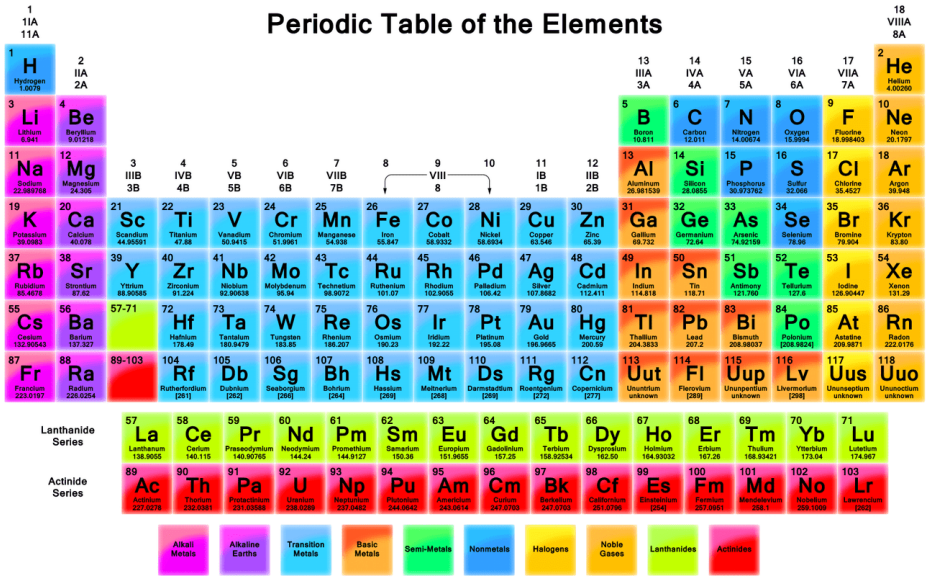
Note:
In diatomic molecules with lighter elements than oxygen

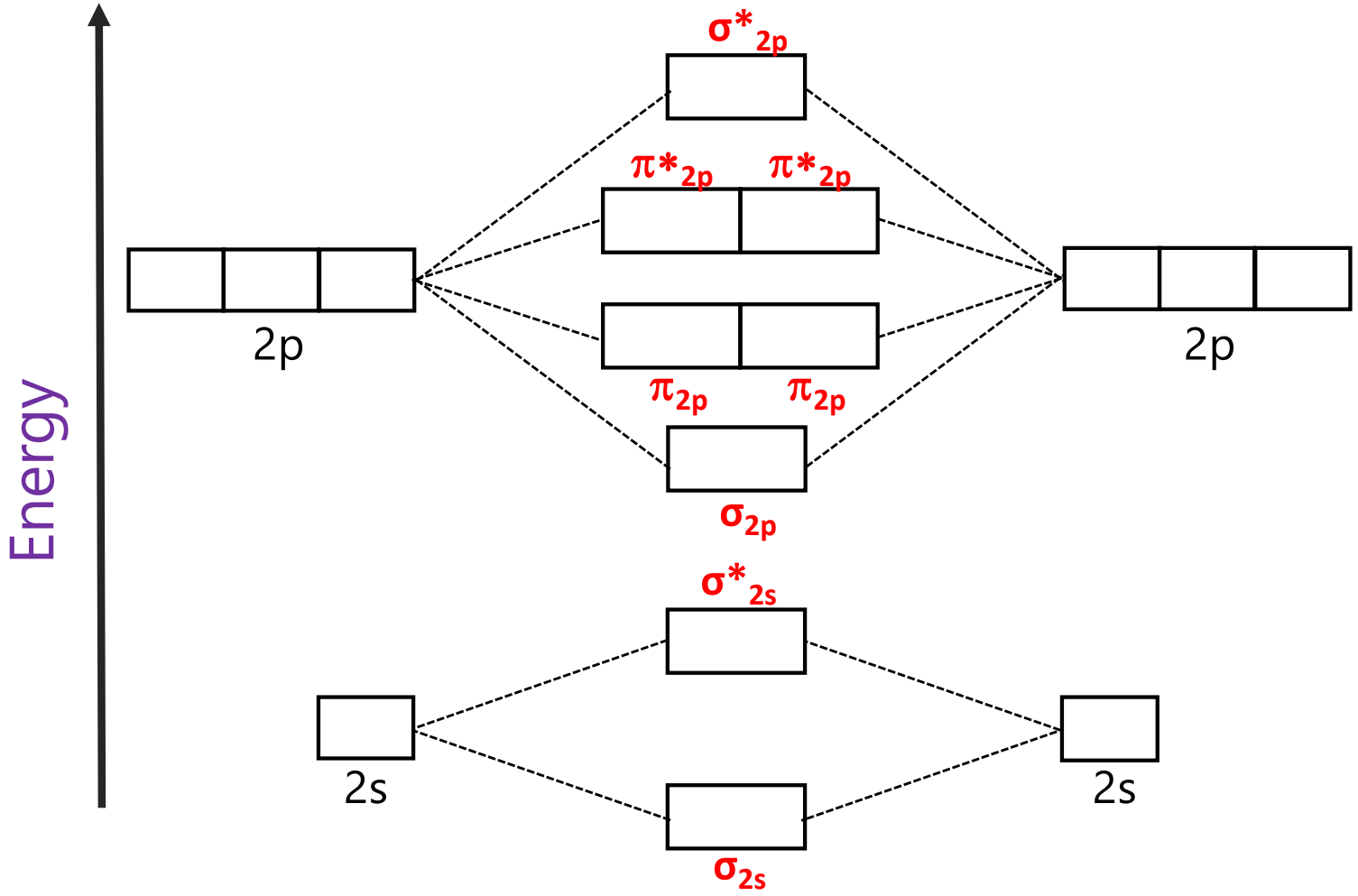
σ_{2p} & π_{2p} ENERGY LEVELS INVERT!

