(20) **Today**

5.3 Heteronuclear Diatomic Molecules

5.4 Polyatomic Molecules

**Next Class** (21)

5.4 Polyatomic Molecules

Chap 6 Acids and Bases

(22) **Second Class from Today**

Chap 6 Acids and Bases

~~**Third Class from Today**~~ (23)

Test 2 on Chap 4 and 5

Test 2 postponed until Nov. 6.

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

~~Diatomic Molecules and Orbital Mixing~~

~~Heteronuclear Di~~atomic Molecules

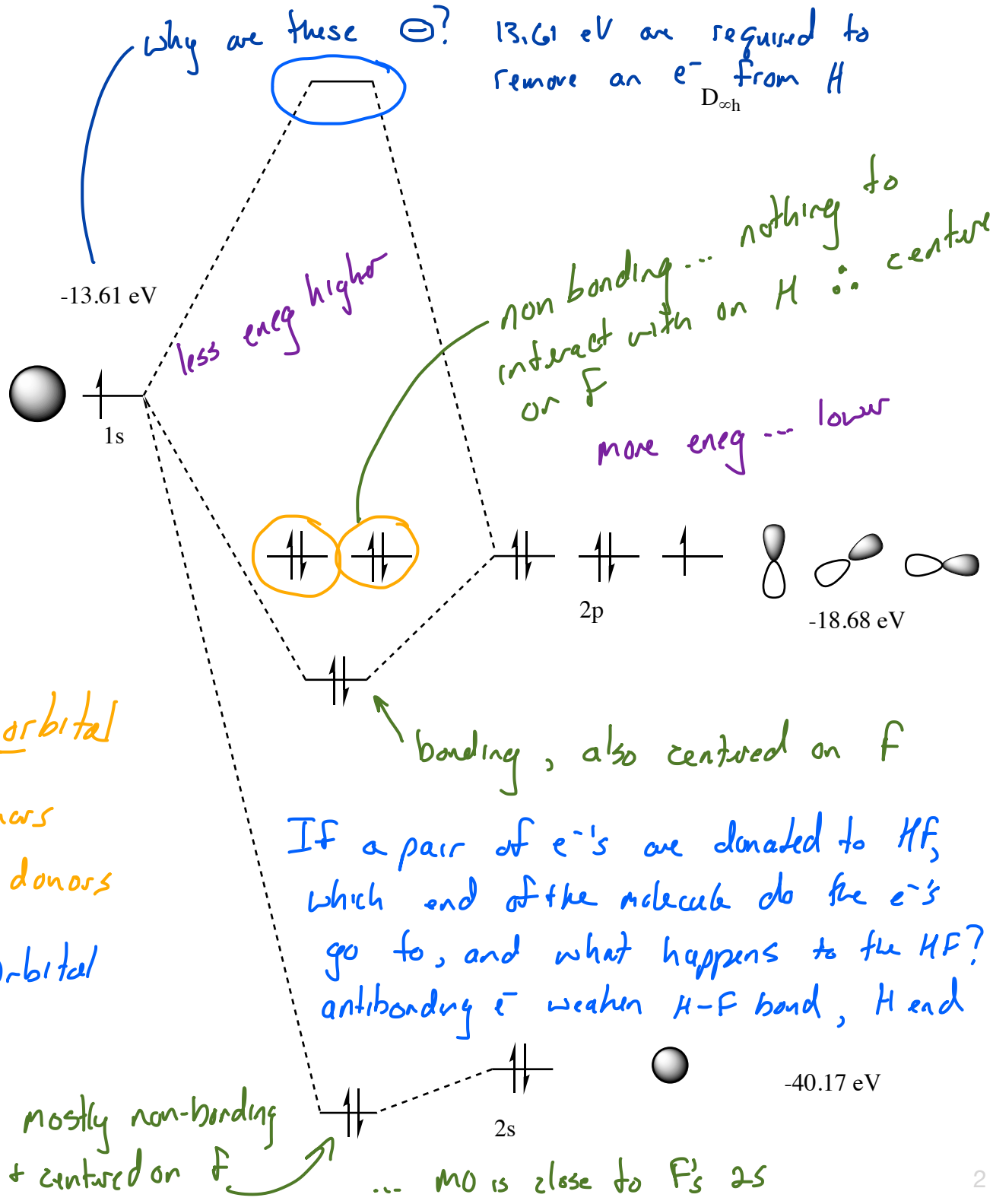
Polyatomic molecules

## Interpreting the MO diagram HF

Energy levels are drawn higher on the page for High E $e^-$ ... and Lower for low E $e^-$

