Remainder of Ch 7

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# Remainder of Ch 7

Oct 10, 2016

## Ex: Multi-Central Atom Lewis Structures Isomers of C2H4O

* Acetaldehyde: CH3CHO,
* Ethenol (aka vinyl alcohol): CH2CHOH
* oxirane (aka ethylene oxide): CH2OCH2

## Molecular Orbital (MO) Theory: Electron Delocalization

* In MO theory:
  + Applies Schrödinger’s wave equation to the molecule to calculate a set of *molecular orbitals*
    - The equation solution is estimated.
    - The estimated solution is evaluated and adjusted until the energy of the orbital is minimized.
* In this treatment, the electrons belong to the whole molecule, so the orbitals belong to the whole molecule.
  + Delocalization

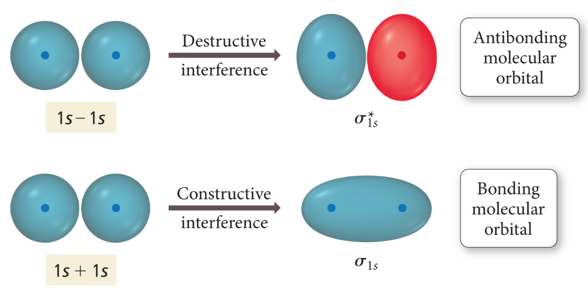
## LCAO: Linear Combination of Atomic Orbitals

* The simplest guess starts with the atomic orbitals of the atoms adding together to make molecular orbitals; this is called the *linear combination of atomic orbitals (LCAO)* method.
  + Weighted sum
* Because the orbitals are wave functions, the waves can combine either *constructively* or *destructively*.

## Molecular Orbitals

* When the wave functions combine constructively, the resulting molecular orbital has less energy than the original atomic orbitals
  + Called a *bonding molecular orbital*
  + Designated: σ, π
  + Most of the electron density between the nuclei
* When the wave functions combine destructively, the resulting molecular orbital has more energy than the original atomic orbital.
  + Called an antibonding molecular orbital
  + Designated: σ*, π*
  + Most of the electron density outside the nuclei
  + Nodes between nuclei

## Interaction of 1s Orbitals

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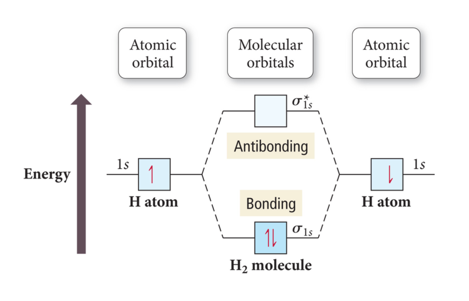
## Molecular Orbital Theory

* Use Aufbau approach for MO’s (as we did for individual atoms)
* electrons go into lowest energy MO’s first
* pair up when they have to

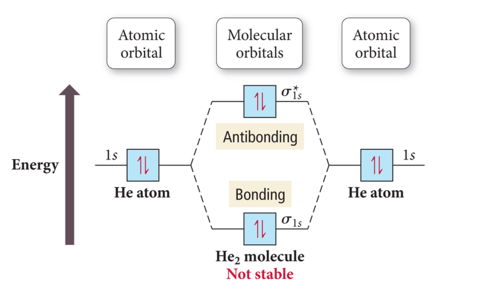
## Molecular Orbital Theory

* Electrons in bonding MOs are stabilizing.
  + Lower energy than the atomic orbitals
* Electrons in antibonding MOs are destabilizing.
  + Higher in energy than atomic orbitals
  + Electron density located outside the internuclear axis
  + Electrons in antibonding orbitals cancel stability gained by electrons in bonding orbitals.

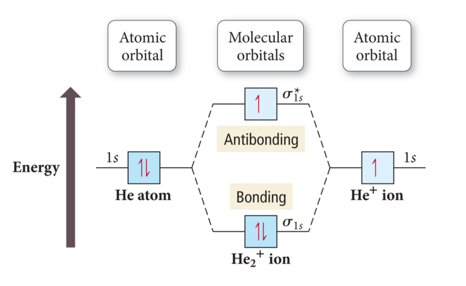
## MO and Properties

* Bond order = ½ (# Bonding Electrons – # Antibonding Electrons)
* Bond order = difference between number of electrons in bonding and antibonding orbitals
  + Only need to consider valence electrons
  + May be a fraction
  + Higher bond order = stronger and shorter bonds
  + If bond order = 0, then the bond is unstable compared to individual atoms and no bond will form.
* A substance will be paramagnetic if its MO diagram has unpaired electrons.
  + If all electrons are paired, it is diamagnetic.
* 
* Bond order = ½ (# Bonding Electrons – # Antibonding Electrons)
* Bond Order H2 = ½ (2 – 0) = 1

