(19) **Today**

5.2 Homonuclear Diatomic Molecules

5.3 Heteronuclear Diatomic Molecules

Next Class (20)

5.3 Heteronuclear Diatomic Molecules

5.4 Polyatomic Molecules

(21) **Second Class from Today**

5.4 Polyatomic Molecules

Chap 6 Acids and Bases

Third Class from Today (22)

Chap 6 Acids and Bases

Office hours today are canceled

~~Introduce MOs (s, p, d orbital interactions)~~

Diatomic Molecules and Orbital Mixing

Heteronuclear Diatomic Molecules

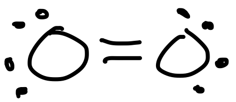
Polyatomic molecules

O_2

O Atom's orbitals

Graphical Representation of O2's MOs

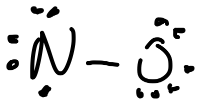
O Atom's orbitals



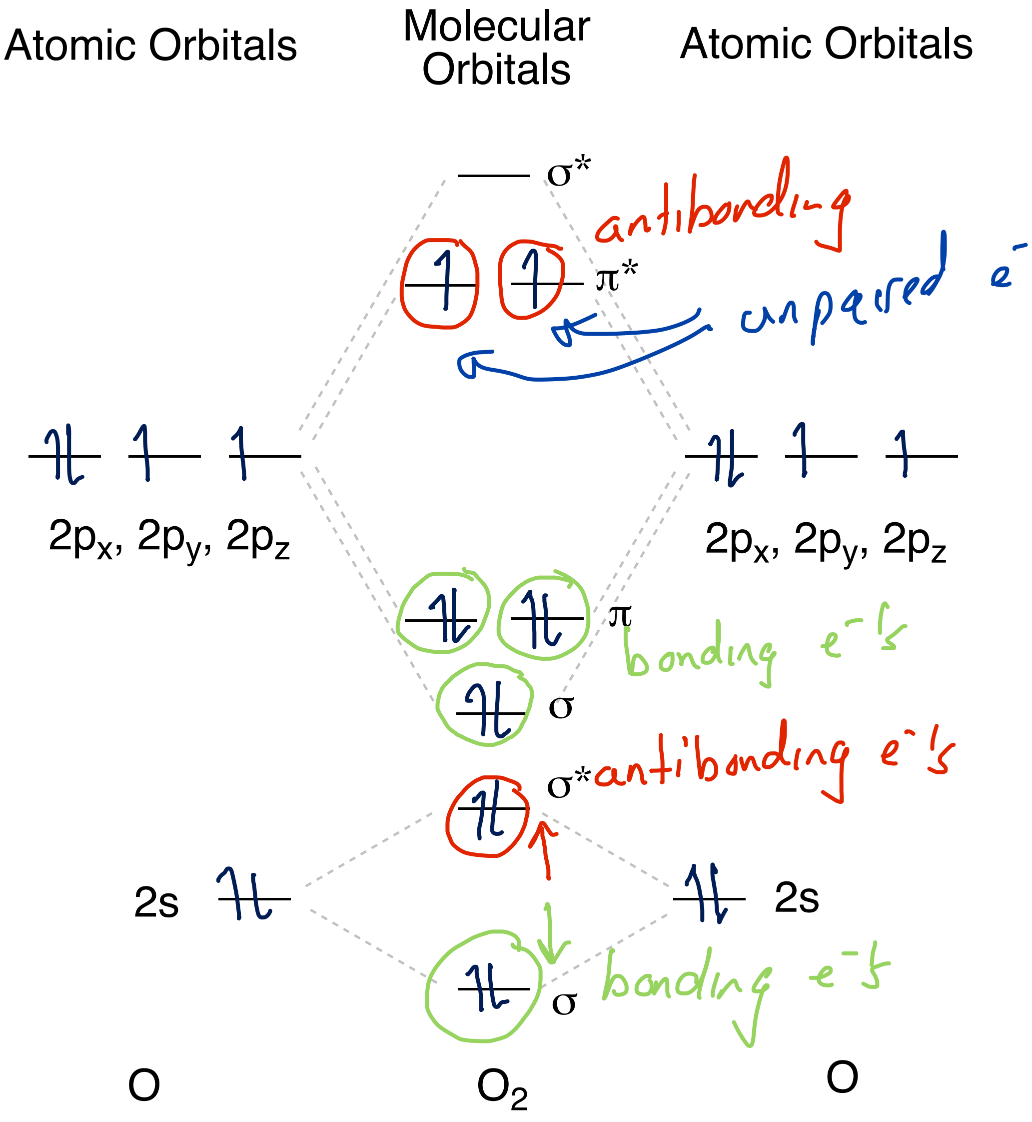
Lewis structures predict that O_2 will have 2 bonds + paired e^-'s

oxygen molecules are attracted to magnetic fields which wouldn't be true if the prediction made by the Lewis structures was

