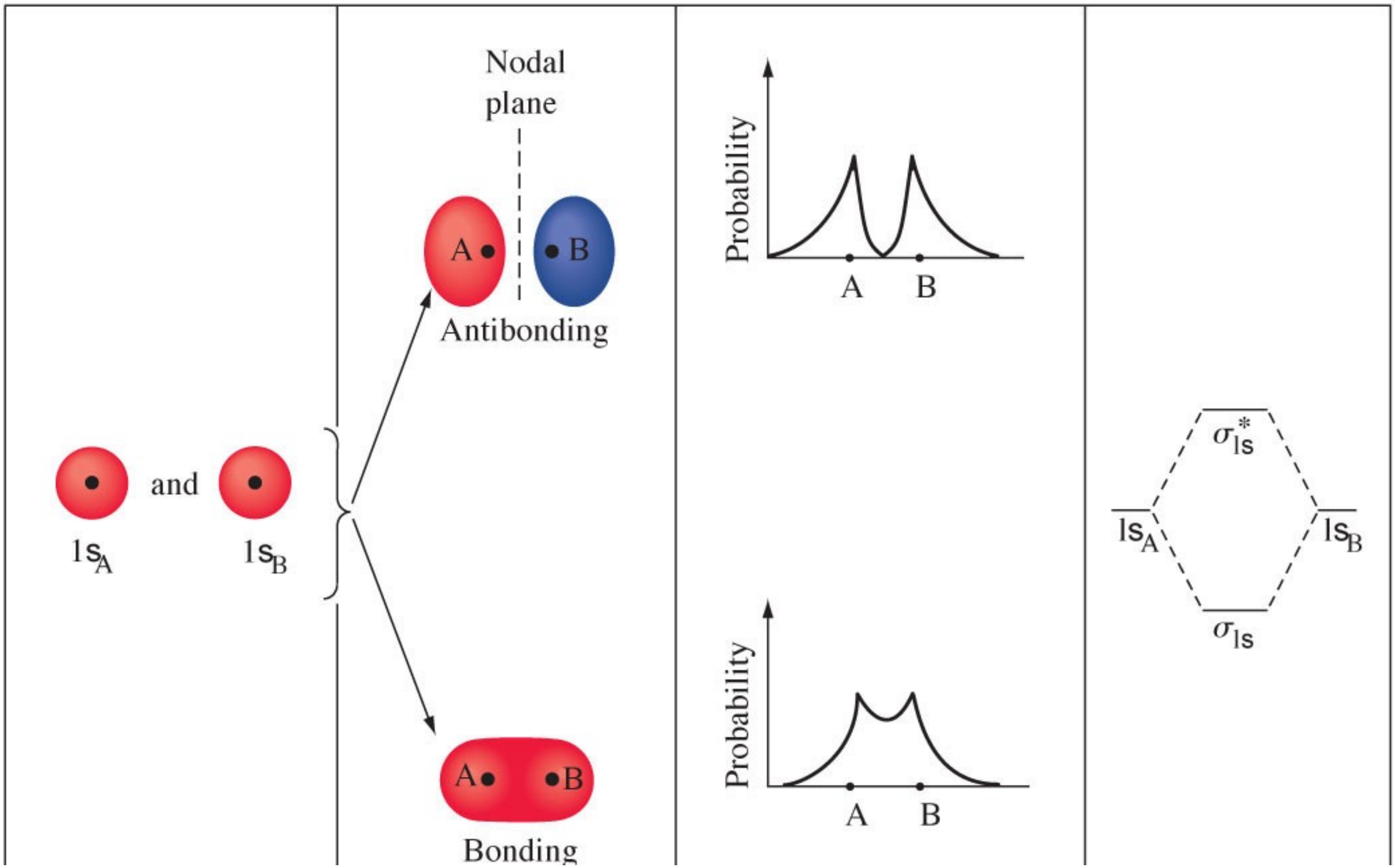
MO diagram



Nodal
plane
A
B
Antibonding
and
1s_A
1s_B
Probability
A
B
σ^*_{1s}
1s_A
1s_B
σ_{1s}
A
B
Bonding
Probability
A
B

But what about more complex molecules with s and p orbitals?

