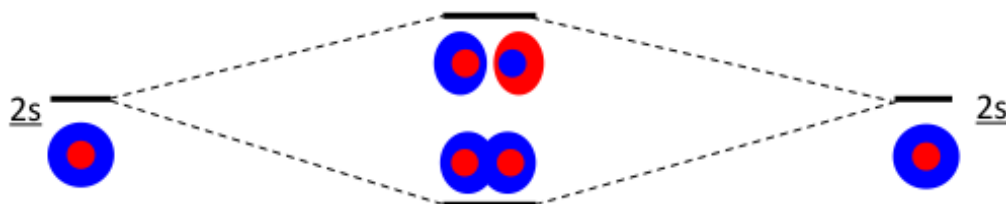


## Lecture 1 – Worksheet: Molecular Orbitals and Bonding

### Model 1: Bonding in s-Block Diatomics

The molecular orbital diagram for a diatomic made up of two 2s elements is shown below.



Once the *valence* electrons have been added to the diagram, the *bond order* can be worked out by first counting up the number of bonding and anti-bonding electrons and then calculating:

$$\text{bond order} = \frac{1}{2} (\text{number of bonding electrons} - \text{number of anti-bonding electrons})$$

### Critical thinking questions

1. Use the MO diagram and the definition of the bond order to complete the table below.

Species	Bond order	Is the species stable?
$\text{Li}_2^+$		
$\text{Li}_2$		
$\text{Be}_2^+$		
$\text{Be}_2$		

2. What is the *maximum* bond order that is possible between two s-block elements?

### Model 2: Bonding in p-Block Diatomics

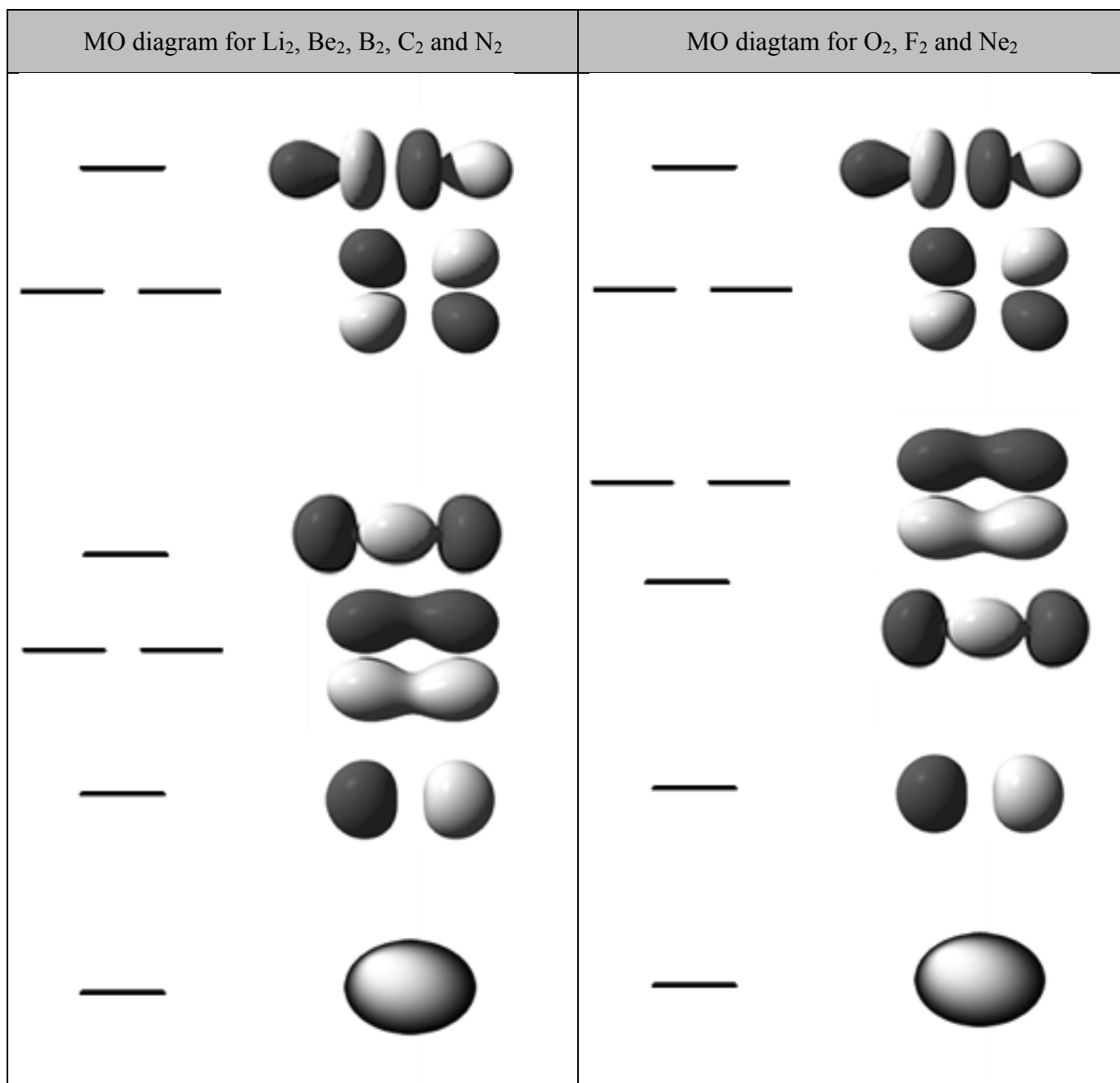
#### $\sigma$ and $\pi$ orbitals

$\sigma$  orbitals are symmetric around a line joining the two nuclei.  $\pi$  orbitals have a node along this line:

#### Bonding and Anti-Bonding Molecular Orbitals

When electrons occupy a *bonding orbital*, they strengthen the bond. When electrons occupy an *anti-bonding orbital*, they weaken the bond. Anti-bonding orbitals have a nodal plane between the nuclei. An asterisk (“\*”) is added to the  $\sigma$  or  $\pi$  label to show this.

The MO diagrams for homonuclear diatomics made from 2p elements are shown overleaf. Two energy sequences are found and the sequence adopted depends on the element involved.



### Critical thinking questions

- Label the orbitals on the diagram as  $\sigma$ ,  $\sigma^*$ ,  $\pi$  or  $\pi^*$ .
- Calculate the bond order in the molecules below.
  - C<sub>2</sub>
  - N<sub>2</sub>
  - O<sub>2</sub>
- Which of the following species has the stronger bond?
  - C<sub>2</sub> or C<sub>2</sub><sup>-</sup>
  - N<sub>2</sub> or N<sub>2</sub><sup>+</sup>
  - O<sub>2</sub> or O<sub>2</sub><sup>+</sup>
- What is the *maximum* bond order that is possible between two *p*-block elements?