NO? odd # of e^-



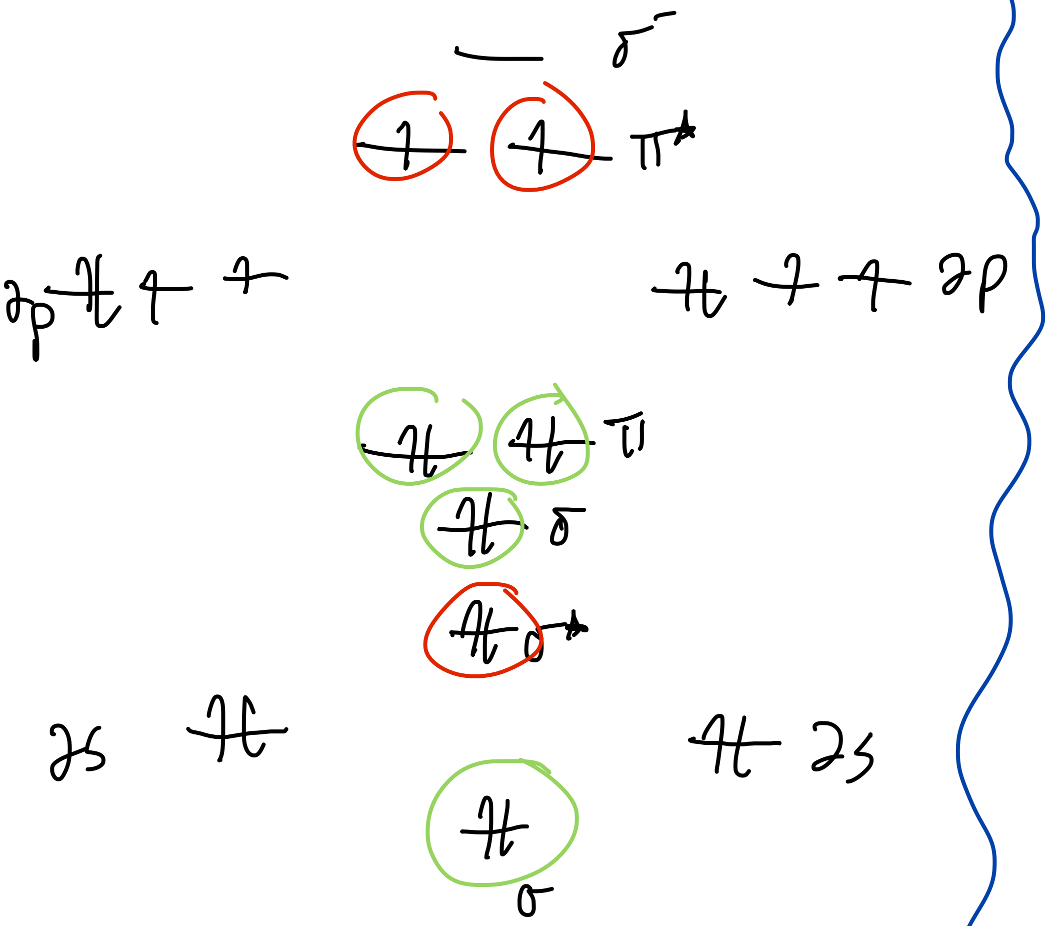
Molecular Orbital Diagram



Bond Order for Diatomic molecules – estimate of the strength of the bond

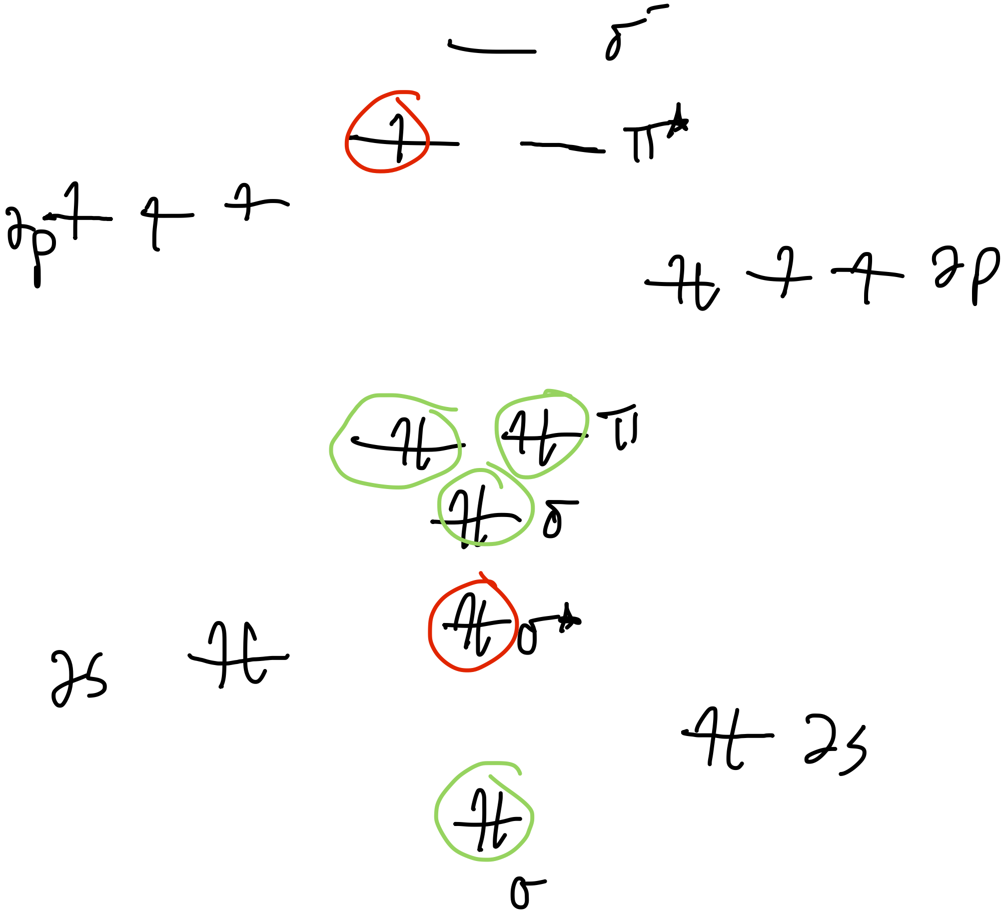
O_2

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



NO

$$BO = \frac{8-3}{2} = 2.5$$

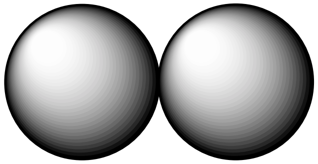


$NO \rightarrow NO^+ + 1e^-$ BO ↑ to 3

Molecular Orbitals (mixing)

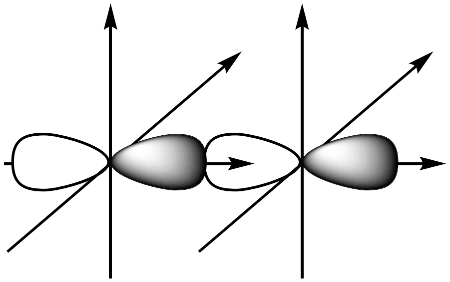
appropriate symmetry, close in E, close in space

