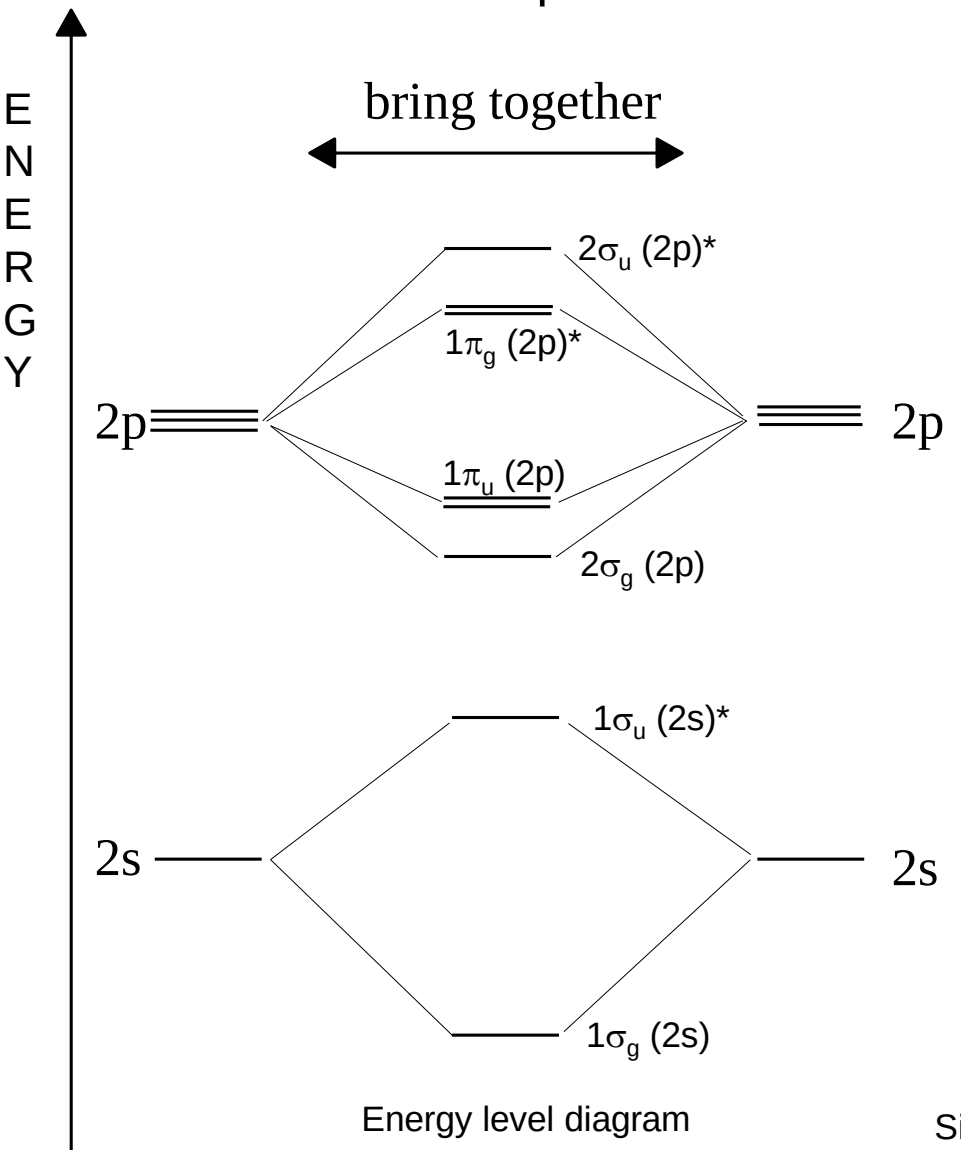
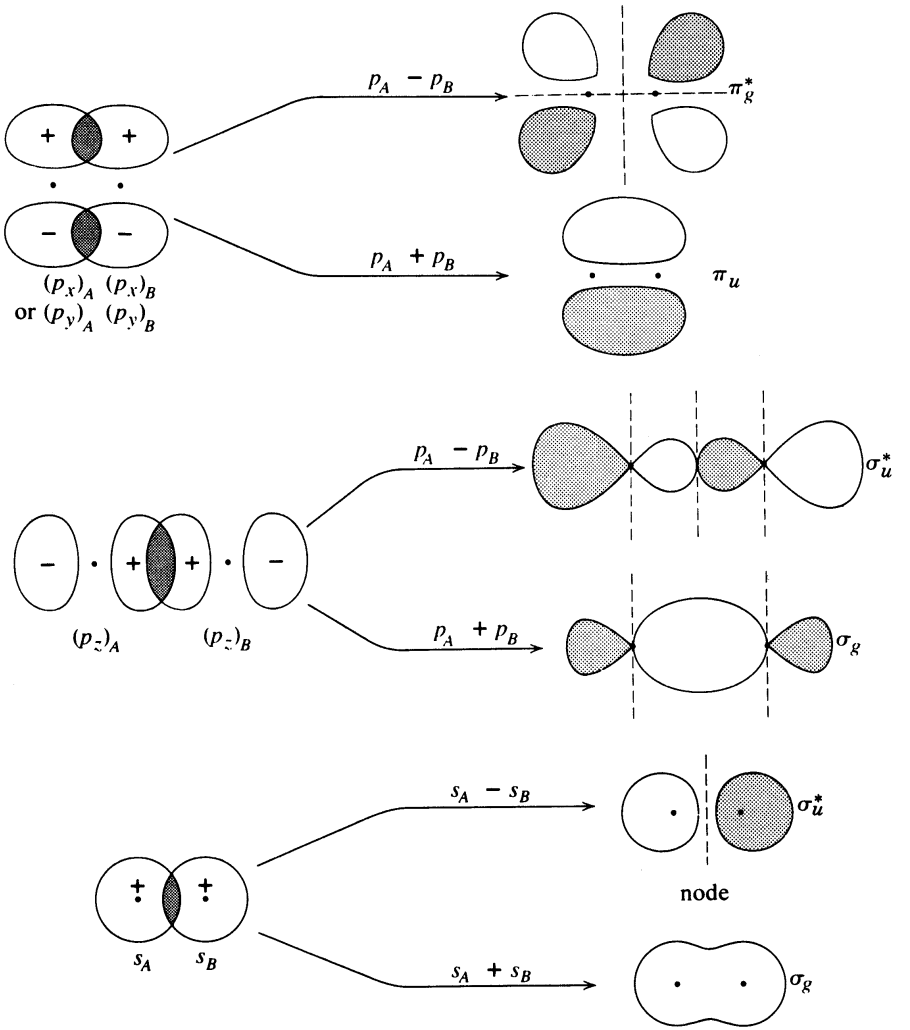
# MO Bonding

