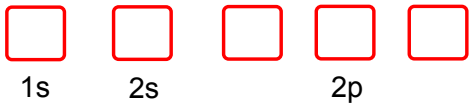
CONCEPT: MOLECULAR ORBITAL THEORY

Electron Orbital Diagrams

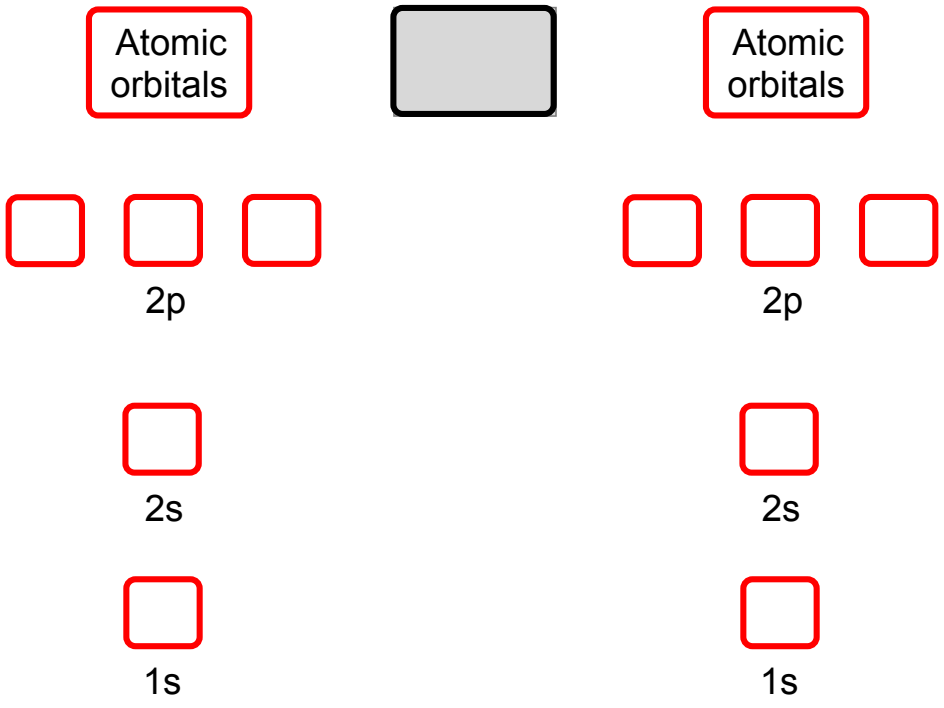
- Recall, electrons are distributed (1s, 2s, 2p …) within orbitals using the _____ Principle.
  - □ Electron orbital diagrams show electrons as residing within _____ orbitals.
    - **Pauli Exclusion Principle:** An orbital can hold a maximum of ____ electrons that have opposite spins.
    - **Hund's Rule:** Same energy (degenerate) orbitals are first _____ -filled before they are totally filled.

EXAMPLE: Provide the electron orbital diagram for a nitrogen atom (Z = 7).



- When atoms _____ their electrons the electron orbital diagrams are shown vertically.
  - □ Use the same three principles to draw these vertical electron orbital diagrams.

EXAMPLE: Fill in the electron orbital diagrams for two oxygen atoms that are combining their electrons.

