This Class

5.2 Homonuclear Diatomic Molecules

5.3 Heteronuclear Diatomic Molecules

Next Class

5.3 Heteronuclear Diatomic Molecules

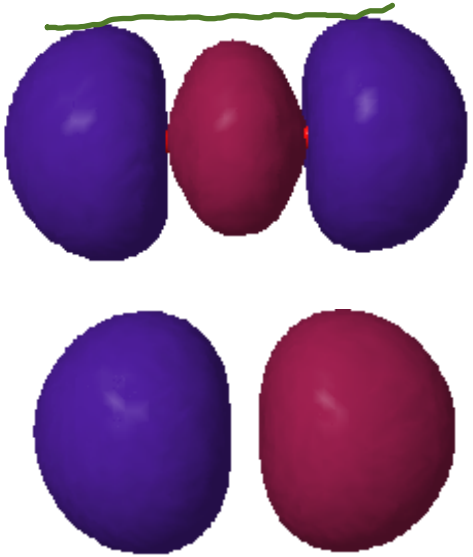
5.4 Polyatomic Molecules

Orbital Mixing in Diatomic Molecules

Heteronuclear Diatomic Molecules

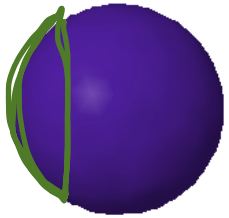
Polyatomic molecules

why are these lobes bigger?