DUE TO MIXING OF s & p ORBITALS

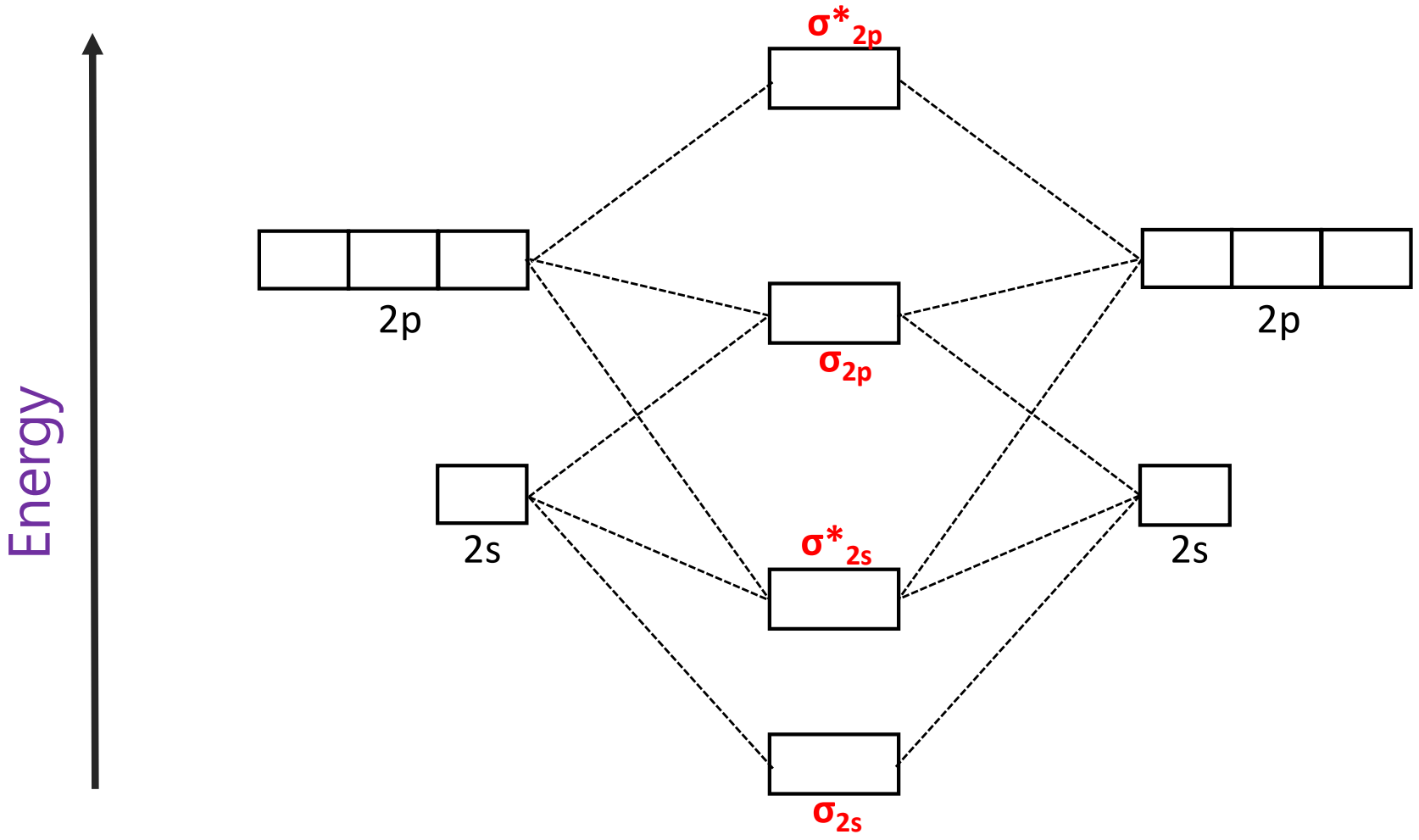


McGill