We will start by determining MOs for F_2 molecule

MO Diagram: F_2 molecule

Fluorine atom

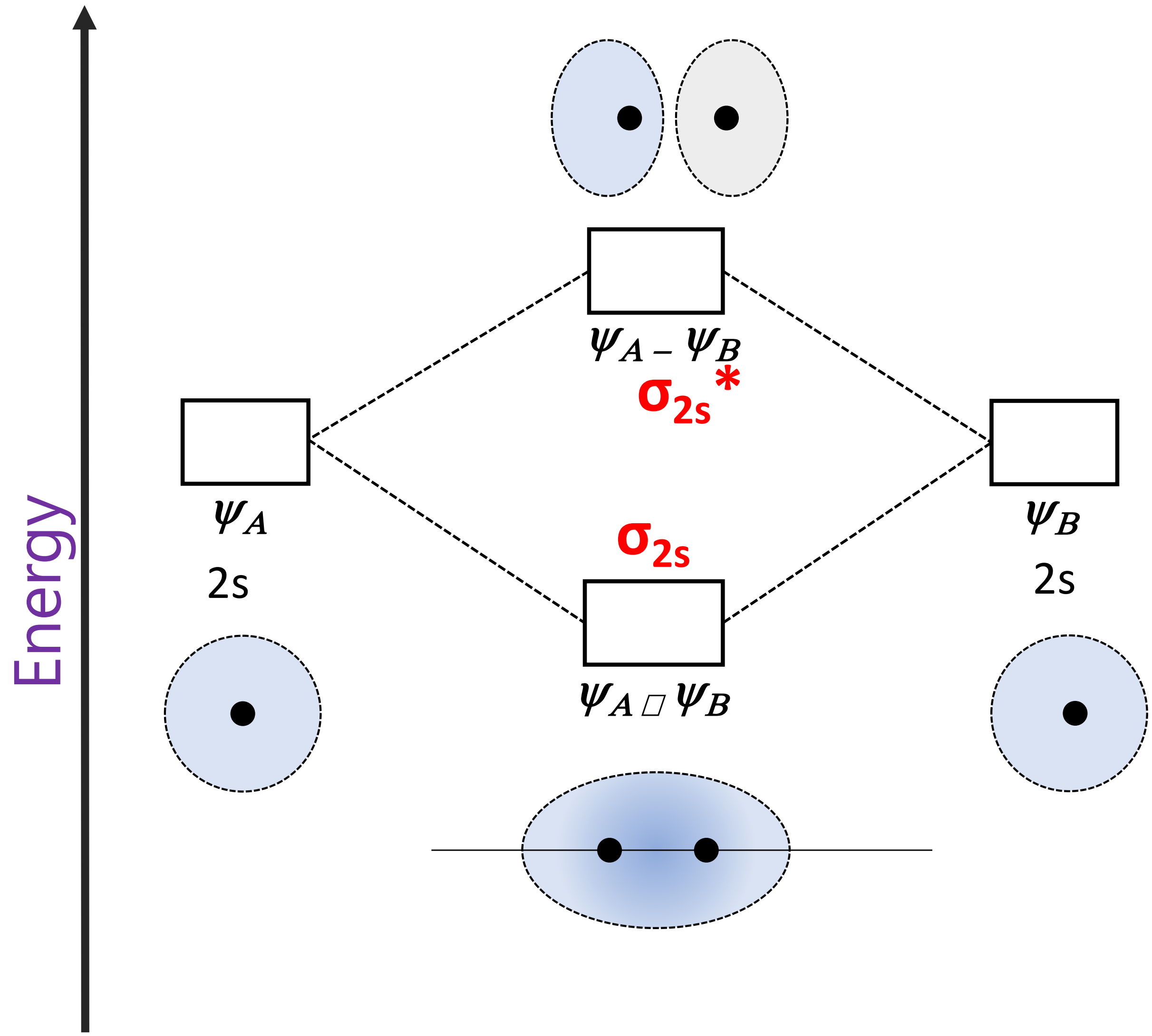
	x	y	z
2p	↑↓	↑↓	↑
2s	↑↓		

Fluorine atom

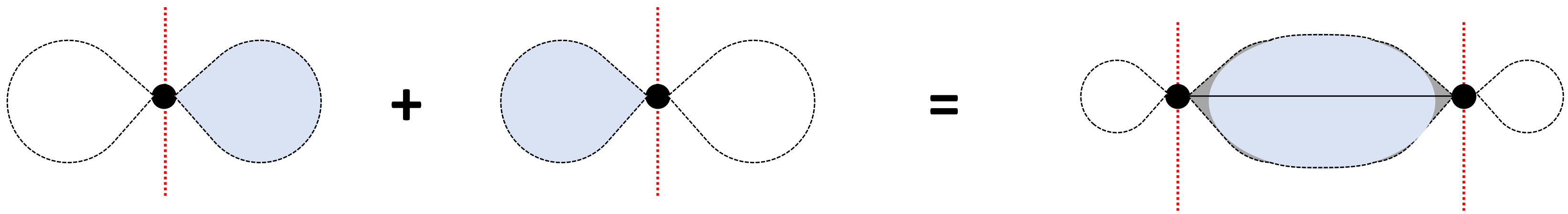
	x	y	z
2p	↑↓	↑↓	↑
2s	↑↓		

1. **Consider only valence orbitals**
2. **4 atomic orbitals + 4 atomic orbitals = 8 molecular orbitals**
3. **Combine the same orbitals i.e linear combination of 2s orbital on one F atom with 2s orbital on the other F atom**

