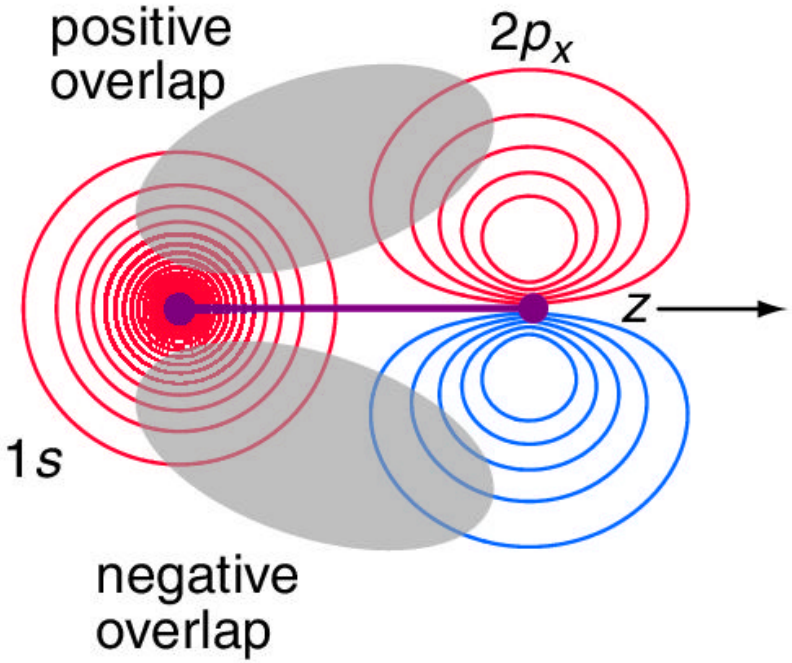
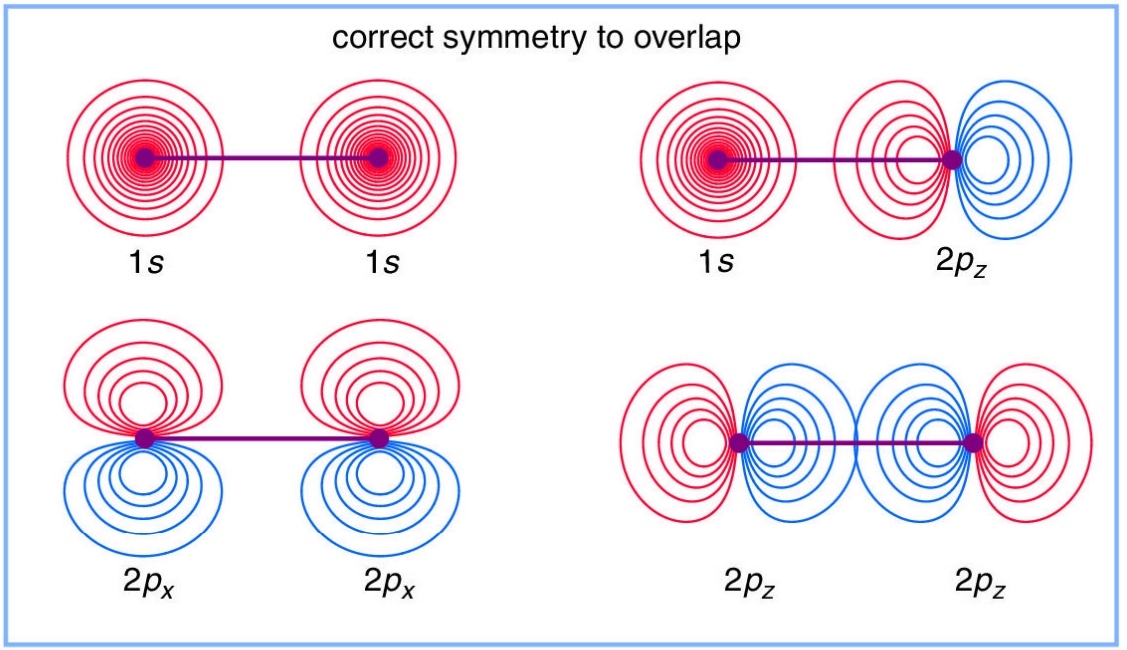
Rules for Forming MOs: 1

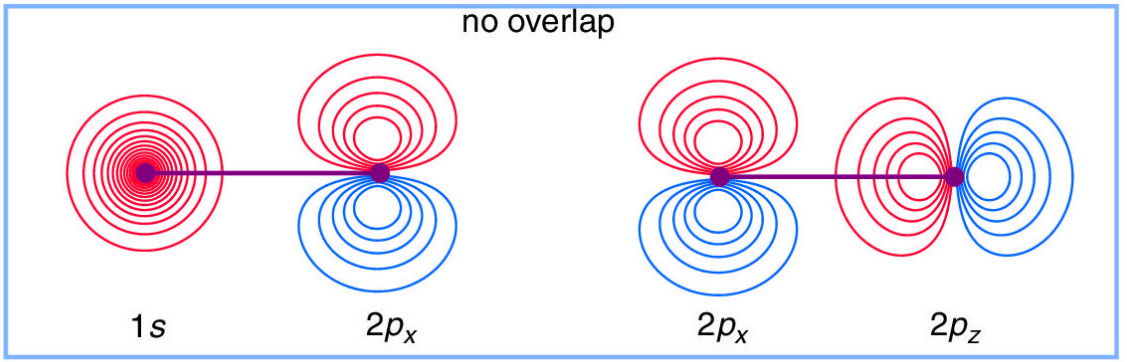
Combining certain number of AO's produces the same number of MO's e.g. combining 4 AOs give 4 MOs