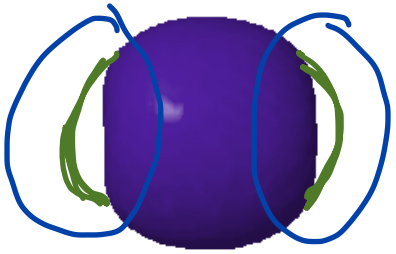


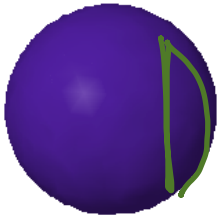
σ_g made from

$2p_z - 2p_z$



2s orbital



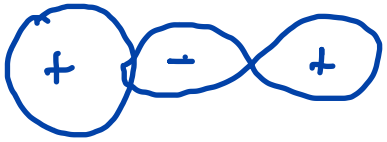


2s orbital

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

it's not this simple

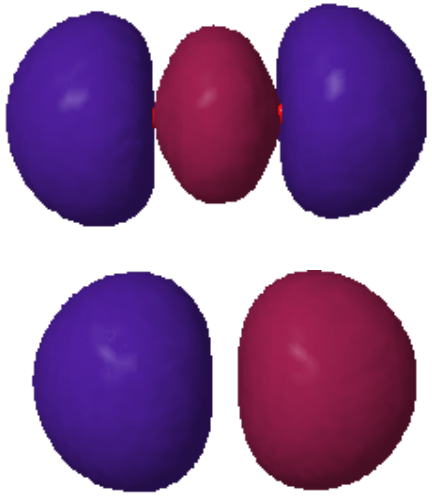
s 2pz

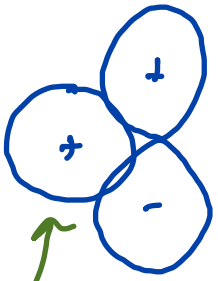


yes

+ lobe of s interacts with 1 lobe of the 2pz

2s orbital





no + of 1 orbital interacts with

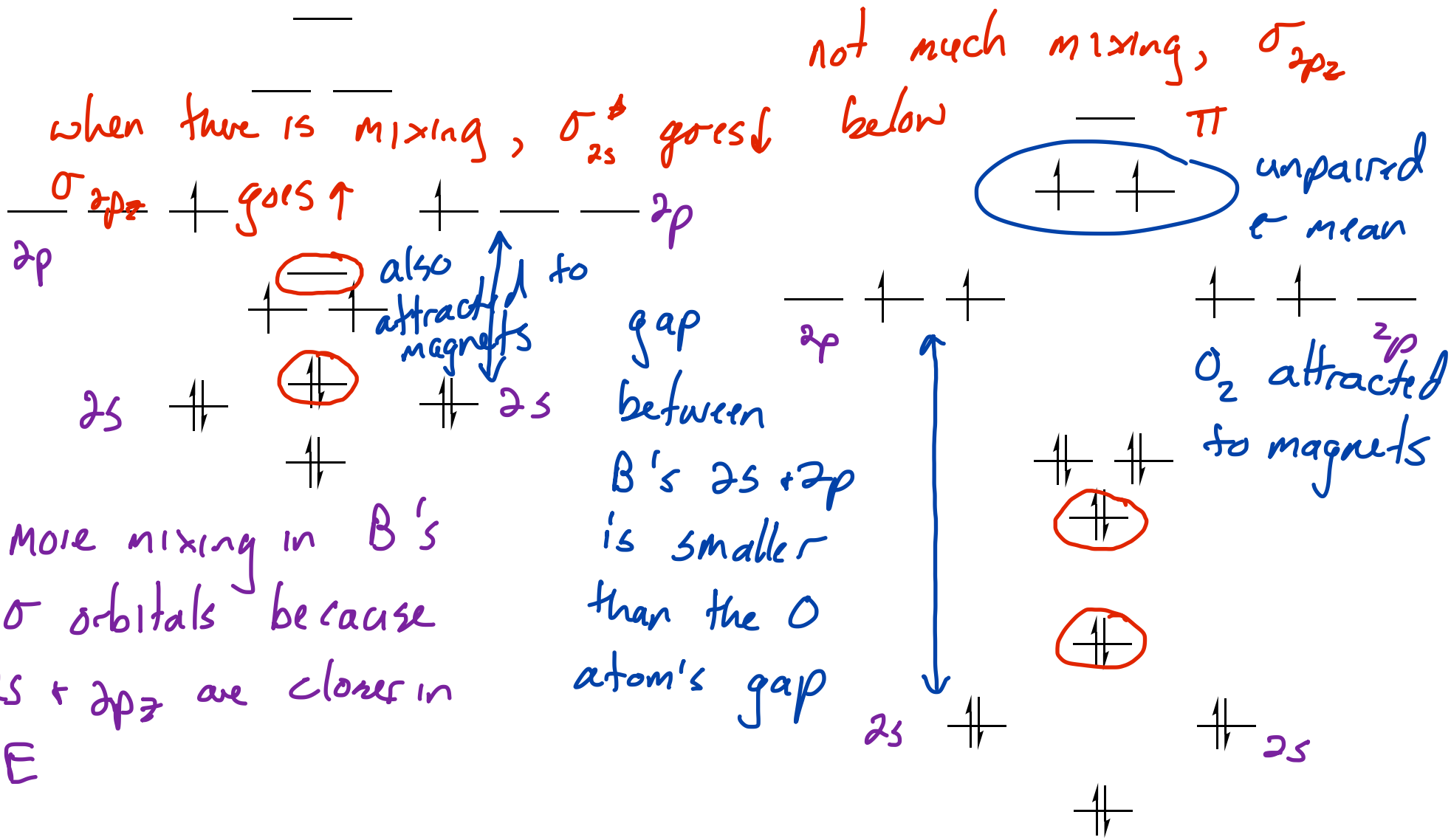
2s orbital

+ + − of the other

σ orbitals s + 2pz orbitals have to be used

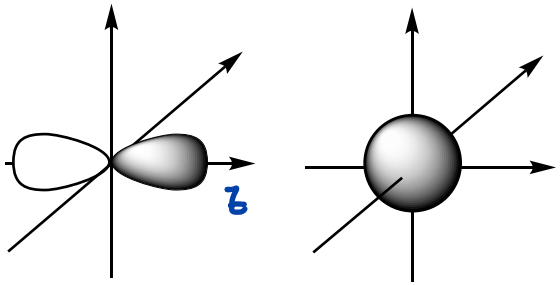
$$\Psi(\sigma_g(s)) = N[c_a\psi(2s_a) + c_b\psi(2s_b) + c_c\psi(2p_a) + c_d\psi(2p_b)]$$ – mixing

