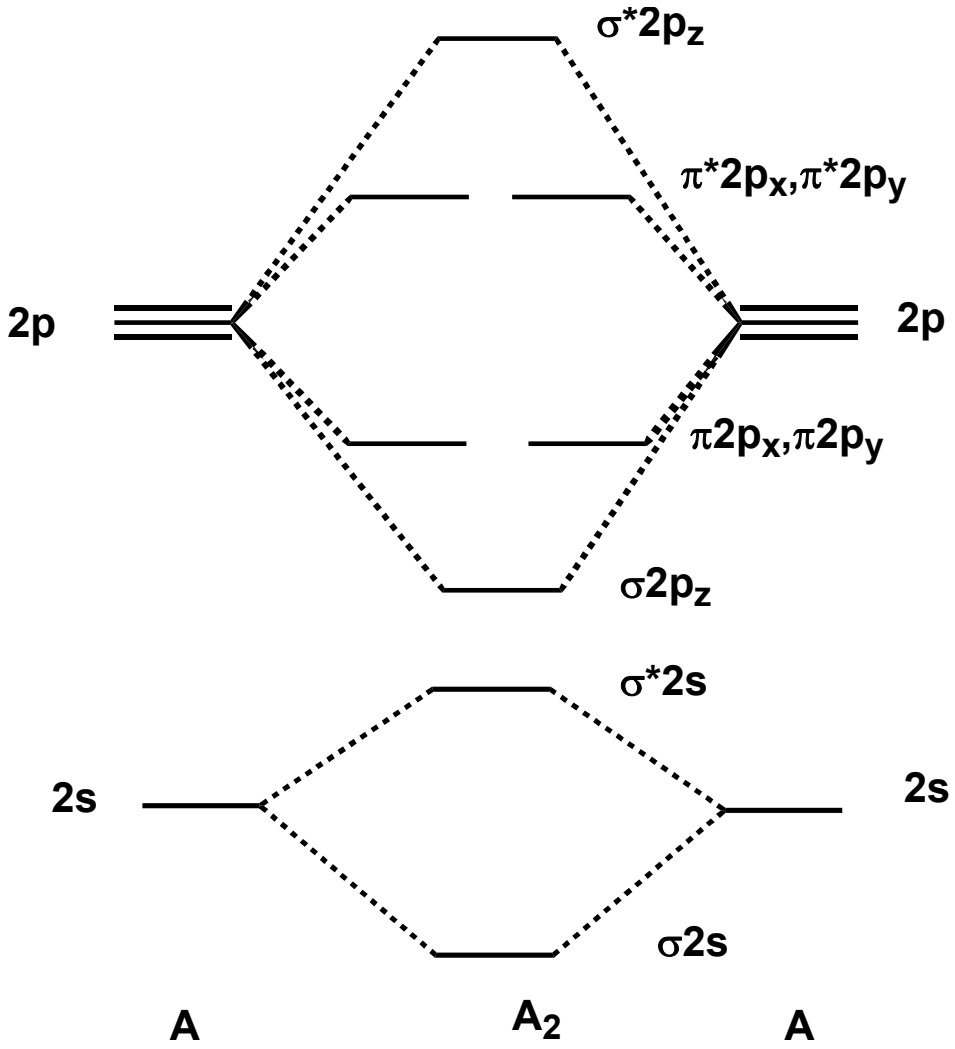
Lecture 16 MO Theory for Heteronuclear Diatomics

M.O.Energy Level Diagram for A_2 (A = O)



"No mixing of 2s and 2p"