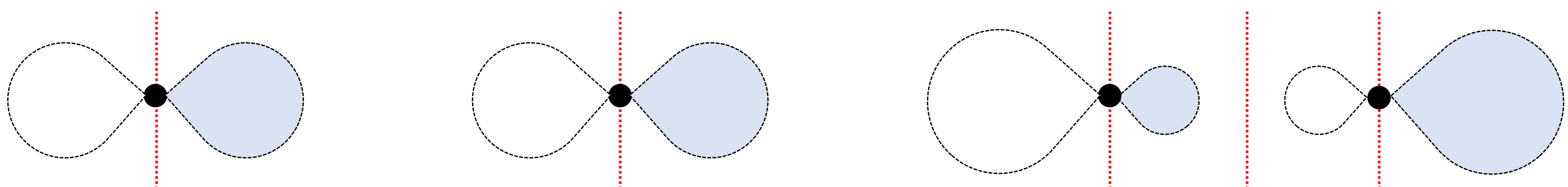
F_2 molecule : LCAO 2s orbital



F_2 molecule : LCAO $2p_x$ orbital

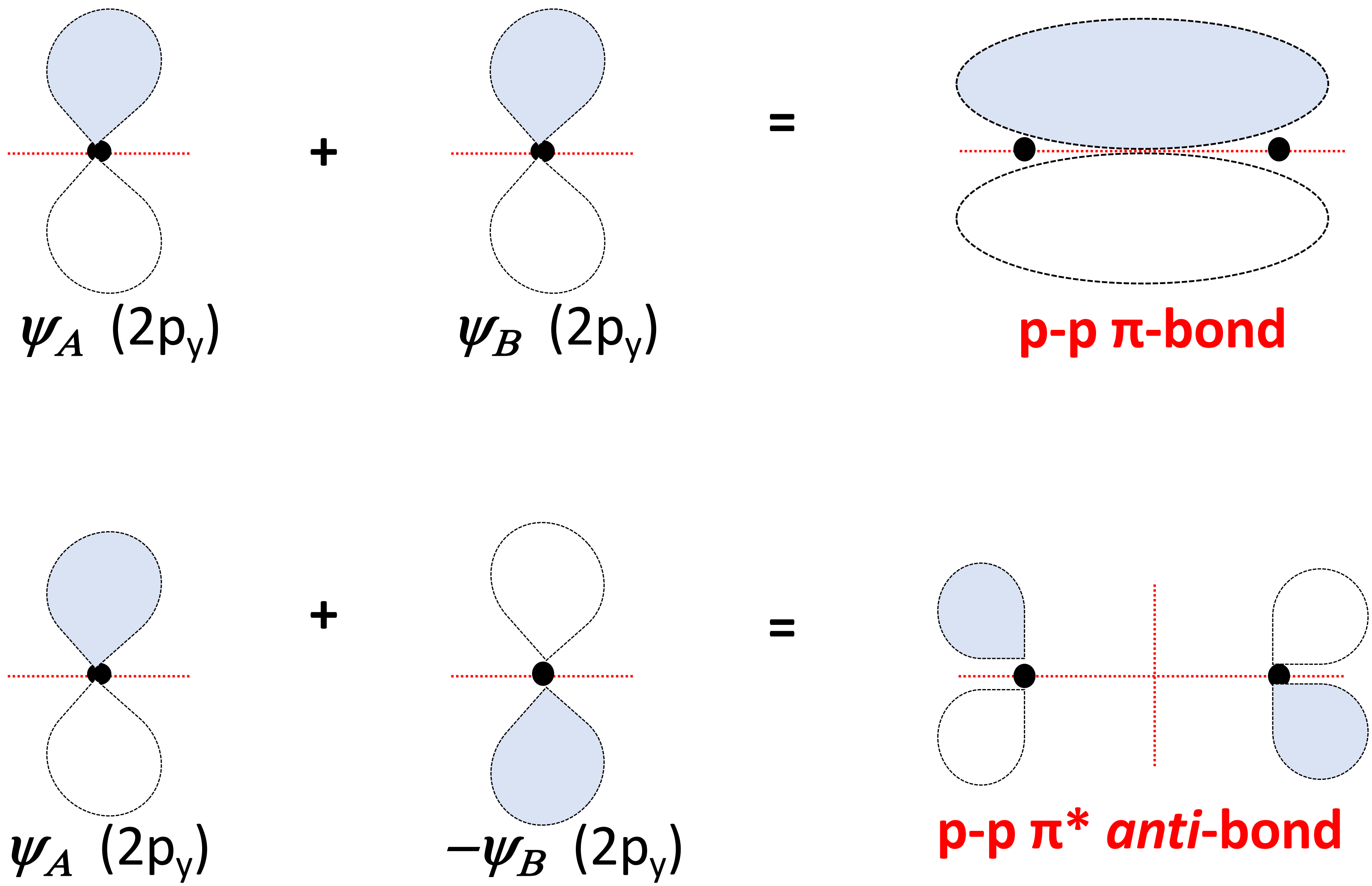


ψ_A ($2p_x$) ψ_B ($2p_x$) **p-p σ-bond**

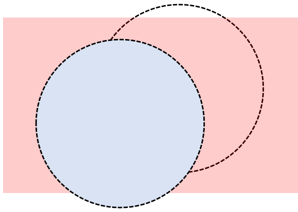