MO description of 2nd row homonuclear diatomic molecules

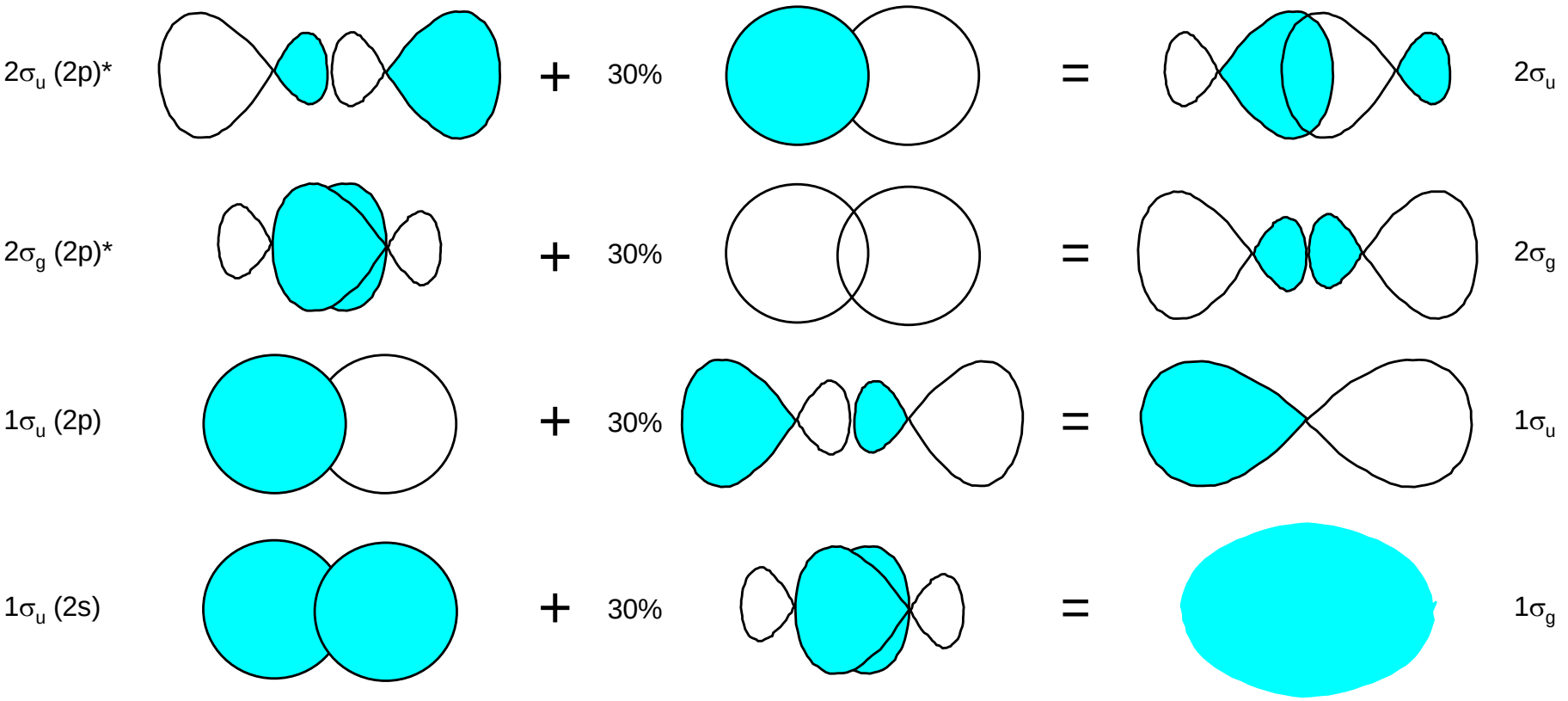



Energy level diagram

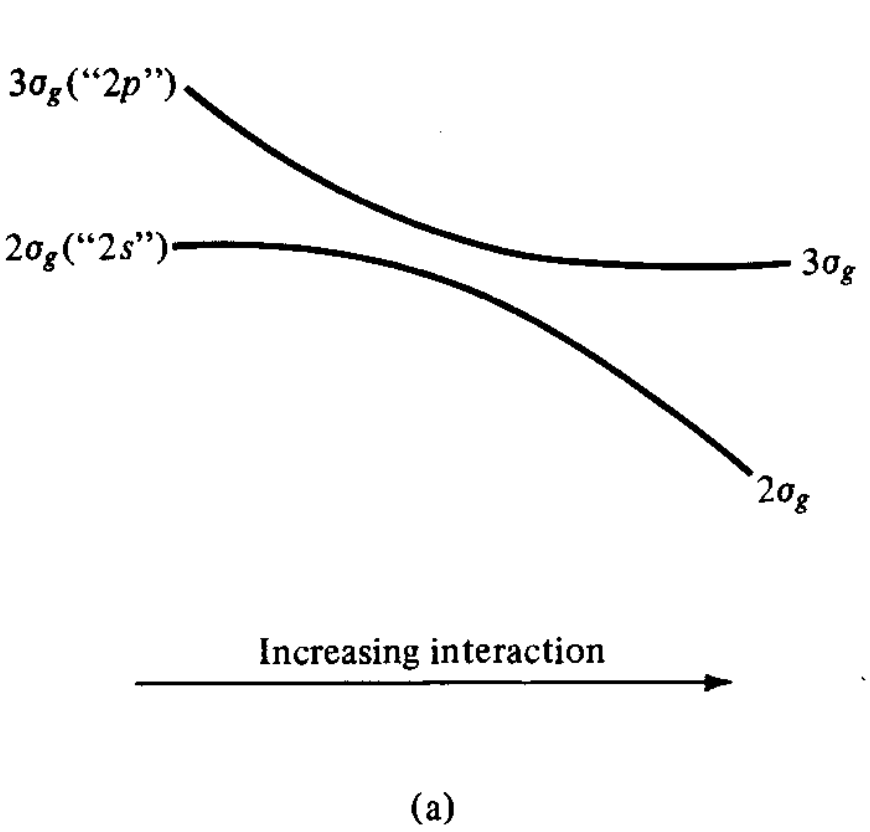



