

Use the localized electron model to describe the bonding in  $\text{CCl}_4$ .

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10-17

### Molecular Orbitals (MO)

- Above models don't always work (carbonate, NO examples)
- "Analogous to atomic orbitals for atoms, MOs are the quantum mechanical solutions to the organization of valence electrons in molecules."
  - Orbitals hold two electrons with opposite spins
  - Square of MO wave indicates electron probability

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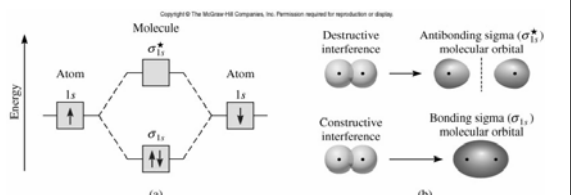
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10-18

### For $H_2$

Fig. 10.23 Chang, 9<sup>th</sup> Ed.

- Recall that waves can add and subtract
- Peak + trough = node
- $MO_1 = 1s_A + 1s_B$
- $MO_2 = 1s_A - 1s_B$




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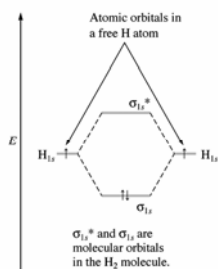
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10-19

### For $H_2$

Fig. 9.26 Zumdahl and Zumdahl, 6<sup>th</sup> Ed.

- Recall that waves can add and subtract
- Peak + trough = node
- $MO_1 (\sigma) = 1s_A + 1s_B$
- $MO_2 (\sigma^*) = 1s_A - 1s_B$
- $\sigma$  = bonding orbital: lower in energy than the atomic orbitals from which it is composed.
- $\sigma^*$  = antibonding orbital: higher in energy than the atomic orbitals from which it is composed.




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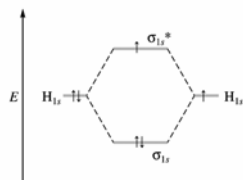
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10-20

### What Would $H_2^-$ and $H_2^{2-}$ Look Like?

- Think like aufbau




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10-21

### Bond Order (BO)

- Difference between the number of bonding electrons and number of antibonding electrons divided by two.

$$BO = \frac{\# \text{ bonding electrons} - \# \text{ antibonding electrons}}{2}$$

Larger bond order means greater bond strength.

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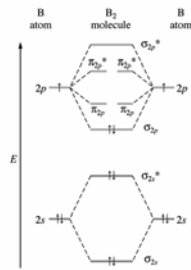
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10-22

### For Large Atoms

Fig. 9.36 Zumdahl and Zumdahl, 6<sup>th</sup> Ed.

- Energy levels are higher
- ∴ 2p higher than 2s
- However,  $\pi^*$  lower than  $\sigma^*$
- Make a change to this figure (next slide)




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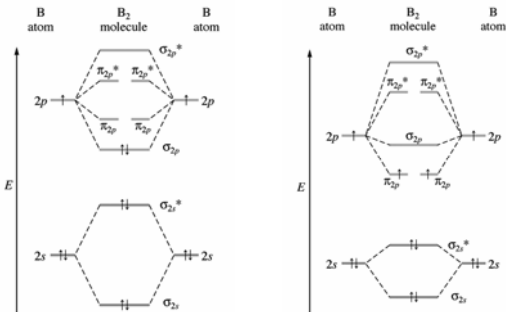
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10-23

### Expected vs. Actual Energies

Fig. 9.36 (expected, left) and 9.38 (actual, right) Zumdahl and Zumdahl, 6<sup>th</sup> Ed.




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10-24

### Outcomes of MO Model

1. As bond order increases, bond energy increases and bond length decreases.
2. Bond order is not absolutely associated with a particular bond energy.
3.  $N_2$  has a triple bond, and a correspondingly high bond energy.
4.  $O_2$  is paramagnetic. This is predicted by the MO model, not by the LE model, which predicts diamagnetism.

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10-25

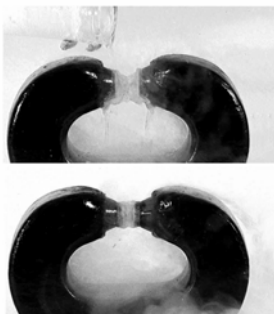
### Paramagnetism

Fig. 9.40 Zumdahl and Zumdahl, 6<sup>th</sup> Ed.

Paramagnetic- substance attracted to magnetic field because of unpaired electrons. The more unpaired electrons, the stronger the attraction.

much stronger than *diamagnetism*

Diamagnetic- substance weakly repelled by magnetic field because all electrons are paired.




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10-26

### O, N, F

Table 10.5 Chang, 9<sup>th</sup> Ed.

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	$Li_2$	$B_2$	$C_2$	$N_2$	$O_2$	$F_2$	
$\sigma_{2p}^*$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	$\sigma_{2p}^*$
$\pi_{2p}^*, \pi_{2p}^*$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	$\pi_{2p}^*, \pi_{2p}^*$
$\sigma_{2p}$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	$\pi_{2p}, \pi_{2p}$
$\pi_{2p}, \pi_{2p}$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	$\sigma_{2p}$
$\sigma_{2s}^*$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	$\sigma_{2s}^*$
$\sigma_{2s}$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	$\sigma_{2s}$
Bond order	1	1	2	3	2	1	
Bond length (pm)	267	159	131	110	121	142	
Bond enthalpy (kJ/mol)	104.6	288.7	627.6	941.4	498.7	156.9	
Magnetic properties	Diamagnetic	Paramagnetic	Diamagnetic	Diamagnetic	Paramagnetic	Diamagnetic	

\*For simplicity the  $\sigma_{2s}$  and  $\sigma_{2s}^*$  orbitals are omitted. These two orbitals hold a total of four electrons. Remember that for  $O_2$  and  $F_2$ ,  $\sigma_{2p}$  is lower in energy than  $\pi_{2p}$  and  $\pi_{2p}^*$ .

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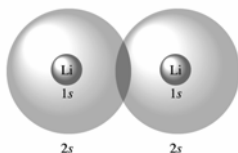
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10-27

## Only Valence Electrons are Involved in Bonding

Fig. 9.31 Zumdahl and Zumdahl, 6<sup>th</sup> Ed.

- In order to participate in MOs, atomic orbitals must overlap in space. (Therefore, only valence orbitals of atoms contribute significantly to MOs.)



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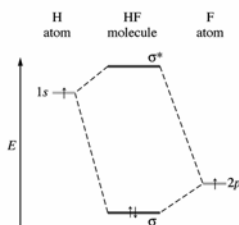
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10-28

## This Model Doesn't Work as Predictably for Heteronuclear Compounds

Fig. 9.43 Zumdahl and Zumdahl, 6<sup>th</sup> Ed.

- Note the lack of symmetry of energy levels compared to previous description.



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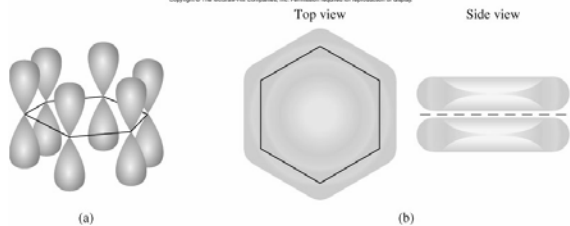
10-29

## Combining LE and MO Models

Fig. 10.29 Chang, 9<sup>th</sup> Ed.

- $\sigma$  bonds *can* be described as being localized.
- $\pi$  bonding *must* be treated as being delocalized.
- Benzene as an example:

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