

## **Today (4)**

Sections 1.11  
An introduction to Molecular Orbital Theory

## **Second Class from Today (6)**

Sections 1.5-1.10  
Valence Bond Theory

## **Next Class (5)**

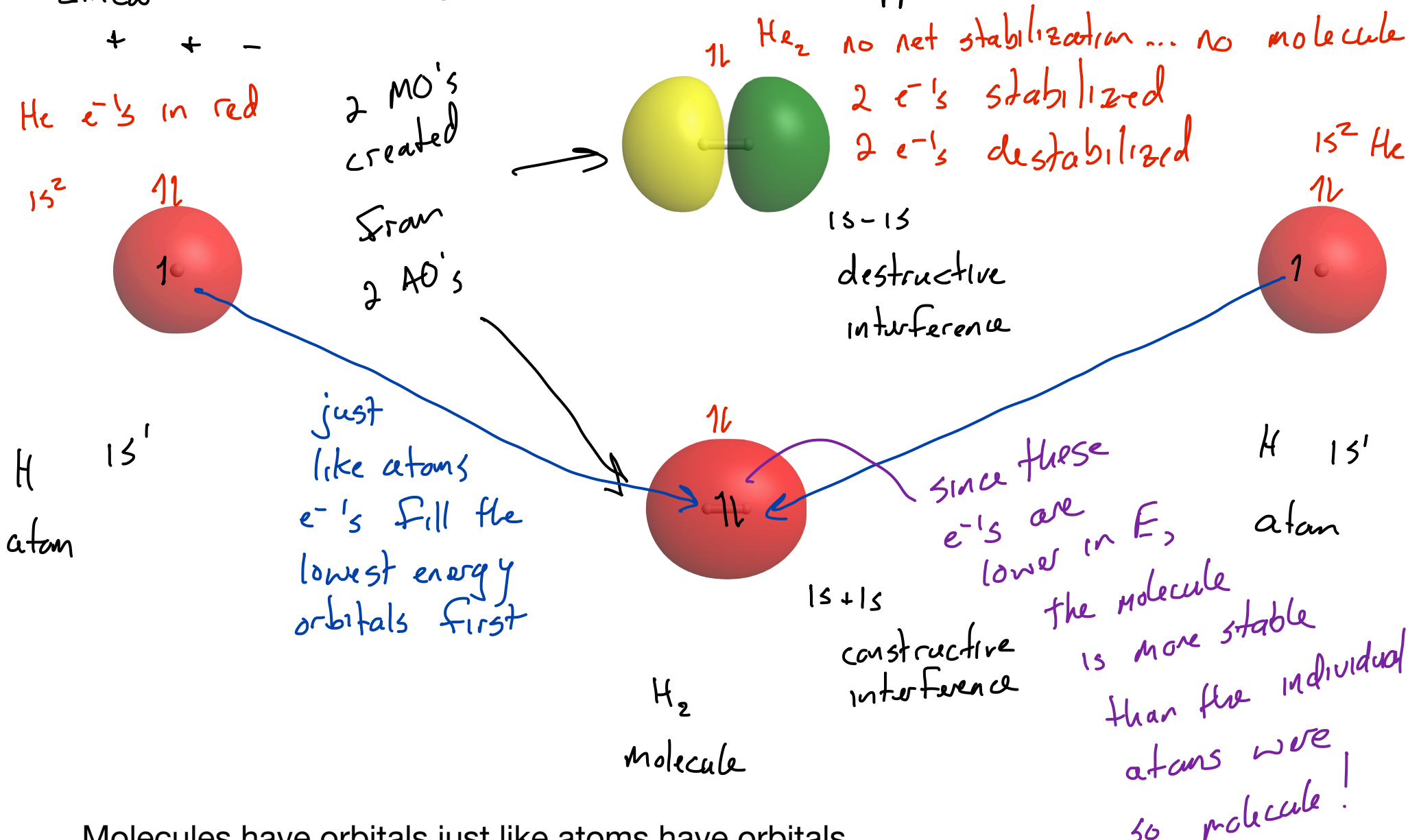
Sections 1.11  
An introduction to Molecular Orbital Theory