Sigma and pi overlap leading to bonding and antibonding MO's

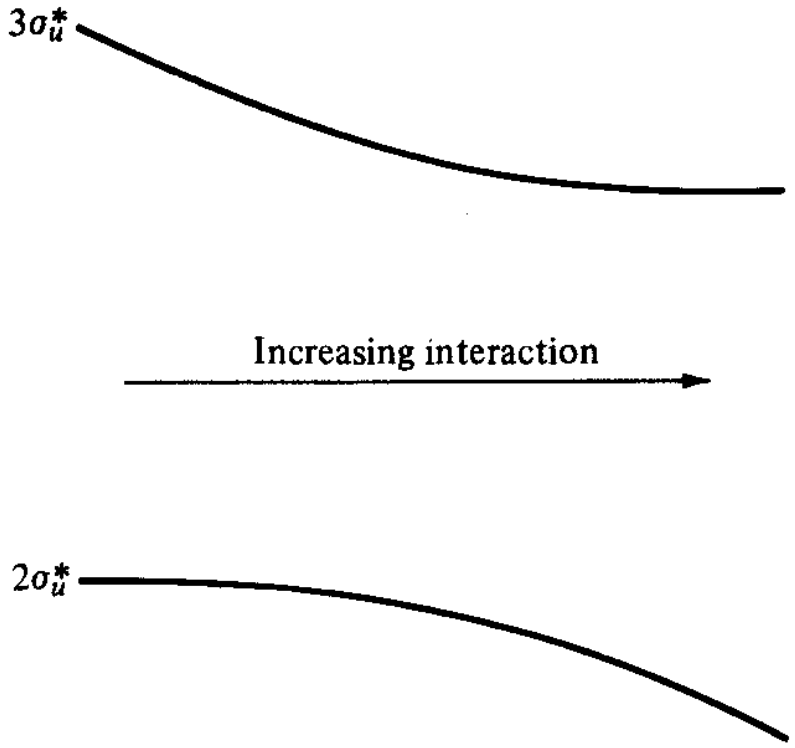
# Mixing of MOs



# Mixing of MOs



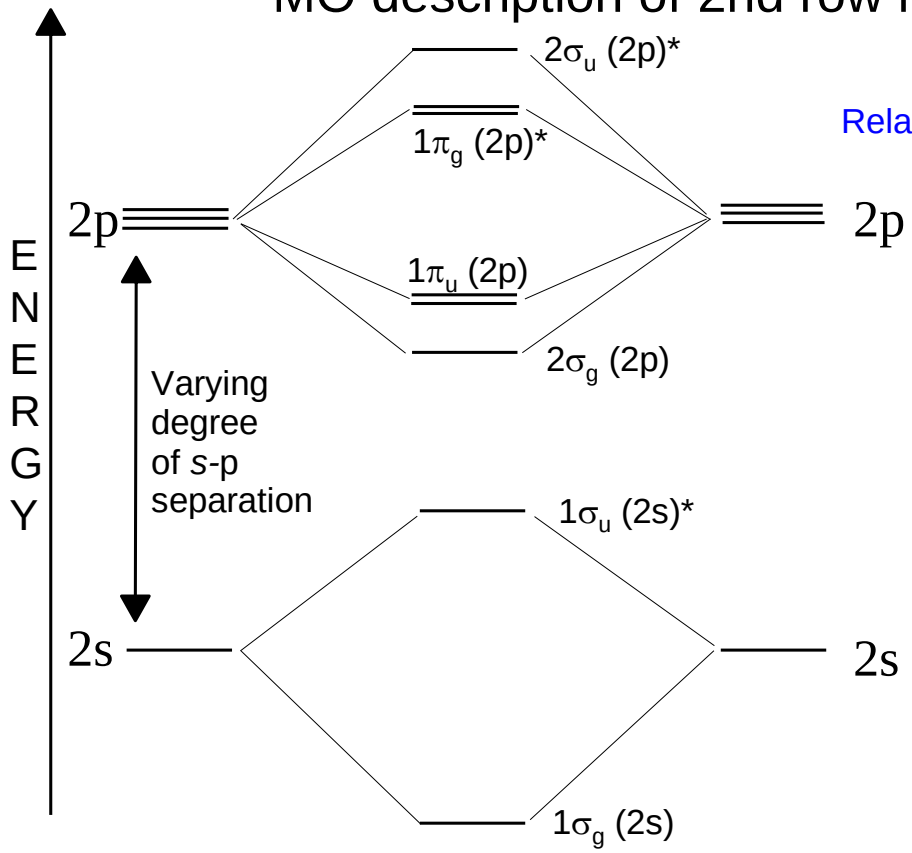

(a)



