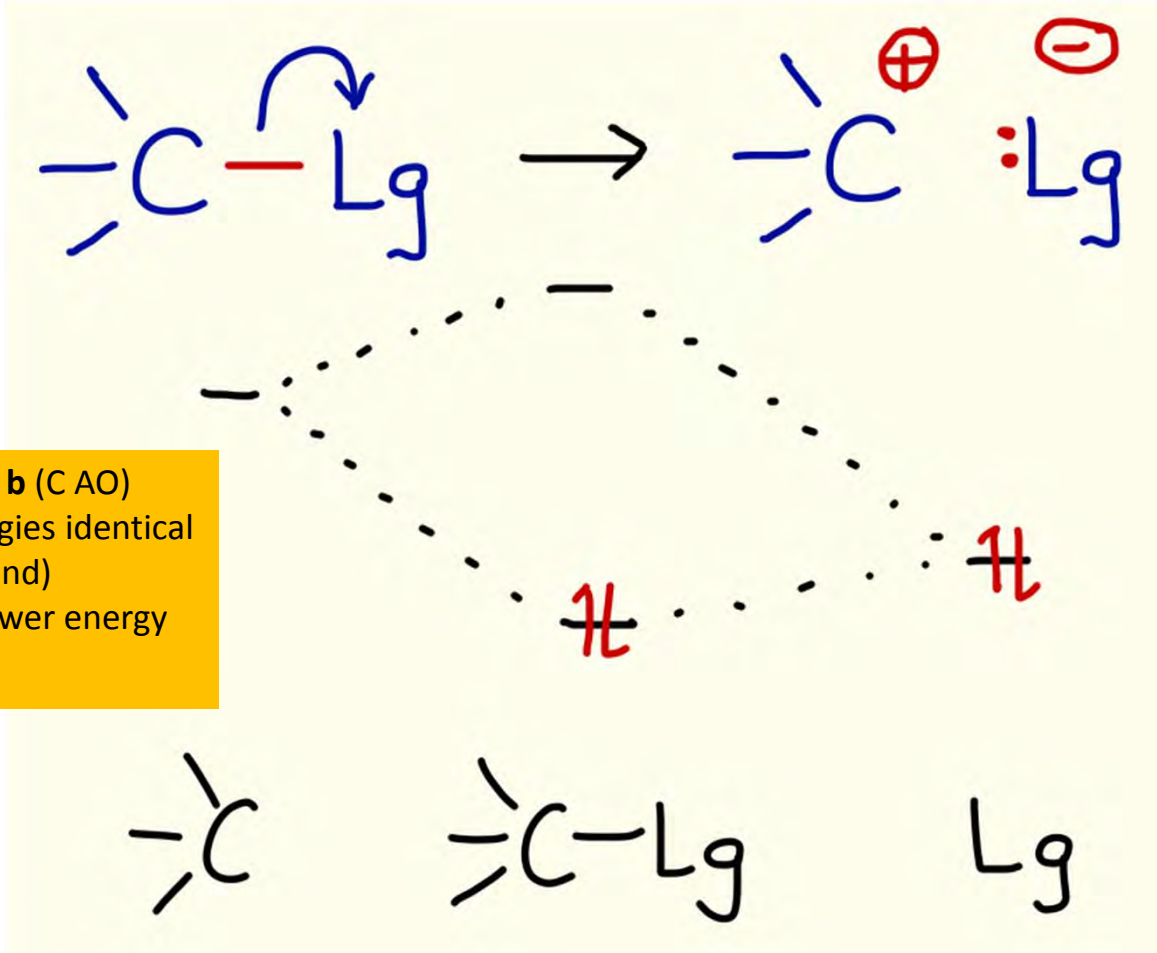
MO of Dissociation Rxns



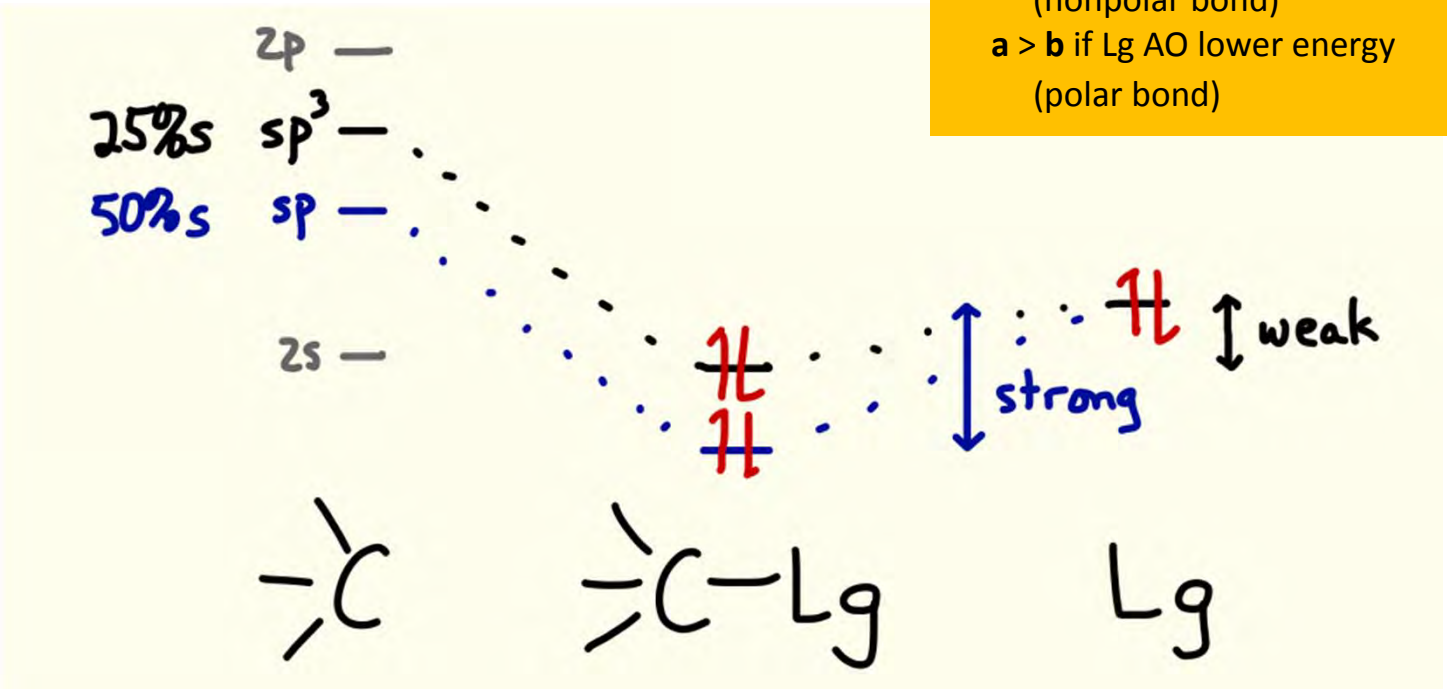
BMO = **a** (Lg AO) + **b** (C AO)

a = **b** if AO energies identical (nonpolar bond)

