

## Announcements – 11/10/00

- **Exam #3** - Wed., 11/15/00, 7pm

*Review/Problem Session:*

**Sunday, 11/12**

**4 - 6 pm**

**B112 Angell**

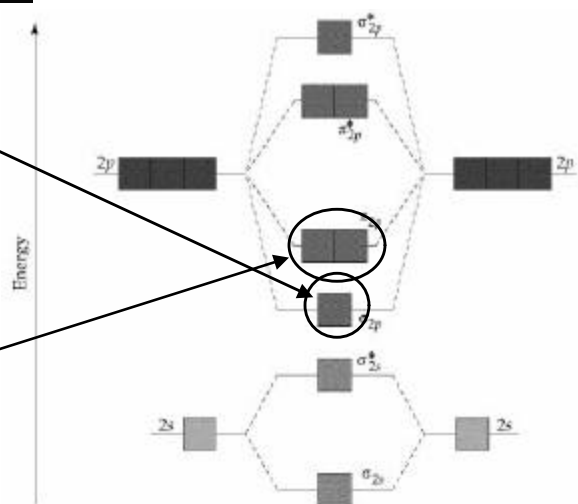
- **Quiz today!**

1

## 2nd Period MO Energies

$\sigma_{2p}$  has lowest energy due to better overlap (end-on) of  $2p_z$  orbitals

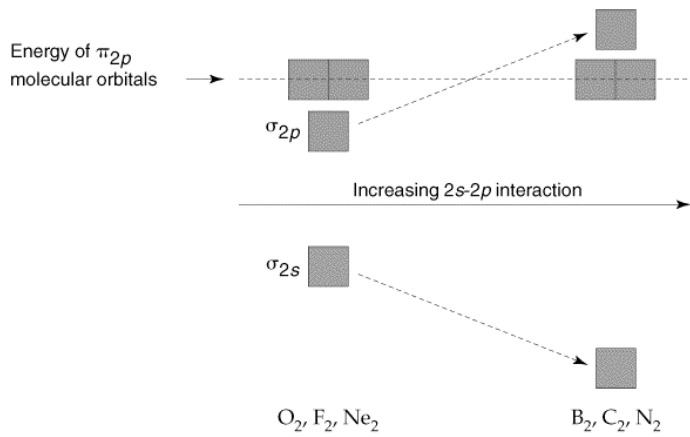
$\pi_{2p}$  orbitals are *degenerate* and at higher energy than the  $\sigma_{2p}$



# 2nd Period MO Energies: Shift!

**For  $Z < 8$ :**

2s and 2p orbitals can interact enough to change energies of the resulting  $\sigma_{2s}$  and  $\sigma_{2p}$  MOs.



3

# 2nd Period Diatomics: $\pi$ first

Note that  $B_2$  has *unpaired electrons* so it must be **paramagnetic**

	$B_2$	$C_2$	$N_2$
$\sigma_{2p}^*$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
$\pi_{2p}^*$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
$\sigma_{2p}$	<input type="checkbox"/>	<input type="checkbox"/>	$\uparrow\downarrow$
$\pi_{2p}$	$\uparrow$ $\uparrow$	$\uparrow\downarrow$ $\uparrow\downarrow$	$\uparrow\downarrow$ $\uparrow\downarrow$
$\sigma_{2s}^*$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
$\sigma_{2s}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$

4

## 2nd Period Diatomics: $\sigma$ first

$O_2$  also has unpaired electrons so it must be *paramagnetic*

	$O_2$	$F_2$	$Ne_2$
$\sigma_{2p}^*$	$\square$	$\square$	$\uparrow\downarrow$
$\pi_{2p}^*$	$\uparrow \quad \uparrow$	$\uparrow\downarrow \quad \uparrow\downarrow$	$\uparrow\downarrow \quad \uparrow\downarrow$
$\pi_{2p}$	$\uparrow\downarrow \quad \uparrow\downarrow$	$\uparrow\downarrow \quad \uparrow\downarrow$	$\uparrow\downarrow \quad \uparrow\downarrow$
$\sigma_{2p}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
$\sigma_{2s}^*$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
$\sigma_{2s}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$

5

## Configurations and Bond Orders: 2nd Period Diatomics

<u>Species</u>	<u>Config.</u>	<u>B.O.</u>	<u>Energy</u>	<u>Length</u>
$Li_2$	$(\sigma_{2s})^2$	1	105 kJ/mol	2.67 Å
$Be_2$	$(\sigma_{2s})^2(\sigma_{2s}^*)^2$	0	9 kJ/mol	2.45 Å
$B_2$	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^2$	1	289 kJ/mol	1.59 Å
$C_2$	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^4$	2	599 kJ/mol	1.24 Å
$N_2$	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^4(\sigma_{2p})^2$	3	942 kJ/mol	1.10 Å
$O_2$	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^2$	2	494 kJ/mol	1.21 Å
$F_2$	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^4$	1	154 kJ/mol	1.41 Å

6

# Heteronuclear Diatomics

---

- Different atoms = different *atomic orbital* energies
  - So, when combining *atomic* orbitals, we don't always combine *like* orbitals
  - And, if we do combine *like* orbitals (e.g., 1s and 1s), they are not necessarily at the same energy, so they combine *unequally*
  - **RESULT: *asymmetry***
    - *Unequal* distribution of electron density between the two atoms
    - Resulting *molecular orbitals* are not symmetrical
    - Bond is *polar* and has a *dipole moment* ( $\mu$ )

7