Li ..... B_2 ..... N_2 O_2



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

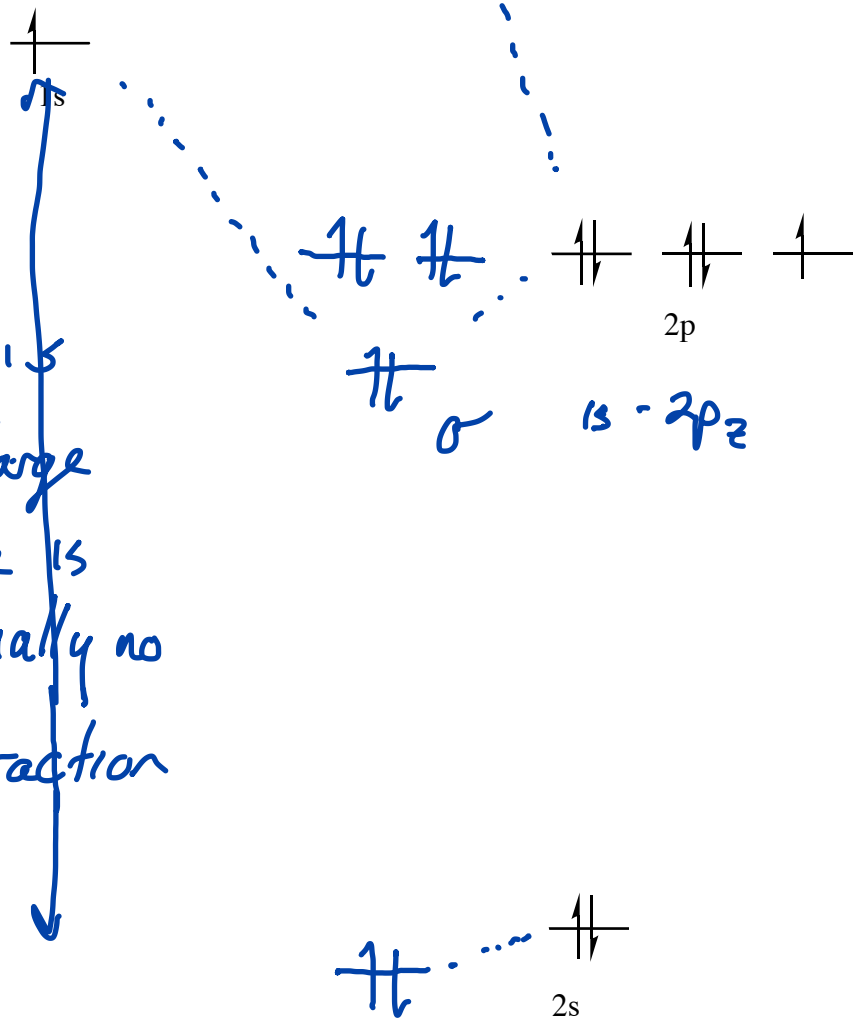
both 2s + 2pz go into determining E of σ MO's
AO's that are closer in E to each other interact more strongly



no p on H

H's 1s + F's 2s are too far apart in E to interact strongly.