Sections 1.5-1.10  
Valence Bond Theory

## **Third Class from Today (7)**

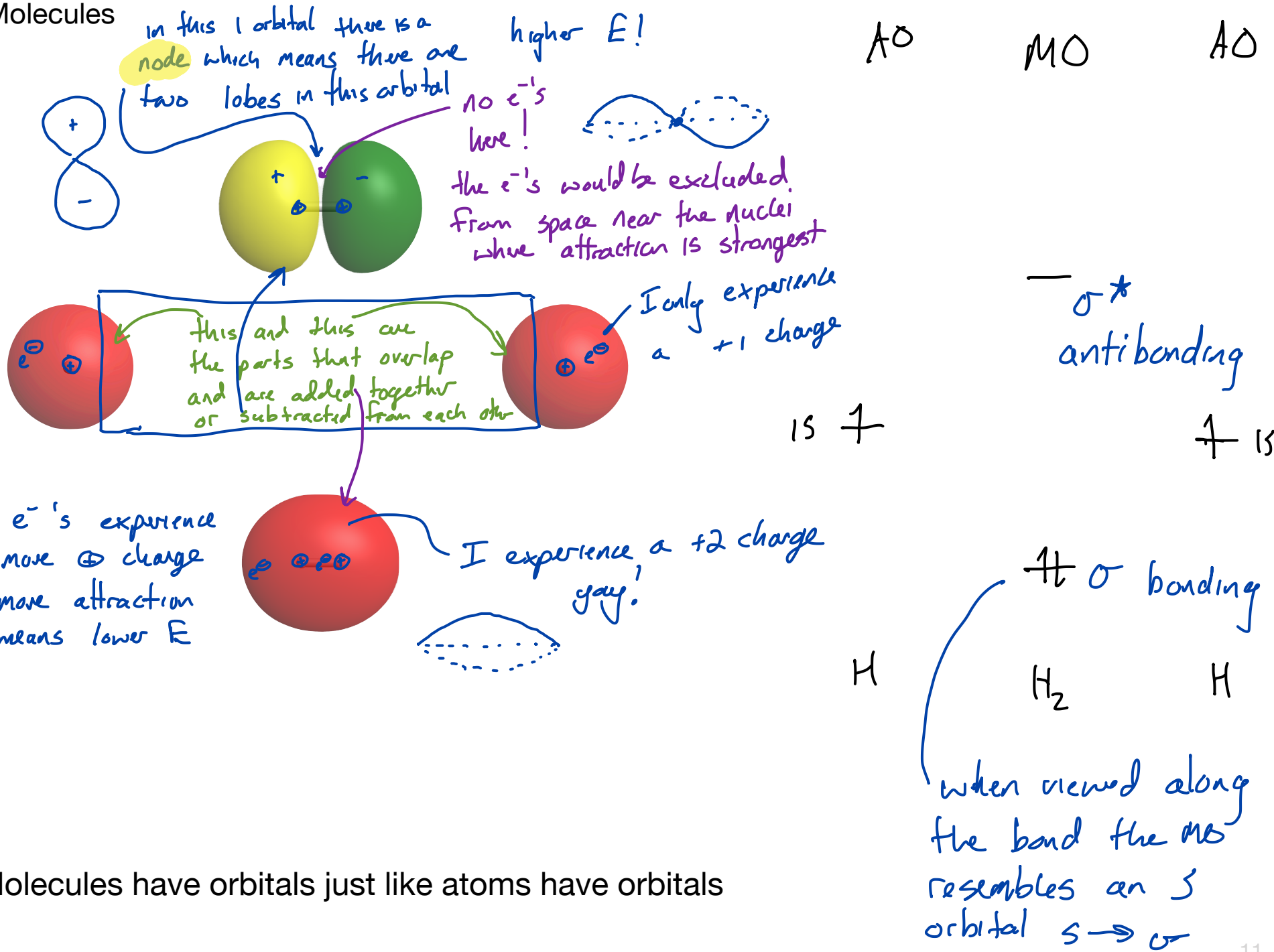
Sections 1.12  
Drawing Chemical Structures

Linear Combinations of Atom Orbitals to approximate molecular orbitals



Molecules have orbitals just like atoms have orbitals

He<sub>2</sub> can be modeled using the same orbital



Molecules have orbitals just like atoms have orbitals

# An Introduction to Molecular Orbital Theory

# Section 1.11

Atomic orbitals

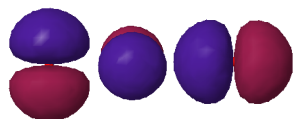
Graphical Representation of MOs

Atomic orbitals

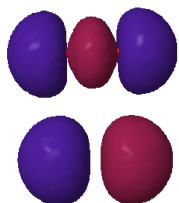
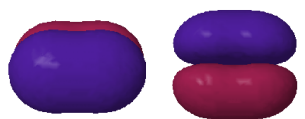
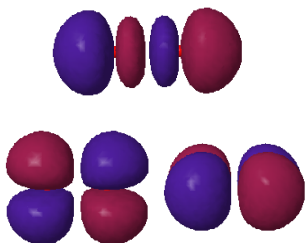
Atomic Orbitals