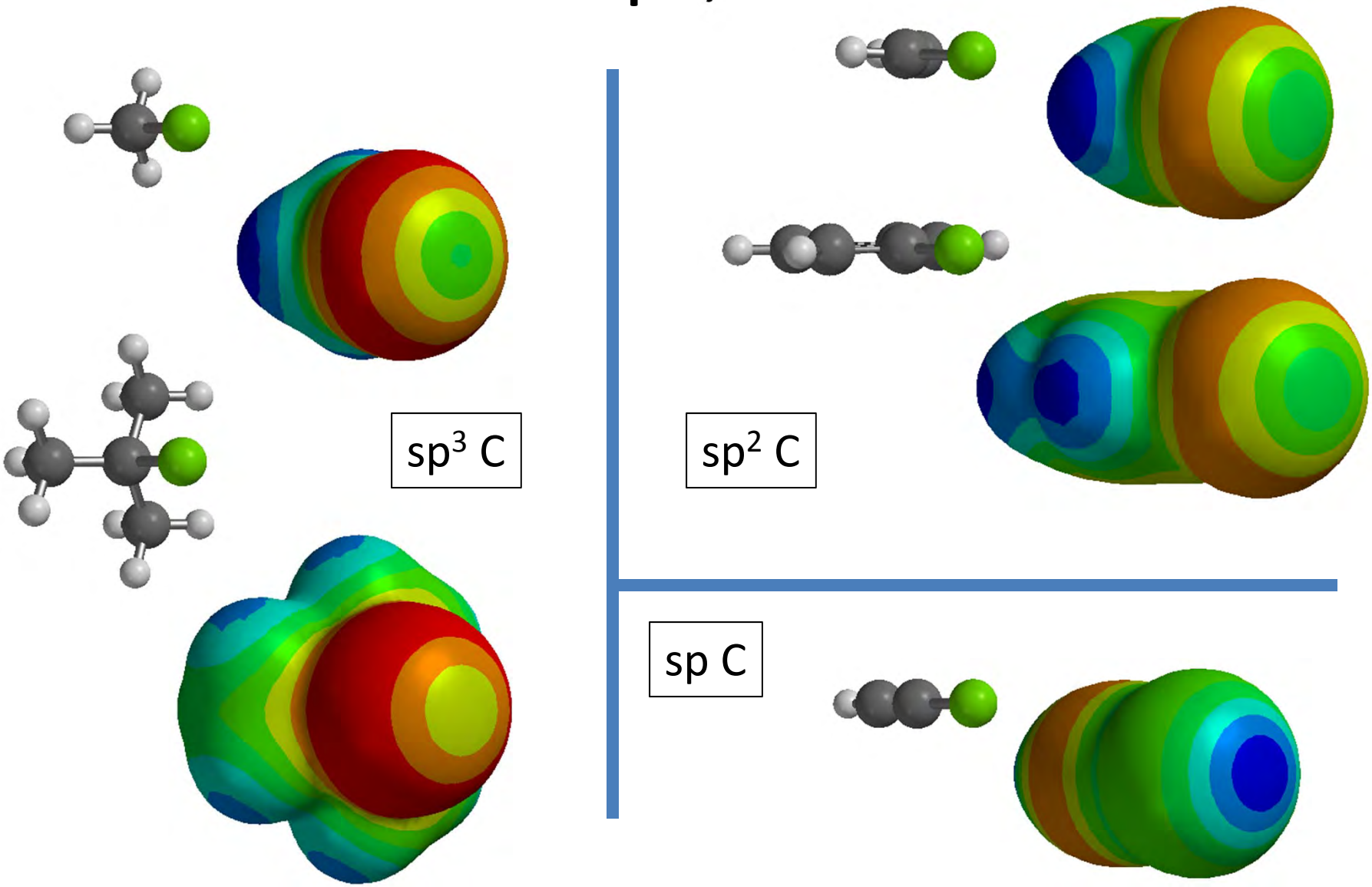
a > **b** if Lg AO lower energy (polar bond)

C Hybridization & BMO Energy

BMO = **a** (Lg AO) + **b** (C AO)
a = **b** if AO energies identical (nonpolar bond)
a > **b** if Lg AO lower energy (polar bond)



Potential Maps, -100 → +100



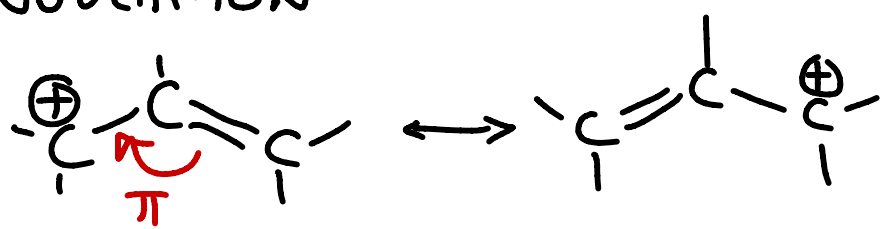
WHAT STABILIZES  ?

