General Chemistry 1

Chem110

Fall 2024

Theories of Covalent Bonding

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Theories covered in Chapter 5

Chapter 5 (Section 5.1 – 5.3)
Valence Bond Theory and Hybridization

Chapter 5 (Section 5.4)
Molecular Orbital Theory
(Using linear combination of Atomic Orbitals)

Theories of Chemical Bonding

What will you be learning? Learning Objectives:

Sections 5.1 to 5.3

- Explain bonding in diatomic molecules in terms of Valence Bond Theory
- Indicate which orbitals' overlap gives sigma (σ) bond and/or pi (π) bonds.
- Sketch pictures of bonding orbitals using valence bond theory.
- Use VSEPR theory to predict hybridization
- Predict hybridization: sp, sp^2, sp^3, sp^3d, sp^3d^2

Section 5.4

- Explain molecular orbital theory (MO theory)
- Understand that the combination of any two AOs creates a bonding & anti-bonding MO pair.
- Prepare MO energy diagrams for simple diatomic molecules (first/second periods).
- Fill MO energy diagrams for simple heteronuclear diatomic molecules.
- Determine bond orders and predict magnetic properties of diatomics.
- Fill π MO energy diagrams for delocalized systems (including benzene and ozone).
- Describe metallic bonding and physical properties using band theory models.

Theories covered in Chapter 5

Concept Video

Formation of covalent bonds (single bonds/ sigma bonds)

Formation of covalent bonds (multiple bonds/ sigma and pi bonds)

