Physics PY4118
Physics of Semiconductor Devices

Molecular Bonds

Bonding Theories

- Valence Bond (VB) theory
  - Focuses on atomic orbits
- Molecular Orbital (MO) theory
  - Focuses on the modules orbitals (thus more complicated)

Valence Bond Theory

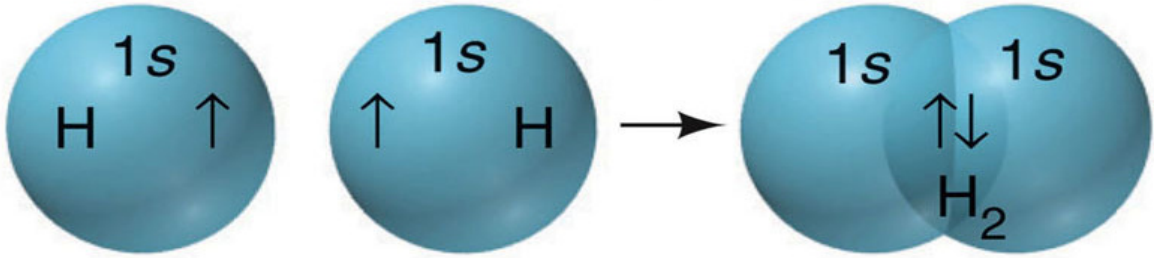
- **Valence Bond Theory** is an attempt to explain the Covalent bond from a Quantum Mechanical view
  - All orbitals of the same type (s, p, d, f) have the same energy
  - According to this theory, a bond forms when two atomic orbitals (s/s s/p p/p) “overlap”
  - The space formed by the overlapping orbitals has a capacity for two electrons that have opposite spins, +1/2 & -1/2 (exclusion principle)
  - Note: Each orbital forming the bond has at least one unfilled slot to accommodate the electron being shared from the other bonding orbital

Valence Bond Theory

- **Valence bond theory (con't)**
  - The bond strength depends on the attraction of the nuclei for the shared electrons
  - The greater the orbital overlap, the stronger (more stable) the bond
  - The extent of the overlap depends on the shapes and directions of the orbitals
  - An s orbital is spherical, but p and d orbitals have more electron density in one direction than in another
  - Whenever possible, a bond involving p or d electrons will be oriented in the direction that maximizes overlap

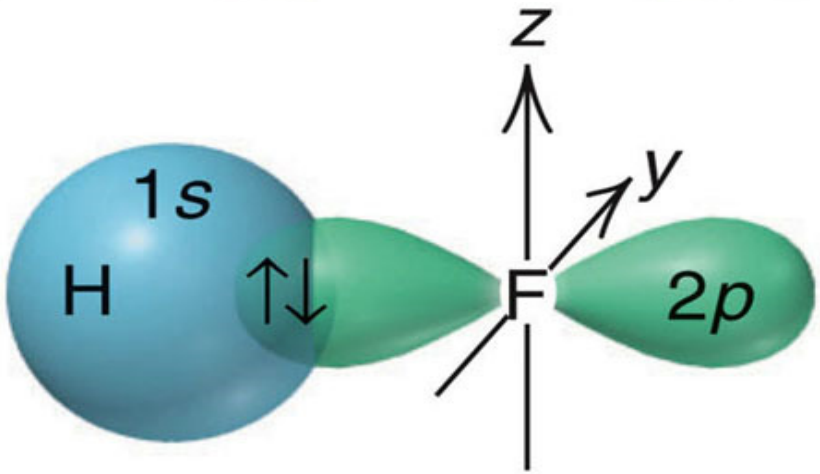
Valence Bond Theory

Hydrogen, H_2 $1s^1$



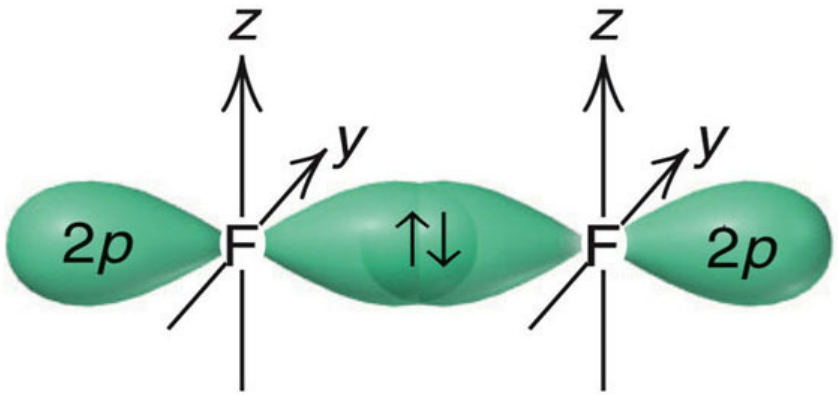
Hydrogen Fluoride, HF $[He]2s^2 2p^5$

To maximize overlap, half-filled H 1s and F 2p orbitals overlap along the long axis of the 2p orbital