## Why Doesn’t the Molecule He2 Exist?

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* Bond order = ½ (# Bonding Electrons – # Antibonding Electrons)
* Bond Order He2 = ½ (2 – 2) =0

## Why Does the Molecule He2+ Exist?

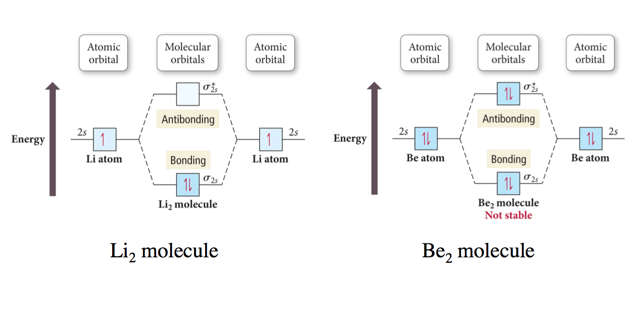
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* Bond order = ½ (# Bonding Electrons – # Antibonding Electrons)
* Bond Order He2+ = ½ (2 – 1) =1/2

## Summarizing LCAO–MO Theory

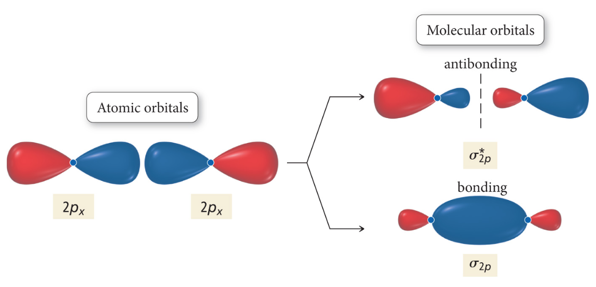
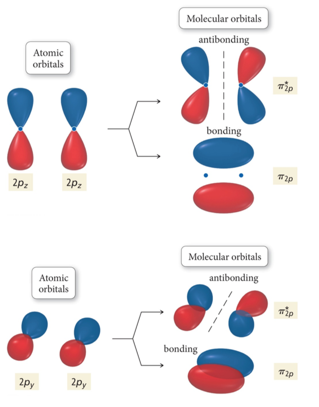
* Molecular orbitals (MOs) are a linear combination of atomic orbitals (AOs).
  + The total number of MOs formed from a particular set of AOs always equals the number of AOs in the set.
* When two AOs combine to form two MOs, one MO is lower in energy (the bonding MO) and the other is higher in energy (the antibonding MO).
* When assigning the electrons of a molecule to MOs, we fill the lowest energy MOs first with a maximum of two spin-paired electrons per orbital.
* When assigning electrons to two MOs of the same energy, Hund’s rule is followed to fill the orbitals singly first, with parallel spins, before pairing.
* The bond order in a diatomic molecule is the number of electrons in bonding MOs minus the number in antibonding MOs divided by two.
  + Stable bonds require a positive bond order (more electrons in bonding MOs than in antibonding MOs).
* MOs are named by type: σ, π, with a subscript to indicate what AOs they were formed from.

## Practice Problem on Bond Order H2-

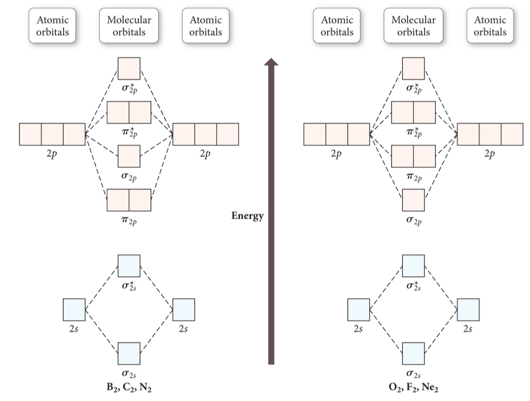
## Period Two Homonuclear Diatomic Molecules

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## Interaction of p Orbitals