ψ_A ($2p_x$) $-\psi_B$ ($2p_x$) **p-p σ* *anti*-bond**

F_2 molecule : LCAO $2p_y$ orbital

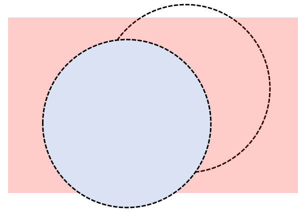


F_2 molecule : LCAO $2p_z$ orbital



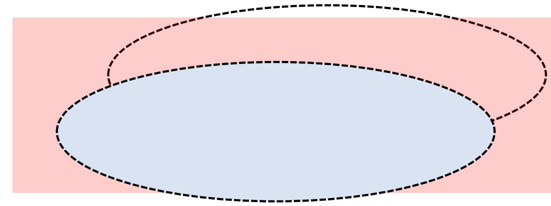
ψ_A $(2p_z)$

+

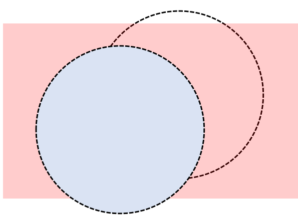


ψ_B $(2p_z)$

=

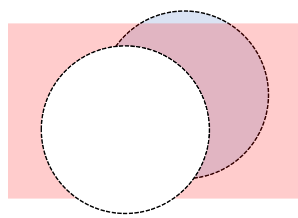


p-p π-bond



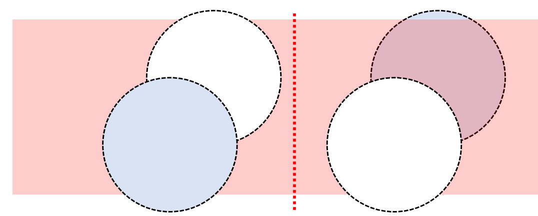
ψ_A $(2p_z)$

+



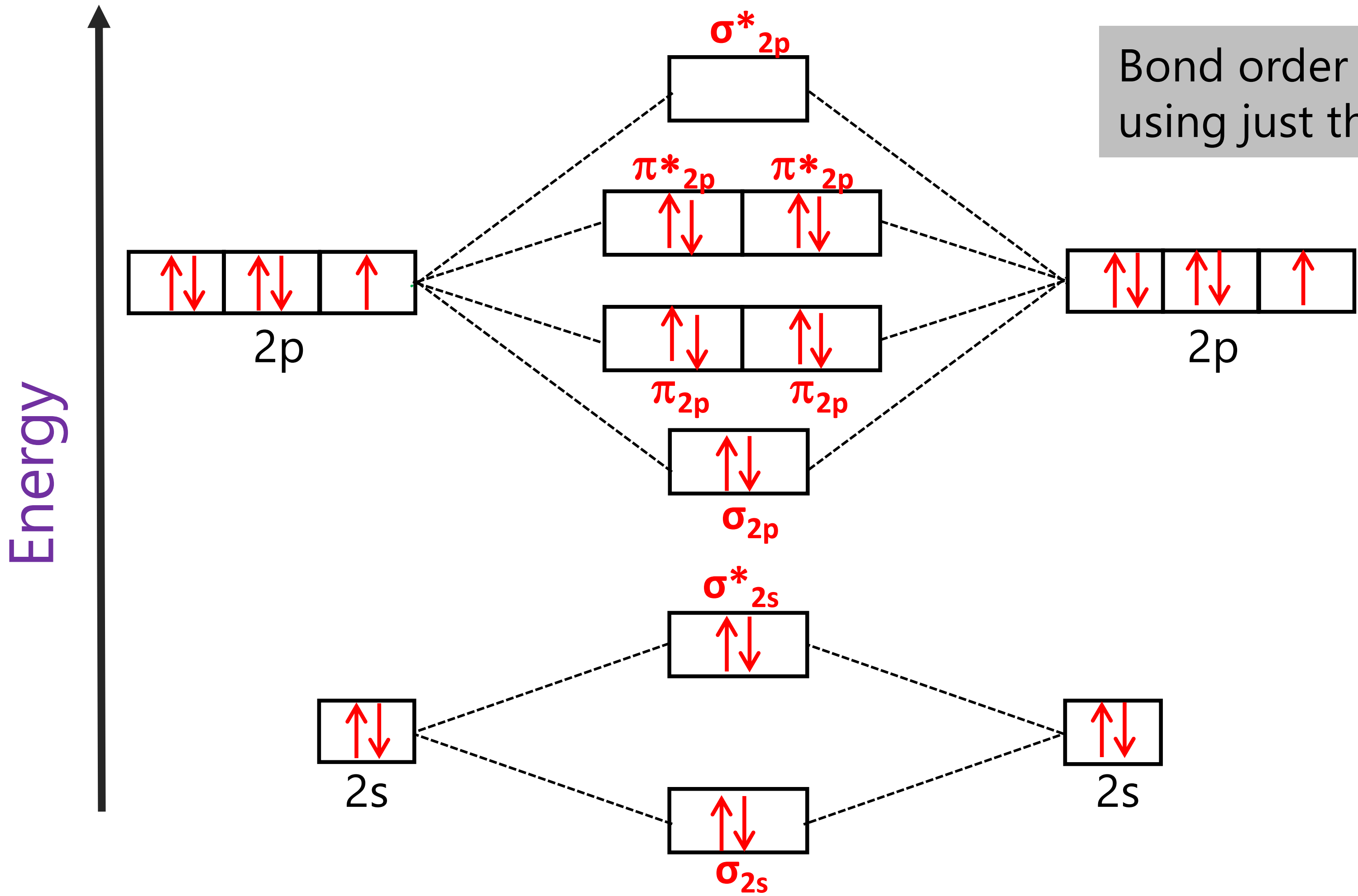
