**Chemistry 362**
**Spring 2018**
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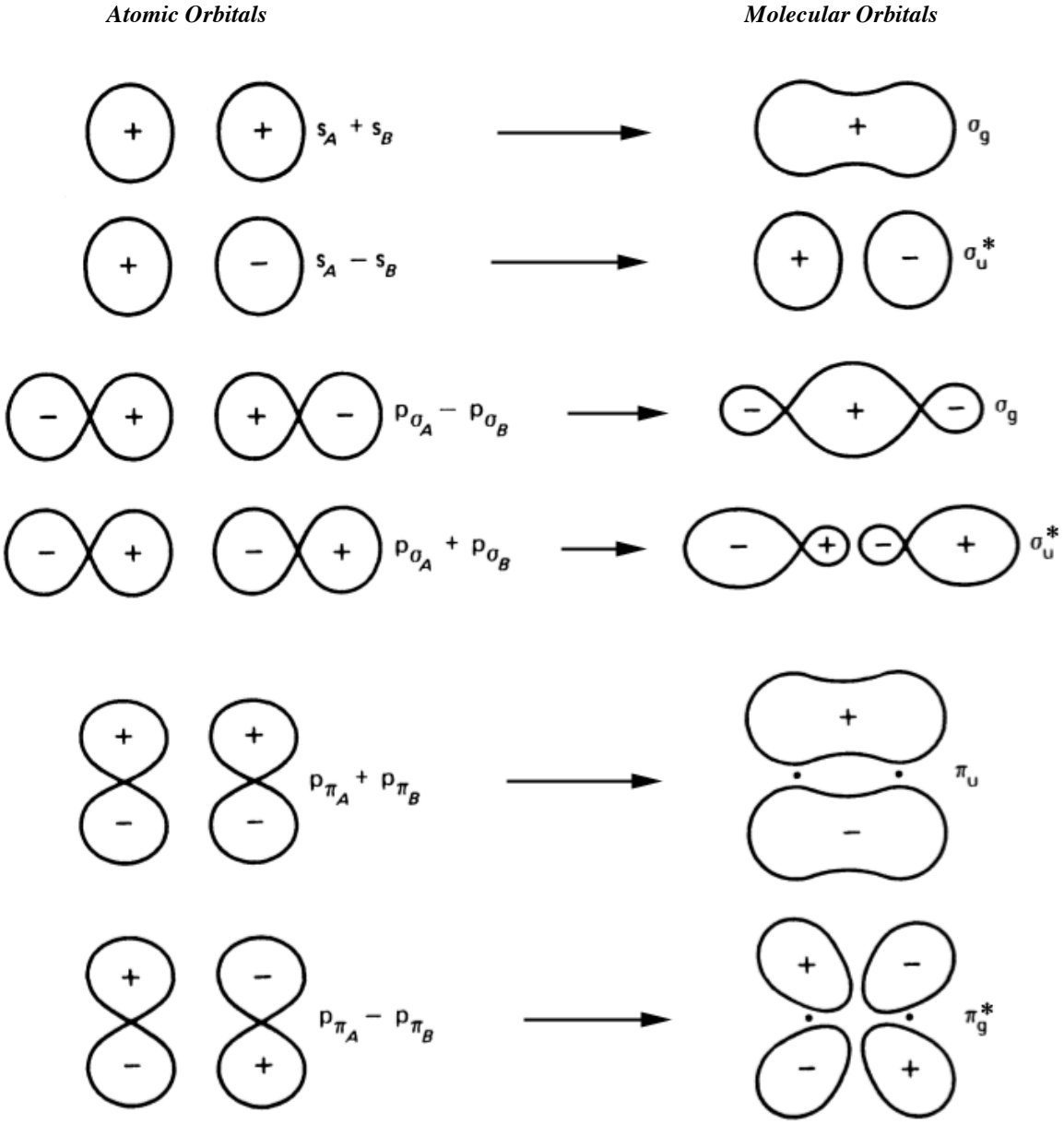
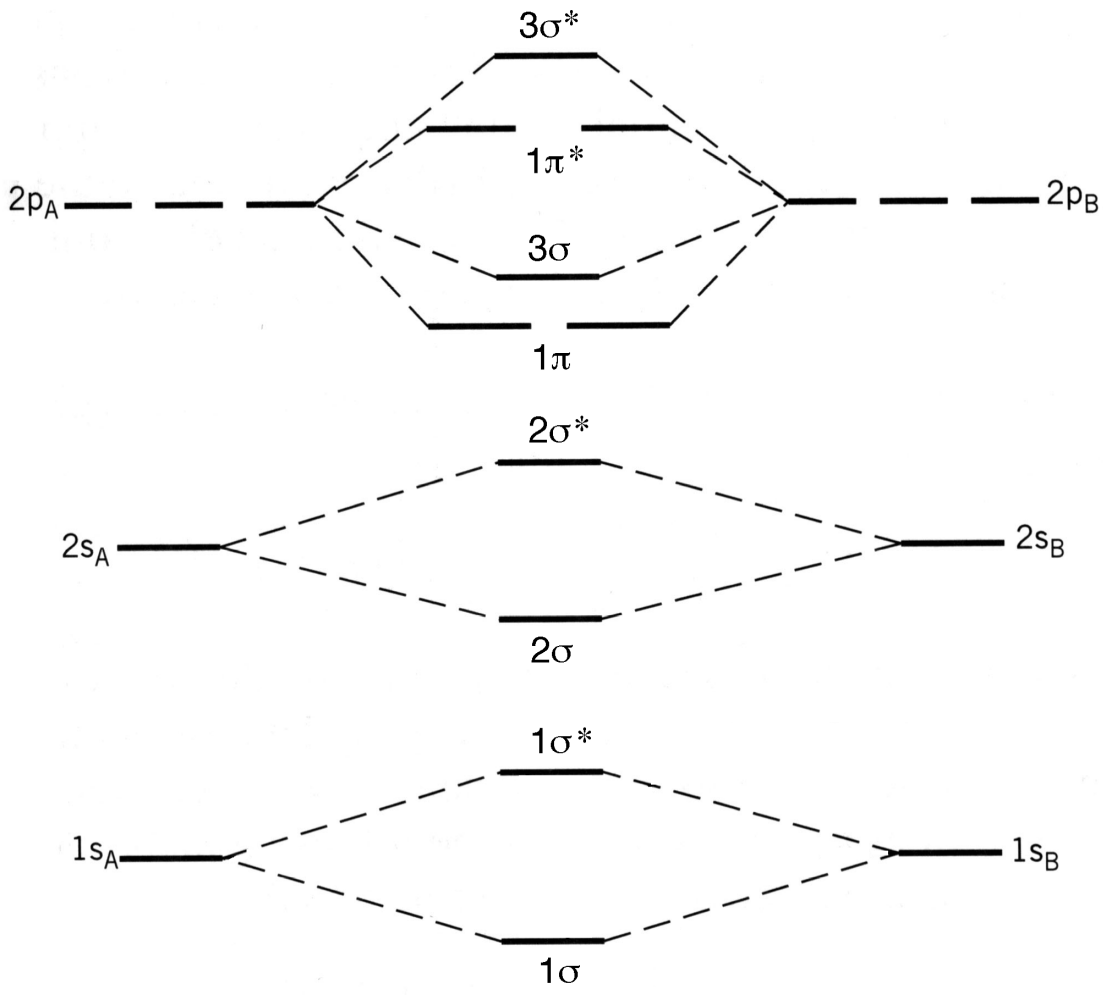
# Molecular Orbitals and Energy Level Diagrams for Diatomic Molecules

## Molecular Orbitals for Diatomic Molecules Formed from a Linear Combination of Atomic Orbitals (the LCAO-MO Approximation)



## Molecular Orbital Energy Diagram for Homonuclear Diatomic Molecules

For diatomic molecules, the atomic orbitals of each atom can be combined using the LCAO-MO method to form molecular orbitals. An approximate energy-ordering scheme is shown below for homonuclear diatomic molecules including $N_2$ and those formed from atoms with lower atomic numbers, including $Li_2$, $Be_2$, $B_2$, and $C_2$. The molecular orbital energy diagram is not shown to scale (that is, the 1s orbitals are the corresponding MOs are much lower in energy than the 2s or 2p orbitals).




For homonuclear diatomic molecules formed from atoms with atomic numbers greater than that of nitrogen, including $O_2$, $F_2$, and $Ne_2$, the energy ordering of the 1π and 3σ molecular orbitals is reversed.