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

Sections 1.6

higher E because e⁻ cannot exist here

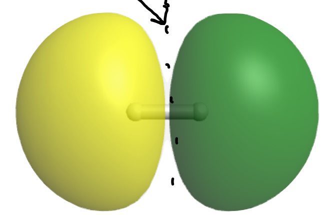
destructive interference

node

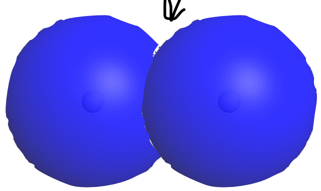
e⁻ can't exist here in the node

1s 1s

subtract

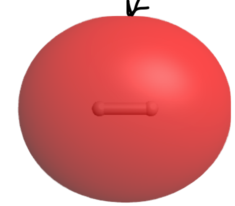


dimple



add

no dimple



Model what happens when H atoms approach each other

lower E because more volume for e⁻ between nuclei

constructive inteference

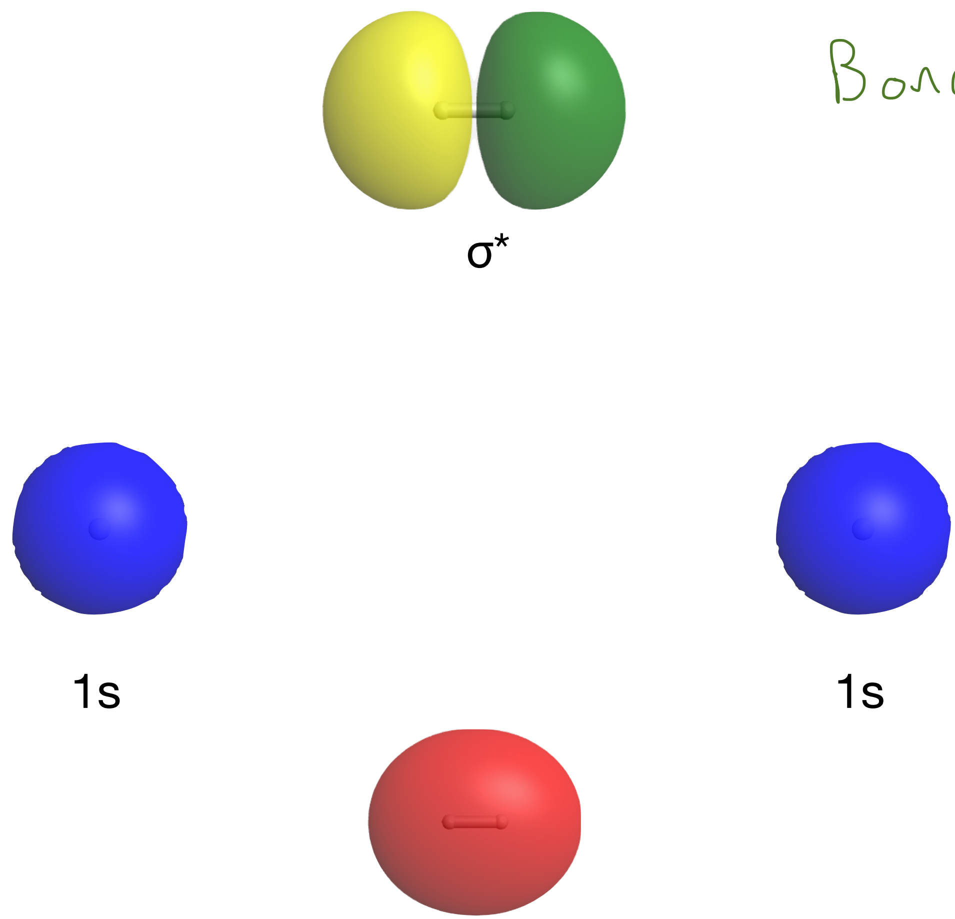
Interpret Molecular Orbitals "dimple... no dimple... dimple... no dimple"; Miguel in Cozo