Rules for Forming MOs: 2

Recall: Only AO's of the correct symmetry will give MOs

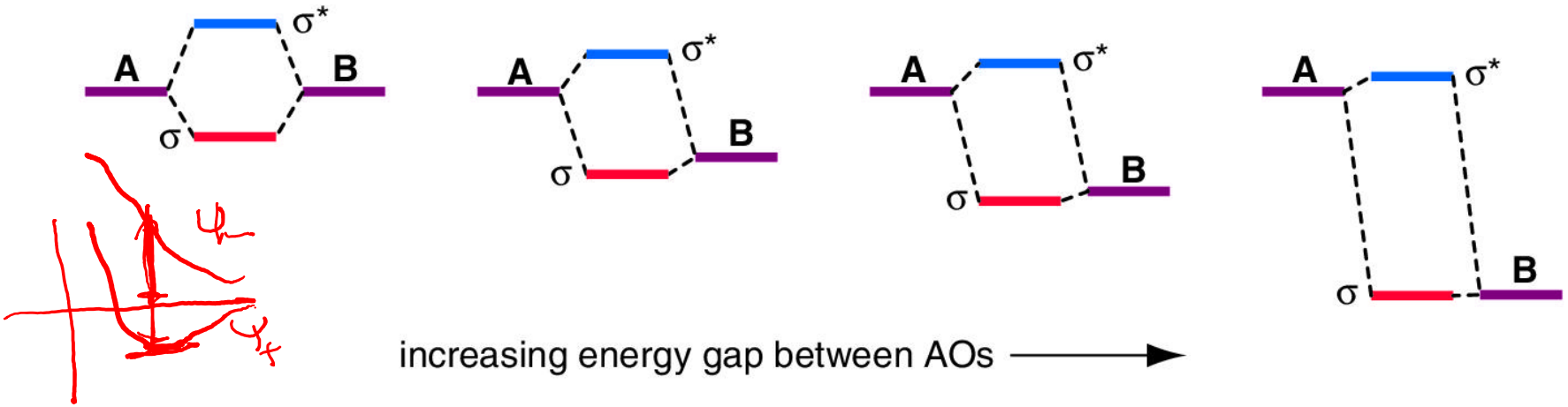






Rules for Forming MOs: 3

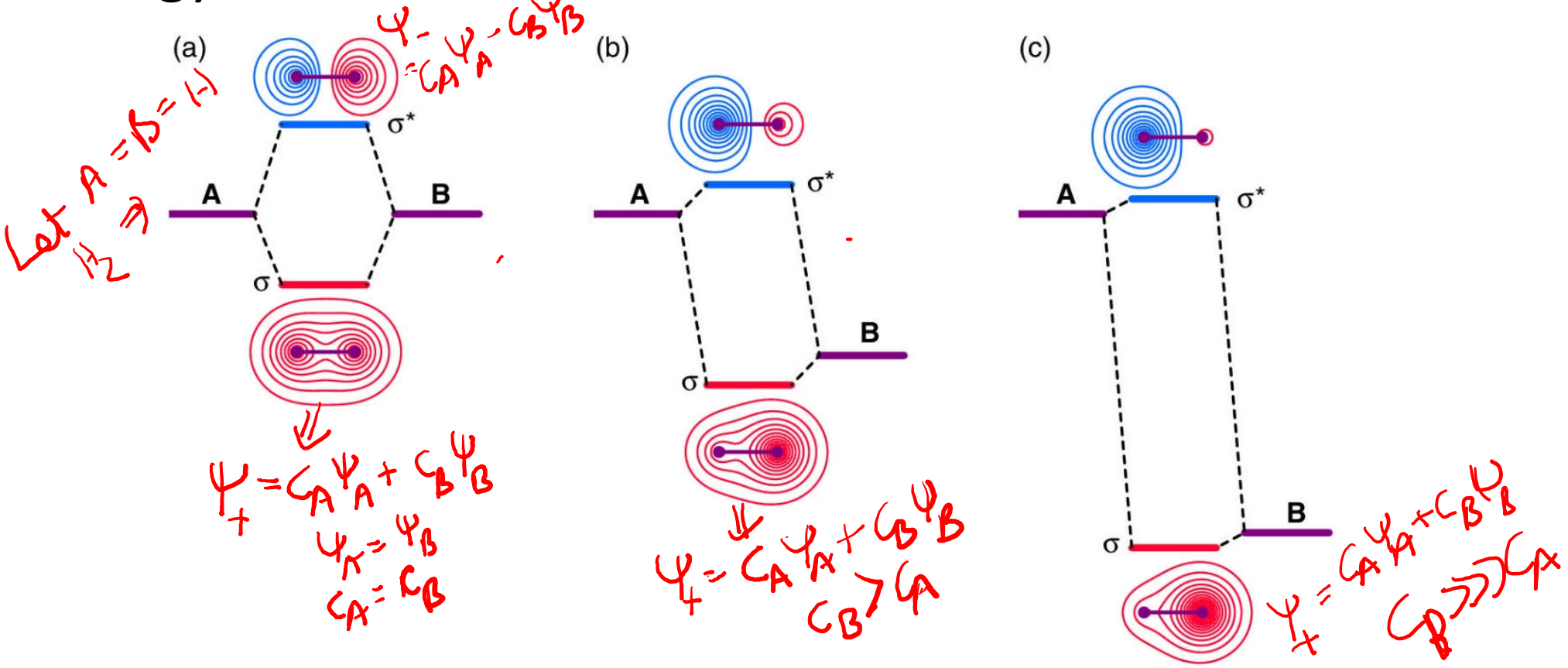
Energy match and contribution from different AOs