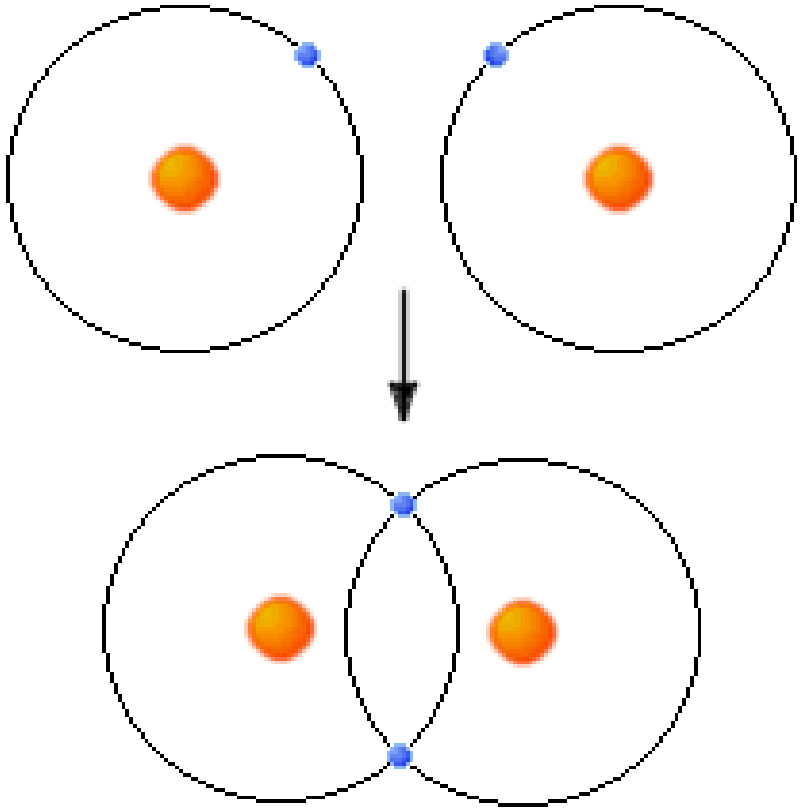
Fluorine, F_2 $[He]\ 2s^2 2p^5$

In F_2, the half-filled 2 p^x orbital on one F atom points end to end toward the half-filled $2p^x$ of the other F to maximize overlap