MO's for H_2

Sections 1.6

Molecular Orbital diagram

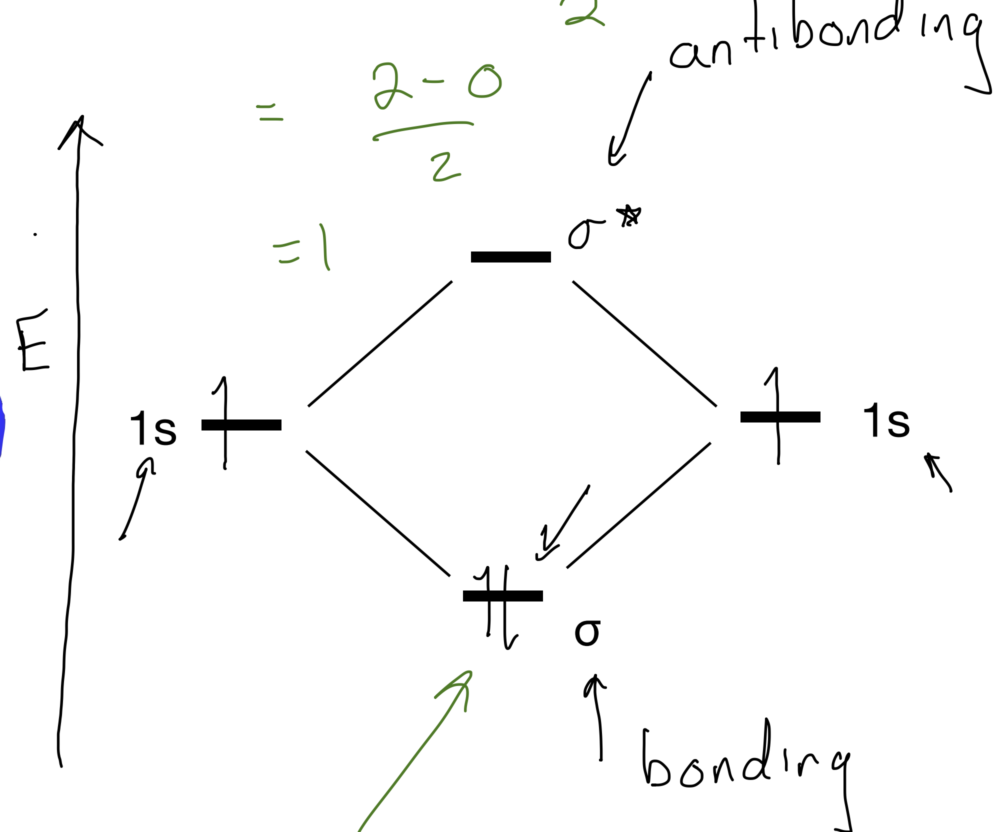
H H_2 H



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

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

$$= 1$$



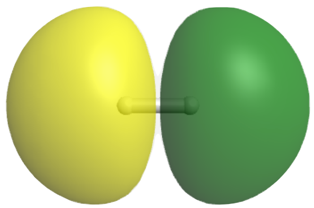
these e^- are lower in E than they used to be on the individual atoms