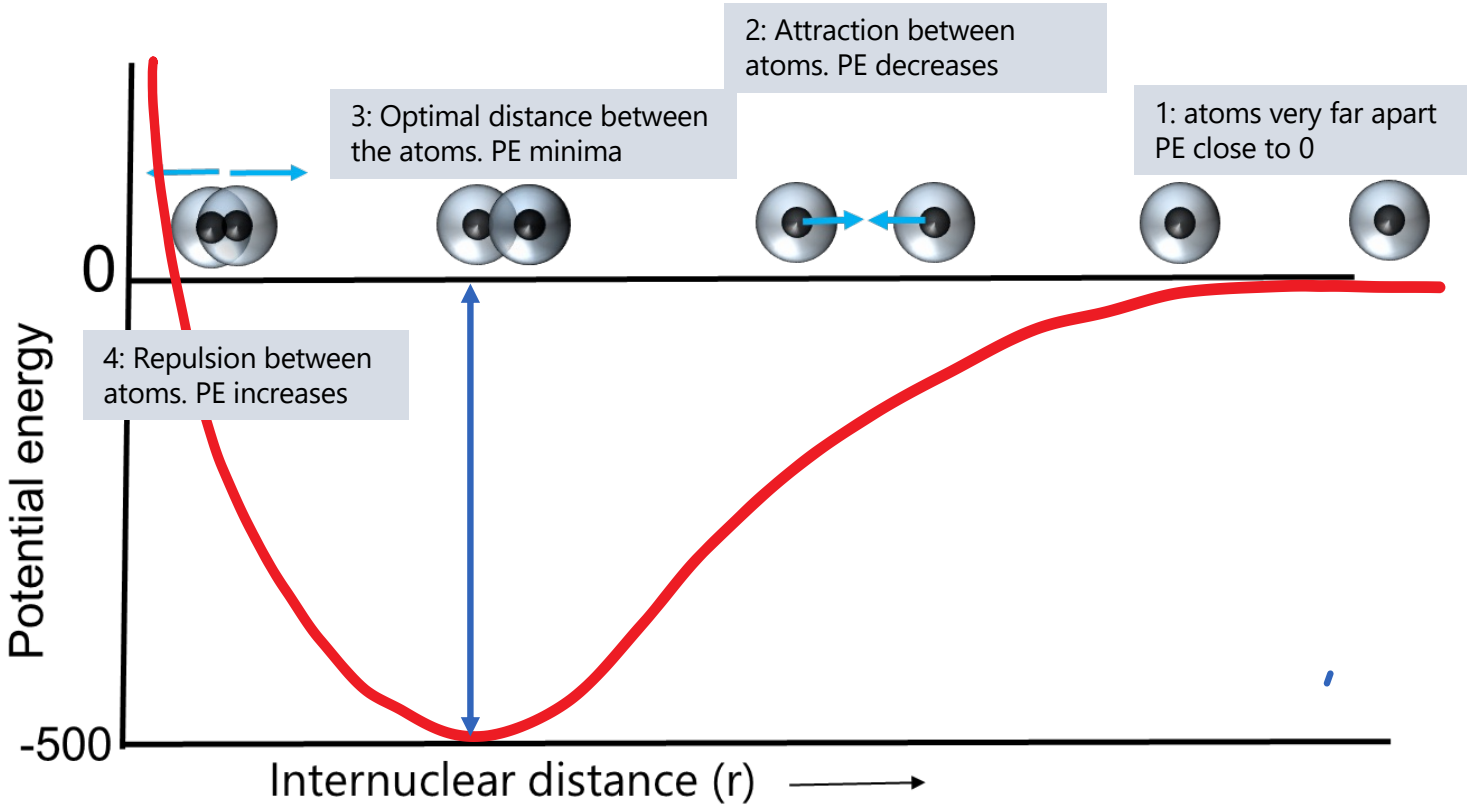
Concept Video

Hybridization of orbitals 1

Concept Video

Hybridization of orbitals 2

How are covalent bonds formed?



 H atom

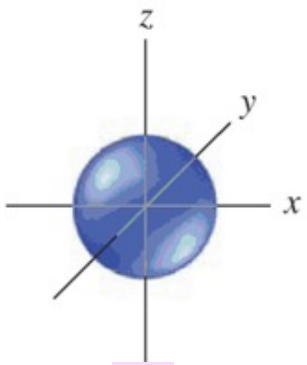
Valence Bond Theory

But how does this bond form?

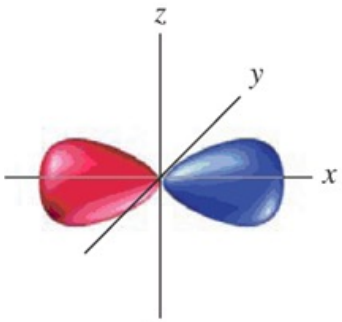
Valence Bond Theory

A covalent bond forms when orbitals of two atoms overlap and a pair of electrons occupy the overlap region

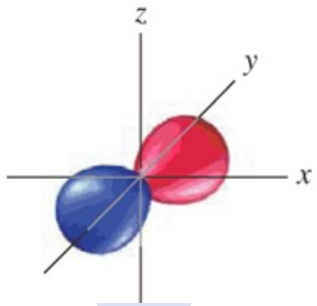
Shapes of Orbitals (Review)



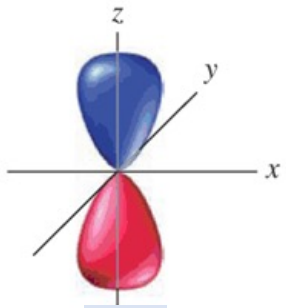
s



p_x



p_y



p_z

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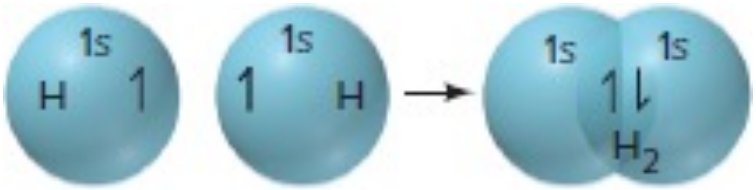
Valence Bond Theory: Making single bonds (H_2)

A covalent bond forms when orbitals of two atoms overlap and a pair of electrons occupy the overlap region



The two **valence** atomic orbital (1s and 1s) combine to have maximum overlap creating a σ-bond (sigma bond).