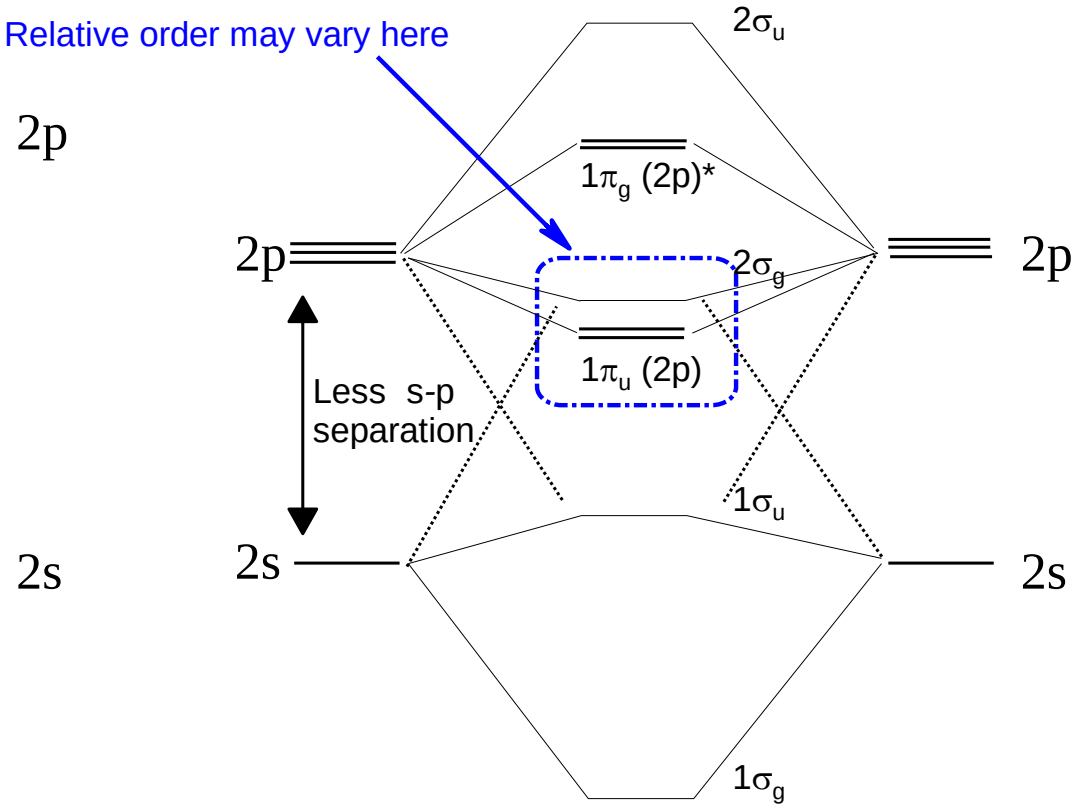

(b)