Interpret Molecular Orbitals

MO's for He_2

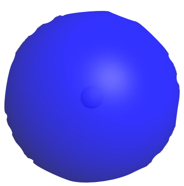
He

He_2 vs He_2^+

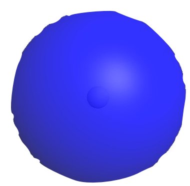


σ*

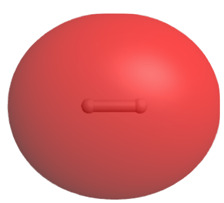
He or He^{2+}



1s



1s

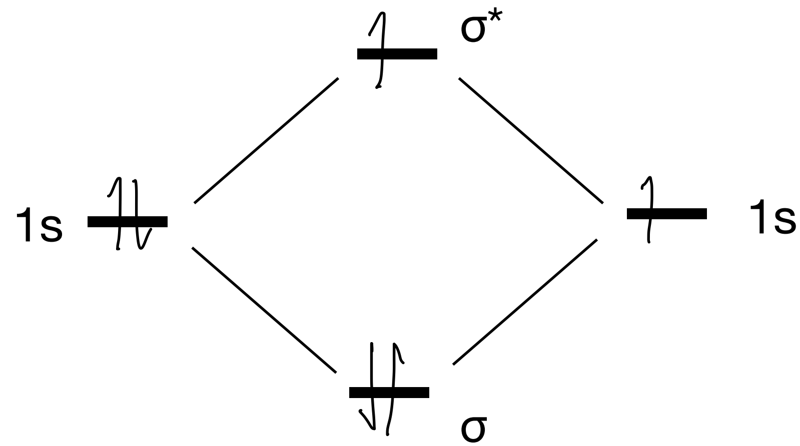


σ

He_2

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

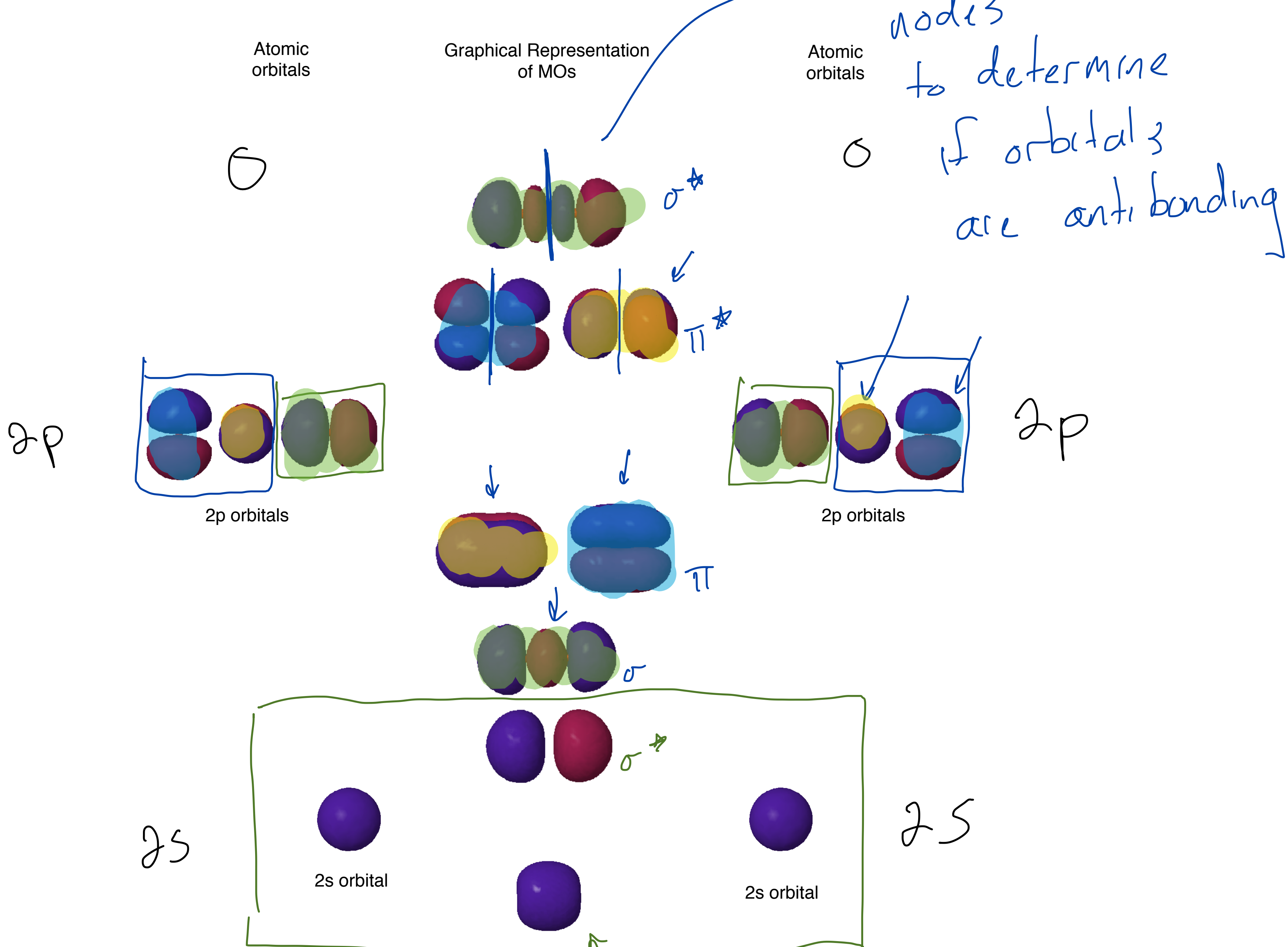
$$He_2^+ = \frac{2-1}{2} = 0.5$$



He: $He^{\cdot\,+}$

$[He:He^{\cdot}]^+$?