Molecular Orbitals

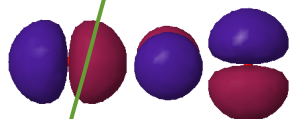
Atomic Orbitals



2p orbitals



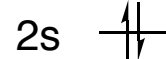
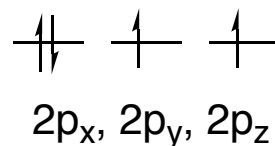
2s orbital



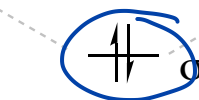
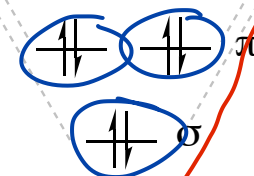
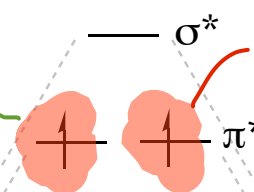
2p orbitals



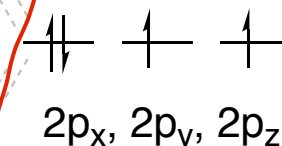
2s orbital



O



O<sub>2</sub>

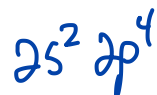


O

MO Theory predicts unpaired e<sup>-</sup>'s which is correct

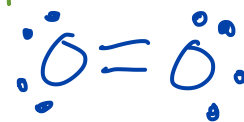
antibonding

making the atoms form



both models predict that 4 e<sup>-</sup>'s are involved in making the atoms form a molecule... MO Theory net stabilization of 4 e<sup>-</sup>'s

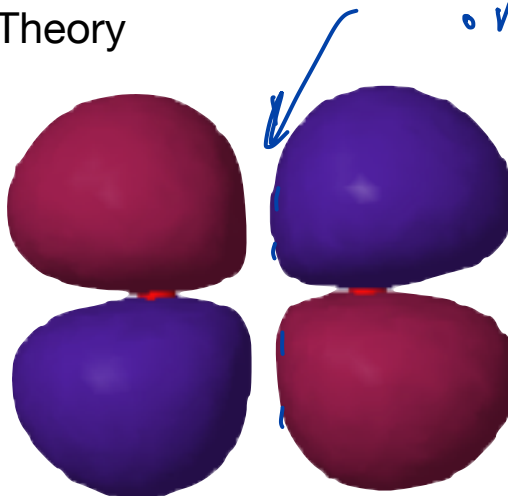
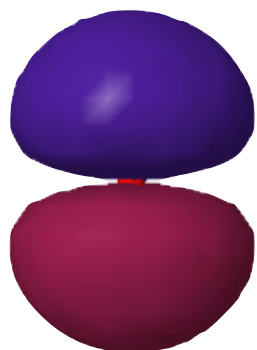
Lewis structure predicts paired e<sup>-</sup>'s which is not correct



<https://www.westfield.ma.edu/cmasi/organic/mo-plain/mo1.html>

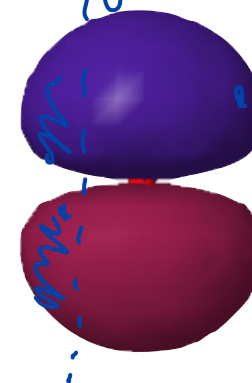
Lewis Theory 4 e<sup>-</sup>'s shared in 2 bonds

$\pi^*$  a.k.a.  
 $\pi$  antibonding orbital

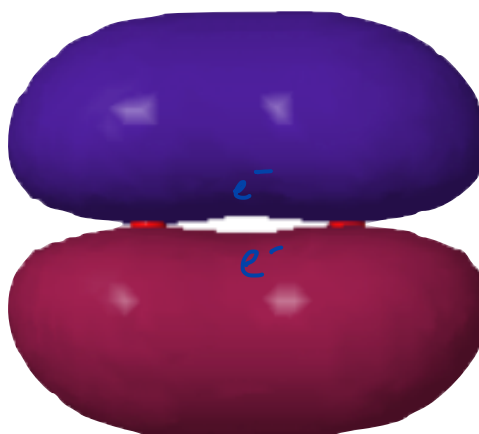


• more nodes

• prime real estate close to the  $\oplus$  of the nucleus is lost  
 •  $e^-$ 's in this orbital would be higher in  $E$



$\pi$  bonding orbital



no increase in the # of nodes

$e^-$  can exist almost directly between nuclei...

lower in  $E$