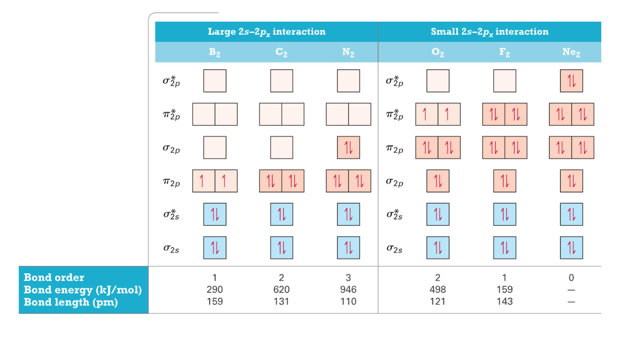
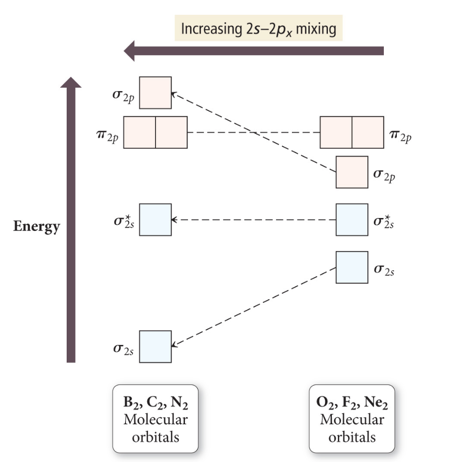
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## Molecular Orbital Energy Ordering

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## Practice Problem on Molecular Orbital Theory N2- ion. Determine the electron configuration, and whether the ion is para or diamagnetic

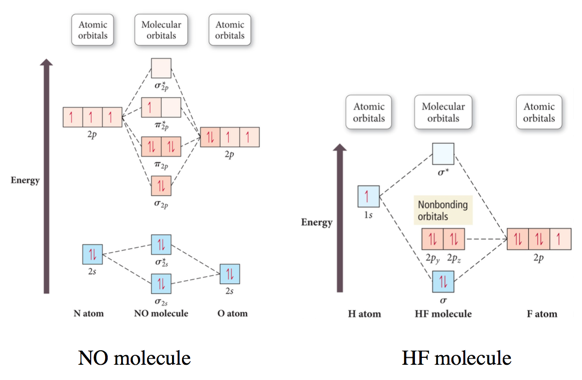
## Molecular Orbital Energy Diagrams for SecondPeriod-p-Block Homonuclear Diatomic Molecules

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## Heteronuclear Diatomic Molecules and Ions

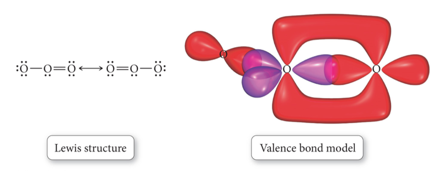
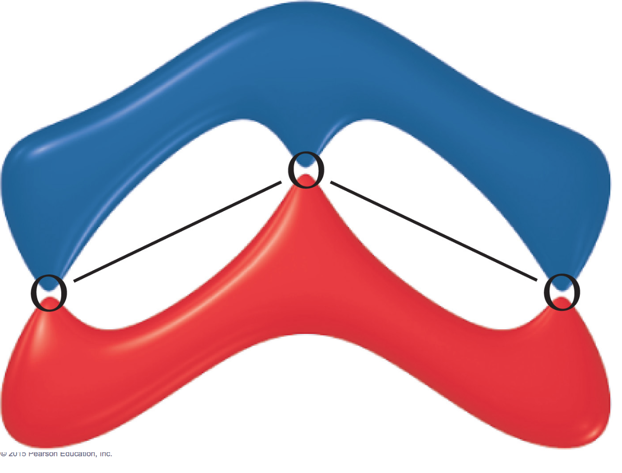
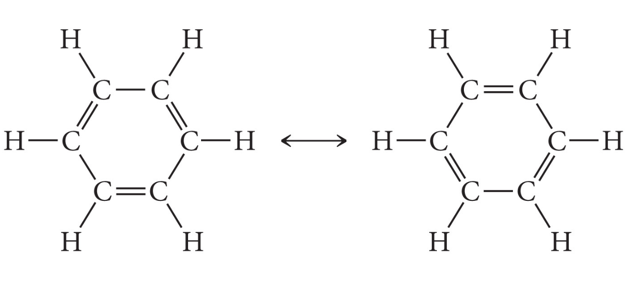
* When the combining atomic orbitals are identical and of equal energy, the contribution of each atomic orbital to the molecular orbital is equal.
* When the combining atomic orbitals are different types and energies, contributions to the MOs are different:
* The more electronegative an atom is, the lower in energy are its orbitals.
* Lower energy atomic orbitals contribute more to the bonding MOs.
* Higher energy atomic orbitals contribute more to the antibonding MOs.
* Nonbonding MOs remain localized on the atom donating its atomic orbitals.