O_2

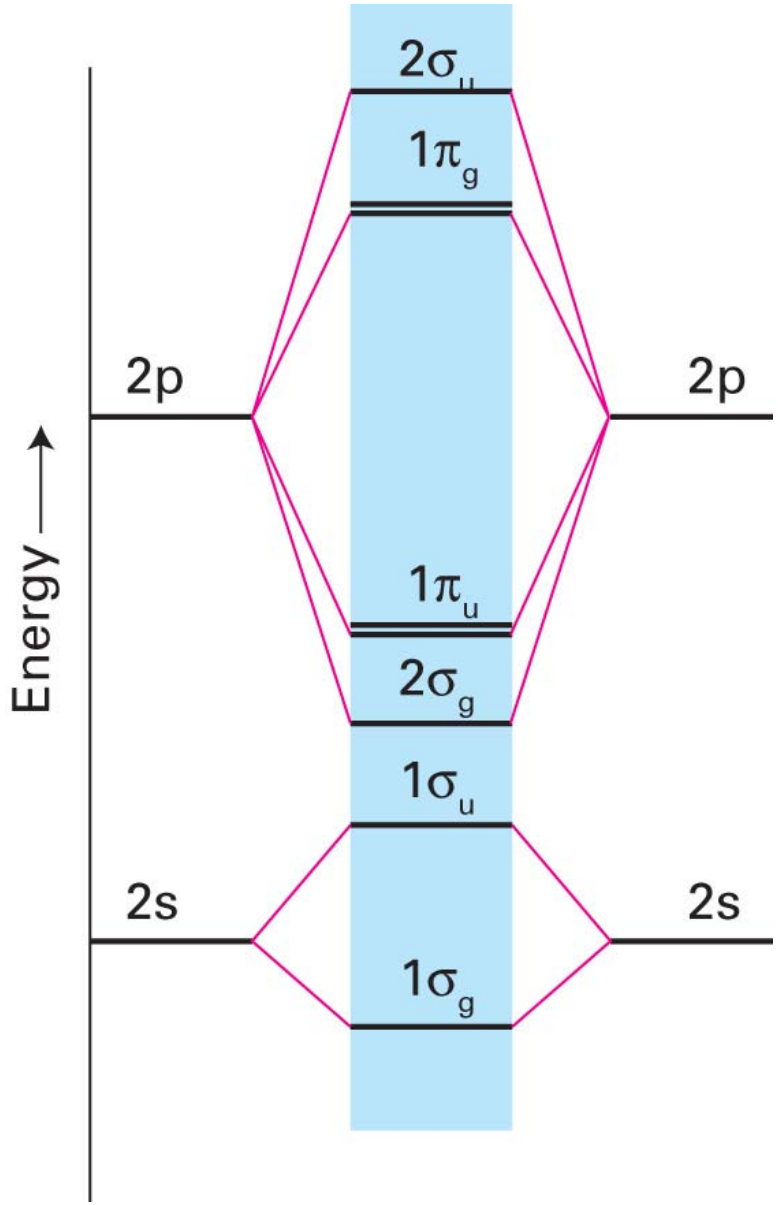
Electronic configuration: $\sigma_s^2 \sigma^*_s{}^2 \sigma_{pz}^2 \pi_{px}^2 \pi_{py}^2 \pi^*_{px}{}^1 \pi^*_{py}{}^1$

Note Hund's rule again! **Bond order = (8 - 4)/2 = 2 (double bond) and PARAMAGNETIC.**