- When AOs are closely matched in energy, the bonding and anti-bonding MOs lie significantly above and below the AOs
- The bonding MO lies closer in energy to that of the lower energy AO
- The anti-bonding MO lies closer in energy to that of the higher energy AO

Rules for Forming MOs: 4

Energy match and contribution from different AOs

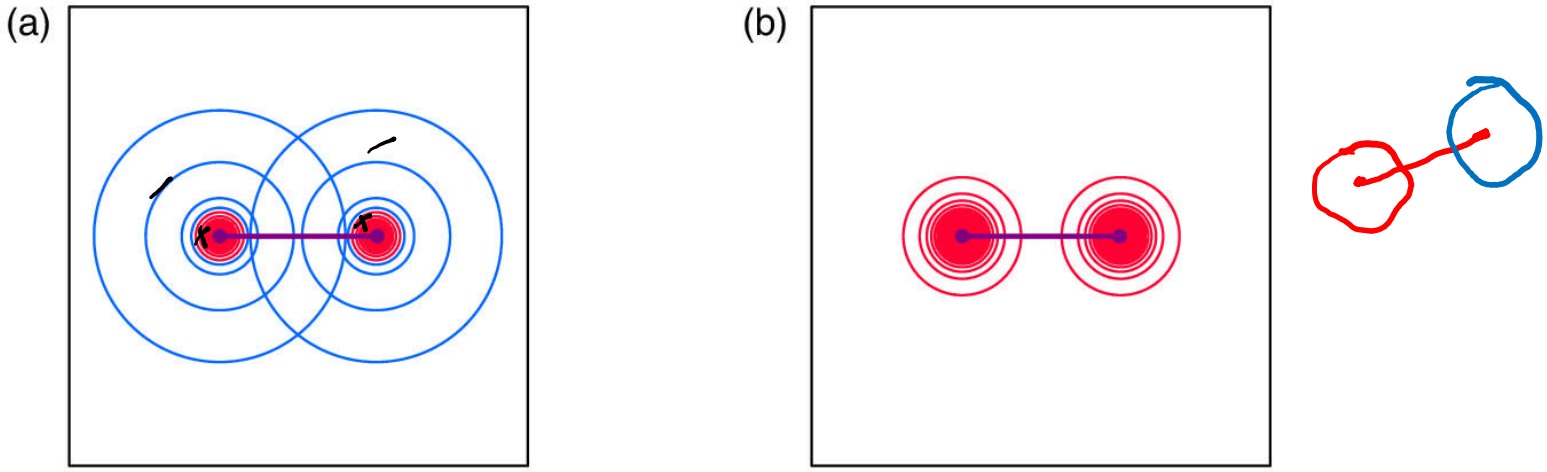


- Contribution to the bonding MO from the lower energy AO increases, while from the higher energy AO decreases
- Contribution to the anti-bonding MO from the higher energy AO increases, while from the lower energy AO decreases

Rules for Forming MOs: 4

Size: In order to interact for form MOs, the AOs must overlap significantly- high S

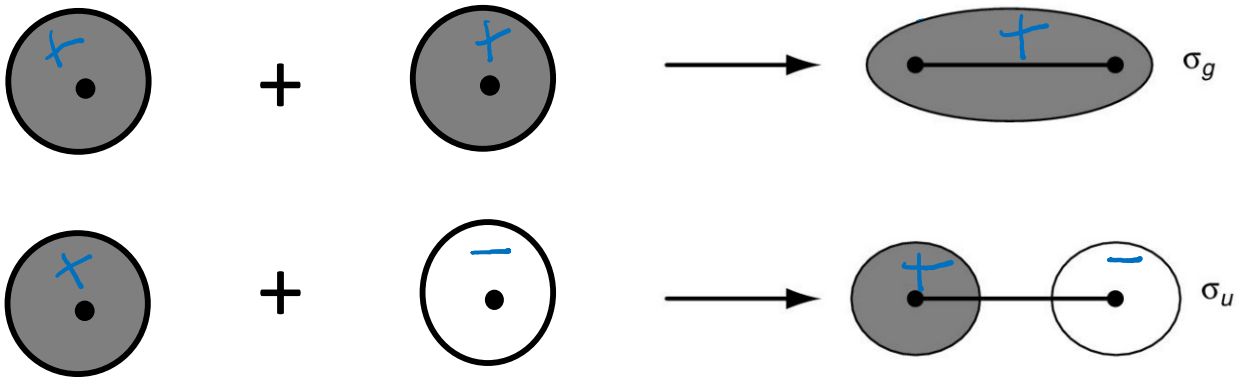
Example: Look at the MO formed from 2s AO's and 1s AO's of Li