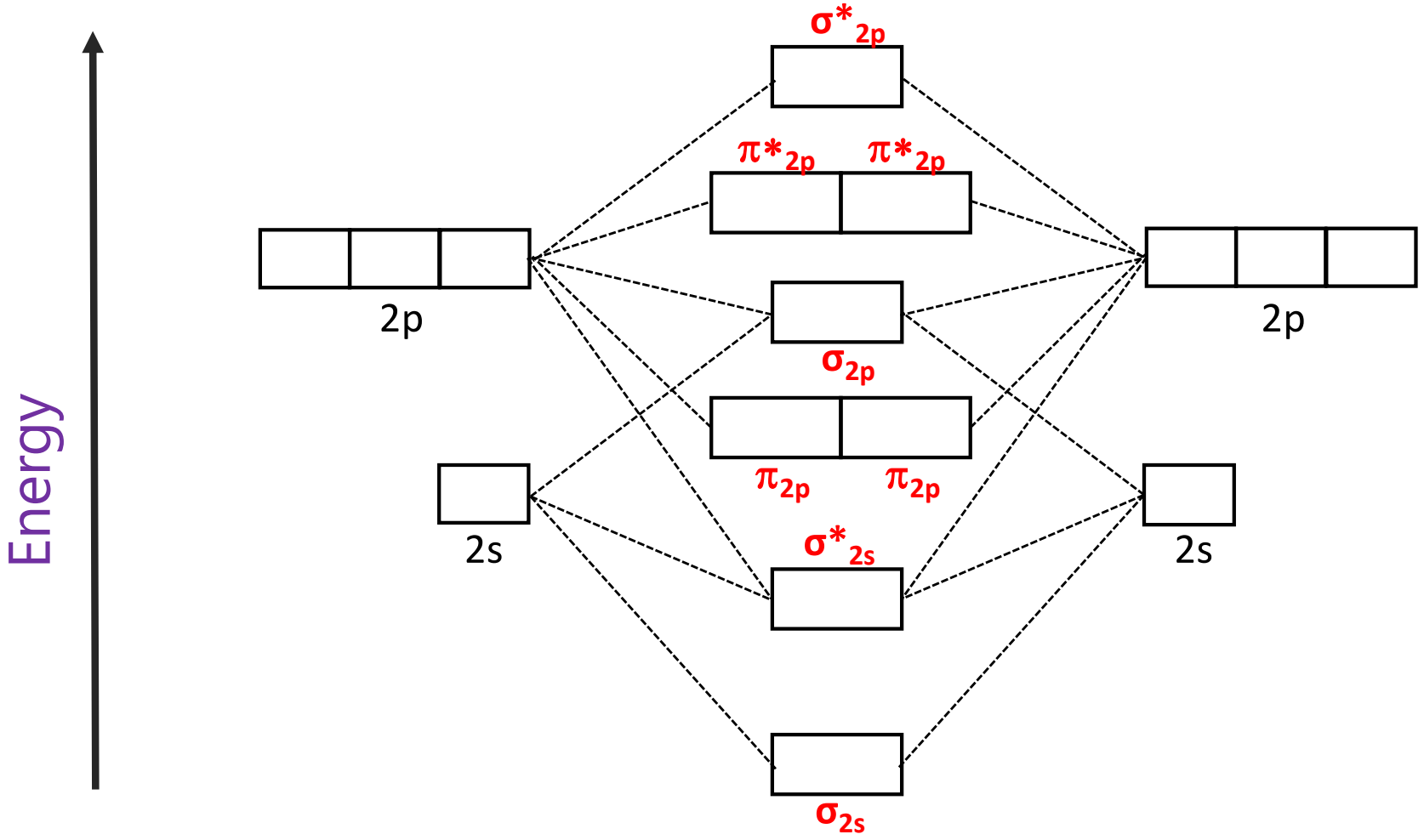
MO diagram for O_2 to F_2