## Second-Period Heteronuclear Diatomic Molecules

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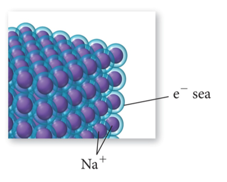
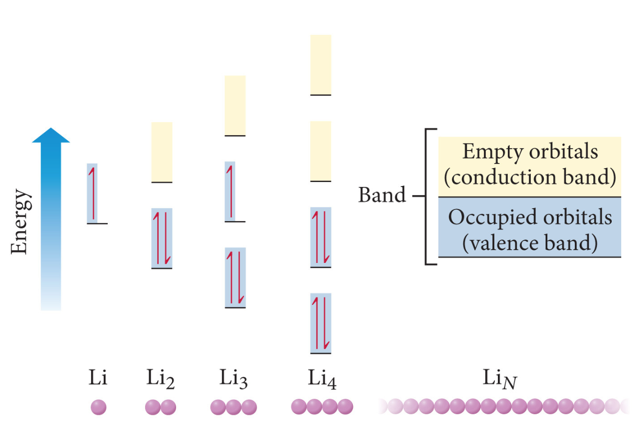
## Practice Problem on Molecular Orbital Theory CN-

## MO and Polyatomic Molecules

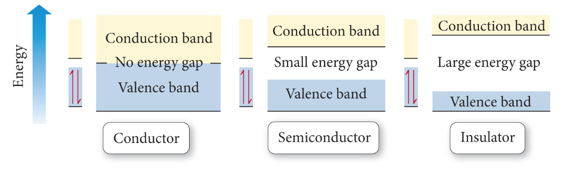
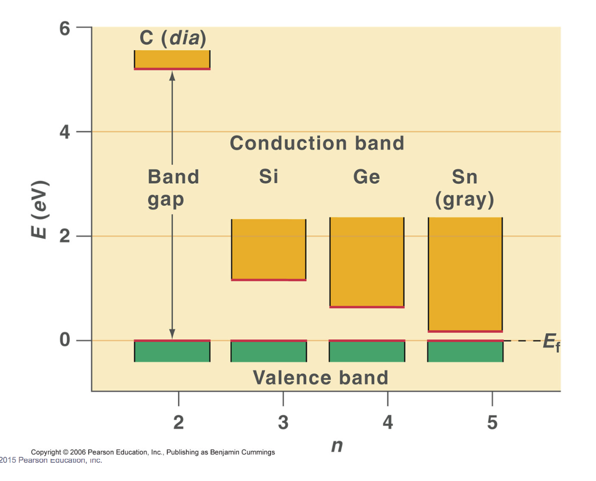
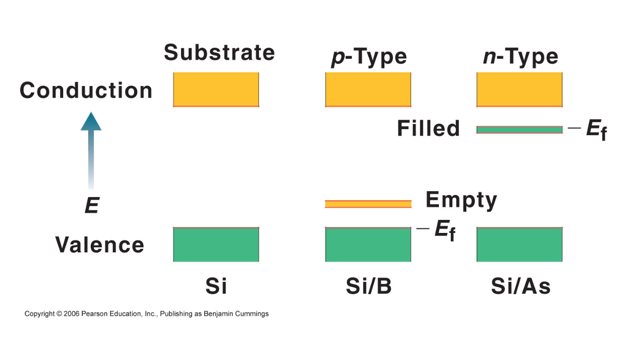
* When many atoms are combined together, the atomic orbitals of all the atoms are combined to make a set of molecular orbitals, which are delocalized over the entire molecule.
* Gives results that better match real molecule properties than either Lewis or valence bond theories
* 
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## Bonding in Metals and Semiconductors

## Bonding in Metals and Semiconductors

* The simplest theory of metallic bonding involves the metal atoms releasing their valence electrons to be shared as a pool by all the atoms/ ions in the metal.
  + An organization of metal cation islands in a sea of electrons
  + Electrons delocalized throughout the metal structure
* Bonding results from attraction of cation for the delocalized electrons.
  + 
* 

## Semiconductors and Band Theory

* Band Theory:
* Electrons become mobile when they make a transition from the highest occupied molecular orbital into higher energy empty molecular orbitals.
* These occupied molecular orbitals are referred to as the valence band.
* The unoccupied orbitals the conduction band.
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# Vocab

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## CH101-008 UA Fall 2016

* CH101-008 UA Fall 2016
* [jmbeach1@crimson.ua.edu](mailto:jmbeach1@crimson.ua.edu)
* jmbeach
* hey\_beach

Notes and study materials for The University of Alabama's Chemistry 101 course offered Fall 2016.