This Class

Finsh 5.1 Formation of Molecular Orbitals

5.2 Homonuclear Diatomic Molecules

5.3 Heteronuclear Diatomic Molecules

Next Class

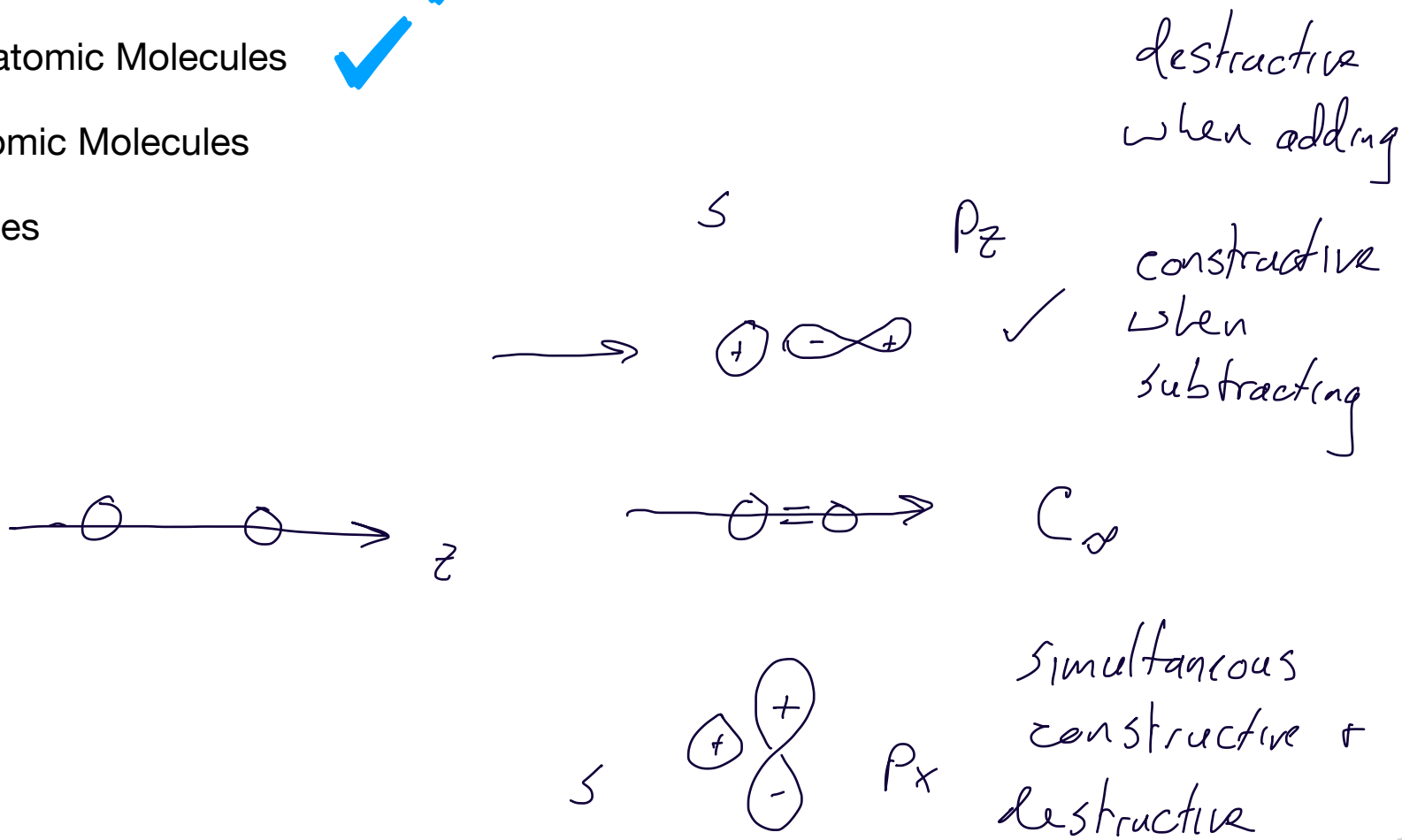
5.3 Heteronuclear Diatomic Molecules

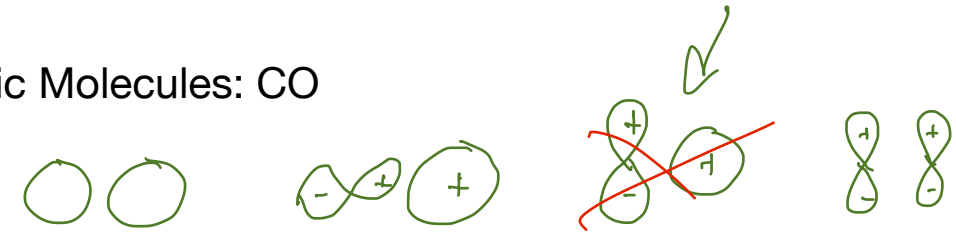
Introduce MOs s, p, d orbital interactions) ✓