# MO Bonding

## MO description of 2nd row homonuclear diatomic molecules



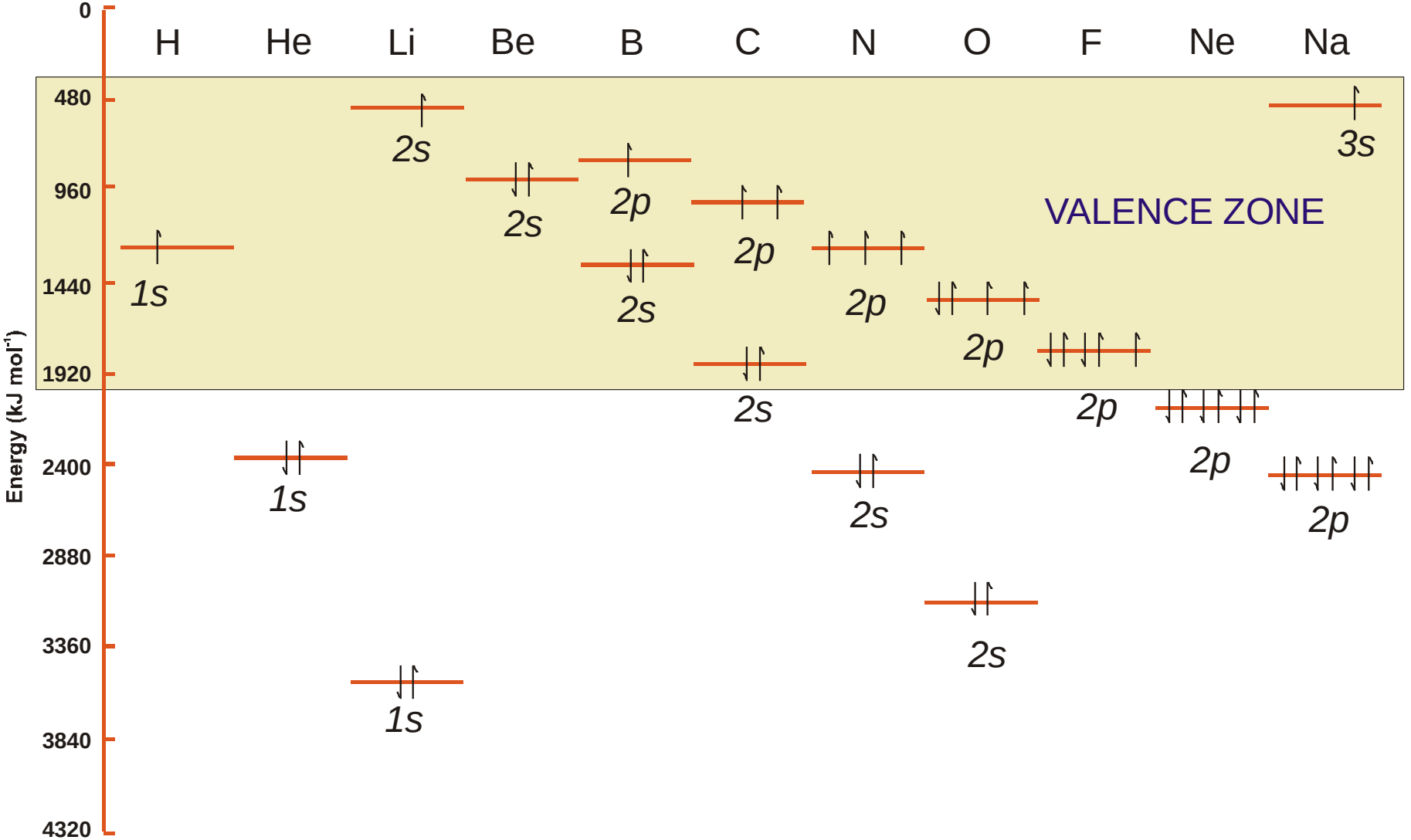

Energy levels in original diatomic construction