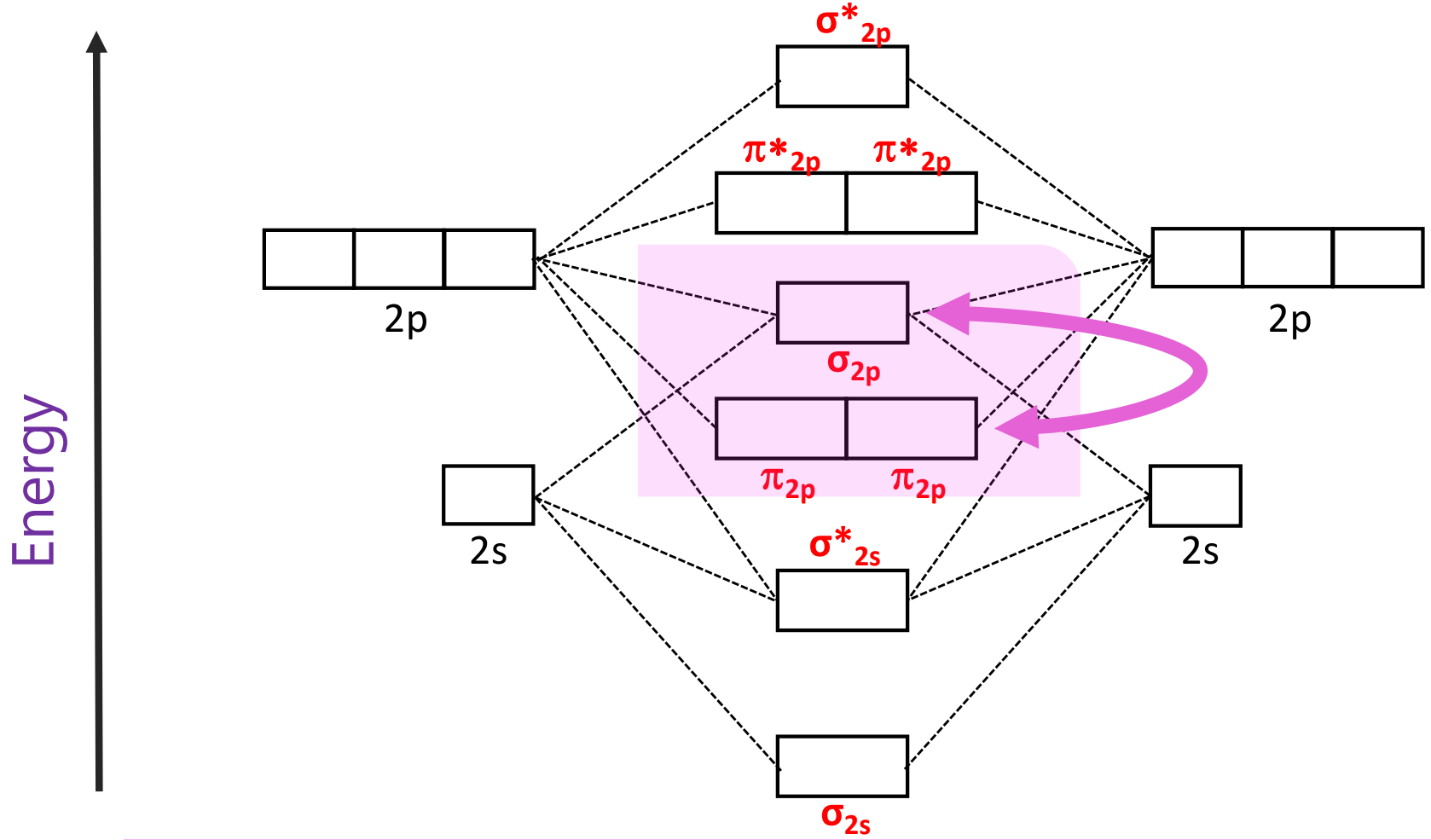
MO diagram for Li_2 to N_2 (sigma MOs only)