σ-bond – formed from overlap of two orbitals. Is cylindrically symmetrical around bond axis

- The two electrons move over to the new **σ-bonding** orbital
- The two electrons in the bonding orbital have opposite spin (Pauli's exclusion principle still followed)

Valence Bond Theory: Making single bonds (H_2)

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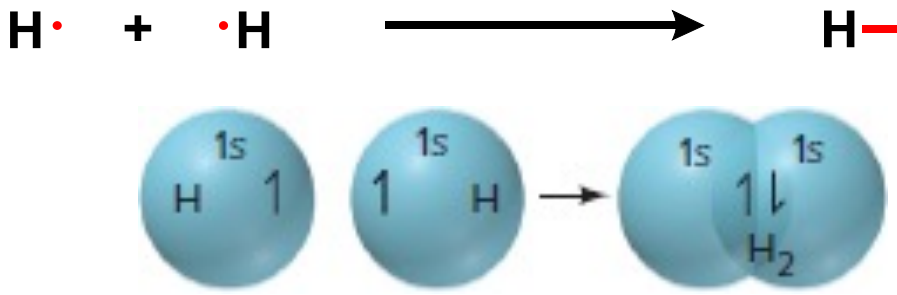
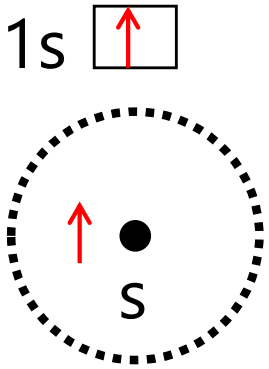
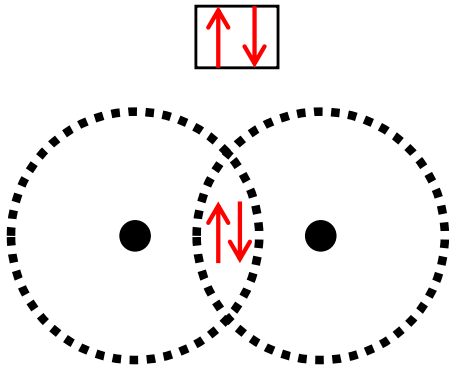