F's $2p_z$ has appropriate sym to interact with H's 1s



this gap is so large there is virtually no interaction

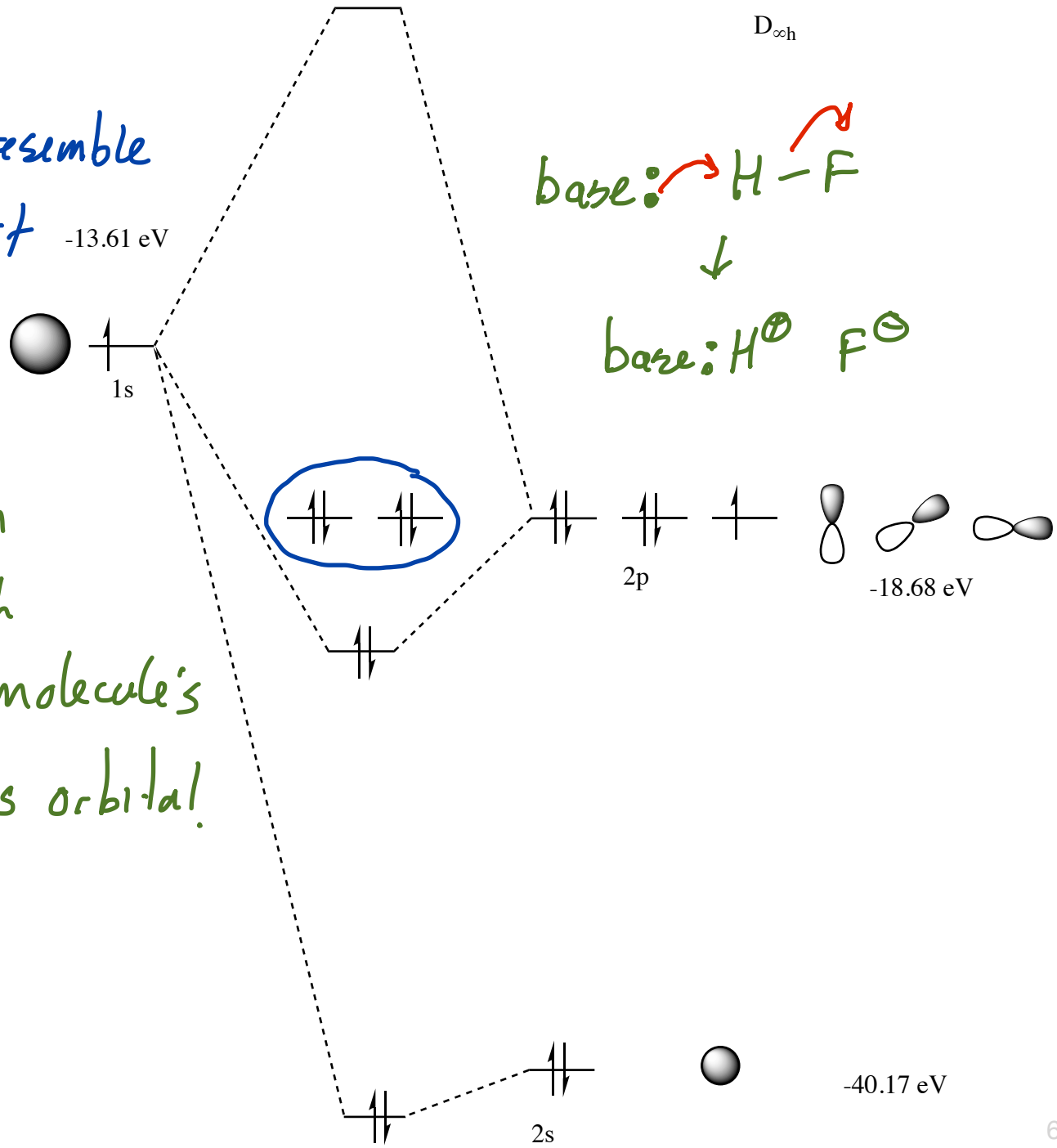
Interpreting the MO diagram

HOMO's are F based
MO's most strongly resemble AO's they are closest to in E.

LUMO is based on the H atom. When reacting with e⁻ rich molecules, the other molecule's e⁻'s will go into this orbital!