① REPLACE H w/ R

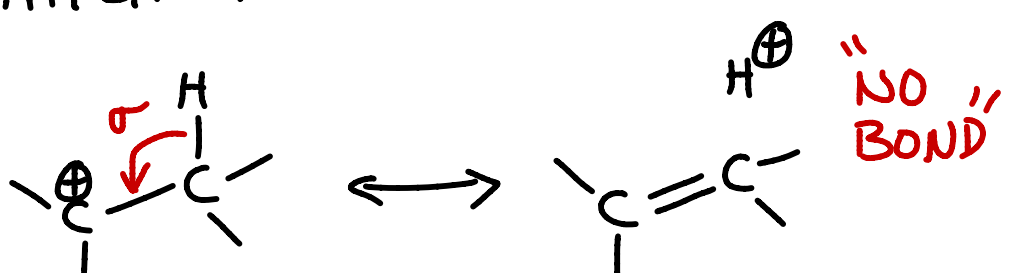
② REPLACE H w/ VINYL OR ARYL

RESONANCE PICTURE

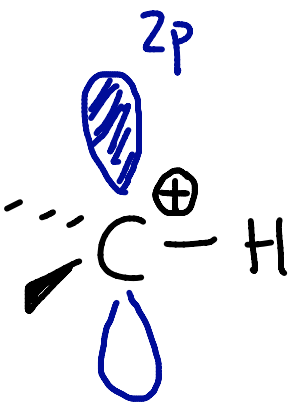
CONJUGATION



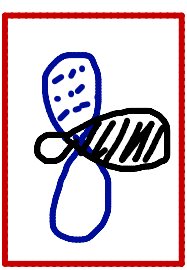
HYPERCONJUGATION



MO MODEL SAYS C–H σ BOND IS A SPECTATOR (CHANGING TO C–C WON'T AFFECT PE)