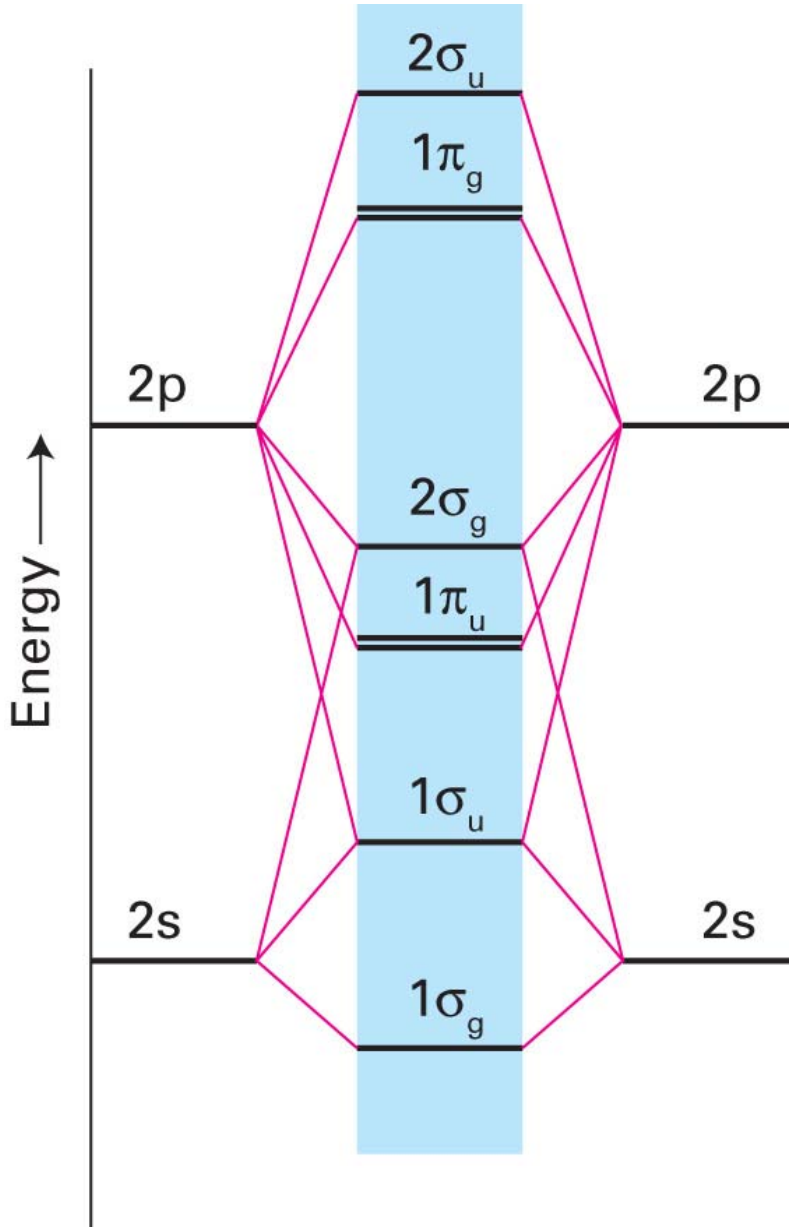
V.B. theory could not explain paramagnetism.