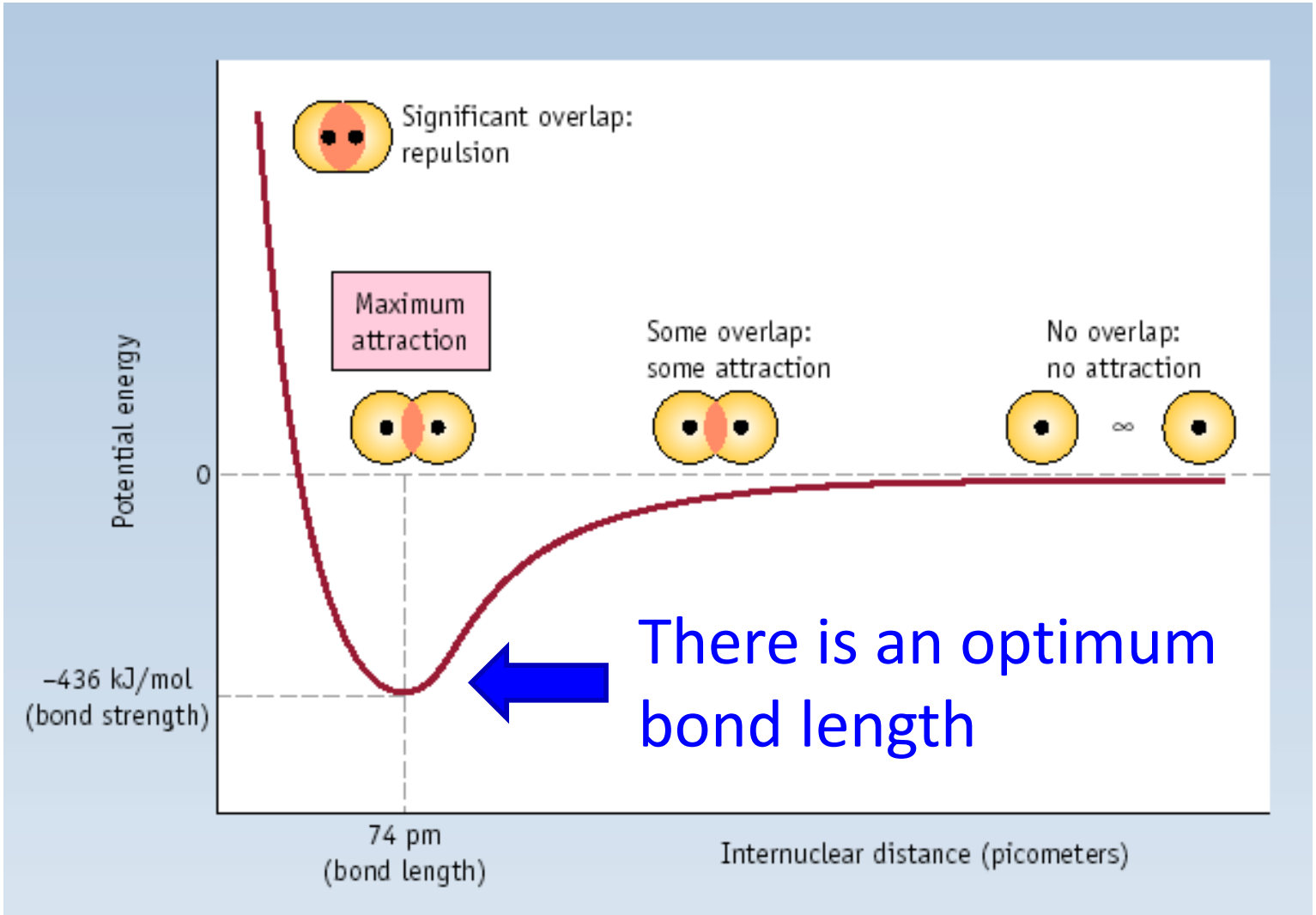


Molecular Orbital Theory (1)

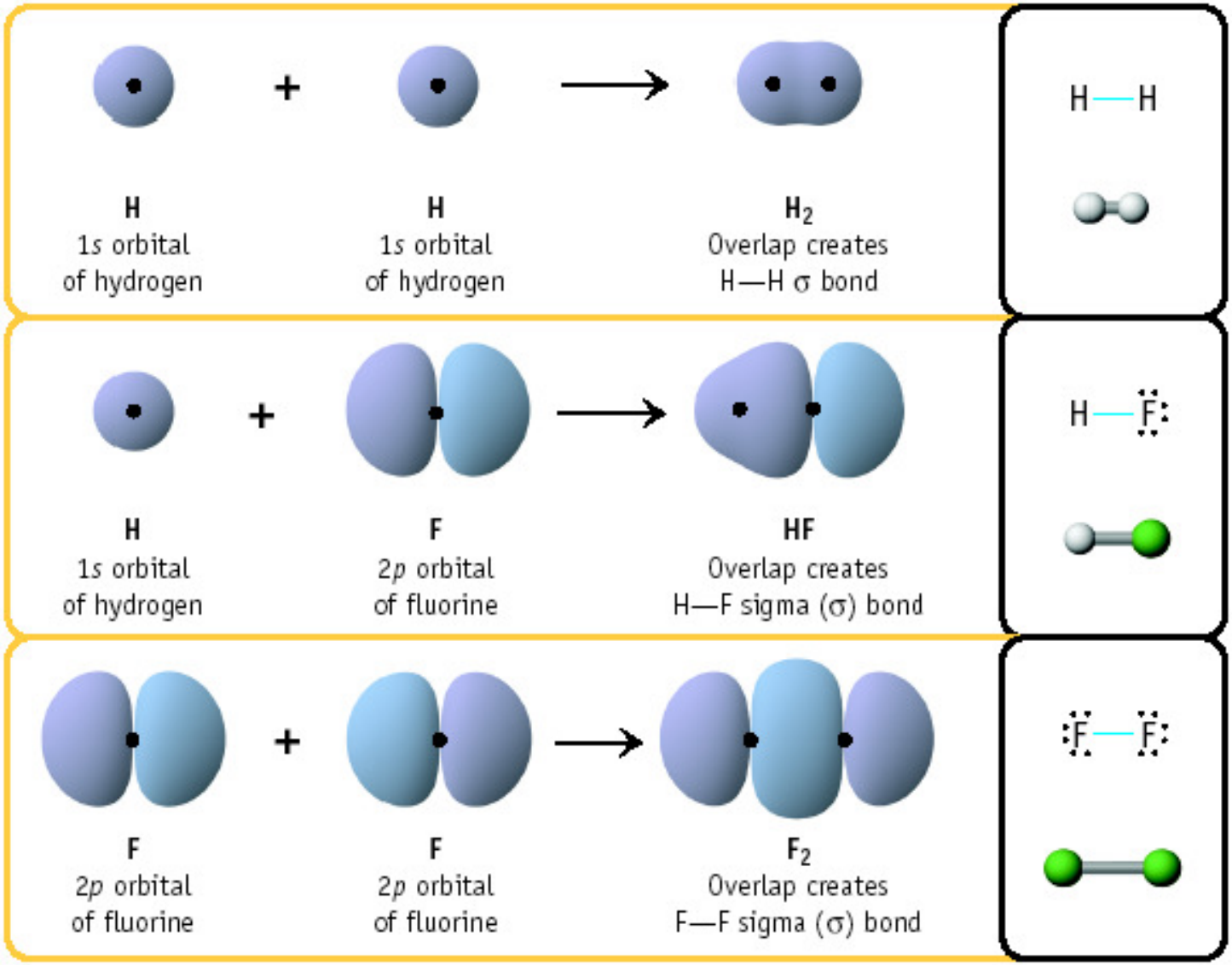
- Electrons are shared in a molecule when:
  - They have similar energy levels.
  - They overlap well.
  - They are close together.