2s 1s

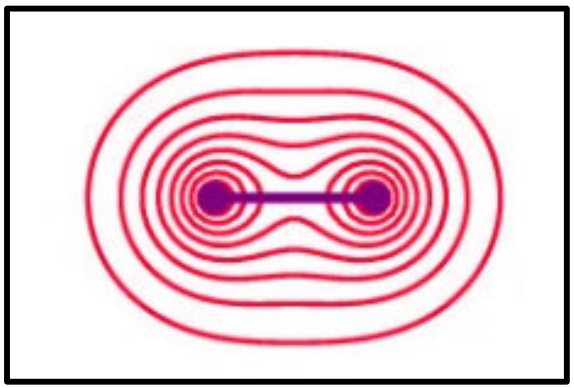
- The 2s AO's overlap significantly- the resulting bonding and anti-bonding MO will be significantly shifted from the energy of AO's
- For the 1s's, even though symmetry is correct to overlap, S will be zero

Types of MO formed from 1s

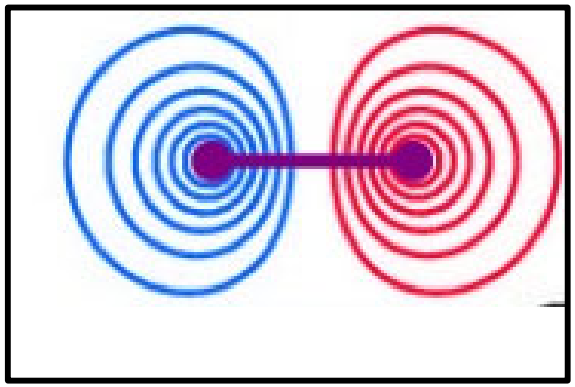


bonding σ_g

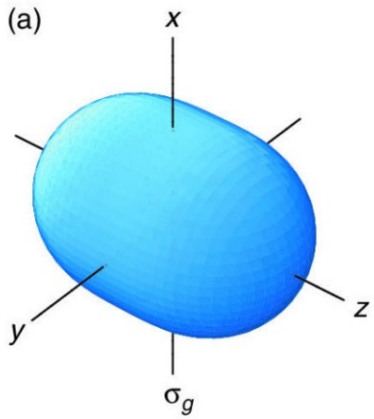