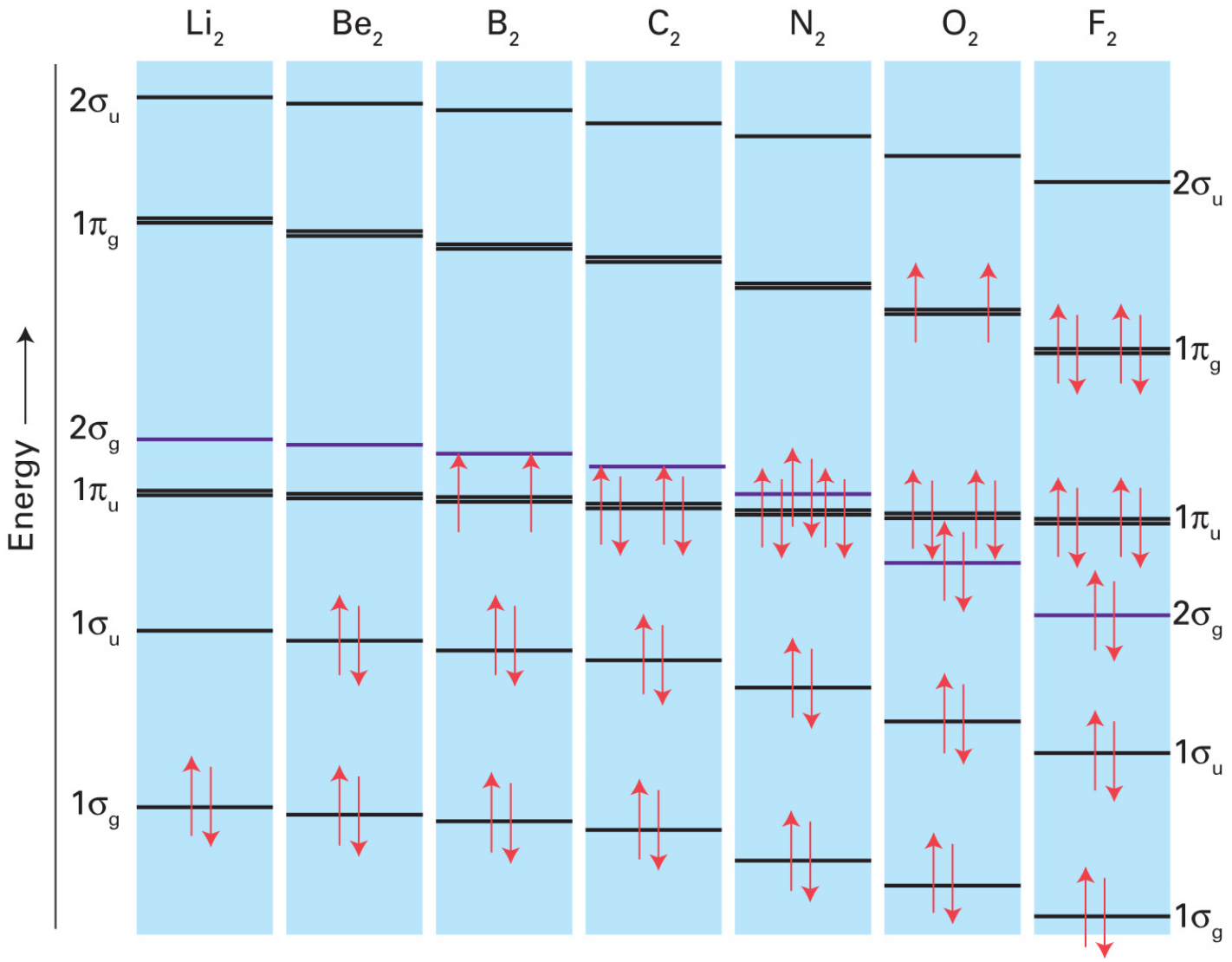
Lecture 16 begins here

MO energy level diagram for O_2 and F_2



MO energy level diagram for Li_2 through N_2