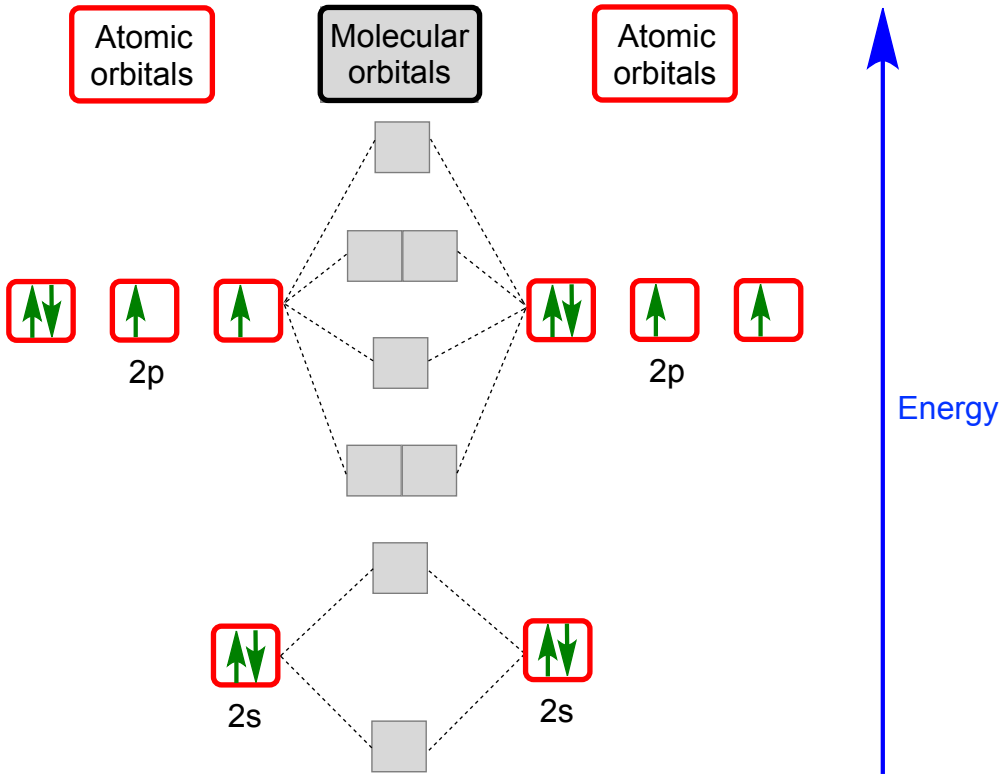


CONCEPT: MOLECULAR ORBITAL THEORY

Molecular Orbital Diagrams

- Show chemical bonding as the combining of _____ electrons from atomic orbitals of elements into *molecular orbitals*.
  - □ **Molecular Orbitals:** set of orbitals created from the combining of electrons _____ 2 elements.

EXAMPLE: Fill in the molecular orbital diagram for when two carbon atoms combine their valence electrons.



Filling in a Molecular Orbital Diagram

STEP 1: If it's not given, determine the number of valence electrons for both elements.

STEP 2: Construct the Molecular Orbital Diagram based on the location of the valence electrons.

- □ Period 1 elements start with ____ , Period 2 elements start with _____ , Period 3 elements start with _____

STEP 3: Following the 3 principles, fill in the molecular orbitals based on increasing energy.

CONCEPT: MOLECULAR ORBITAL THEORY

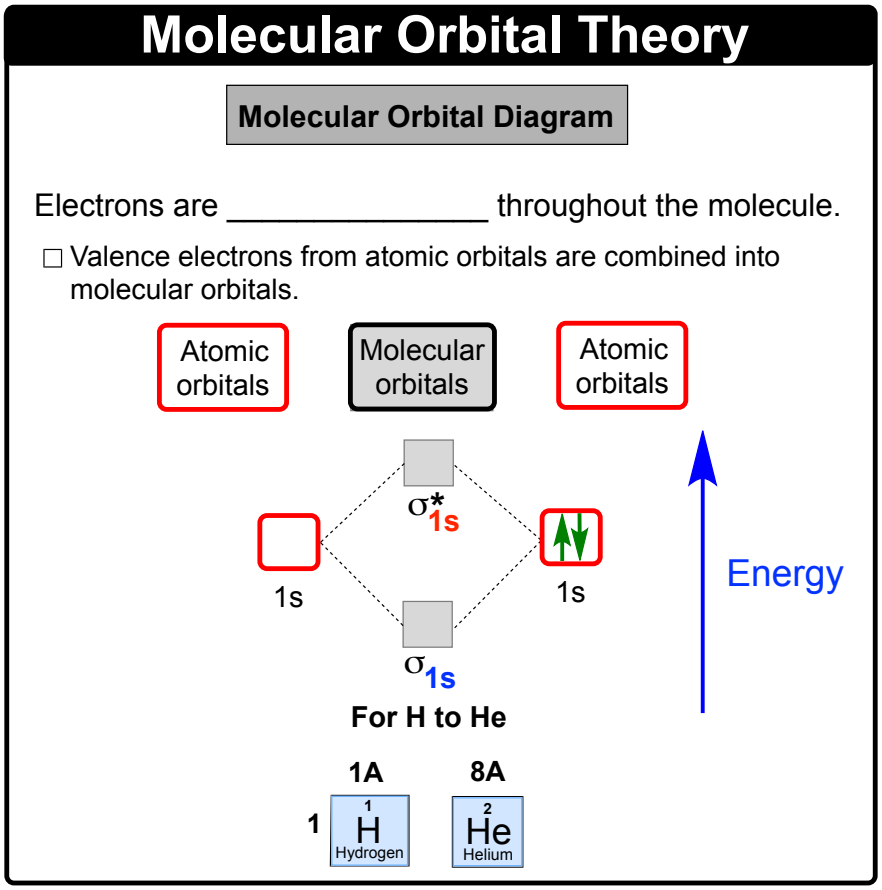
Bonding vs. Anti-bonding Molecular Orbitals

● When combining the valence electrons between there are two types of molecular orbitals involved.

□ **Bonding Molecular Orbital**: region of ____ electron density between elements that promotes bond formation.

□ **Anti-bonding Molecular Orbital (__)**: region with ___ electron density (node) that prevents bond formation.

- Filled bonding molecular orbitals ____ stability and filled anti-bonding molecular orbitals ____ stability.



EXAMPLE: Construct the Molecular Orbital Diagram for the dihelium cation, He_2^+.

Filling in a Molecular Orbital Diagram

STEP 1: Determine the number of valence electrons for both elements.

STEP 2: Construct the Molecular Orbital Diagram based on the location of the valence electrons.

□ Period 1 elements start with ____ , Period 2 elements start with _____ , Period 3 elements start with _____

STEP 3: Following the 3 principles, fill in the molecular orbitals from the bottom to the top.