anti-bonding σ_u

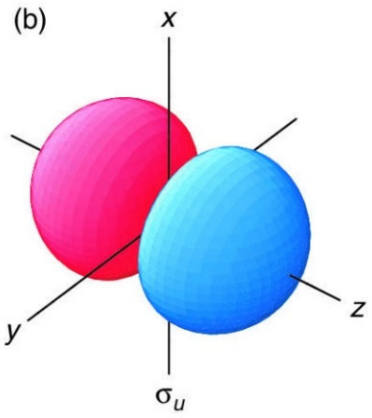


bonding σ_g

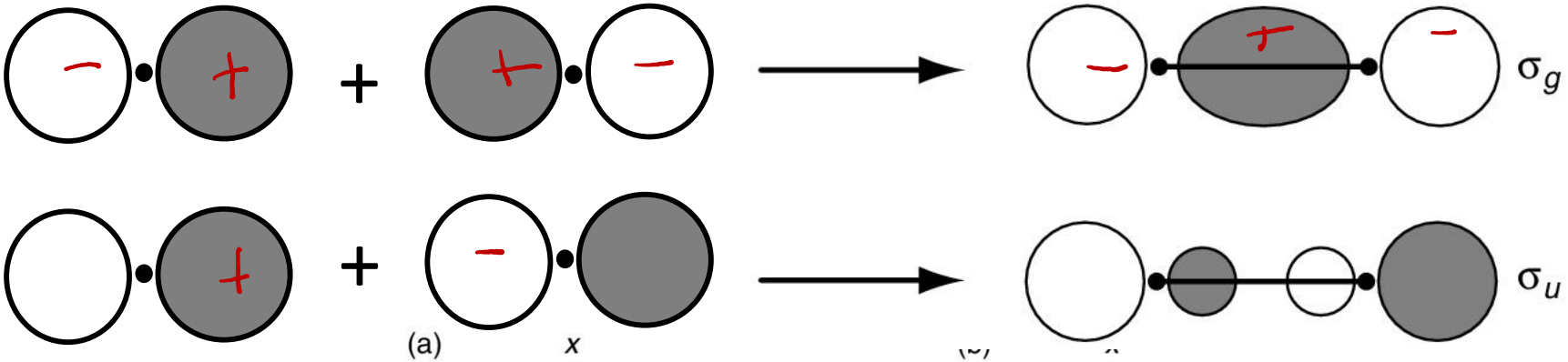


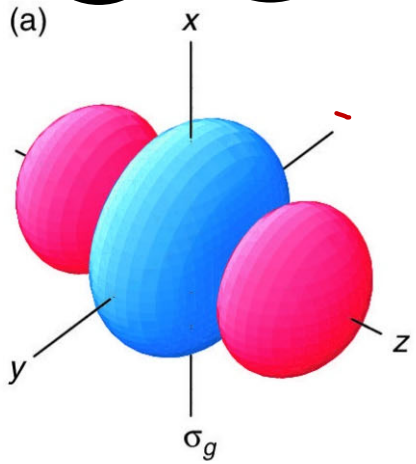
anti-bonding σ_u

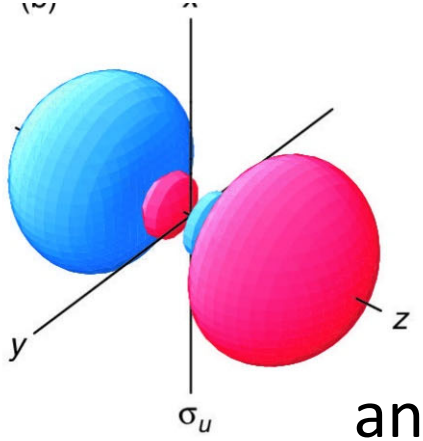




MO formed from $2p_z$ σ overlap

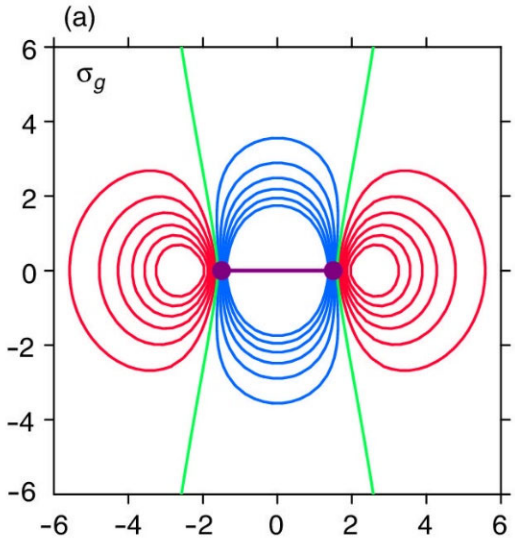


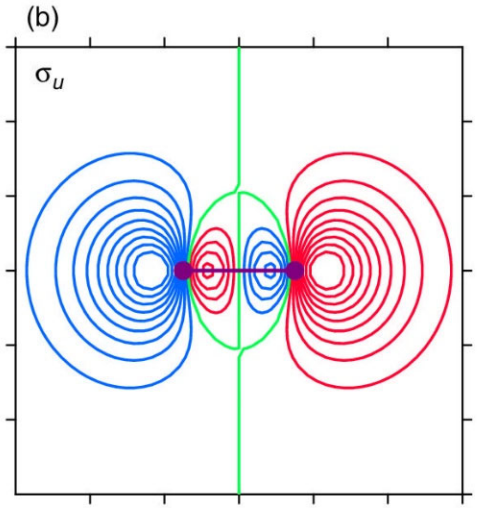