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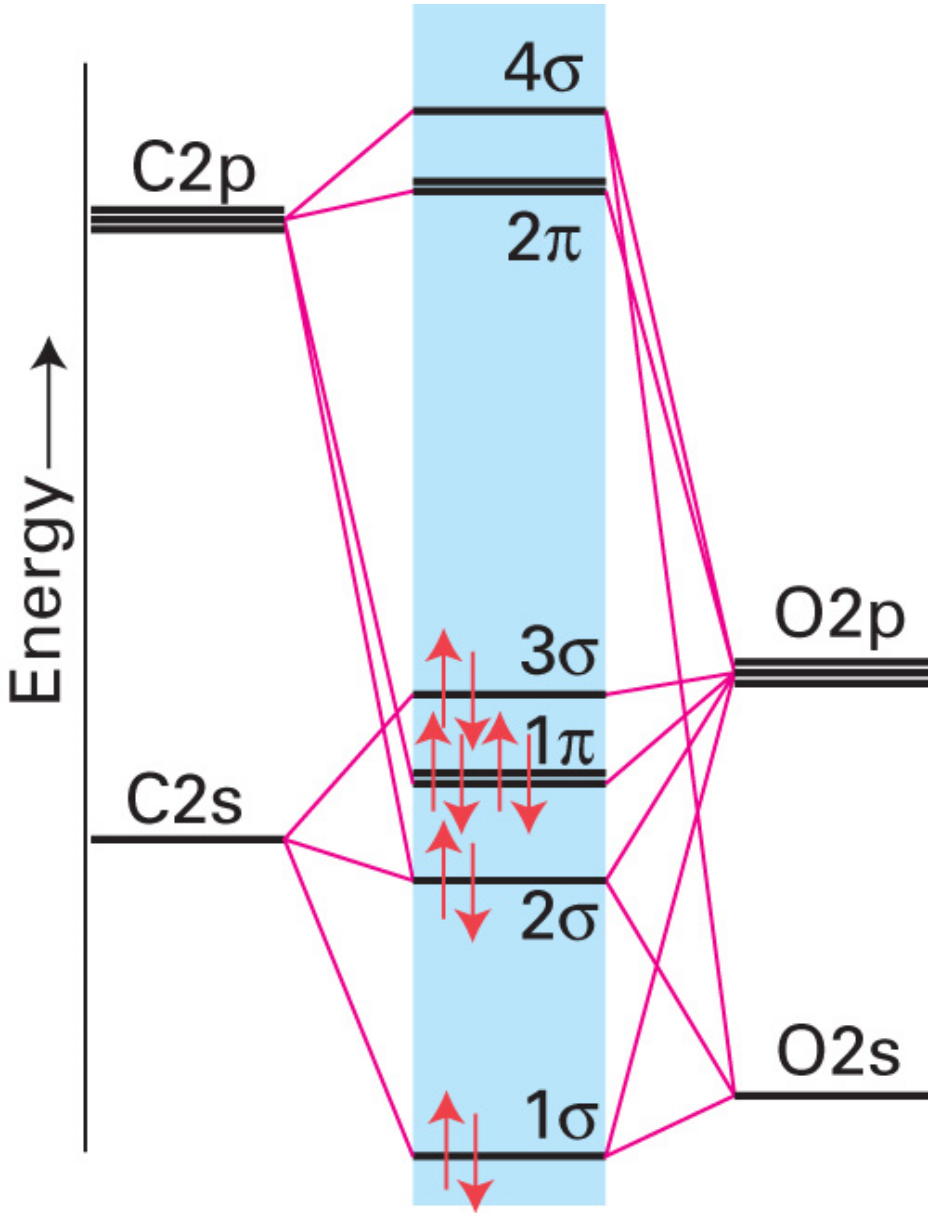
MO energy level diagram for CO



