This Class

5.1 Formation of Molecular Orbitals

5.2 Homonuclear Diatomic Molecules

Next Class

5.3 Heteronuclear Diatomic Molecules

Introduce MOs s, p, d orbital interactions)

Orbital Mixing in Diatomic Molecules

Heteronuclear Diatomic Molecules

Polyatomic molecules

 are to molecules as orbitals are to atoms

Schrödinger Equation

$H\Psi = E\Psi$ but $H^+ \; e^-$ $He \; e^- \; e^-$

$H^+ \; e^- \; e^- \; H^+$

LCAO

(start with hydrogen-like atomic orbitals

linear combinations of atomic orbitals will be used to create MO's (add + subtract)

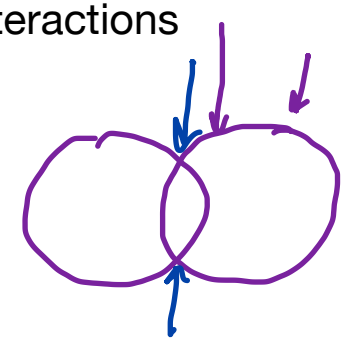
Symmetry must be such that regions with the same sign or opposite sign overlap but not regions of both signs

The energies of the orbitals must be similar

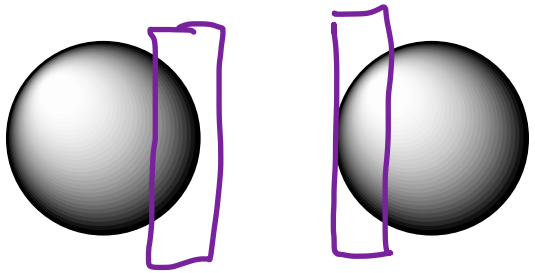
When the energies are significantly different, the overlap is ineffective in substantially lowering the energy of the electrons

→ The distance between the atoms must be short enough to allow for good overlap

s orbital interactions



L - R

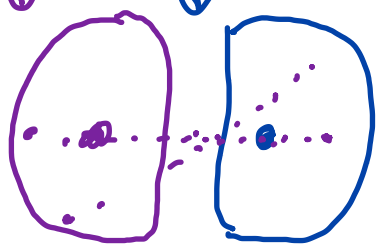


+ - 0

0 - +

higher E because node

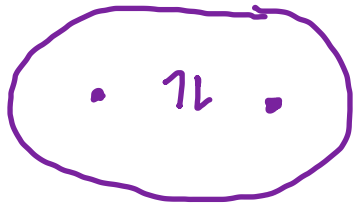
subtraction



σ_u^*

orbitals destructively interfere and cancel out. A new node has formed.

add



σ_g

constructive interference creates an orbital that e^-'s can be placed between nuclei