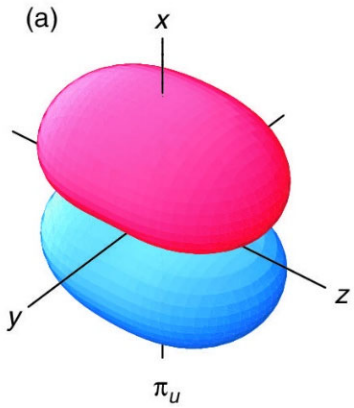
bonding σ_g

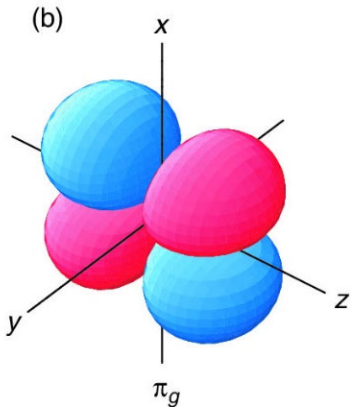
anti-bonding σ_u

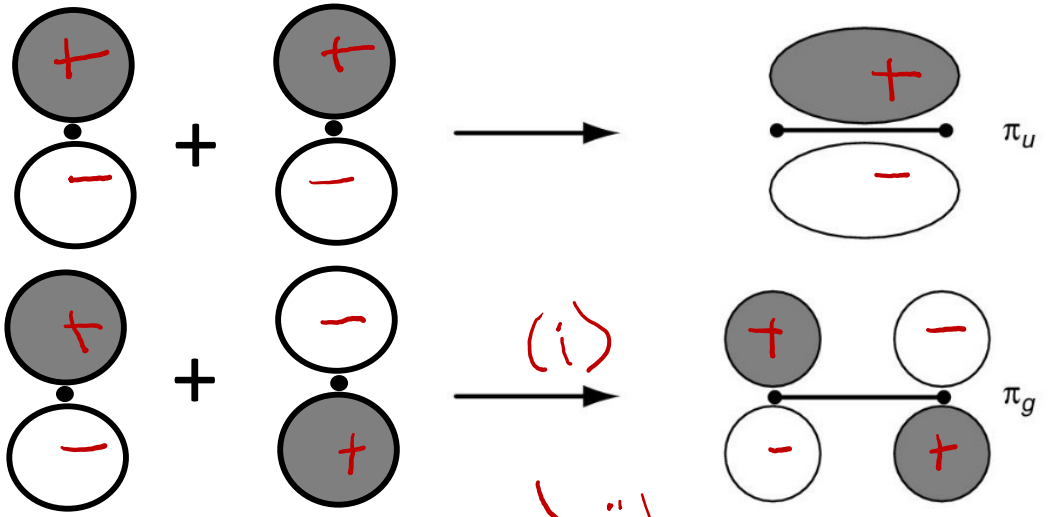


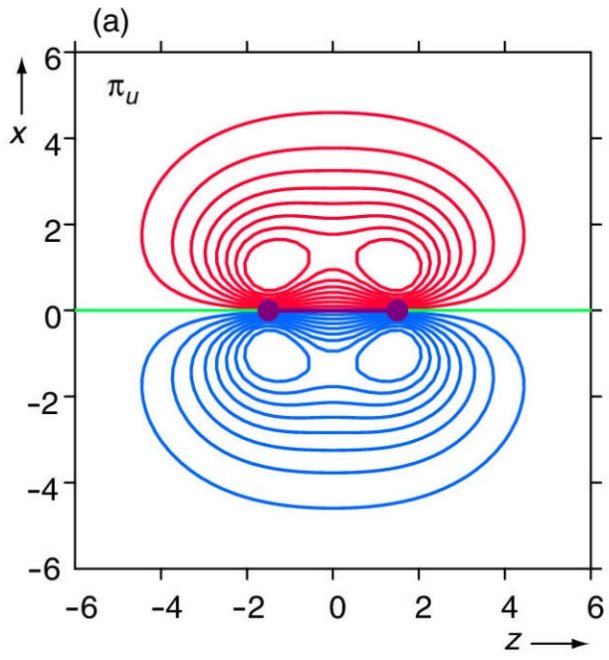


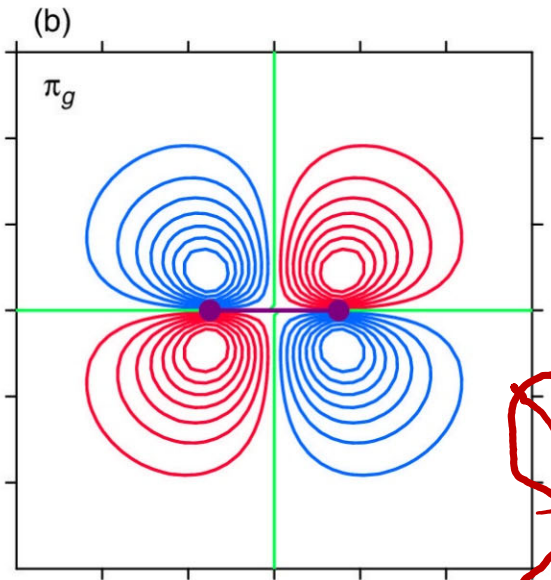
MO formed from $2p_y$ π overlap

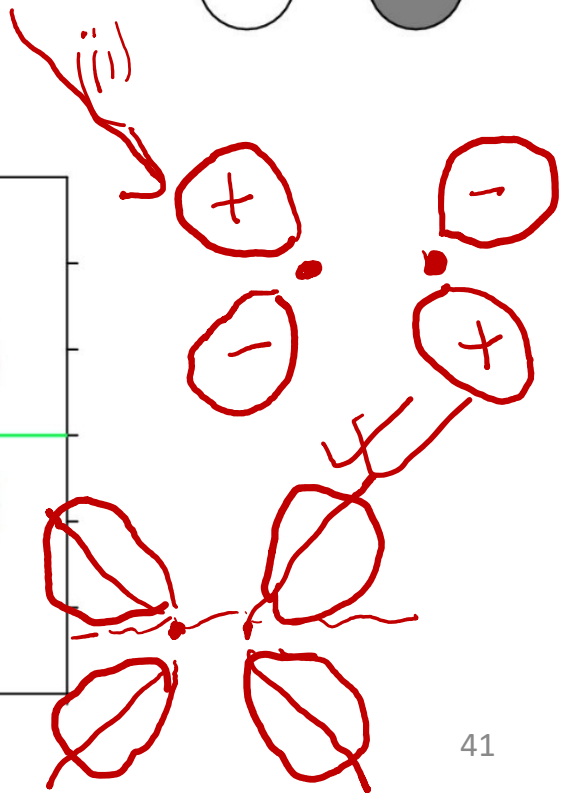




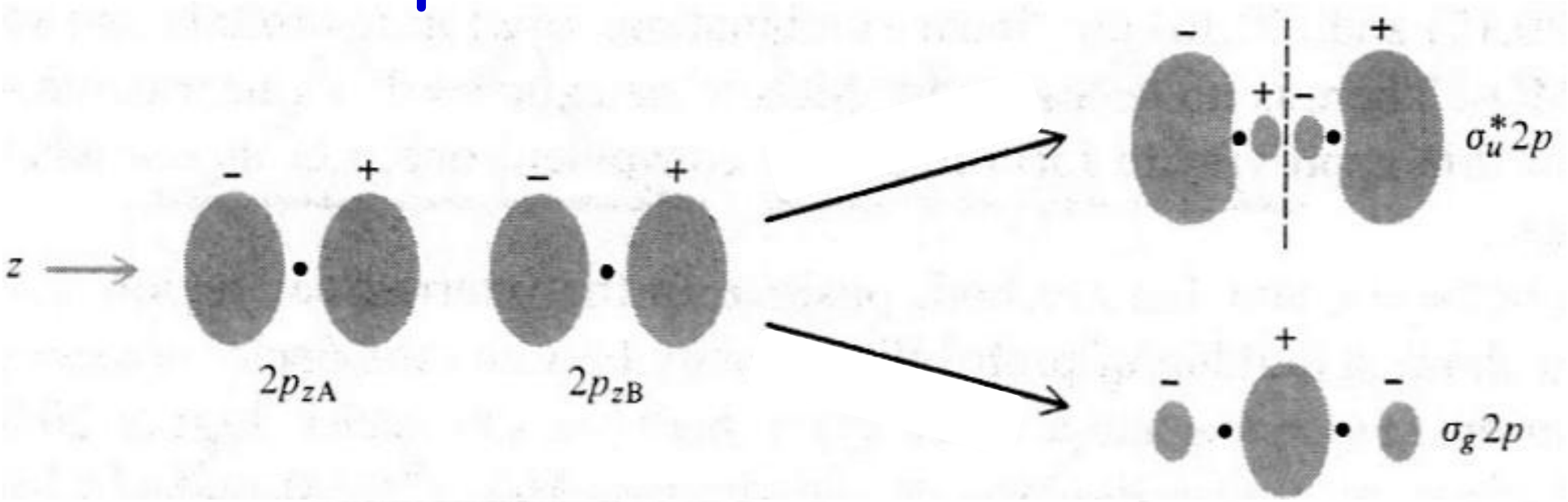