Molecular Orbital Theory (2)

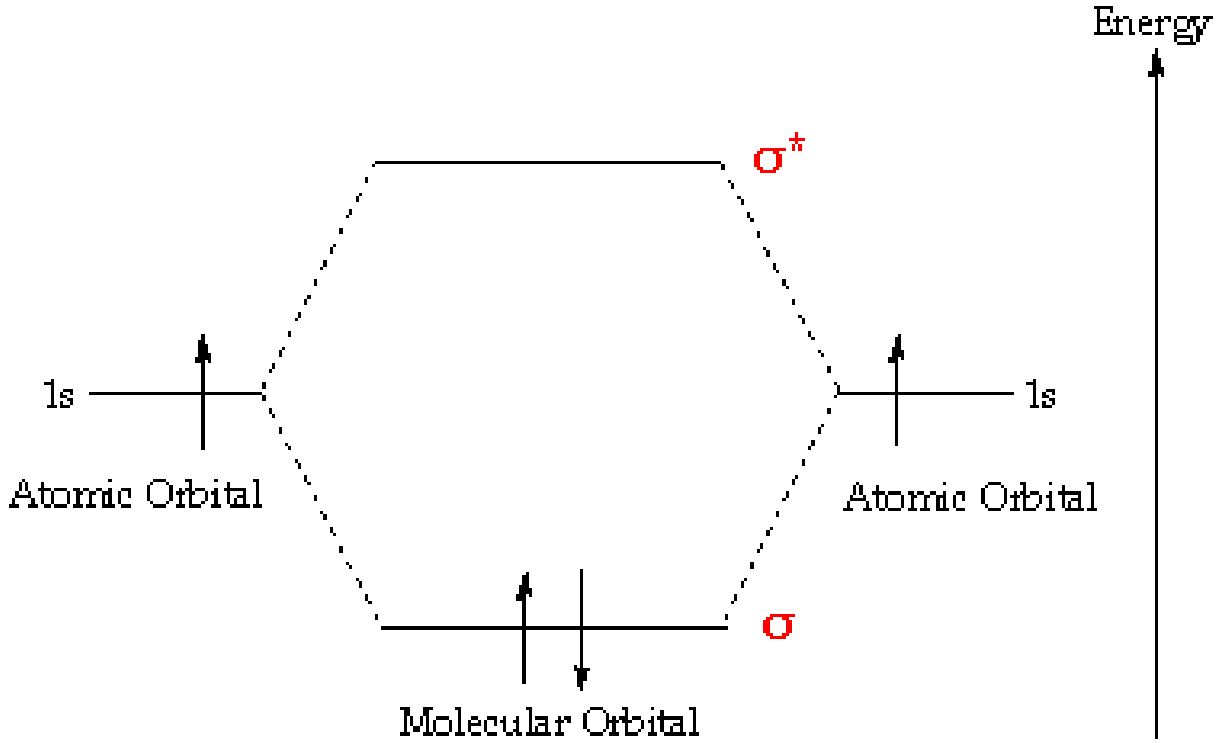


Molecular Orbital Theory (3)



Molecular Orbital Theory (4)

- Two similar atomic orbitals combine to form two molecular orbitals, one bonding (σ) and one antibonding (σ*).