$-\psi_B$ $(2p_z)$

=



p-p π* *anti*-bond

F_2 molecule MO energy diagram



Bond order can be calculated using just the valence electrons

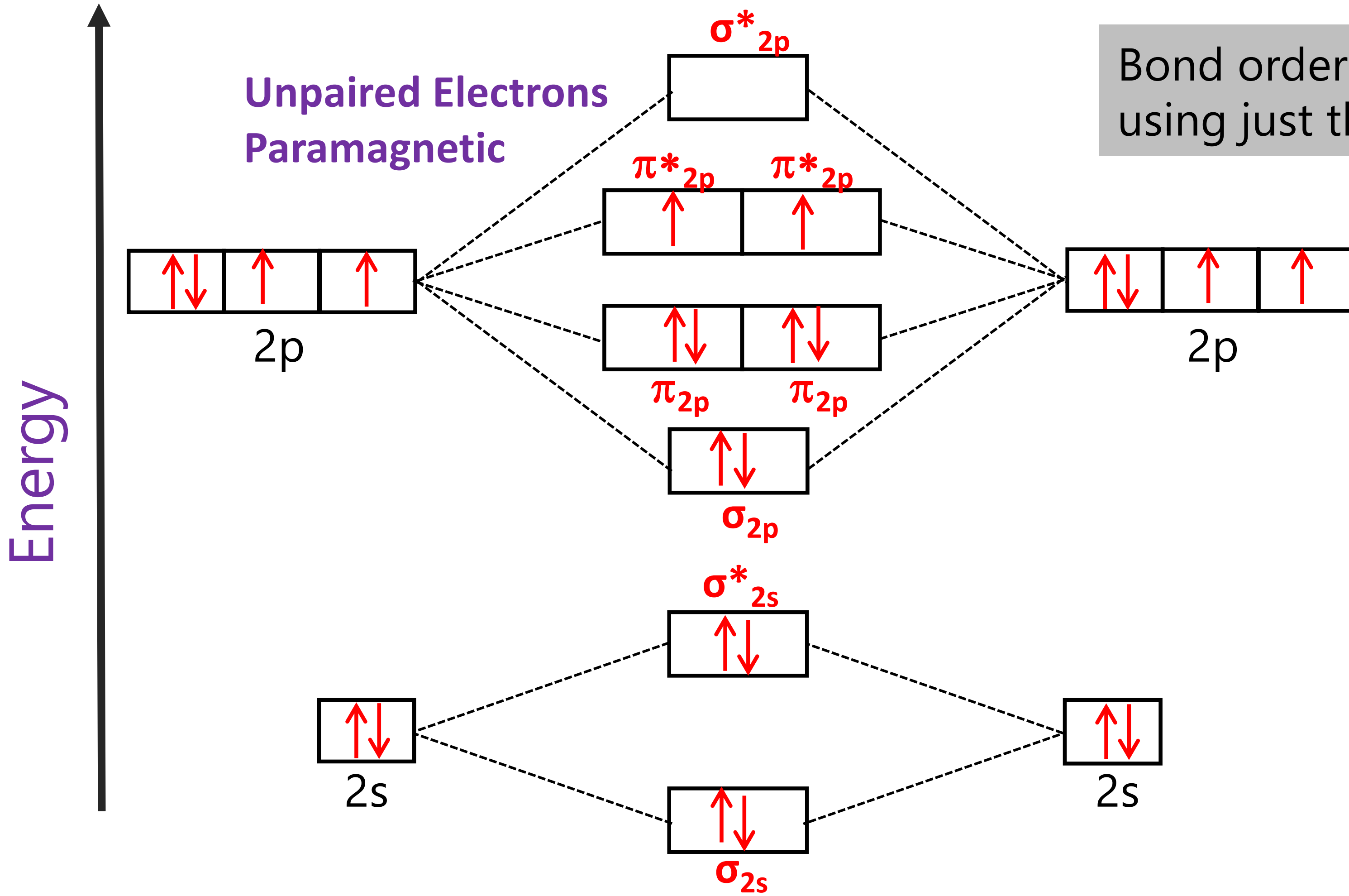
F_2 bond order: **BO in F_2 = ½ (8 - 6) = 1**

