

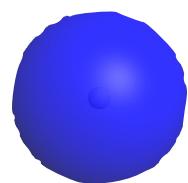
Today

Section 1.6: An Introduction to MO Theory
Sections 1.7-1.15: An Introduction to Valence Bond Theory

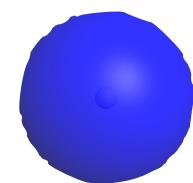
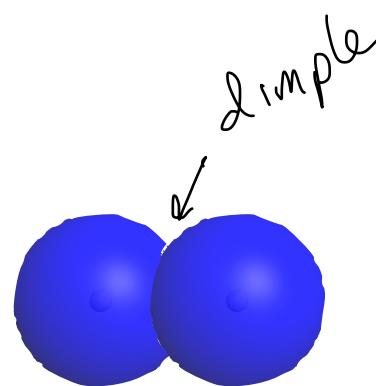
Next Class

Sections 1.7-1.15
An Introduction to Valence Bond Theory

An Introduction to Molecular Orbital Theory



1s



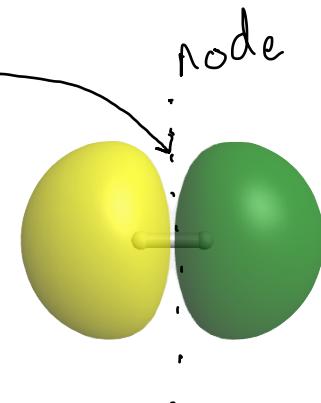
1s

higher E
because e^-
cannot exist
here

subtract

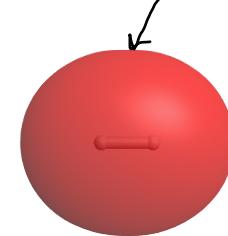
add

destructive
interference



e^- can't
exist
here in
the
node

dimple



lower E because
more volume for e^-
between nuclei

constructive
interference

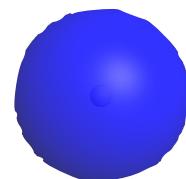
Interpret Molecular Orbitals "dimple... no dimple... dimple... no dimple", Miguel in
Coco

Sections 1.6

MO's for H₂

H

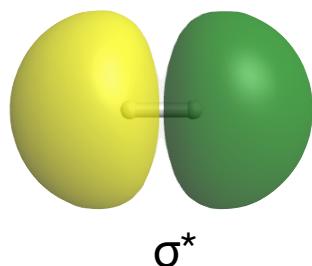
H₂



1s



σ

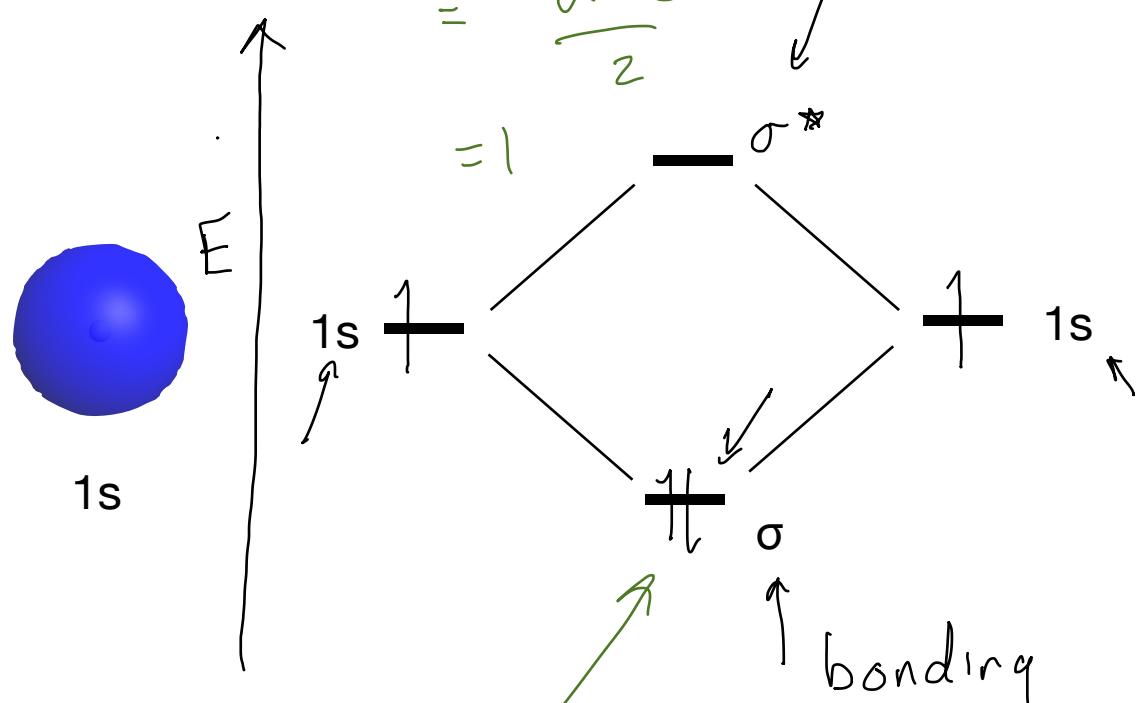


σ*

Molecular Orbital diagram Sections 1.6

H

$$\text{Bond order} = \frac{\# e^- \downarrow \text{in } E - \# e^- \uparrow E}{2}$$