star means anti bonding

this is the normalization factor so $\int_0^\infty [\Psi(\sigma)]^2 = 1$

$$\Psi(\sigma^*) = N[c_a\psi(1s_a) - c_b\psi(1s_b)]$$

$$\Psi(\sigma) = N[c_a\psi(1s_a) + c_b\psi(1s_b)]$$

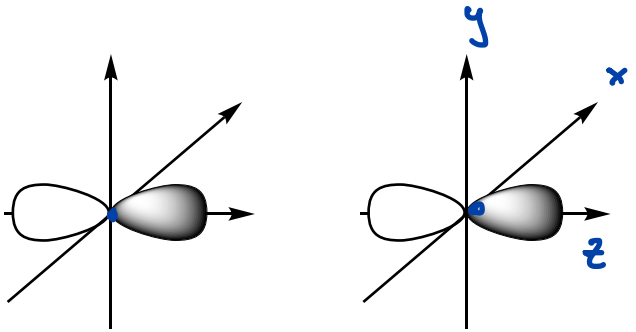
a molecular orbital

H_2

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

σ is cylindrically symmetrical

the p_z orbitals are colinear



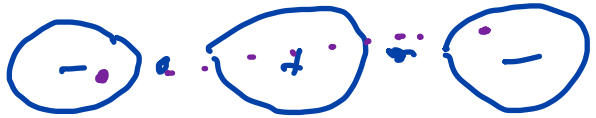
destructive

constructive

high E

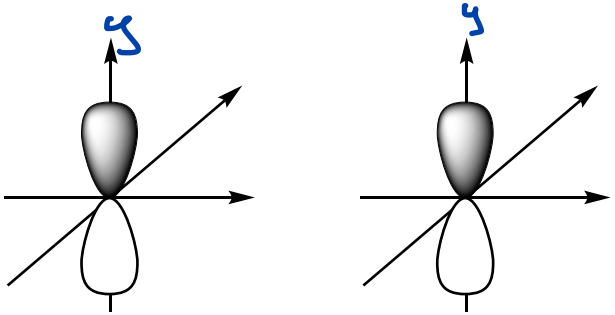
σ_u^*

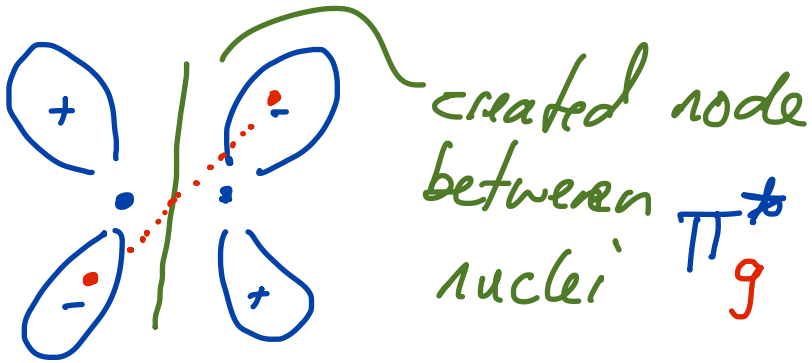
node formed between nuclei



σ_g