F_2 **valence** electron configuration: **$(\sigma\ 2s)^2 (\sigma*\ 2s)^2 (\sigma\ 2p)^2 (\pi\ 2p)^2 (\pi\ 2p)^2 (\pi*\ 2p)^2 (\pi*\ 2p)^2$**

$(\sigma\ 2s)^2 (\sigma*\ 2s)^2 (\sigma\ 2p)^2 (\pi\ 2p)^4 (\pi*\ 2p)^4$

McGill

O_2 molecule MO energy diagram



Bond order can be calculated using just the <u>valence electrons</u>

O: $1s^2\ 2s^2\ 2p^4$

O: $2s^2\ 2p^4$

6 electrons

Two oxygen atoms:
Total 6 x 2 =
12 Valence electrons

O_2 bond order: **BO in O_2 = ½ (8 - 4) = 2**

O_2 **<u>valence</u>** electron configuration: **$(\sigma\ 2s)^2\ (\sigma^*\ 2s)^2\ (\sigma\ 2p)^2\ (\pi\ 2p)^4\ (\pi^*\ 2p)^2$**

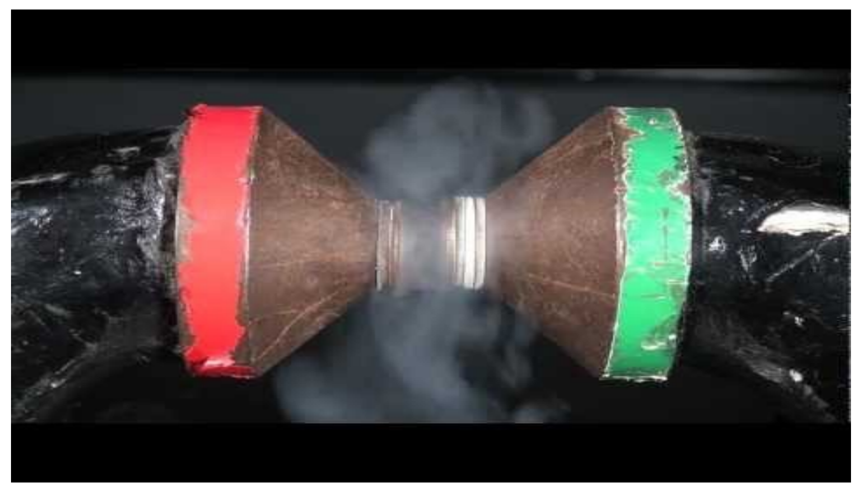
Magnetic Properties of molecules

From the MO Diagram of O_2 – we would predict that O_2 molecule is paramagnetic.

Experimentally – this is how O_2 molecules behave

Some demos videos showing the phenomena are below:

https://www.youtube.com/watch?v=Isd9IEnR4bw



https://www.youtube.com/watch?v=Lt4P6ctf06Q

McGill

Magnetic Properties of molecules

https://www.youtube.com/watch?v=Isd9IEnR4bw