these e^- are lower in E than they used to be on the individual atoms

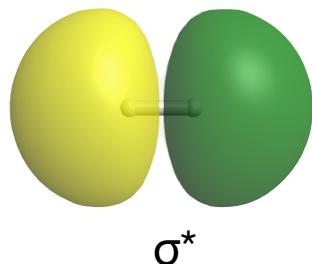
Interpret Molecular Orbitals

MO's for He₂

Sections 1.6

He

He₂ vs He₂⁺



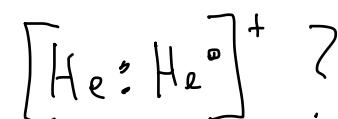
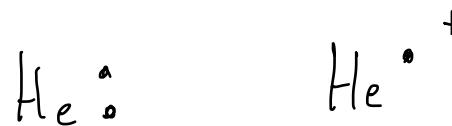
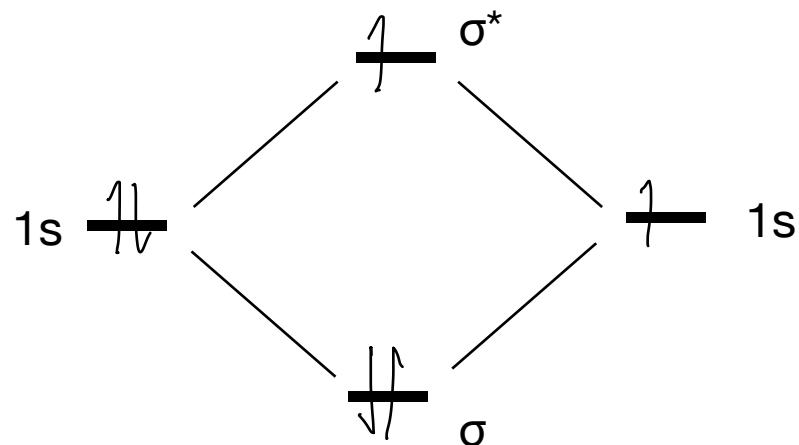
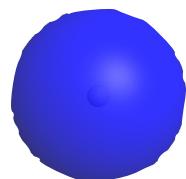
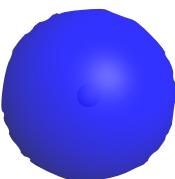
He
or