If you dont have the energies you can use electronegativity trends as a standing

Interpreting




Highest occupied molecular orbital

HOMO nucleophiles - $e^-$ donors

Lewis Bases - $e^-$ pair donors

Lowest Unoccupied Molecular Orbital

LUMO accepts $e^-$ density

electrophiles

Lewis acids

# Interpreting the MO diagram

:C ≡ O: ⟶ z axis

antibonding centred on C

these e⁻'s went down in E bonding

O centred bonding orbitals

HOMO is C centred

LUMO is C centred

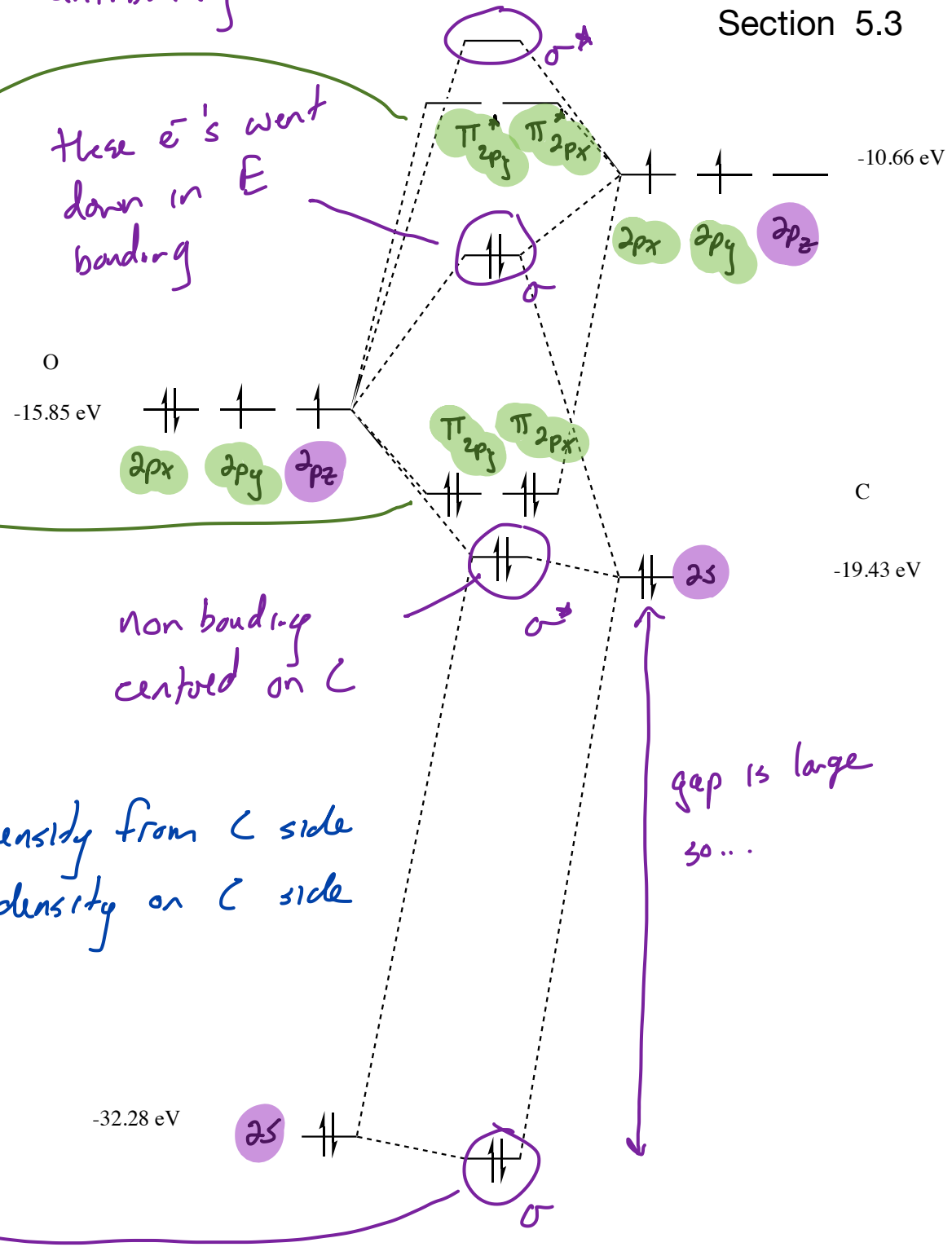
non bonding centred on C

carbon monoxide donates e⁻ density from C side

carbon monoxide accepts e⁻ density on C side

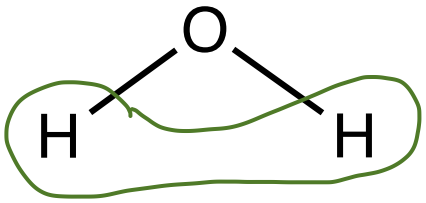
gap is large so...

O centred mostly non bonding



MO Diagram for $H_2O$ - polyatomic molecules






central atom

O

outer atoms

2H

we no longer have 2 atoms 2 sides

—— 

2p ———

group orbitals

"SALC"

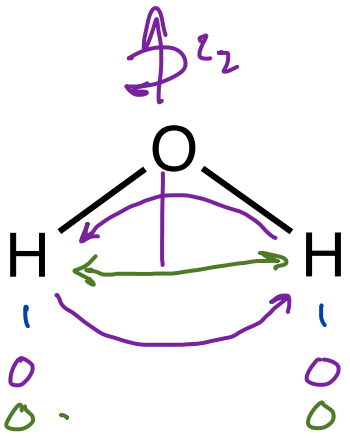
↑

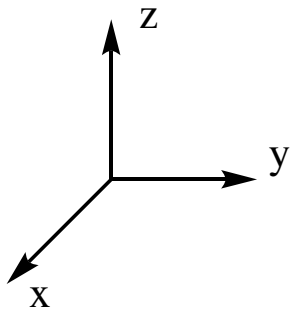
symmetric

2s —

We use character tables to determine the symmetry of the SALC's formed from H's 1s orbitals






| $C_{2v}$ | E | $C_2$ | $\sigma_v(xz)$ | $\sigma_v(yz)$ | | |
|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | z | $x^2$, $y^2$, $z^2$ |
| $A_2$ | 1 | 1 | -1 | -1 | $R_z$ | xy |
| $B_1$ | 1 | -1 | 1 | -1 | x, $R_y$ | xz |
| $B_2$ | 1 | -1 | -1 | 1 | y, $R_x$ | yz |

$\Gamma$ 2 0 0 2

1. Find point group for molecule

$\Gamma = A_1 + B_2$

2. Find reducible representation for orbitals that make up the SALC

3. Find irreducible representations that combine to form the reducible representation

2 1s's ⟶ 2 SALC's with $A_1 + B_2$