(17) **Today**

5.1 Formation of Molecular Orbitals

5.2 Homonuclear Diatomic Molecules

Next Class (18)

5.2 Homonuclear Diatomic Molecules

5.3 Heteronuclear Diatomic Molecules

(19) **Second Class from Today**

5.3 Heteronuclear Diatomic Molecules

5.4 Polyatomic Molecules

Third Class from Today (20)

5.3 Heteronuclear Diatomic Molecules

5.4 Polyatomic Molecules

Please rework test 1 and hand in on Monday, Oct 23

Introduce MOs (s, p, d orbital interactions)

Diatomic Molecules and Orbital Mixing

Heteronuclear Diatomic Molecules

Polyatomic molecules

Schrödinger Equation ↙ Hamiltonian

$H\Psi = E\Psi$ can be solved for $H = 1p^+ + 1e^-$

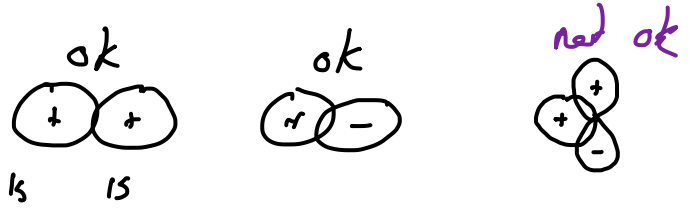
must be approximated for He $2\,p^+ + e^- + e^-$ because $e^- - e^-$ interactions

H^+ e^- e^- H^+

LCAO

↑

linear combination of atomic orbitals - take Hydrogen-like and add + subtract them to make MO's



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

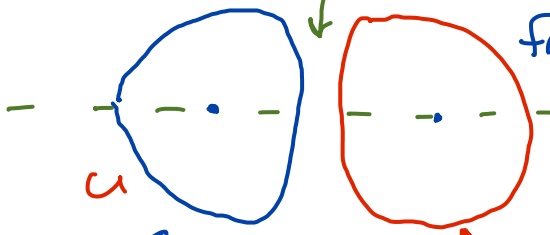
H_2 use 1s orbitals

s orbital interactions

If 2 1s orbitals are being used to make molecular orbitals

2 molecular orbitals must form

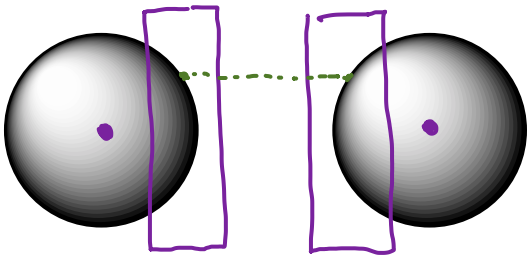
antibonding — Higher in E — a node — lower probability of finding e⁻ near nuclei



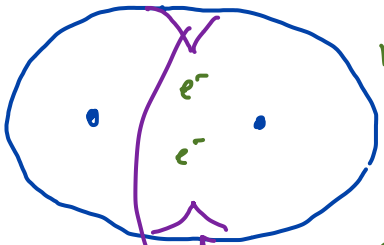
a lobe with a positive phase

a lobe with a negative phase

when viewed along the line connecting the nuclei we saw that the orbitals were cylindrically symmetrical or



2 go in 2 come out



when contructive interference occurs the probability of finding e⁻ directly between 2 ⊕ nuclei increases