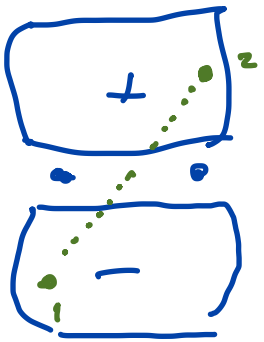
the p_x + p_y orbitals are parallel





created node between nuclei

π_g^*



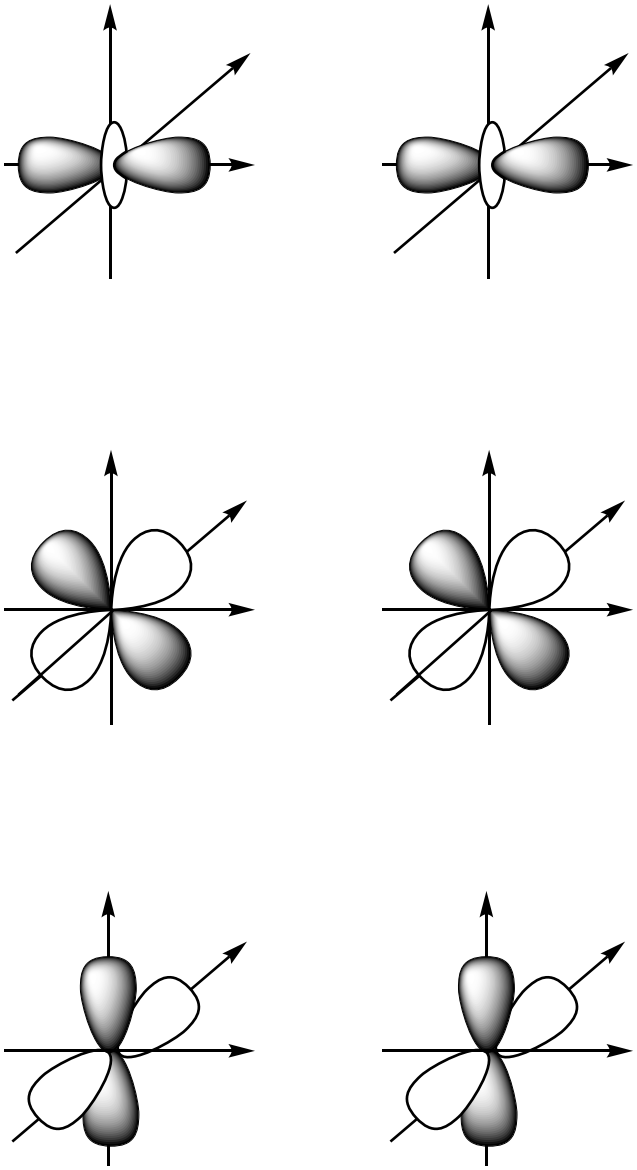
π_u

gerade g even

ungerade u odd

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

do an i sign changes u sign doesn't change g



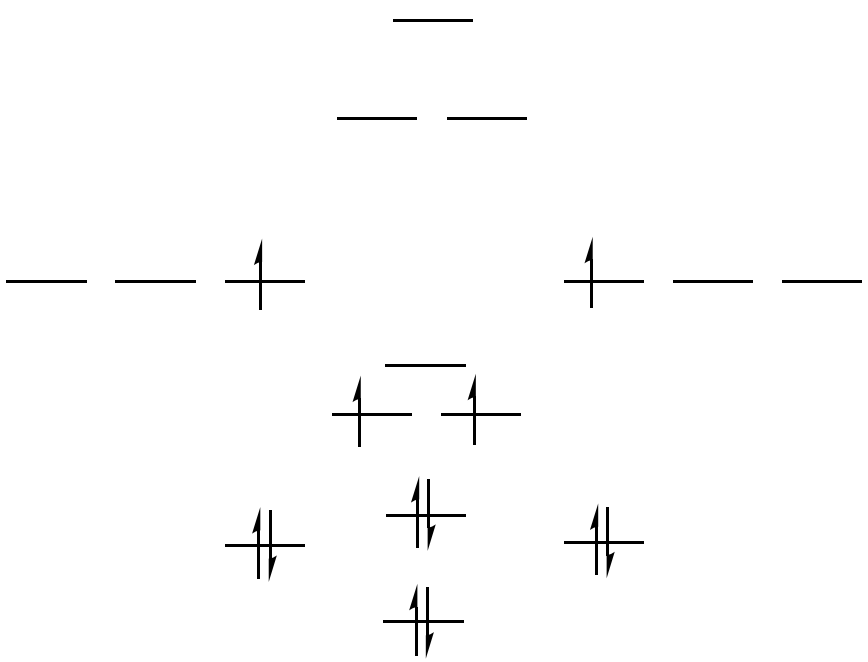
https://www.westfield.ma.edu/cmasi/advinorg/dorbs/dorbsp.html

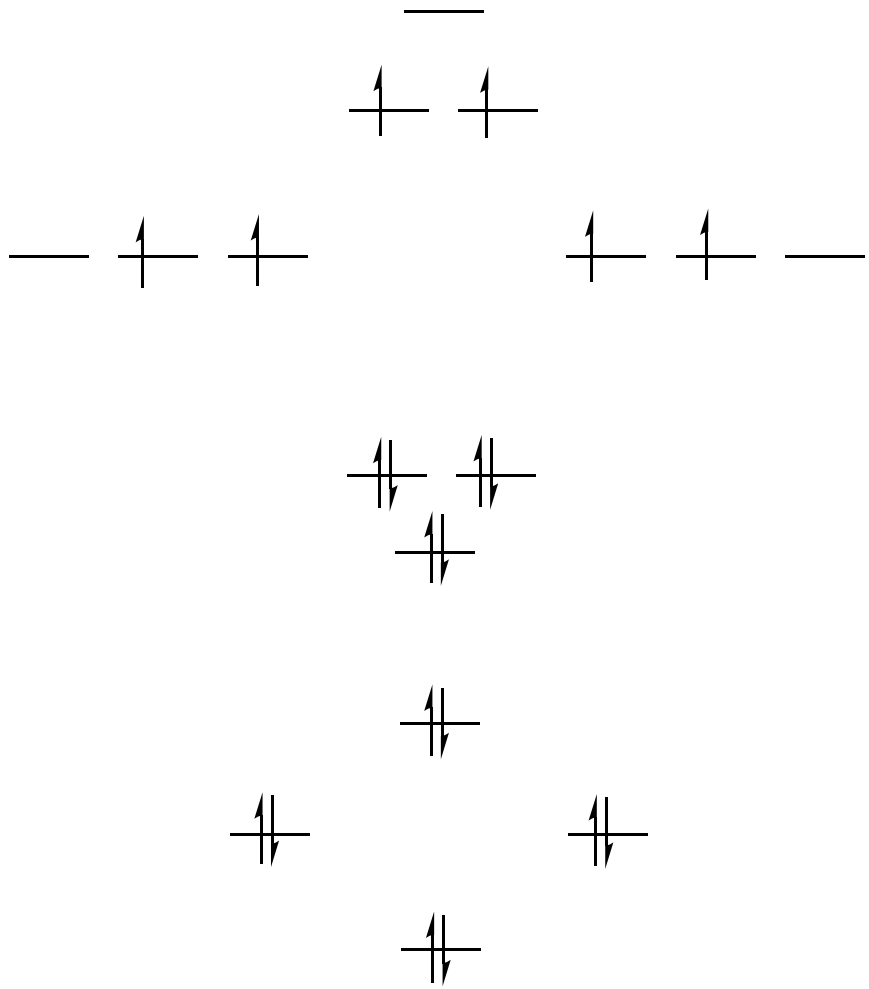
Bonding

Anitbonding

Nonbonding

F_2





$$\Psi(\sigma_g(s)) = N[c_a\psi(2s_a) + c_b\psi(2s_b)]$$

$$\Psi(\sigma_g(s)) = N[c_a\psi(2s_a) + c_b\psi(2s_b) + c_c\psi(2p_a) + c_d\psi(2p_b)]$$