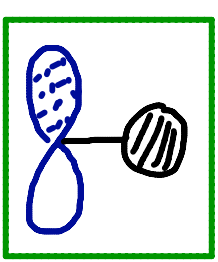


NO OVERLAP BTW



2p & Csp^2

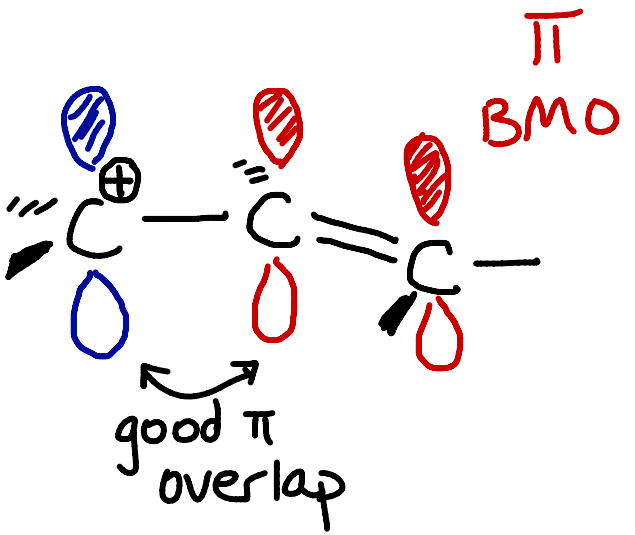
OR BTW

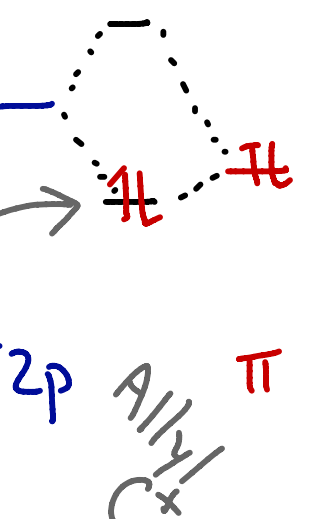


2p & H 1s

SO NO HELP HERE W/ 3°, 2°, 1°

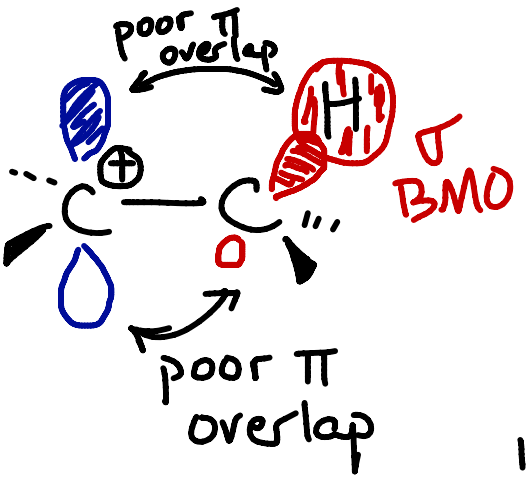
MO CONJUGATION

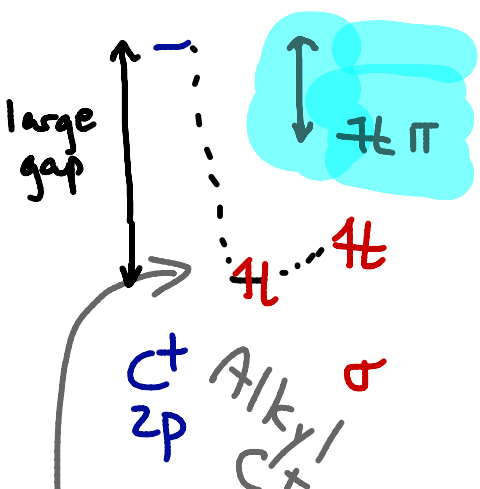




3 atom
MO
2e⁻ spread over 3C

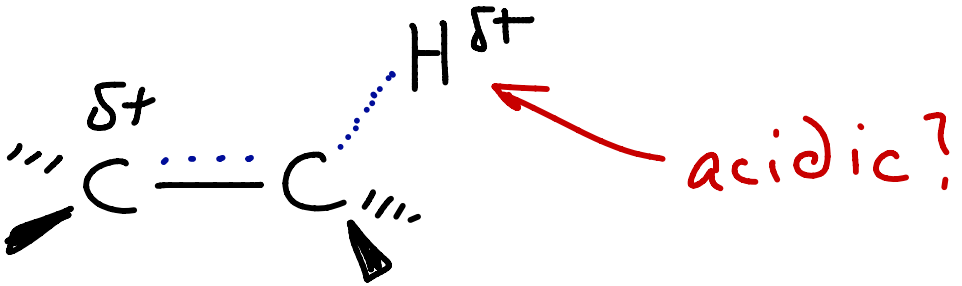
HYPERCONJUGATION

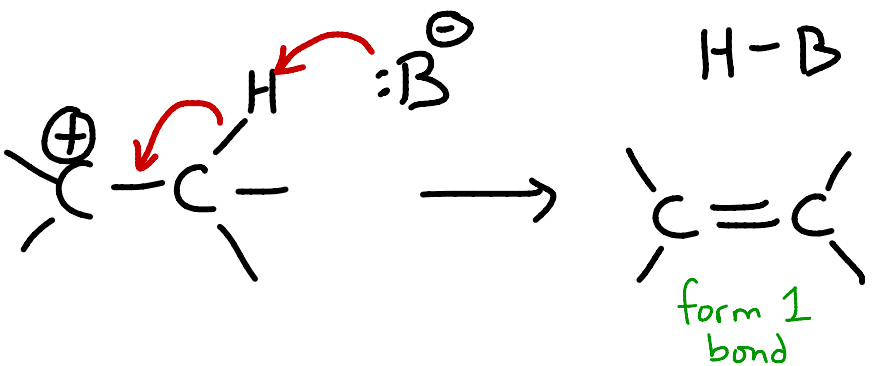




3 atom MO

2e⁻ spread over C–C–H





vs.