Section 5.1

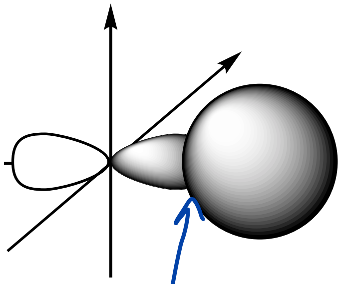


s orbitals interact with s orbitals

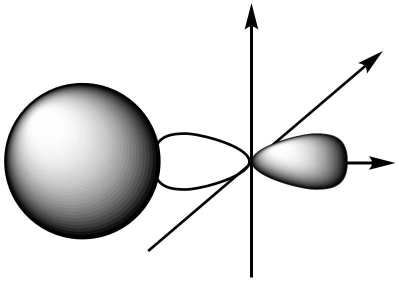
all 4 orbitals interact



p_z orbitals interact with p_z orbitals



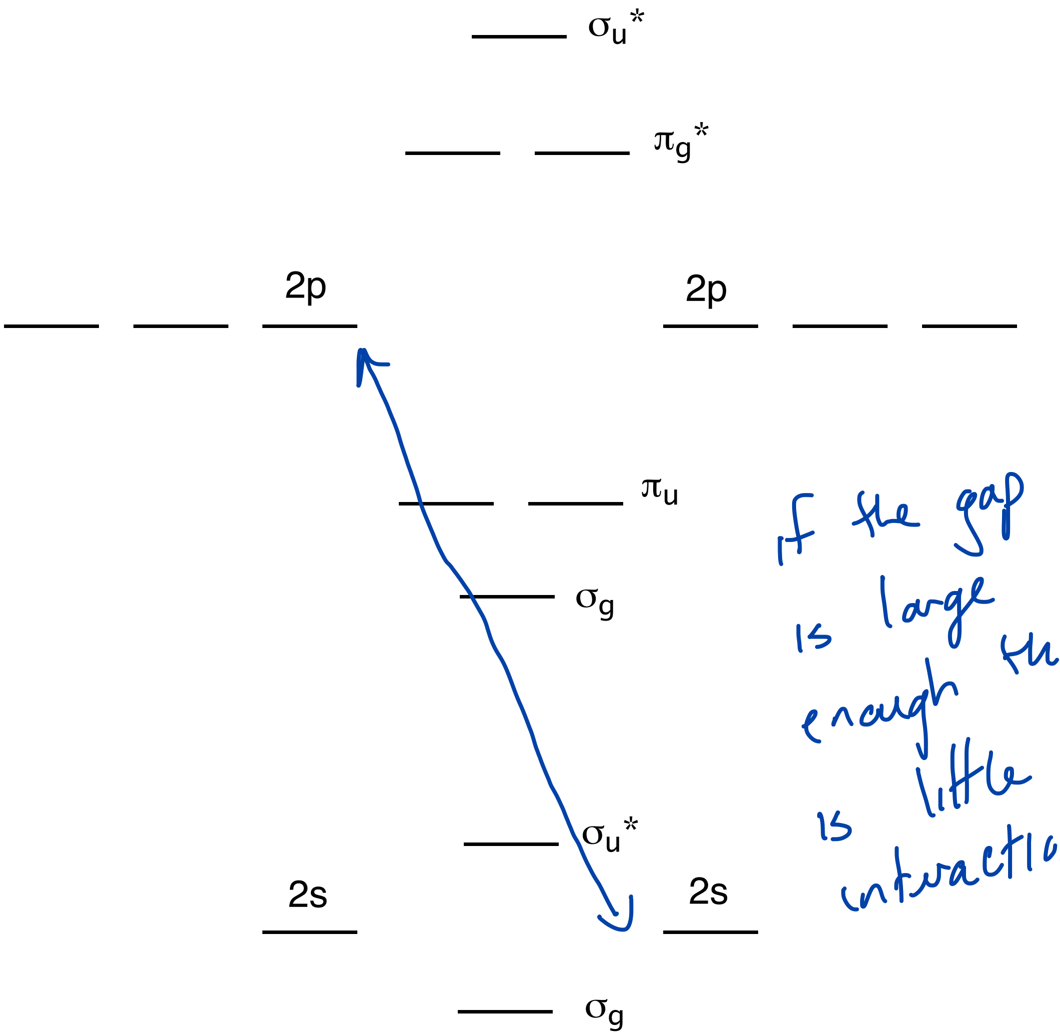
