But it’s not that simple…

The 2s and 2p orbitals on each atom overlap in space and can be “mixed” to yield new hybrid orbitals. We saw this in Valence Bond Theory.

This type of thing happens here as well. In this case, this mixing lowers the energies of the lower energy orbitals and raises the energies of the higher energy orbital, as shown at right.

This leads to the more correct M.O. Theory energy diagrams shown in the textbook.
Bond Order = \((6-4)/2 = 1\)

10 electrons

Bond Order = \((6-4)/2 = 1\)

5 electrons

2p_y  2p_x  2p_z

2s

1s

5 electrons

2p_z  2p_x  2p_y
Bond Order = \( \frac{8-4}{2} = 2 \)

12 electrons

6 electrons

6 electrons

2p_y 2p_x 2p_z

2p_z 2p_x 2p_y

2s

2s

1s

1s
Bond Order = \( \frac{10-4}{2} = 3 \)

14 electrons

7 electrons
Bond Order = \( \frac{(10-6)}{2} = 2 \)

16 electrons

8 electrons

2p\text{y}  
2p\text{x}  
2p\text{z}

2s

1s
Bond Order = (10-8)/2 = 1

18 electrons

9 electrons

2p_y  2p_x  2p_z

2s

1s

9 electrons

2p_z  2p_x  2p_y
Bond Order = \( \frac{(10-10)}{2} = 0 \)