He²⁺

He₂

$$BO = \frac{2 - 2}{2} = 0$$

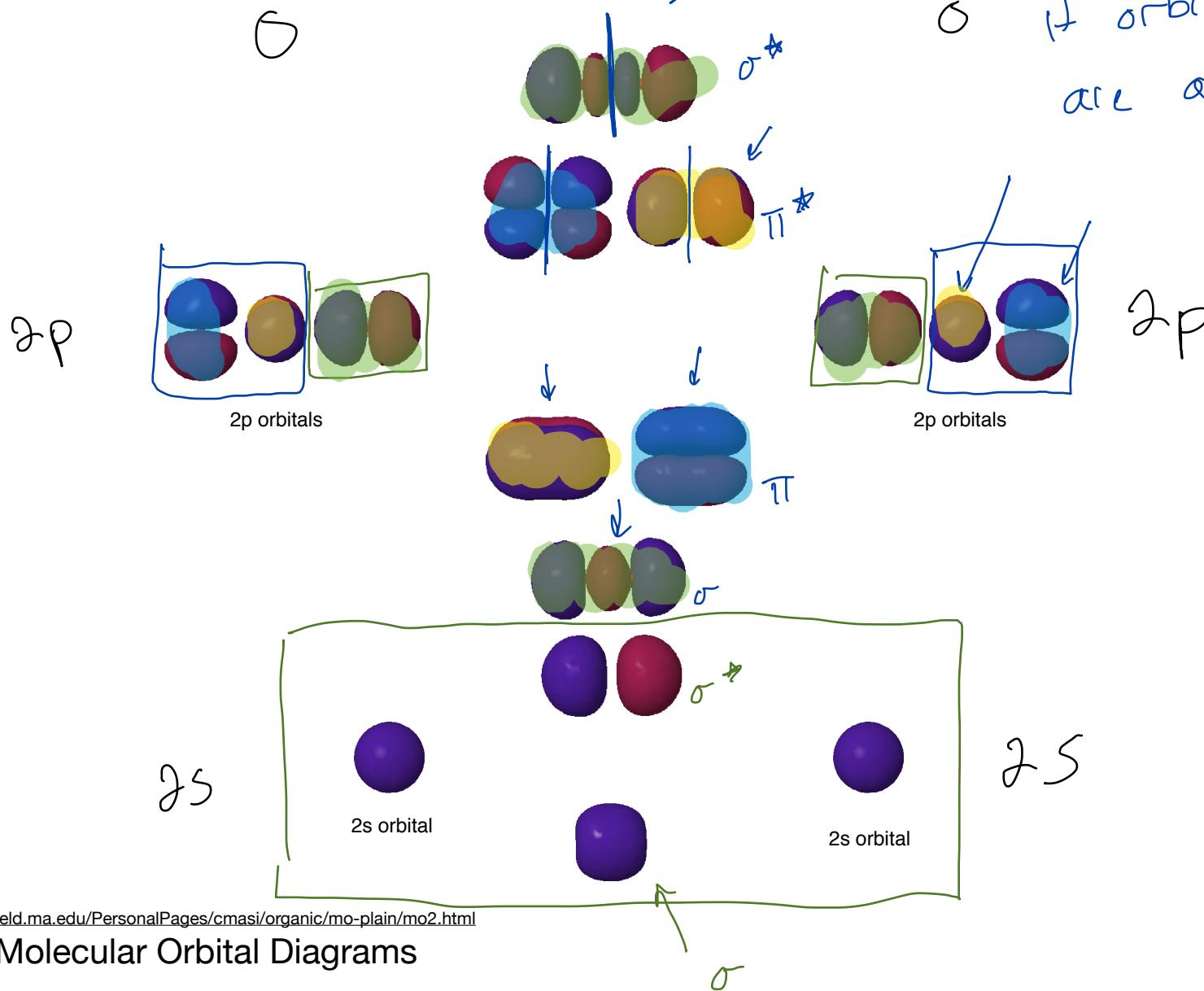
$$He_{2+} = \frac{2 - 1}{2} = 0.5$$



Interpret Molecular Orbitals

An Introduction to Molecular Orbital Theory: O₂

Section 1.6



<https://www.westfield.ma.edu/PersonalPages/cmasi/organic/mo-plain/mo2.html>

Interpret Molecular Orbital Diagrams

An Introduction to Molecular Orbital Theory: O₂

Section 1.6

O ~~NH~~ $2s^2 2p^4$

concentrate on valence e's

not Atomic orbitals 201e e^-_5 MO diagram for n=2 orbitals

MO diagram for
n=2 orbitals

Atomic orbitals

Graphical Representation of MOs



The diagram illustrates the formation of a molecule through the combination of two atoms. On the left, two separate atoms are shown, each with a pair of overlapping purple and red lobes representing p-orbitals. An arrow points from these individual atoms towards the center. In the center, the two sets of p-orbitals overlap significantly, forming a larger, more complex orbital system. This central region contains several large, semi-transparent blue spheres, representing the resulting molecular orbitals. To the right, a yellow vertical shape with the number '11' is positioned above a horizontal line, likely indicating the atomic number of the element involved.

Atomic orbitals $2p$ e^- 's MO diagram for $n=2$ orbitals

Atomic orbitals $2p$ e^- 's

σ^*

σ

π^*

π

unpaired make O_2 paramagnetic

1

1

$2p$ orbitals

1

1

$2p$ orbitals

The diagram illustrates the atomic orbitals of a single atom. It features a central nucleus represented by a small grey sphere. Surrounding the nucleus are three pairs of 2p orbitals, each pair consisting of one purple lobe pointing up and one red lobe pointing down. A blue rectangular box encloses these six 2p orbitals. To the left of the nucleus, a single 2s orbital is shown as a single purple sphere. Another 2s orbital is located at the bottom right.

2p orbitals

2s orbital

$BO = \frac{8 - 4}{2} = 2$

2s orbital

The diagram illustrates a cross-section of a bacterial cell wall. It features two green, rod-shaped structures representing the cytoplasmic membrane. Between them is a yellow oval representing the peptidoglycan layer, which is composed of two orange ovals stacked vertically. A blue arrow points from the label σ to a protein embedded in the peptidoglycan layer. Another blue arrow points from the label Tt to a protein embedded in the outer membrane.

25 

11

2s orbital

2s orbital

25

2s orbital

$$\begin{array}{c} 6 \\ 6 \\ \times 5 \\ \hline 30 \end{array}$$

Interpret Molecular Orbital Diagrams

$$BO = \frac{8 - 4}{2} = 2$$

(2 $2s$ e⁻'s go
down in E
while the other
2 go up

<https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid.html>

Identify atoms that use sp^3 hybrid orbitals to form bonds and hold lone-pair electrons