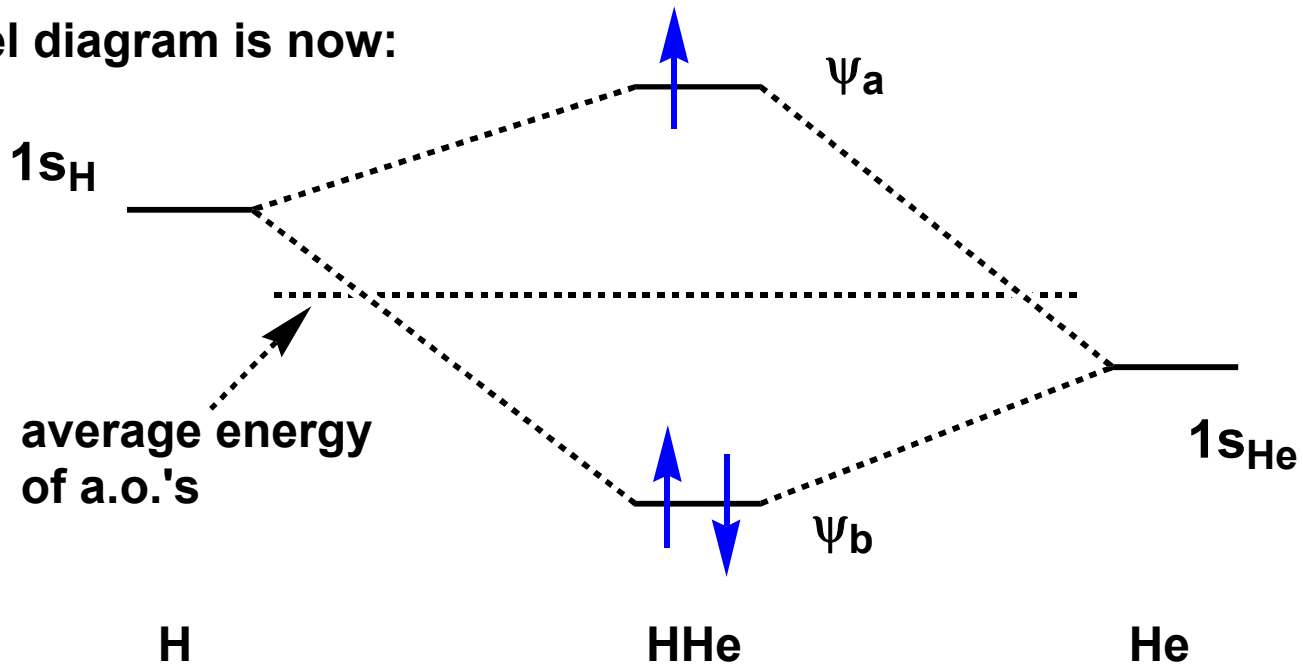
HETERONUCLEAR DIATOMIC MOLECULES

Simplest would be HHe. Differs from H_2 in two ways:

(1) A.O. energies for H, He different. He - greater nuclear charge, electrons more tightly bound.