✓ ⊕ of p_z is interacting with ⊕ of s



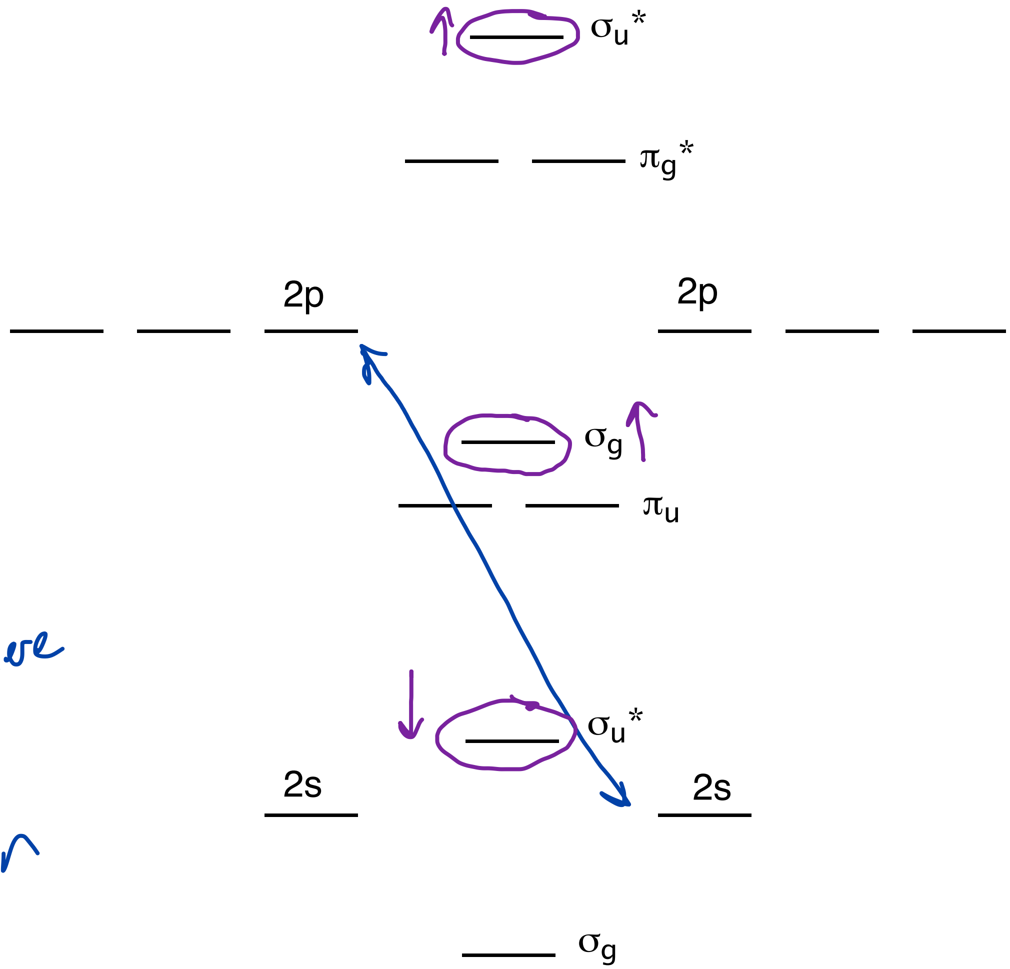
✓ ⊕ of s is interacting with ⊖ of p_z

Molecular Orbitals (mixing)

close in E



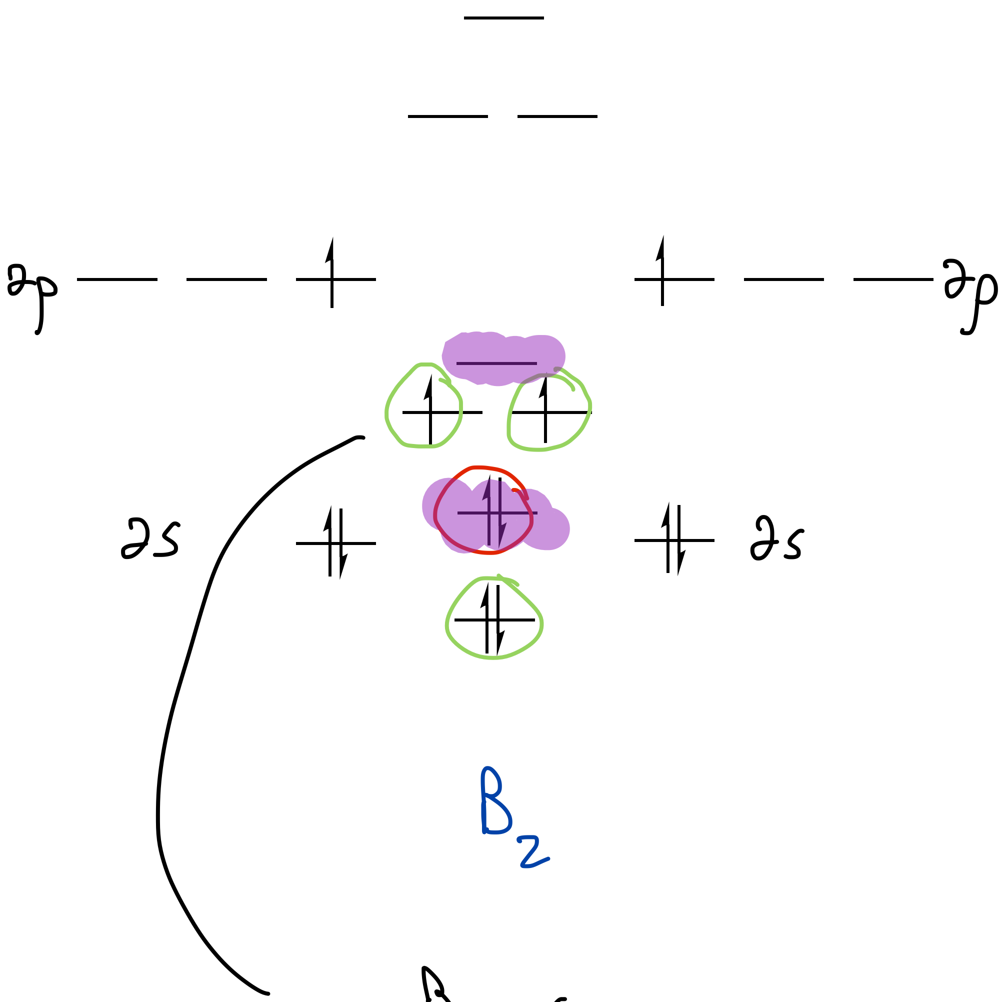
if the gap is large enough there is little interaction