Orbital Mixing in Diatomic Molecules ✓

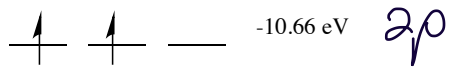
Heteronuclear Diatomic Molecules

Polyatomic molecules





+ 10.66 eV will get the e⁻ out

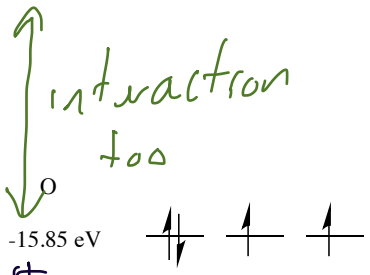


Symmetry

Location ✓

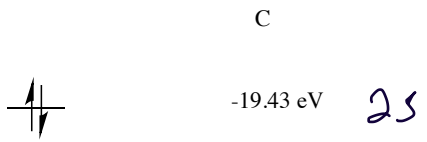
Energy

strong interaction too



stronger interaction between O's 2pz & C's 2s

smaller gap



O's 2pz & C 2s

large gap in E between O 2s & C 2s

only stabilized a little since it doesn't strongly interact

C

Li_2 through Ne_2 be able to draw

O

Interpreting the MO diagram

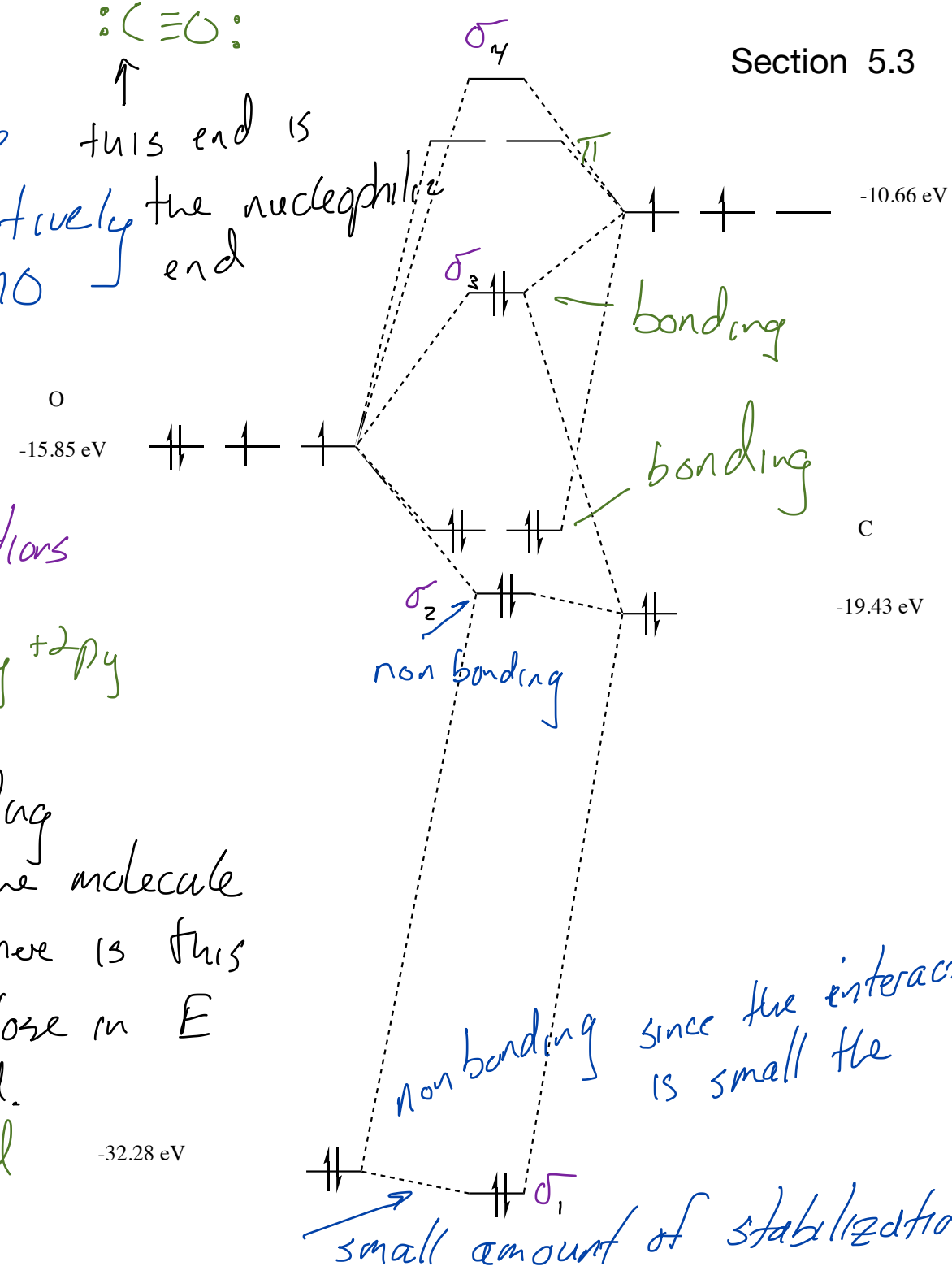
:C≡O:

↑ this end is the nucleophilic end

When strongly interacting atomic orbitals constructively interfere the bonding MO will be stabilized a lot

σ from 2s + 2pz interactions

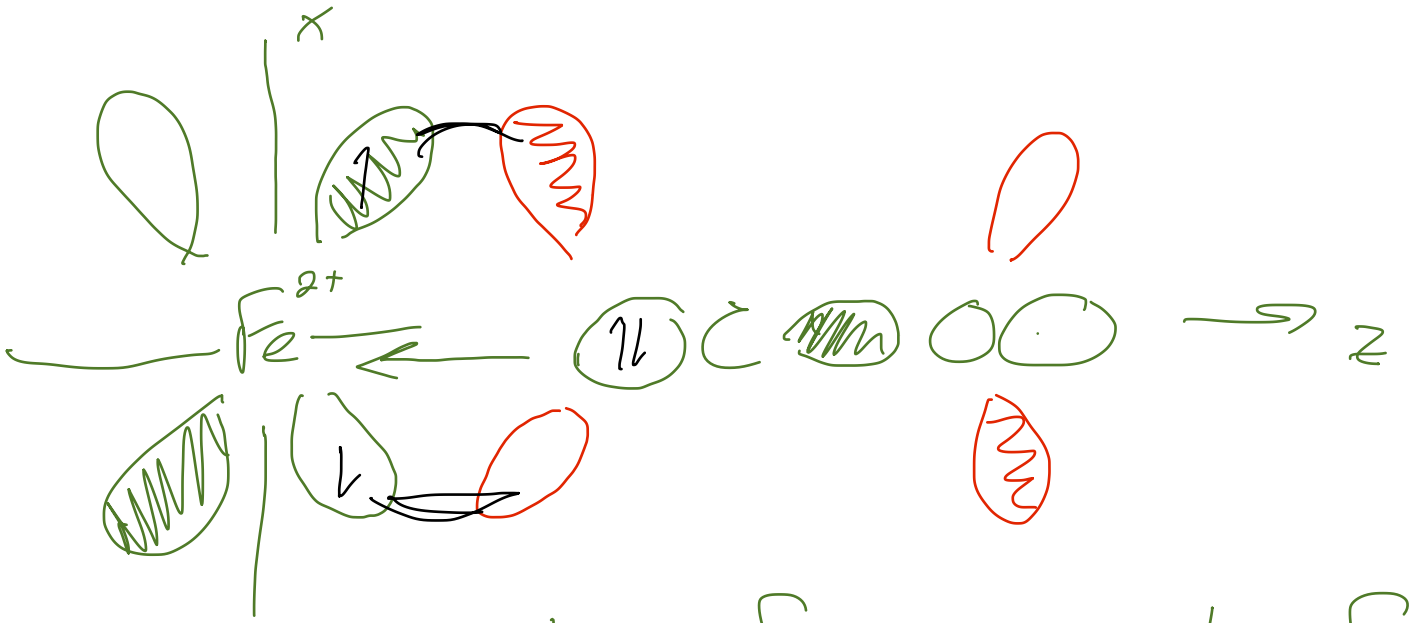
π from 2px + 2px and 2py + 2py interactions



The HOMO is the σ bonding orbital. HOMO is where the molecule donates e⁻'s from. Where is this orbital centered? σ_3 is close in E to C so it is C centered.

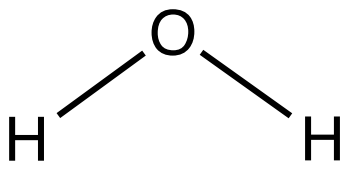
LUMO has π symmetry and is C centered

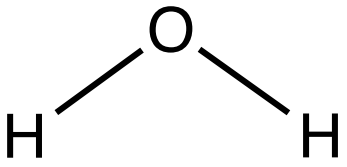
non bonding since the interaction is small the