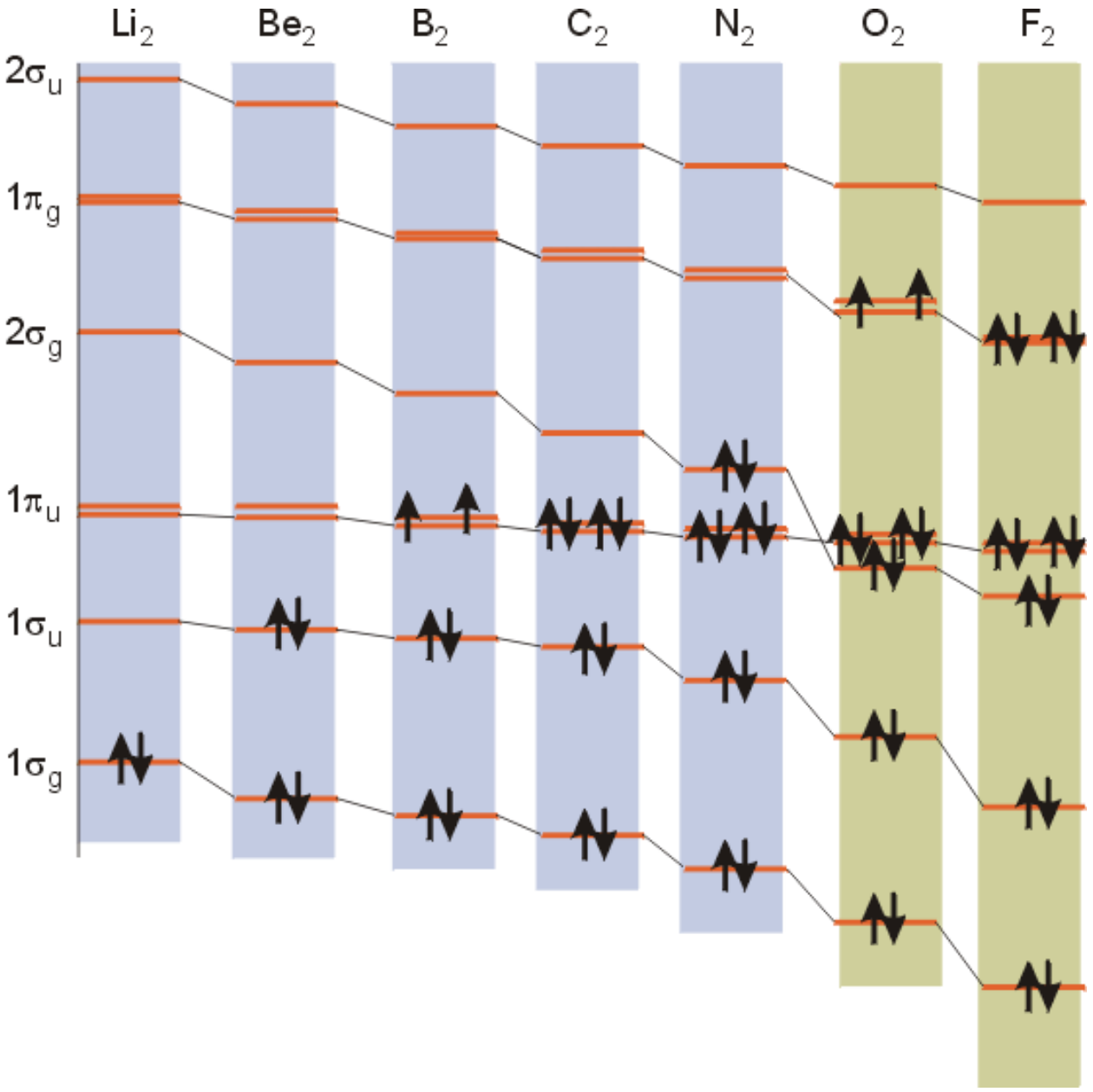

Energy levels in re-mixed diatomic

# Valence AOs

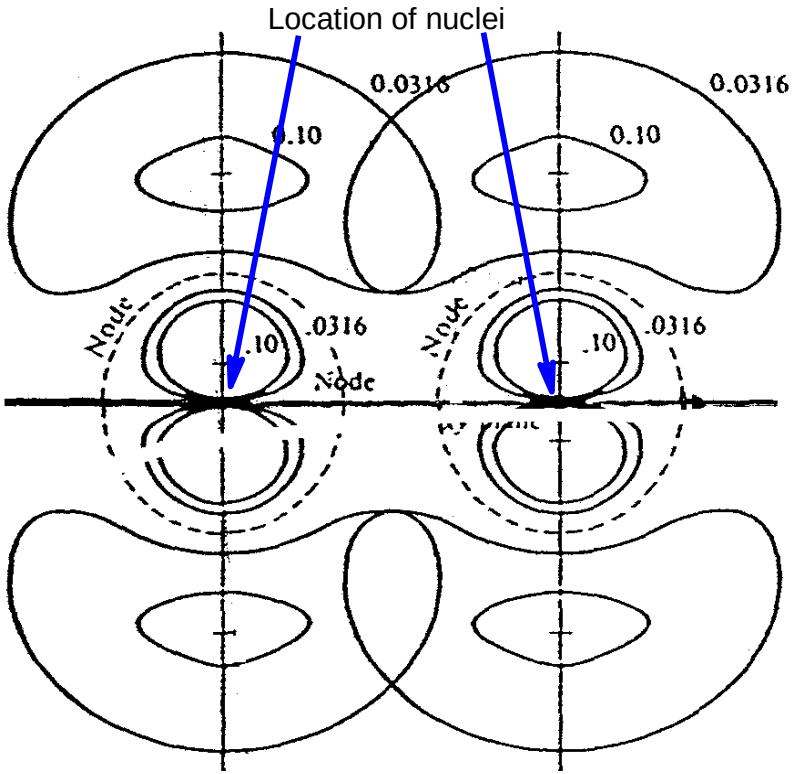
- Valence AOs have the correct properties to interact to form MOs.