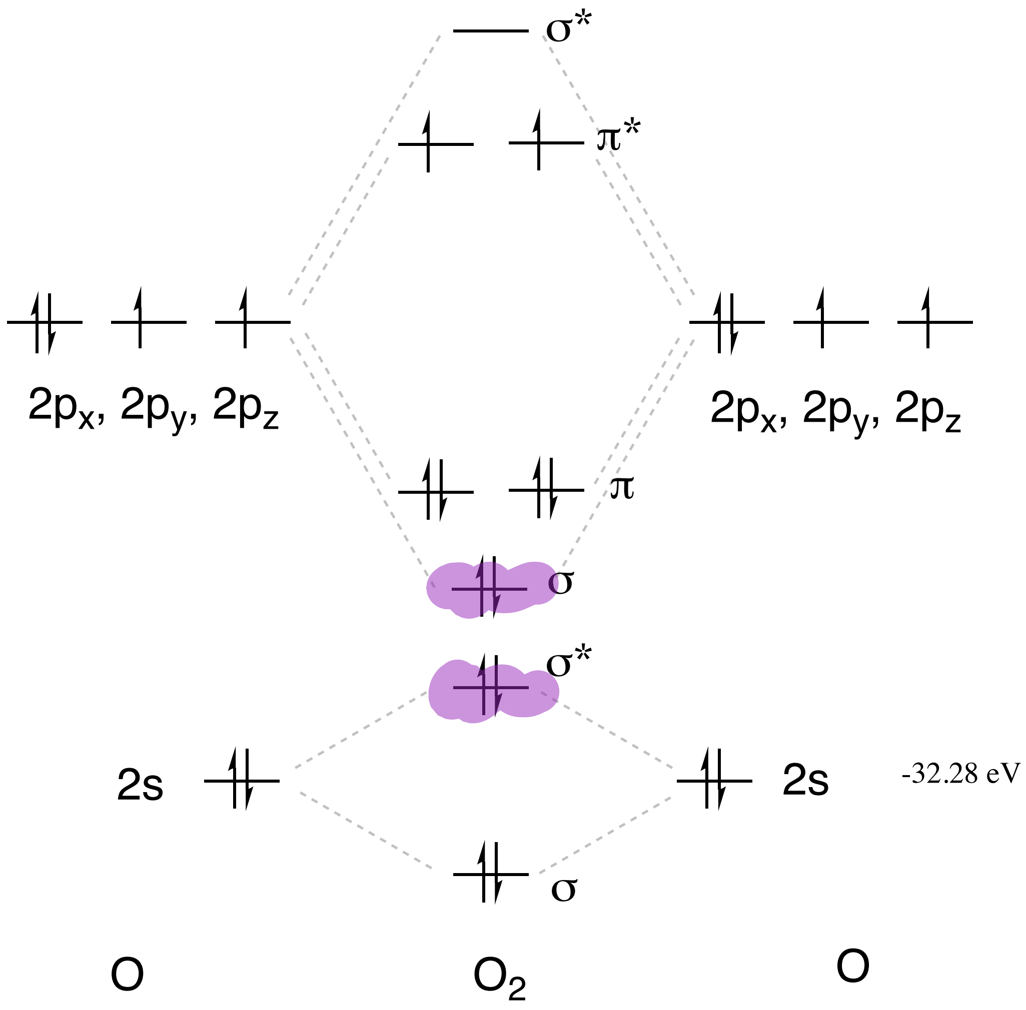
really only O_2 + F_2 where the 2s + 2pz are far enough appart to minimize orbital mixing

when the gap is smaller there is substantial orbital mixing

Molecular Orbitals (mixing)