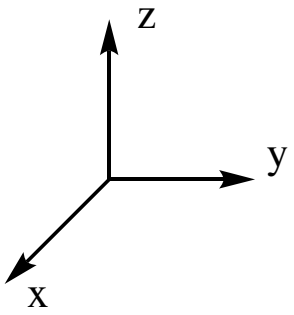


σ donation of e^- density from CO's

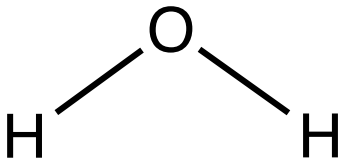
σ symmetry HOMO into Fe d_{z^2}

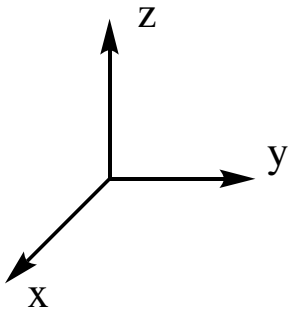

O
H
H

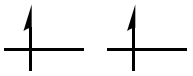




C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz







-13.61 eV

-15.85 eV

2p

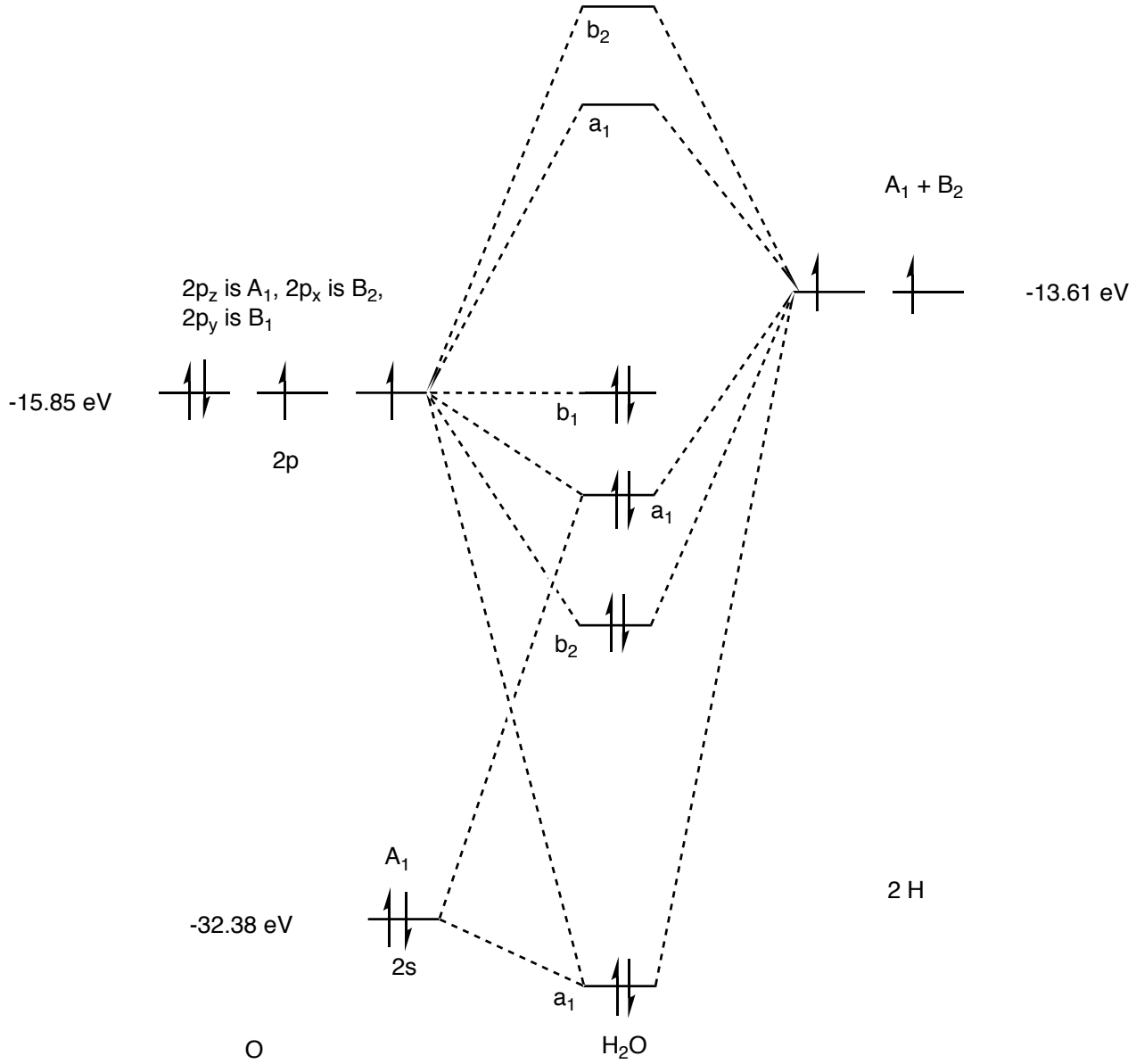
-32.38 eV

2s

O H_2O 2 H

Interpreting the MO Diagram for H_2O

Section 5.3



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