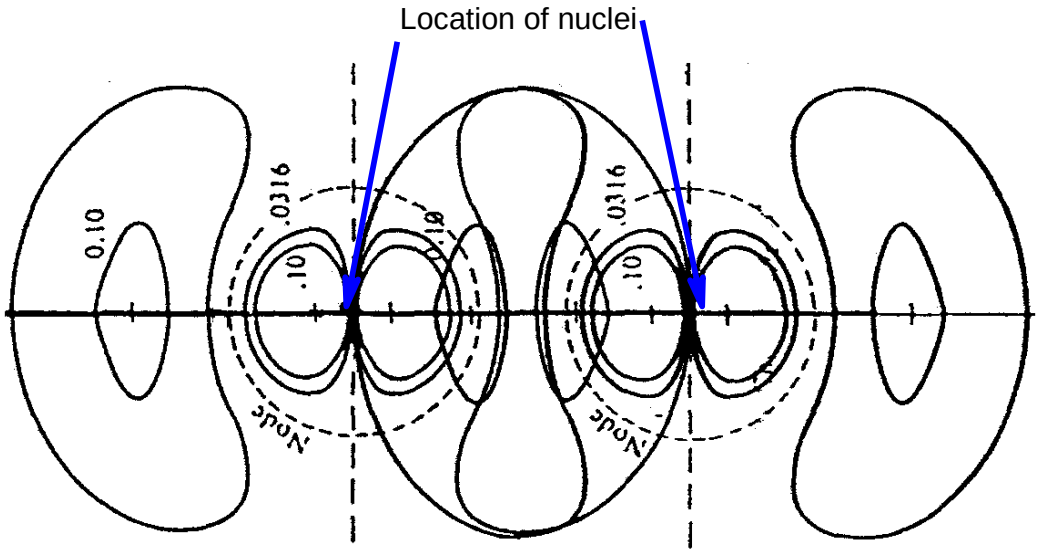
# 2nd Row Diatomics



# σ versus π Overlap for the 3rd Row



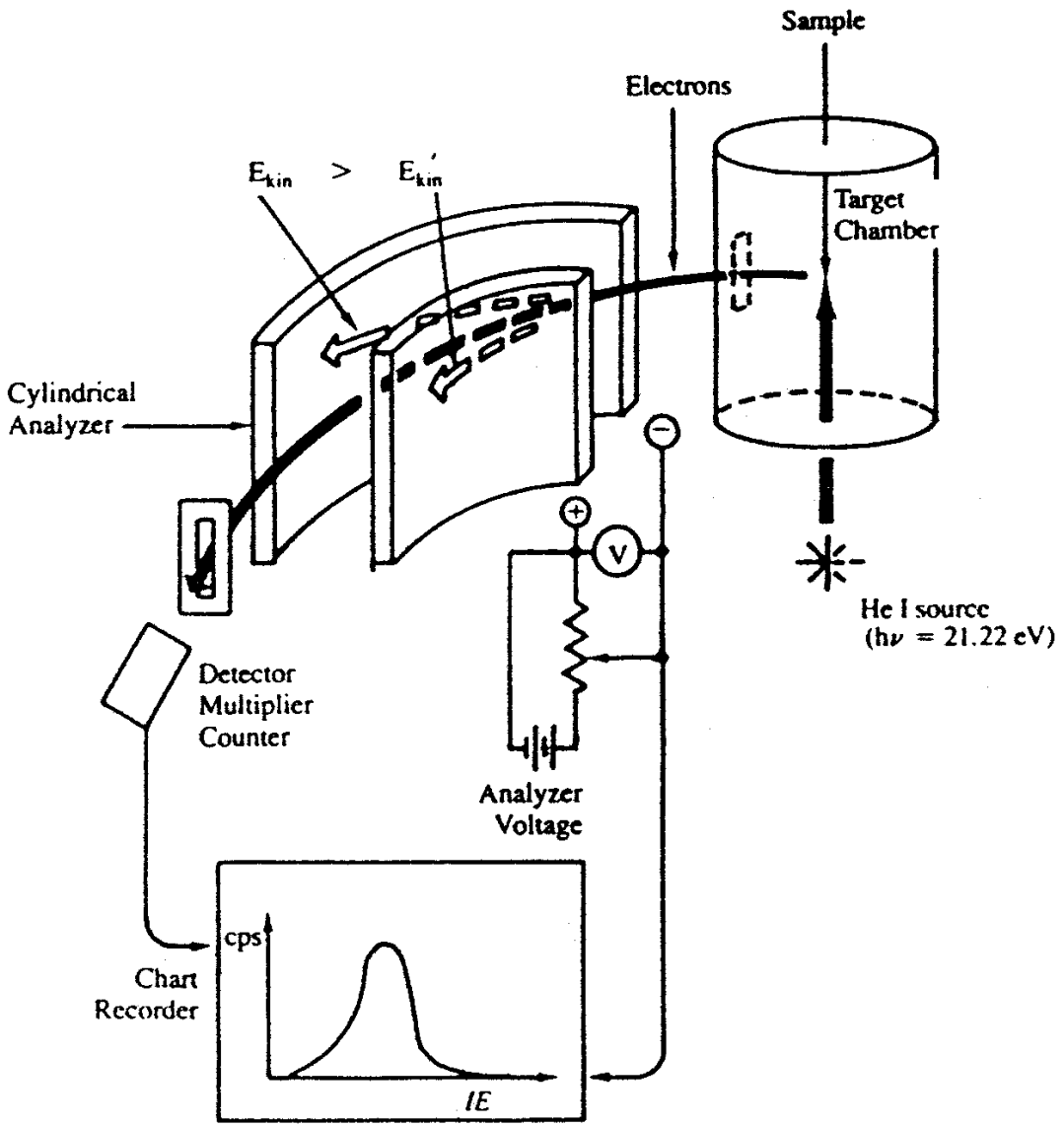

Two *3p* orbitals in π bonding orientation at the distance of a triple bond




Two *3p* orbitals in σ bonding orientation at the distance of a triple bond

- π overlap is generally not favourable for 3rd row and heavier elements.
- Double bond rule.

# Photoelectron Spectroscopy




Sources:

He(I) line of 21.22 eV

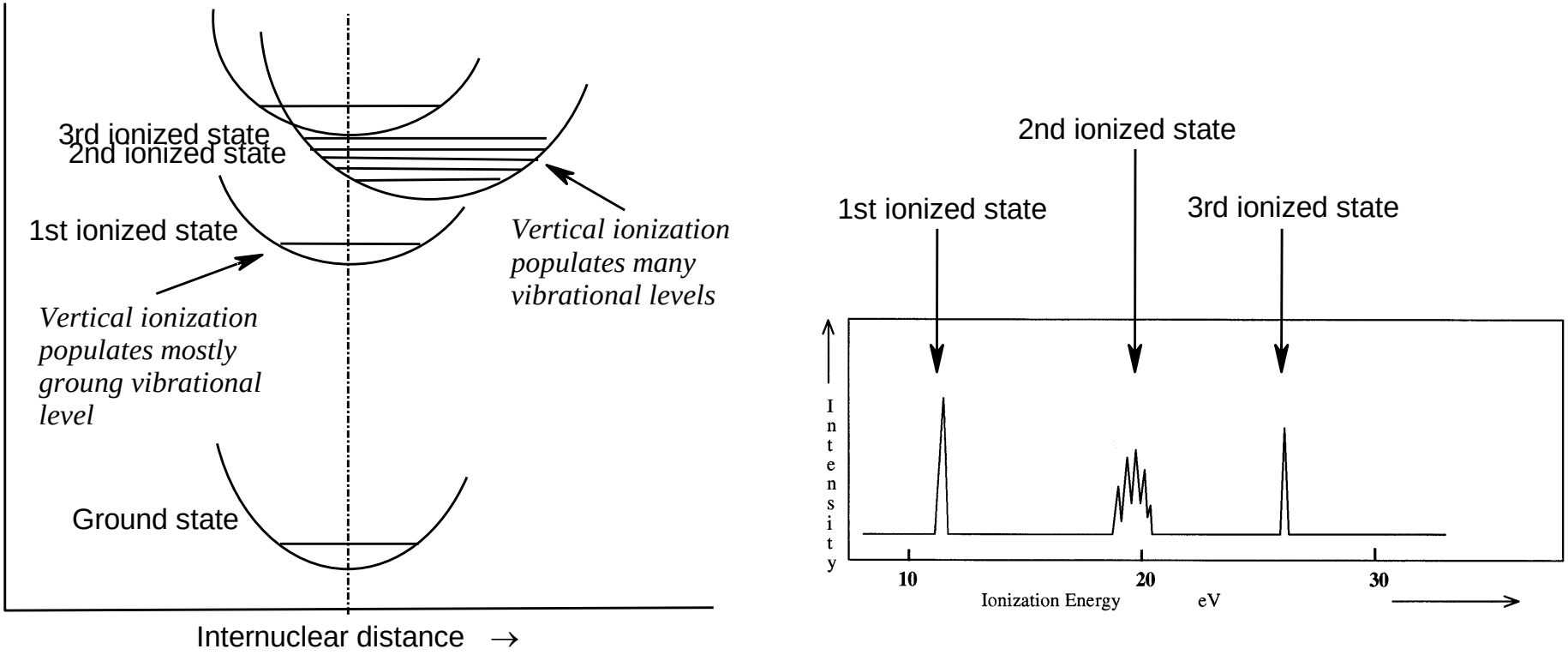
He(II) line of 40.8 eV

$E_{kin} = hv - I_1$

Koopman's Theorem:

