

Answers to Exercise 2.2

Linear Combination of Atomic Orbitals: Homonuclear Diatomics

If you don't need to draw the pictures of the atomic orbitals first (i.e. the pictures on the left of the arrows), that's fine. Unless specifically requested in a question, they're not necessary; they're simply a helpful intermediate step.

1.

(a) $2p_z + 2p_z$ (constructive overlap)



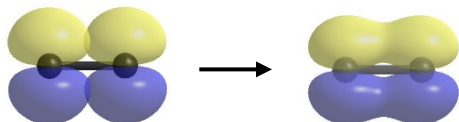
sigma
bonding

$2p_z - 2p_z$ (destructive overlap)



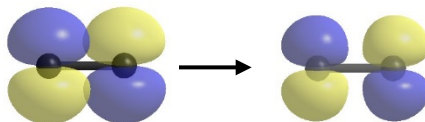
sigma
antibonding

(b) $2p_x + 2p_x$ (constructive overlap)



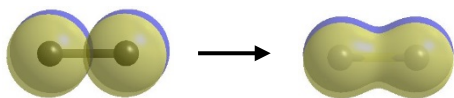
pi
bonding

$2p_x - 2p_x$ (destructive overlap)



pi
antibonding

(c) $2p_y + 2p_y$ (constructive overlap)



pi
bonding

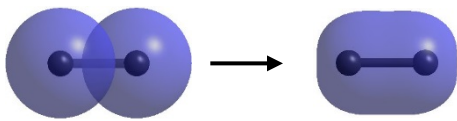
$2p_y - 2p_y$ (destructive overlap)



pi
antibonding

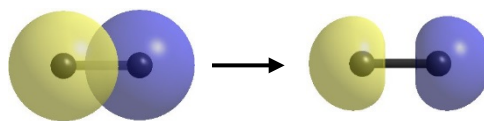
2.

(a) $3s + 3s$ (constructive overlap)



sigma
bonding

$3s - 3s$ (destructive overlap)



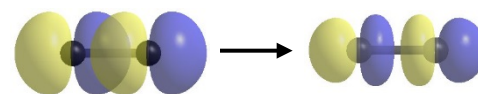
sigma
antibonding

(b) $3p_z + 3p_z$ (constructive overlap)



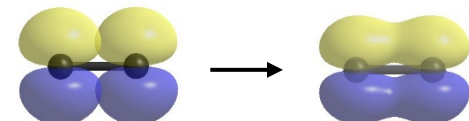
sigma
bonding

$3p_z - 3p_z$ (destructive overlap)



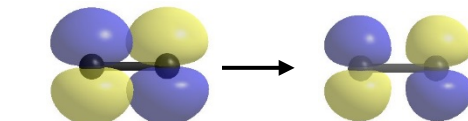
sigma
antibonding

(c) $3p_x + 3p_x$ (constructive overlap)



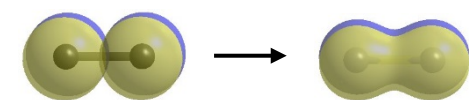
pi
bonding

$3p_x - 3p_x$ (destructive overlap)



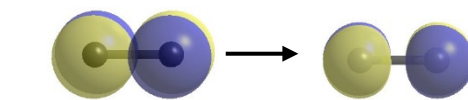
pi
antibonding

(d) $3p_y + 3p_y$ (constructive overlap)



pi
bonding

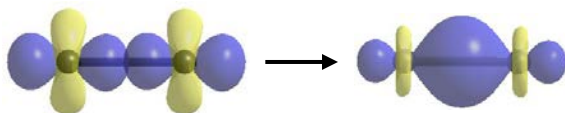
$3p_y - 3p_y$ (destructive overlap)



pi
antibonding

3.

(a) $3d_{z^2} + 3d_{z^2}$ (constructive overlap)



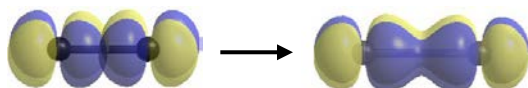
sigma
bonding

$3d_{z^2} - 3d_{z^2}$ (destructive overlap)



sigma
antibonding

(b) $3d_{xz} + 3d_{xz}$ (constructive overlap)



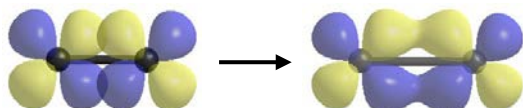
pi
bonding

$3d_{xz} - 3d_{xz}$ (destructive overlap)



pi
antibonding

(c) $3d_{yz} + 3d_{yz}$ (constructive overlap)



pi
bonding

$3d_{yz} - 3d_{yz}$ (destructive overlap)



pi
antibonding

4.

(a)  0 nodes

(b)  3 nodes

(c) The remaining two MOs should have 1 node and 2 nodes. They are drawn below.



Nodes are shown using dashed red lines. You only need to draw nodes if the question asks for them.