Hydrogen atom

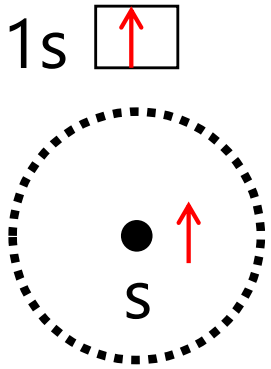


H_2 molecule



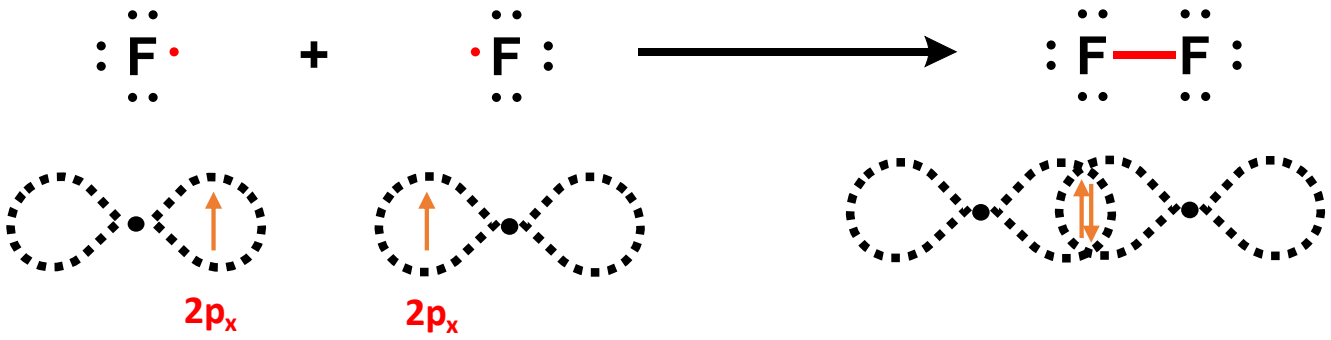
s-s σ-bond

Hydrogen atom

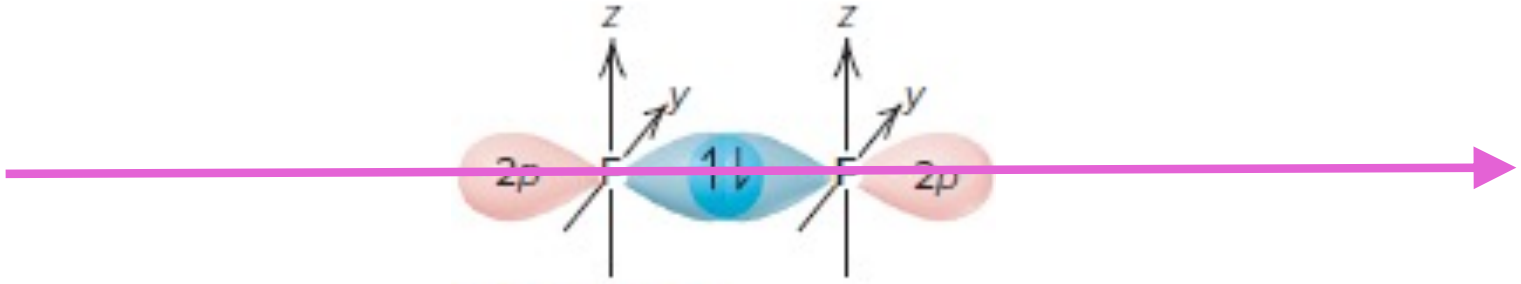


Valence Bond Theory: Making single bonds (F_2)

A covalent bond forms when orbitals of two atoms overlap and a pair of electrons occupy the overlap region



The two **valence** atomic orbitals (2p and 2p) have maximum overlap creating a σ-bond.

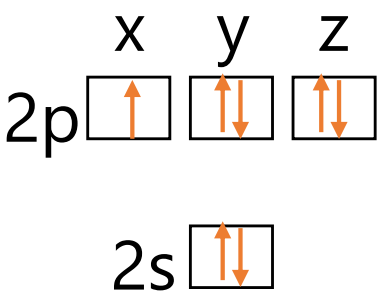


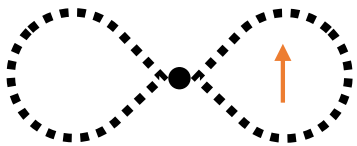
<u>σ-bond</u> – formed from overlap of two orbitals. Is cylindrically symmetrical around bond axis

- The two electrons move over to the new **<u>σ-bonding</u>** orbital
- The two electrons in the bonding orbital have opposite spin (Pauli's exclusion principle still followed)

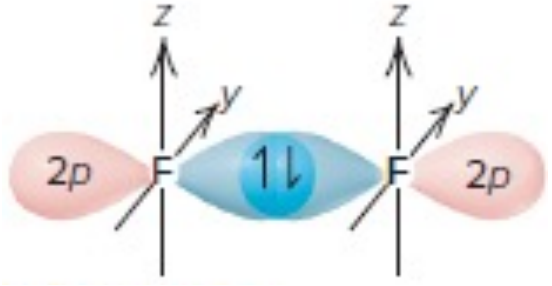
Valence Bond Theory: Making single bonds (F_2)