$I_1 = -$ E(orbital)

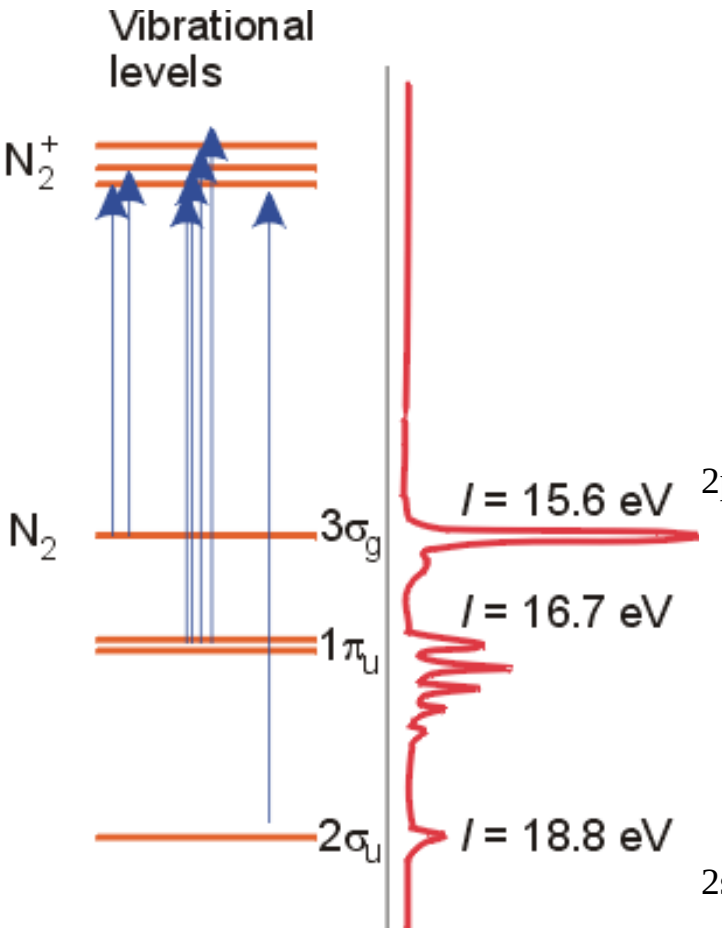
# Photoelectron Spectroscopy

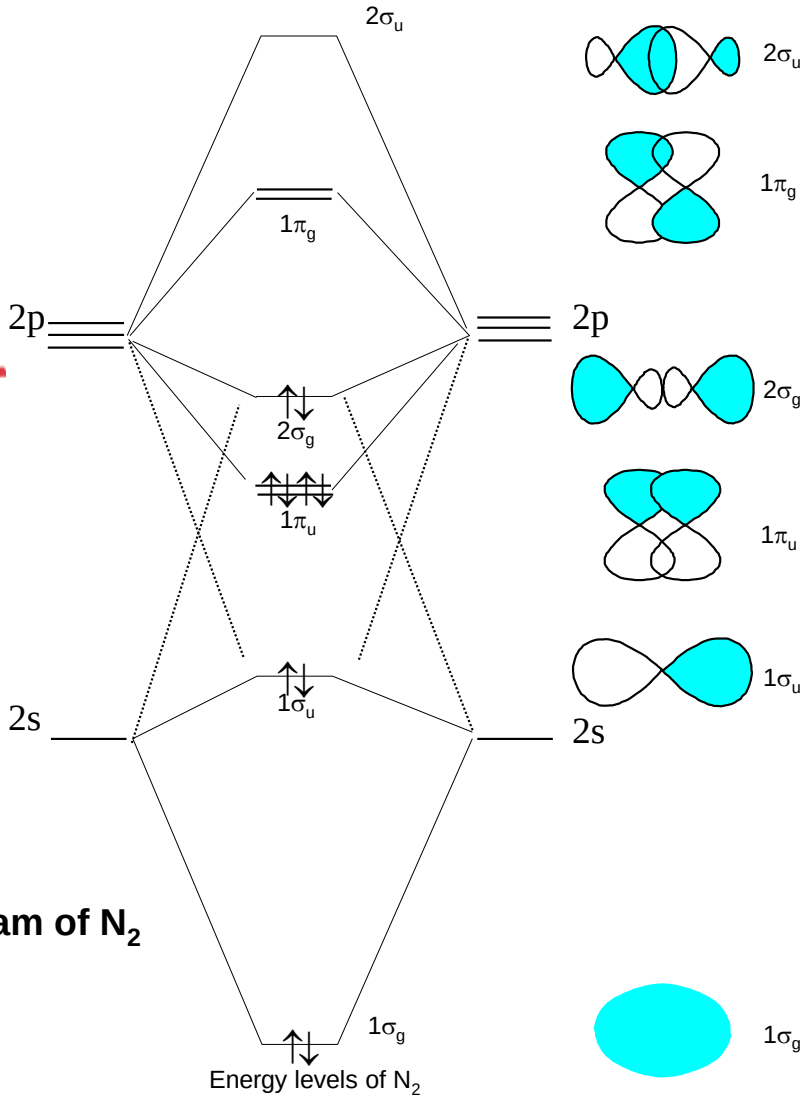



Schematic diagram of the UV-PES experiment and the output

- Vibrational fine structure for bonding and antibonding MOs

# MO Diagram for Dinitrogen




**Using a UV-PES to scale the MO diagram of $N_2$**