MO diagram for Li_2 to N_2 (sigma and pi MO)

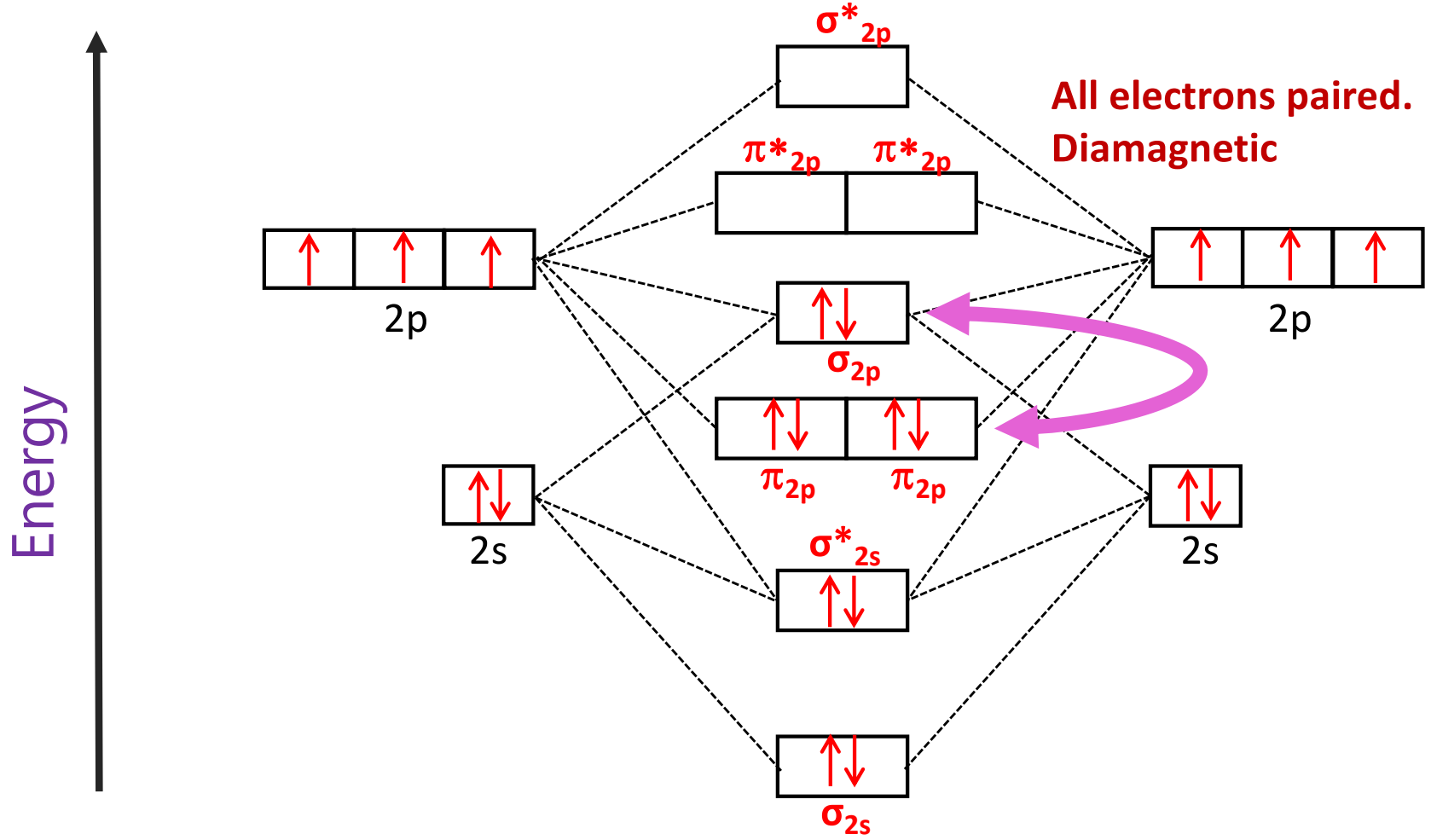


MO diagram for Li_2 to N_2



Compared to MO diagram for O_2 and F_2, mixing of 2s and 2p orbitals result in lower energy of π 2p orbitals as compared to σ 2p orbital