Fluorine atom



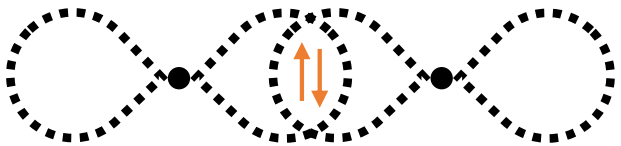


p_x

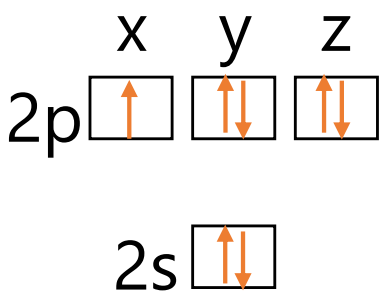


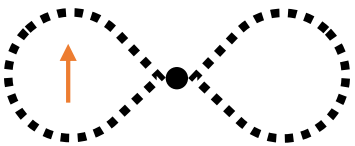
F_2 molecule

p_x-p_x σ-bond



Fluorine atom

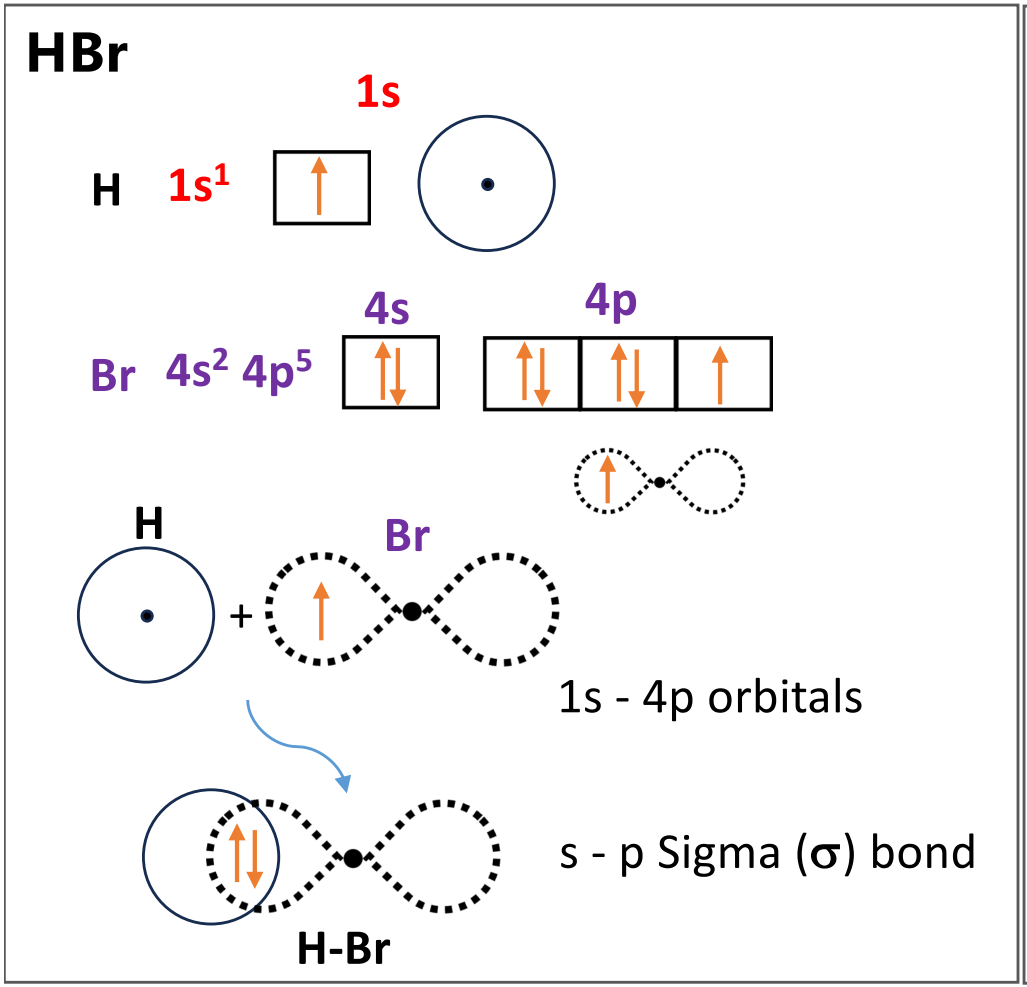


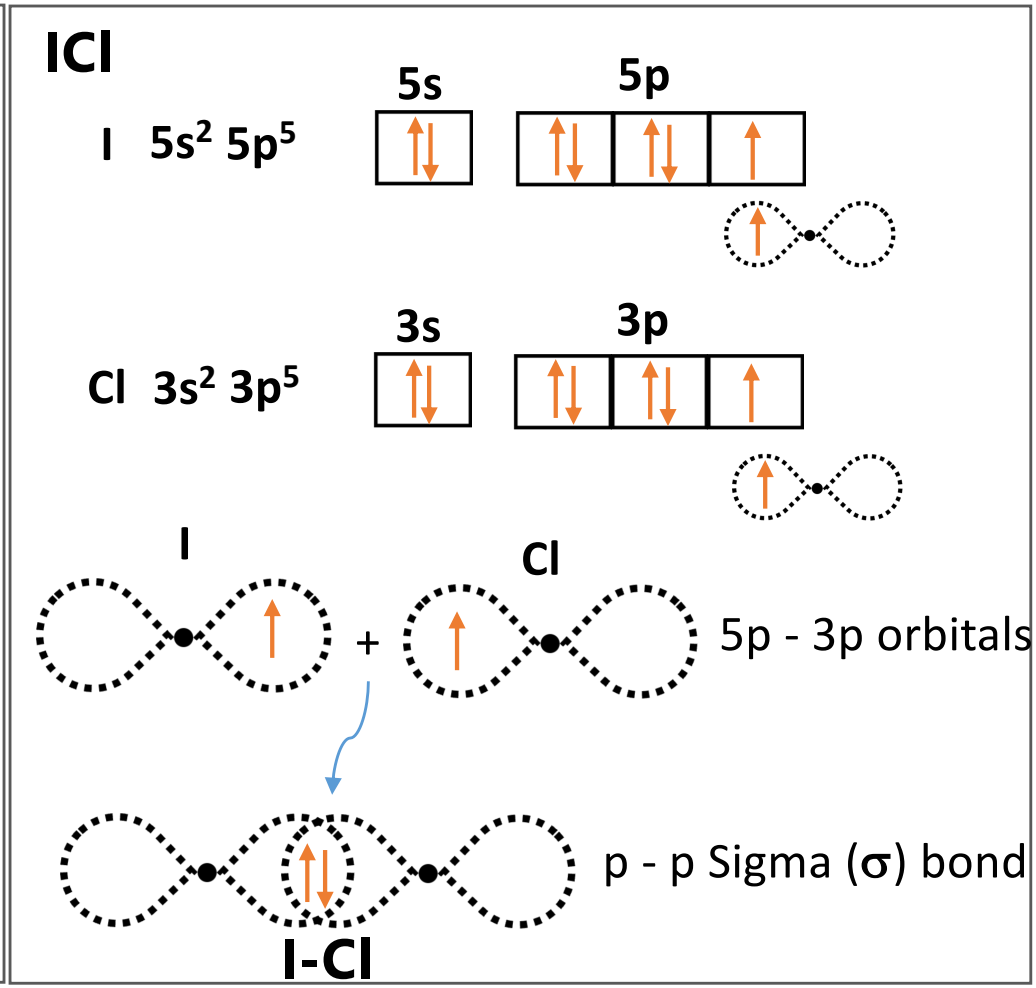


p_x

What about hetero-nuclear molecules (molecules with different atoms)?