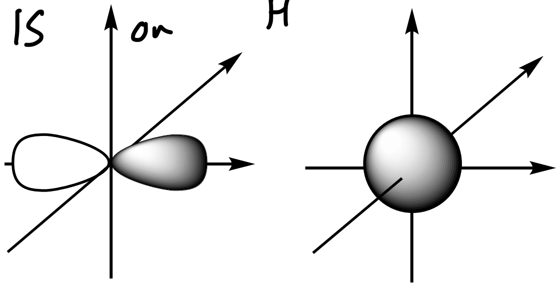
In B_2 a
π interaction
forms before
the σ_{pz} interaction.



Heteronuclear Diatomic Molecules: HF

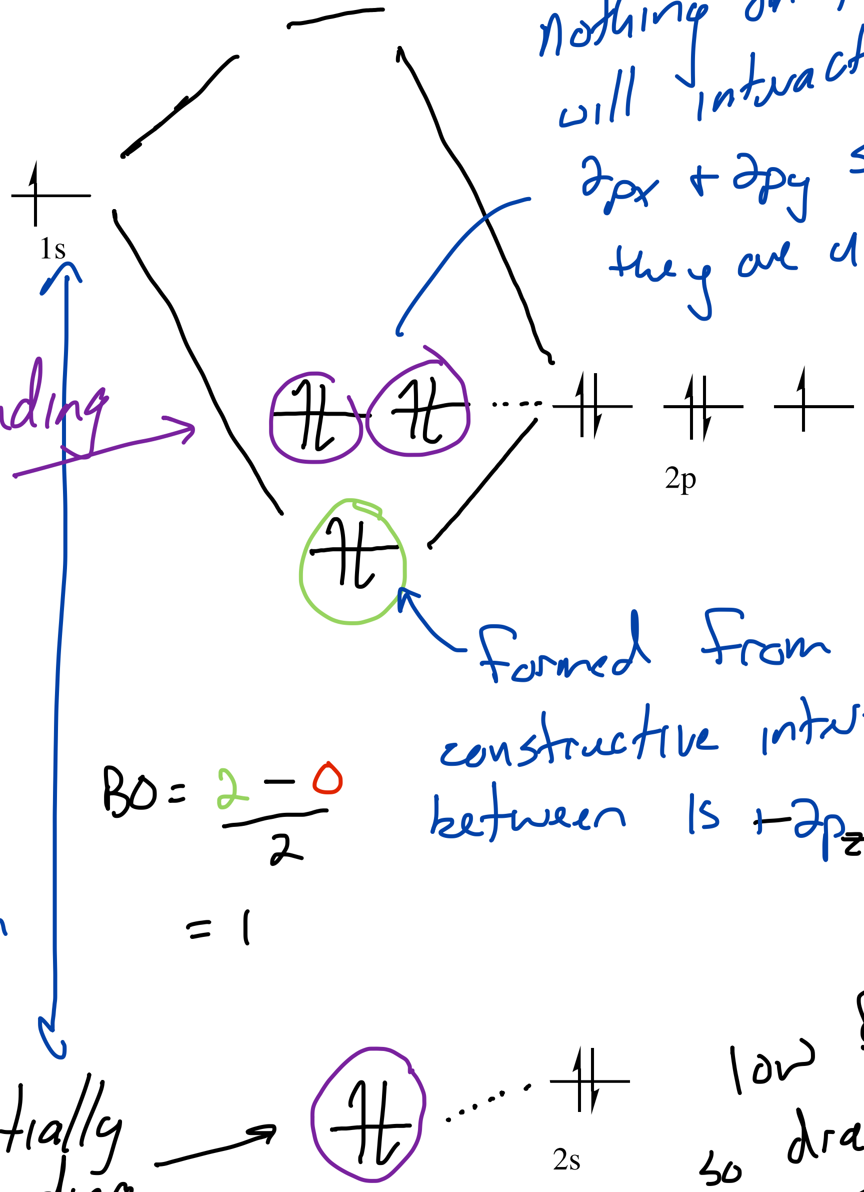
Section 5.3

$2p_z$ on F can interact with 1s on H



H is less eneg... means orbital will be higher in E

so we draw them higher on the page



formed from destructive interference $2p_z$ + 1s

nothing on H will interact with $2p_x + 2p_y$ so they are unchanged

nonbonding

formed from constructive interference between 1s + $2p_z$

$$BO = \frac{2 - 0}{2} = 1$$

