

(18) Today

5.1 Formation of Molecular Orbitals

5.2 Homonuclear Diatomic Molecules

(20) Second Class from Today

5.3 Heteronuclear Diatomic Molecules

5.4 Polyatomic Molecules

Next Class (19)

5.2 Homonuclear Diatomic Molecules

5.3 Heteronuclear Diatomic Molecules

Third Class from Today (21)

5.3 Heteronuclear Diatomic Molecules

5.4 Polyatomic Molecules

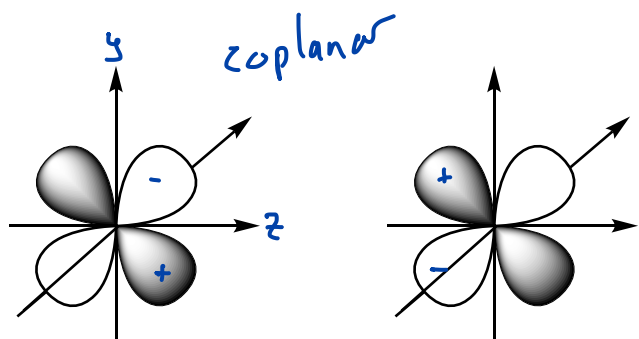
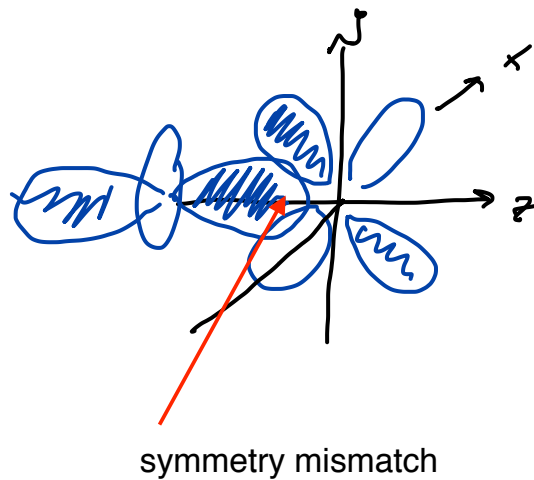
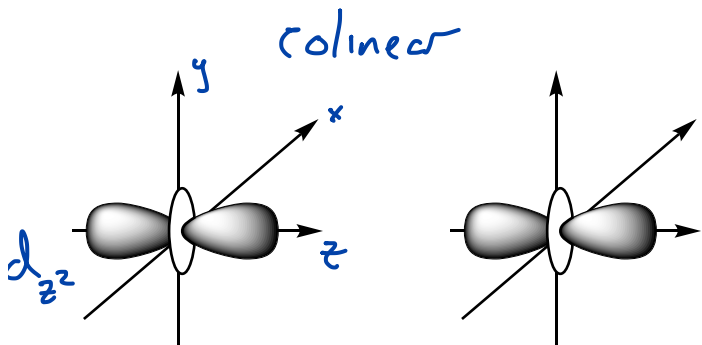
Introduce MOs (s, p, d orbital interactions)