got a little bigger

Lower E

Bonding

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

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

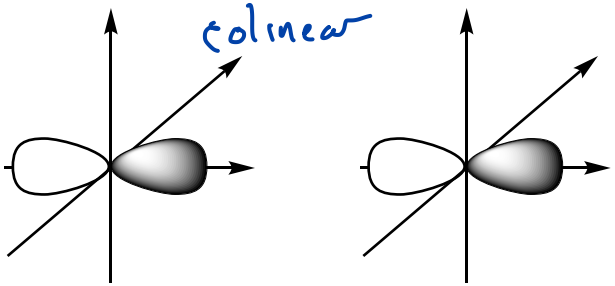
wave function for 1s orbital on H_b

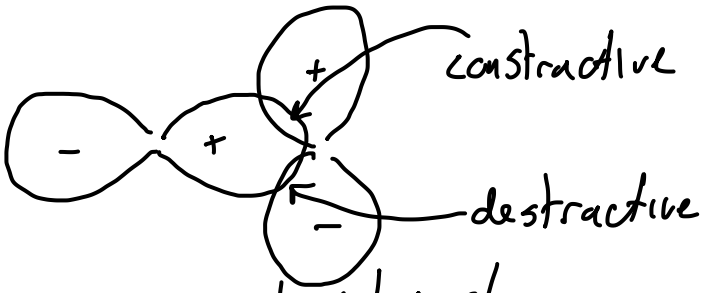
wave function for the 1s orbital on H_a

normalization factor

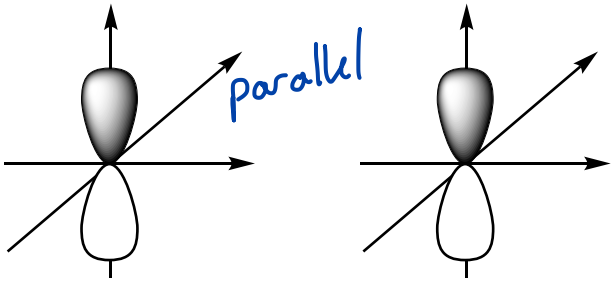
https://www.westfield.ma.edu/cmasi/organic/mo-plain/mo1.html

point at each other



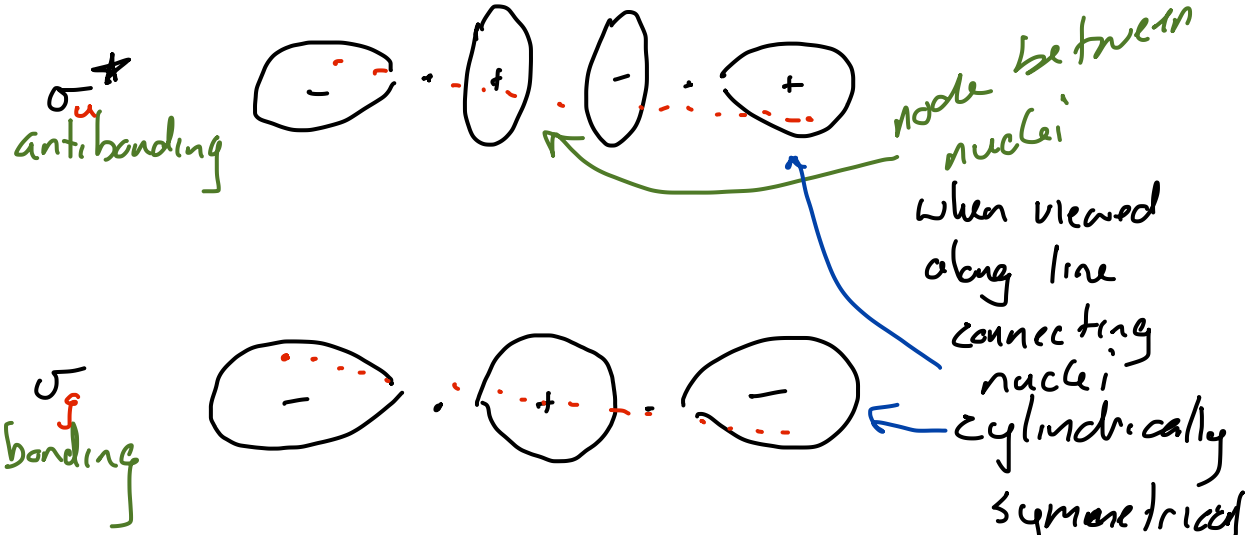


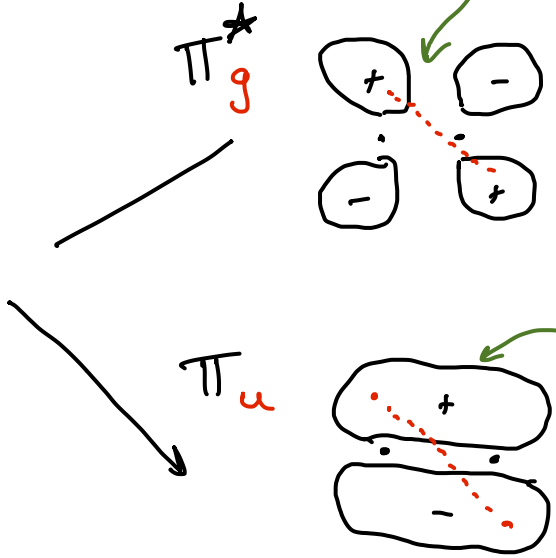
no net interaction



or face each other

2 different interactions





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