(2) Now three electrons to feed into m.o.'s.

Energy level diagram is now:



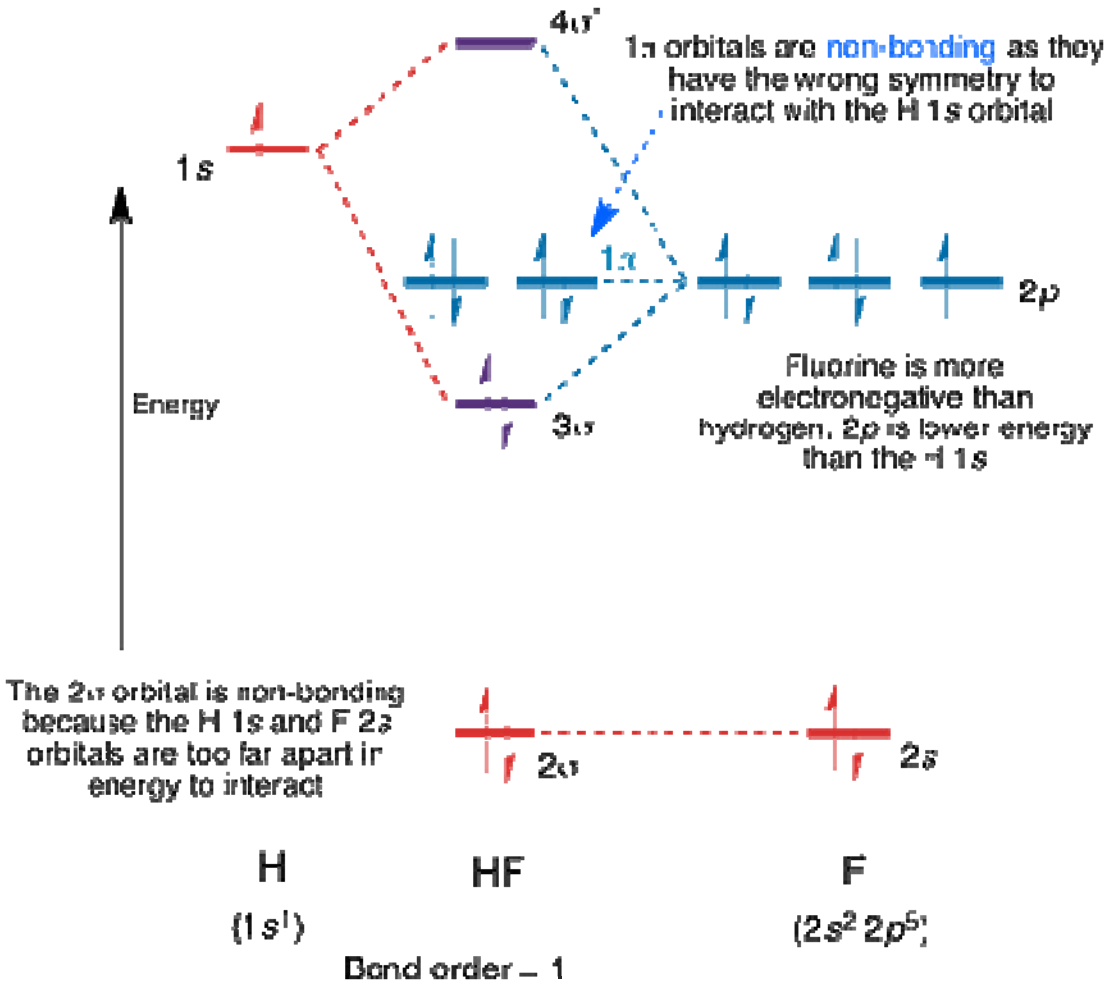
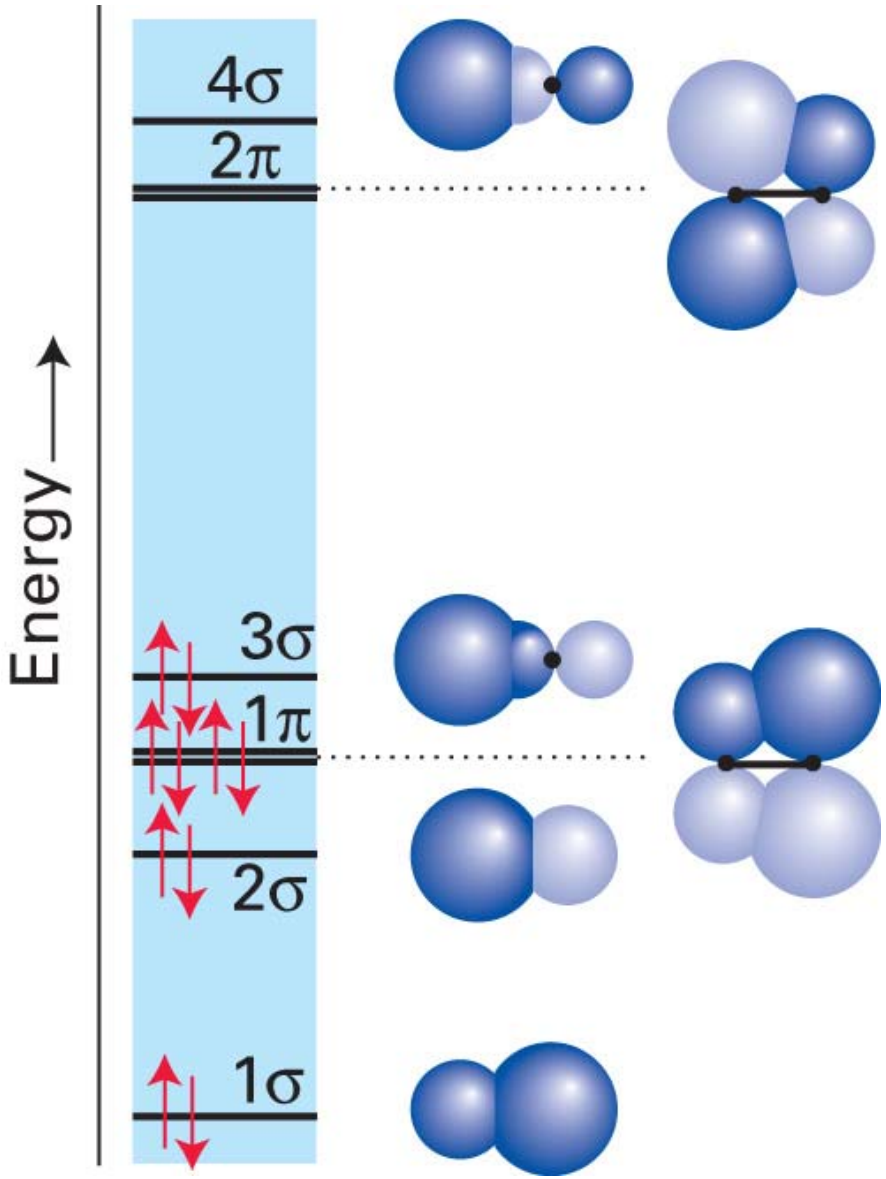
For heteronuclear diatomics, m.o.'s formed symmetrically above and below AVERAGE energy of constituent a.o.'s

For HHe, bond order = (2 - 1)/2 = 1/2 i.e. v. wk. "1/2" bond - not formed under normal conditions - v. unstable.

Unpaired electron, PARAMAGNETIC.

Note for "He_2" - extra electron in antibonding m.o. - therefore bond order = 0. Molecule does not exist - no force to hold atoms together.
He is monatomic gas.

MO for Heteronuclear Diatomics: HF



MO's for CO: the contour plots and significance for Metal Carbonyls