Interpret Molecular Orbitals

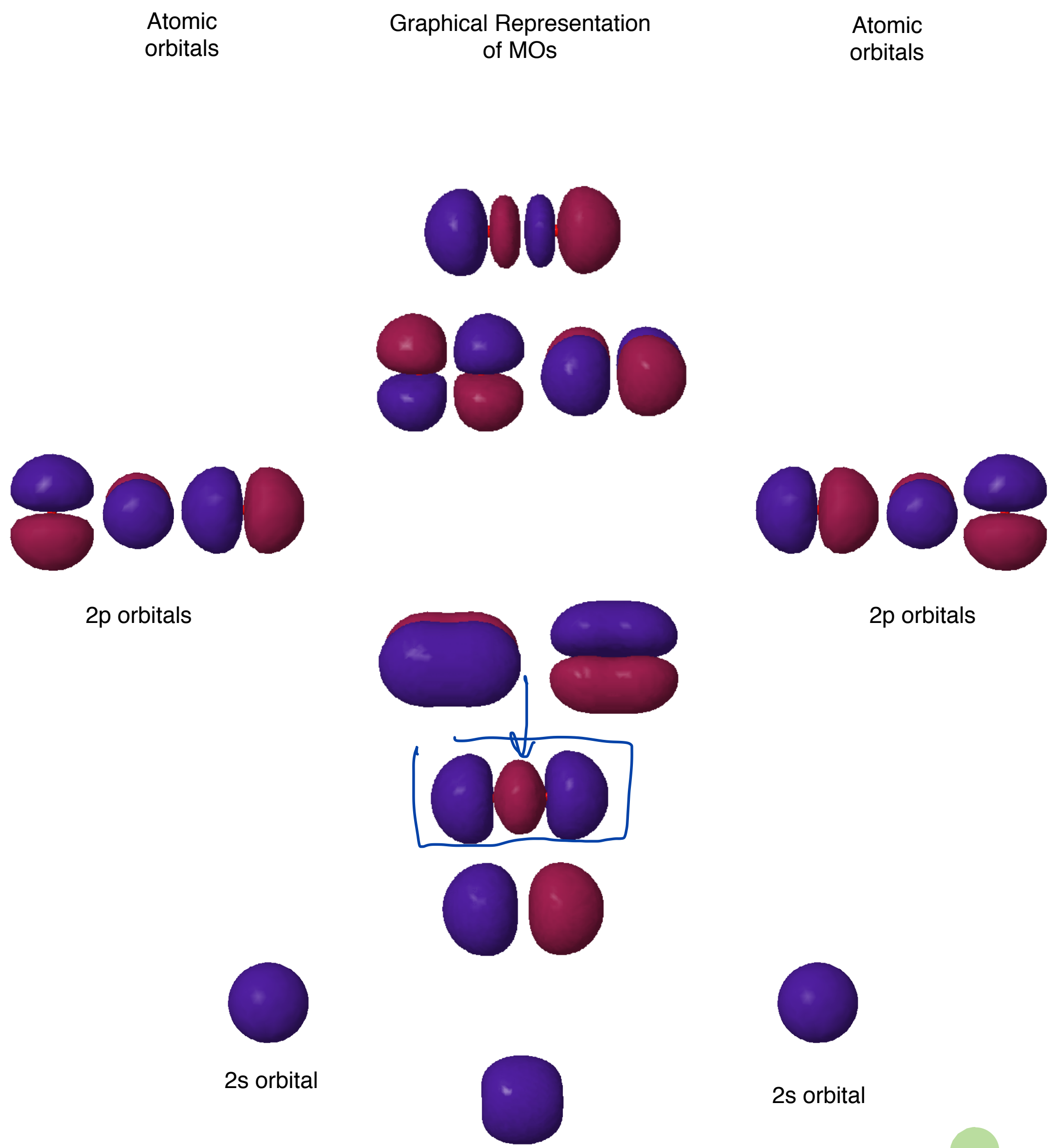


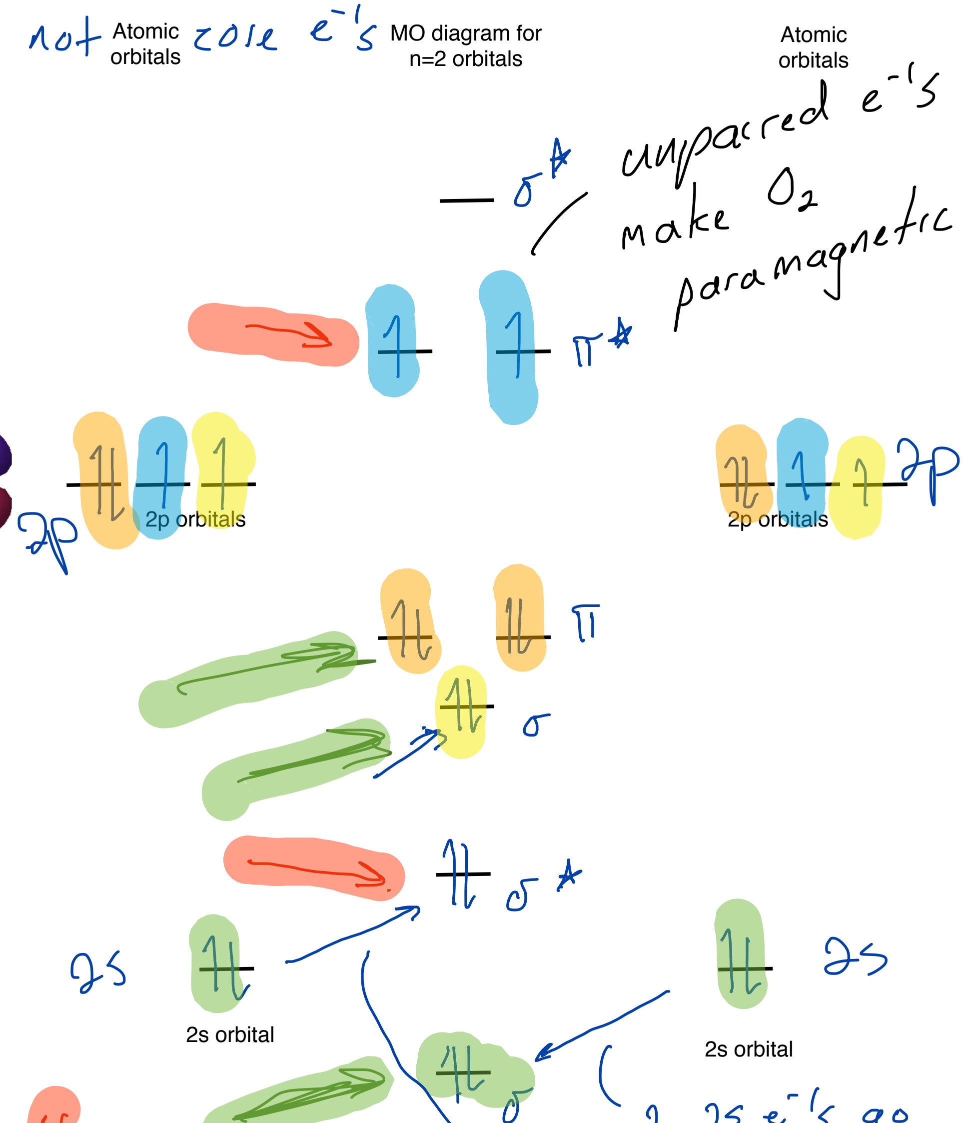
https://www.westfield.ma.edu/PersonalPages/cmasi/organic/mo-plain/mo2.html

Interpret Molecular Orbital Diagrams

O $2s^2 2p^4$

concentrate on valence e^-'s not core e^-'s

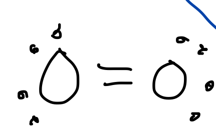




unpaired e^-'s make O_2 paramagnetic

(2 2s e^-'s go down in E while the other 2 go up)

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



Interpret Molecular Orbital Diagrams

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