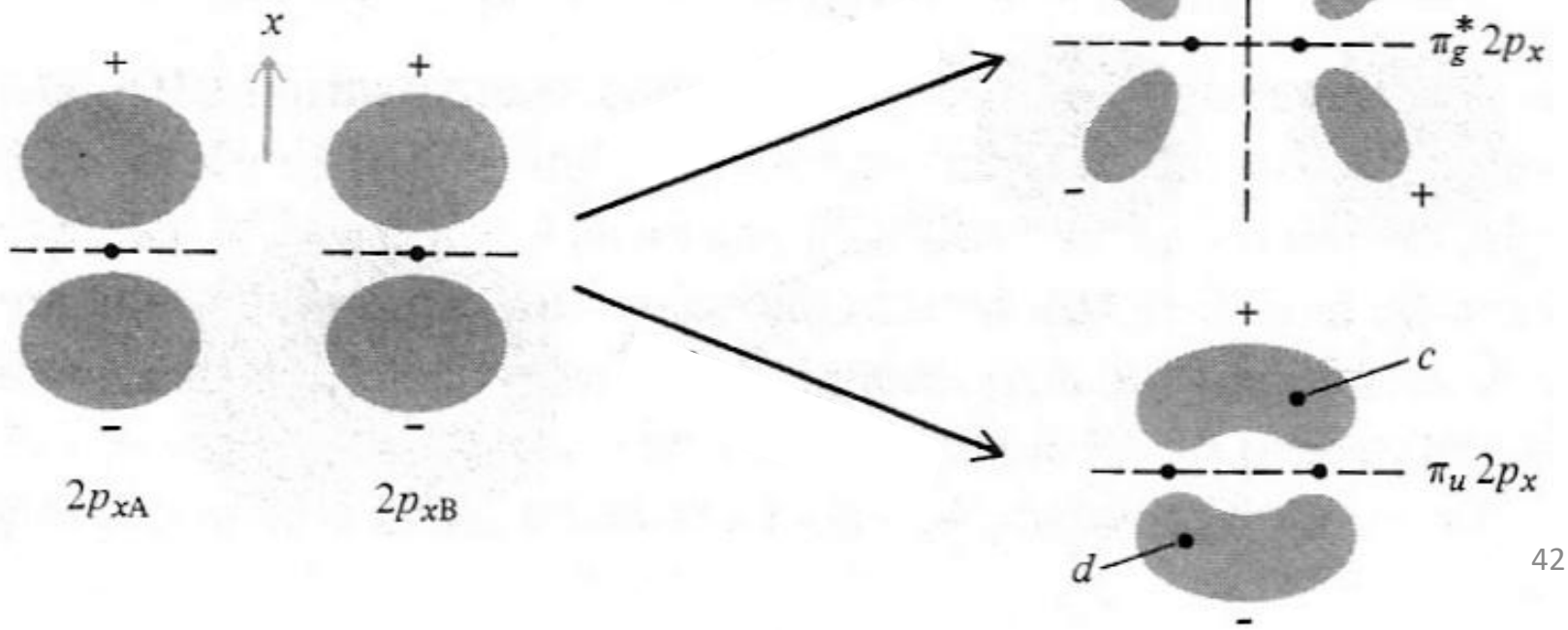




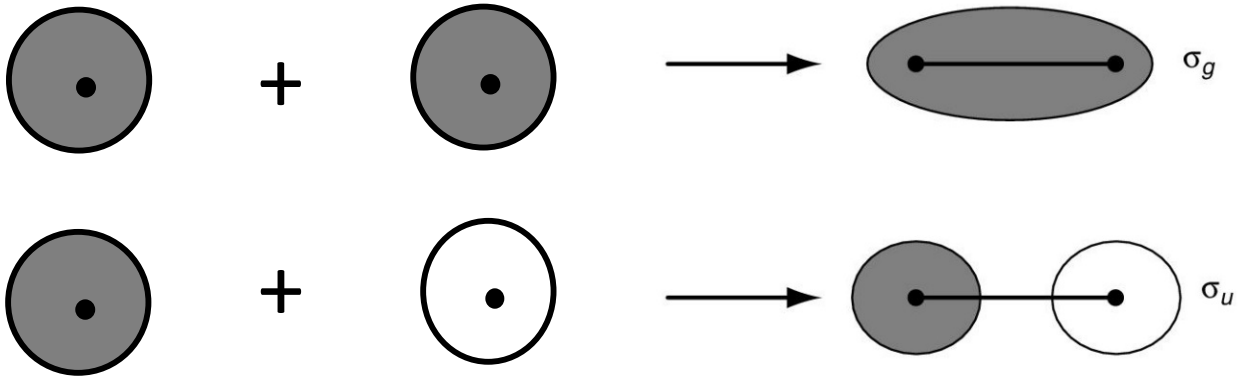
LCAO of p-orbitals: σ- and π- bonds



Note the signs, symmetries and nodes

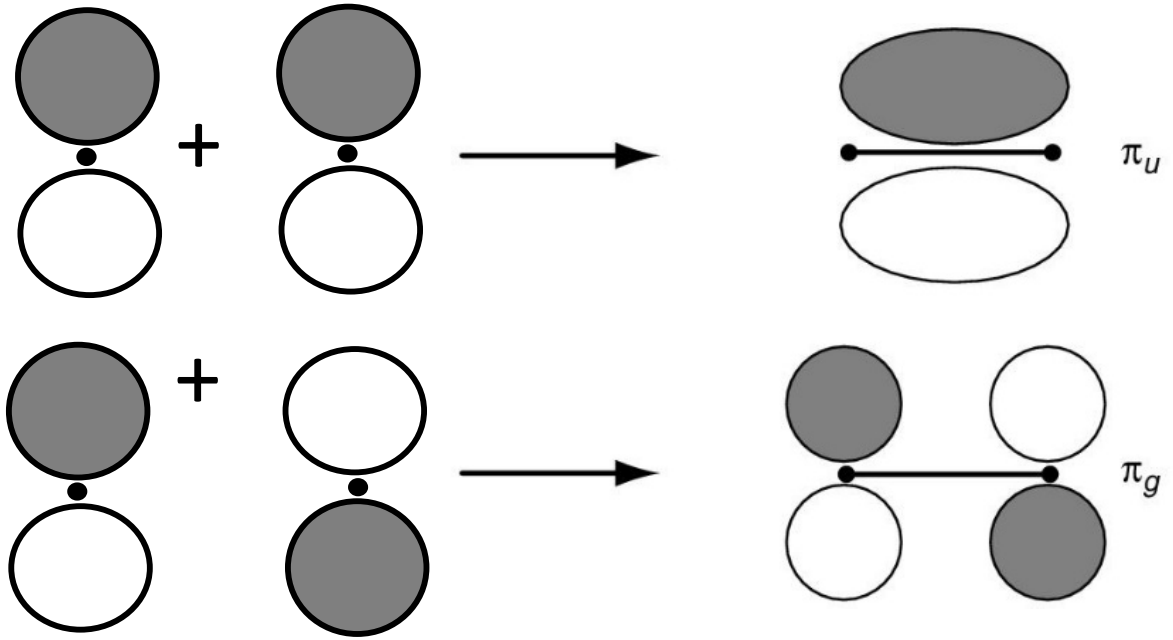


Review



bonding σ_g

anti-bonding σ_u



bonding π_u

anti-bonding π^*_g

Dihydrogen Molecule: Orbital Interaction Diagram

1. Plot atomic valence orbital energies
2. Determine which orbitals can interact (those with S>0).
3. Determine magnitude of each interaction: scales directly with magnitude of overlap; scales inversely with orbital energy difference
4. Plot MO energies and draw orbitals Interaction
5. Use Aufbau principle to fill in electrons

Dihydrogen Molecule: One more electron goes to bonding orbital