essentially non-bonding

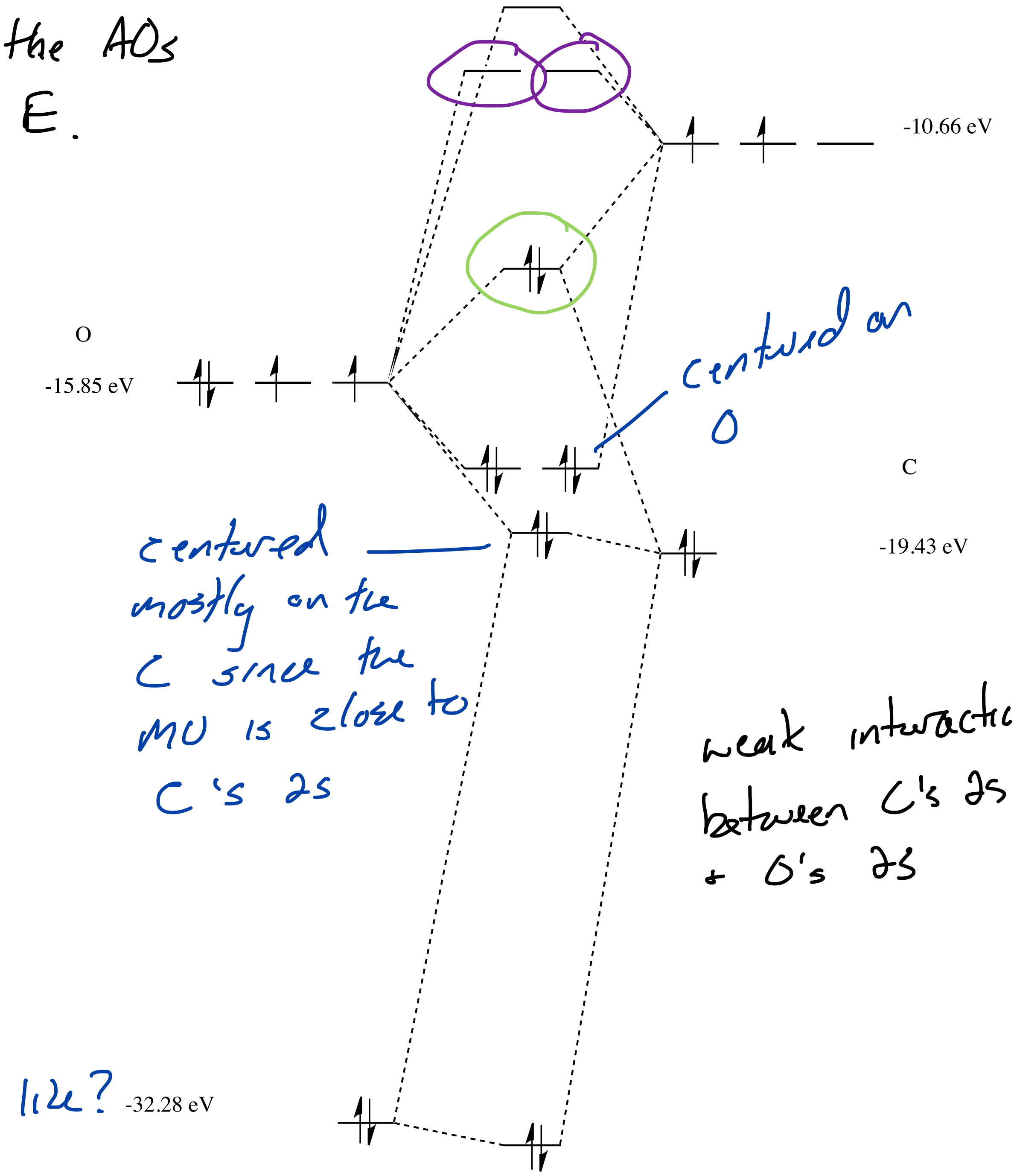
low E so drawn lower

energy gap between 1s on H + 2s on F is very large.... so there is very little interaction

Where are the e^-'s in HF...
where are the nonbonding e^-'s?
centered around F

Heteronuclear Diatomic Molecules: CO

MOs more strongly resemble the AOs that they are close to in E.



centered on O

centered mostly on the C since the MO is close to C's 2s

weak interaction between C's 2s & O's 2s

what does this orbital look like?

The 2s orbital on O