LUMO is more like...

base: → H – F
↓
base: H⊕ F⊖

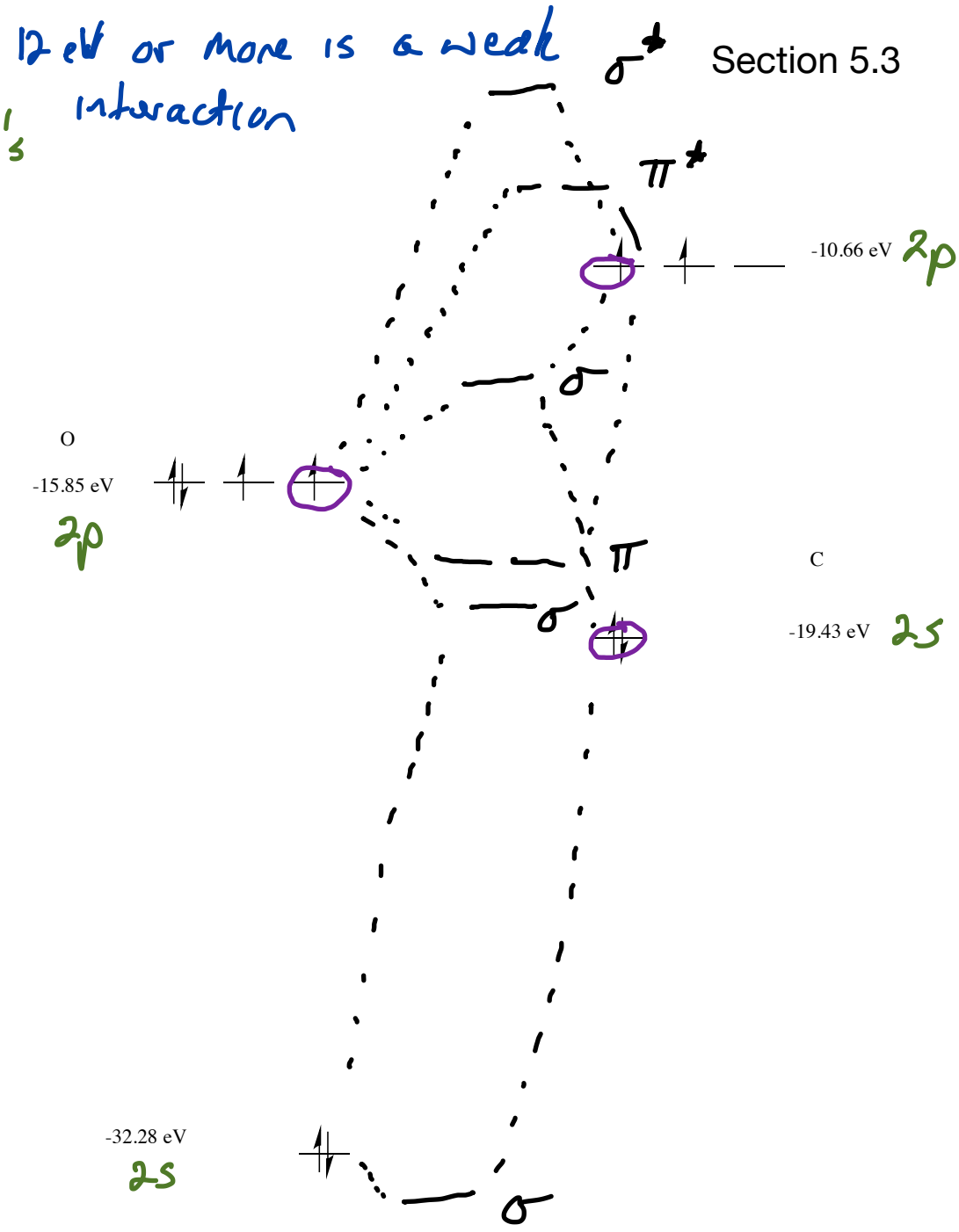


12 eV or more is a weak interaction

Interaction between O's 2s + C's 2s? strong or weak

O's $2p_z$ + C's 2s are much closer in E and will more strongly interact

O $2p_z$ + C $2p_z$ are close too, so they will interact



Interpreting the MO diagram