MO diagram for N_2

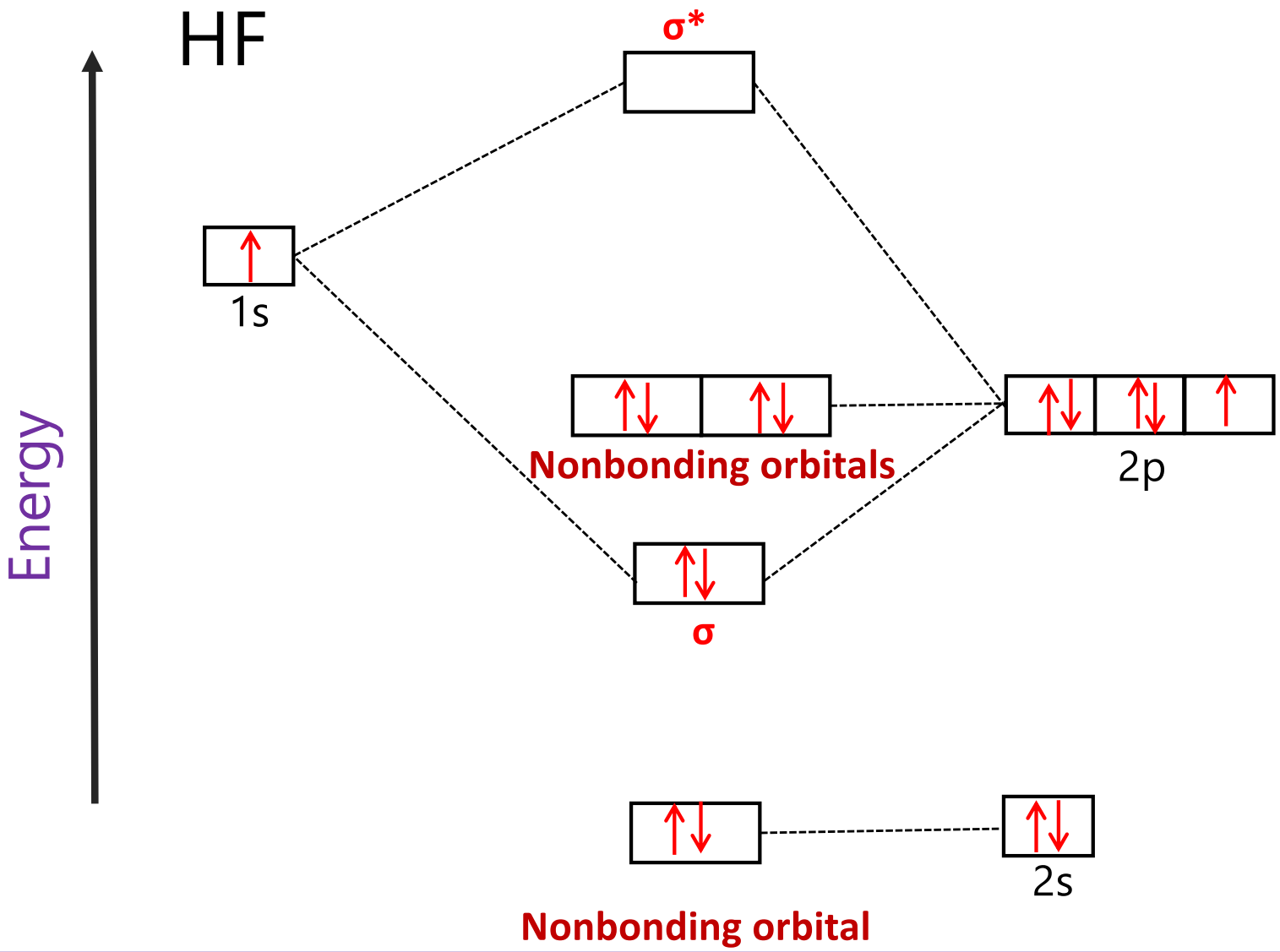


N $1s^2$ $2s^2$ $2p^3$

N $2s^2$ $2p^3$

5 electrons in the valence shell and in total we have 10 electrons

Heteronuclear diatomic molecules



Bond Order = ½ (no. of bonding electrons – no. of antibonding electrons)

BO in HF = ½ (2-0) = 1

Heteronuclear diatomic molecules

NO