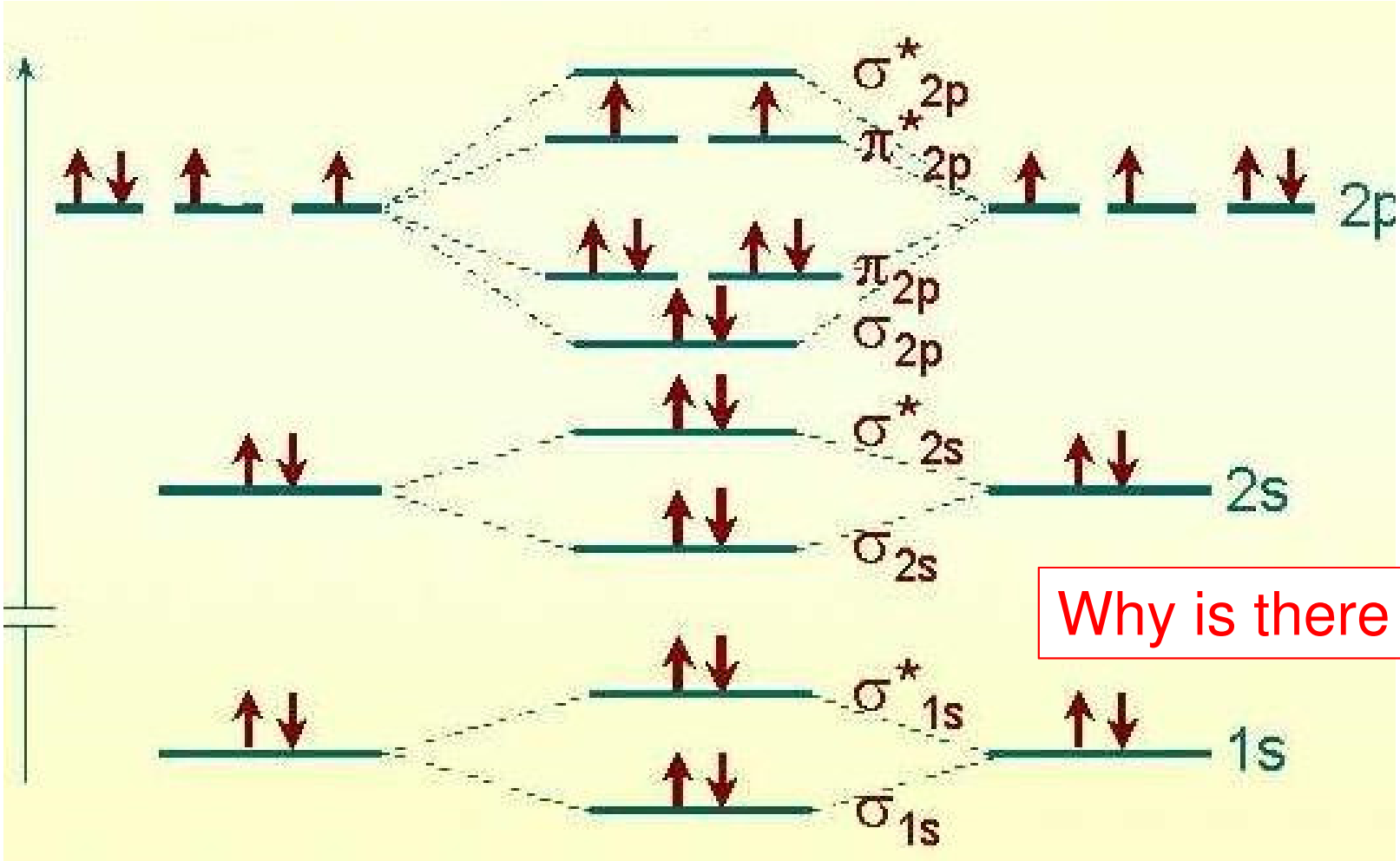
Molecular Orbital Theory (5)

- The electrons fill the molecular orbitals of molecules like electrons fill atomic orbitals in atoms
- Electrons go into the lowest energy orbital available to form lowest potential energy for the molecule.
- The maximum number of electrons in each molecular orbital is two. (Pauli exclusion principle)
- One electron goes into orbitals of equal energy, with parallel spin, before they begin to pair up. (Hund's Rule.)

(With an atom, we used the Aufbau Principle)

Molecular Orbital Theory (6)

MO Diagram for O_2



Why is there no He_2?

Molecular Orbital Theory (7)

MO Diagram for H_2O