Diatomic Molecules and Orbital Mixing

Heteronuclear Diatomic Molecules

Polyatomic molecules

d orbital interactions

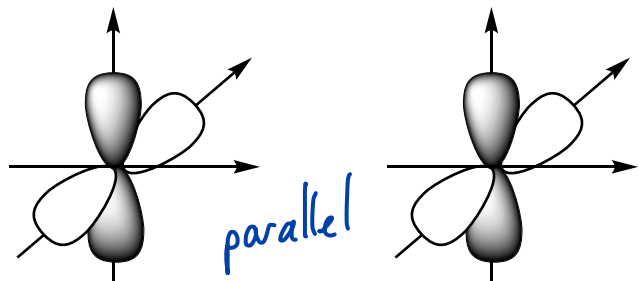


d_{yz}

d_{xz}

d_{yz}

d_{xz}



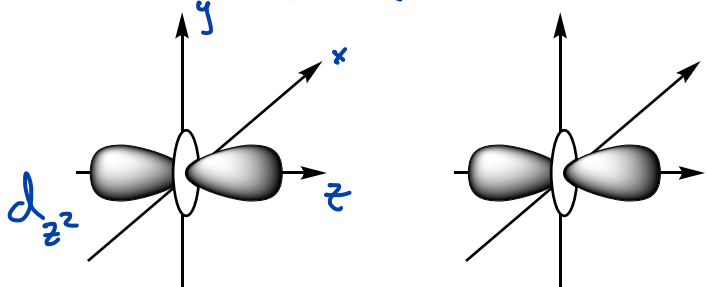
$d_{x^2-y^2}$

d_{xy}

<https://www.westfield.ma.edu/cmasi/advinorg/dorbs/dorbsp.html>

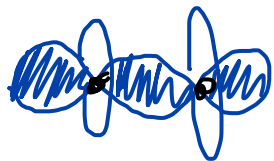
d orbital interactions

colinear



σ_g

constructive interference



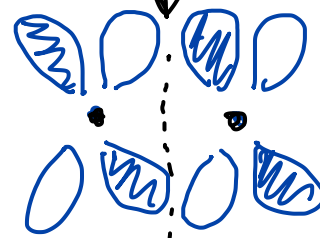
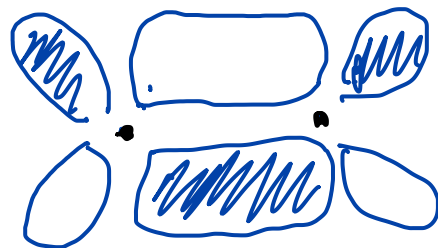
distractive interference Section 5.1/2.1



node formed between nuclei

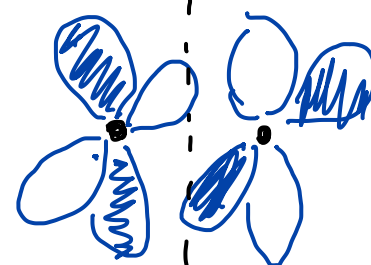
e^- 's between nuclei

π_u



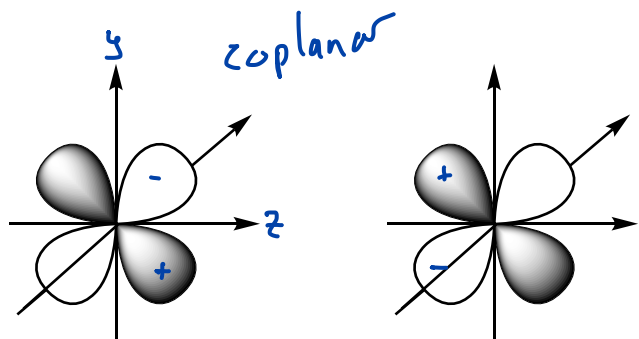
π_g^*

node



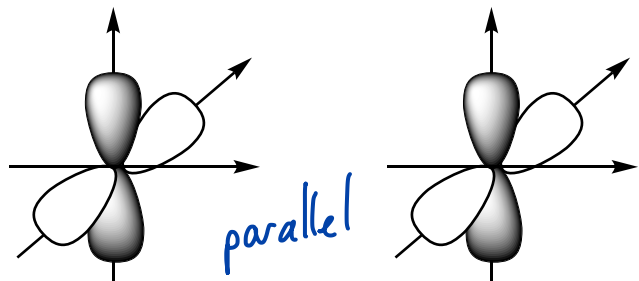
σ_u^*

coplanar



d_{yz}
 d_{xz}

parallel



$d_{x^2-y^2}$ d_{xy}

σ_g



Bonding - constructive interference

Lowers the energy of the e^- 's because they have volume between the 2 nuclei where the e^- 's can experience more \oplus charge as compared to the e^- in the atom

Antibonding - destructive interference

Raises the E of the e^- 's because a node is created and the e^- is excluded from the space near the nuclei where they could have been when part of the atom

Nonbonding

neither stabilizes nor destabilizes the e^- 's

- if there is an AO that doesn't have a symmetry match
- if there is an AO whose E isn't close to the E of an AO on the other atom
- more than 2 orbitals interact and create a non bonding orbital