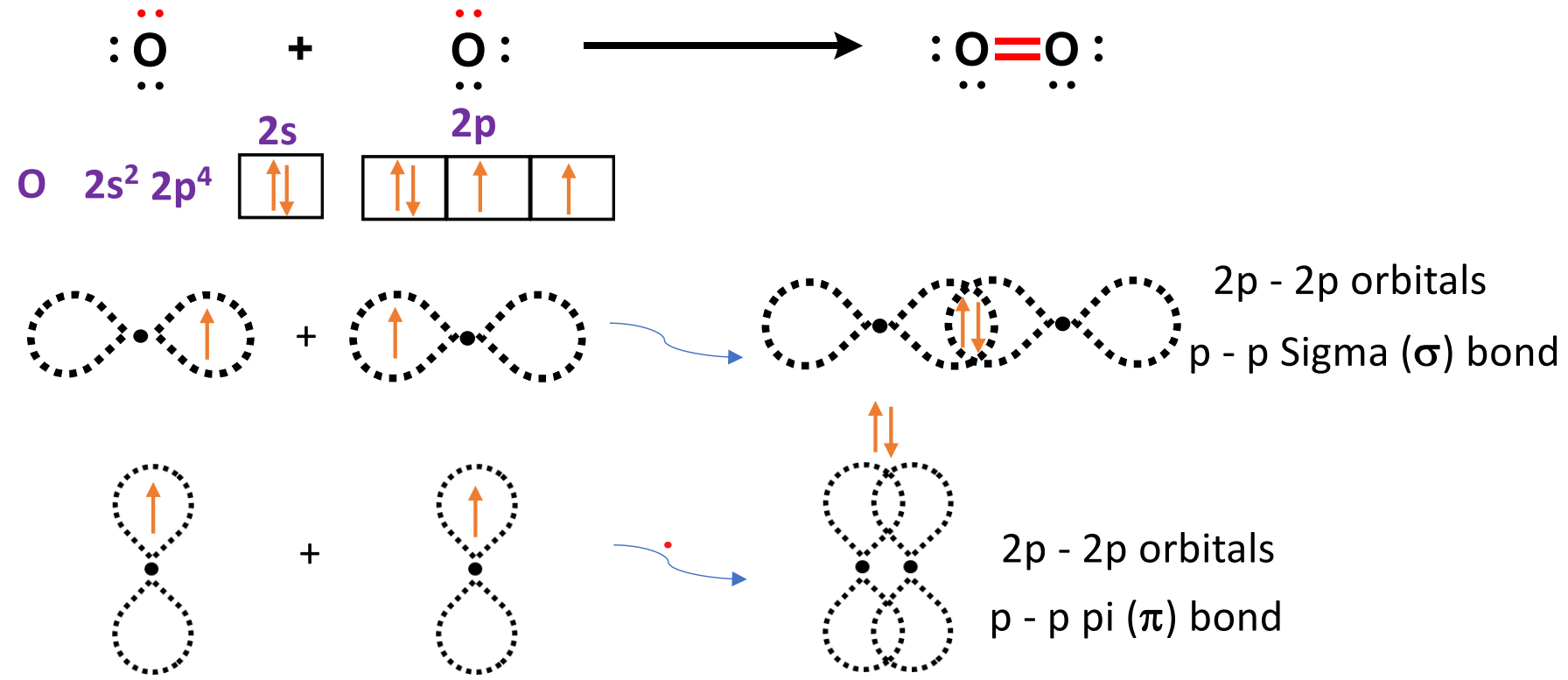
Practice
Use valence bond theory to depict bond formation in the following cases

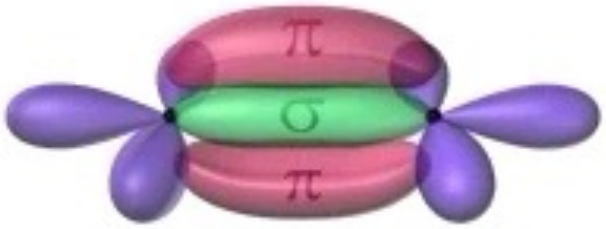




Valence Bond Theory: Making multiple bonds (O_2)

A covalent bond forms when orbitals of two atoms overlap and a pair of electrons occupy the overlap region





O_2

Valence Bond Theory: Making <u>multiple</u> bonds (O_2)

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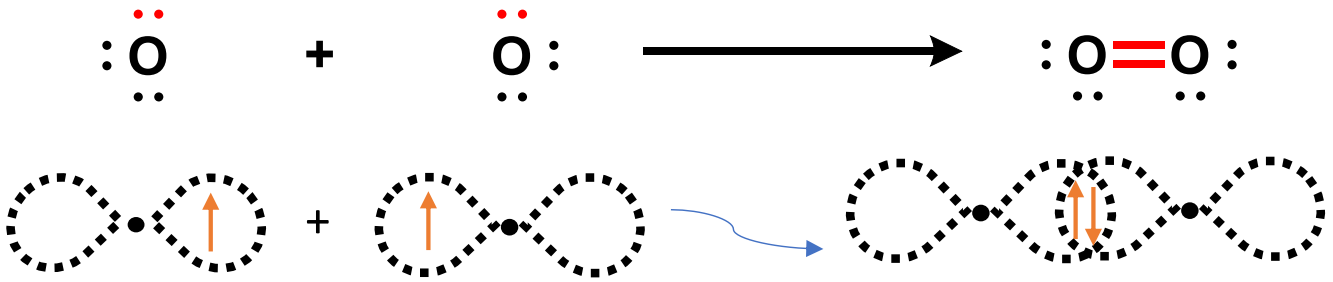
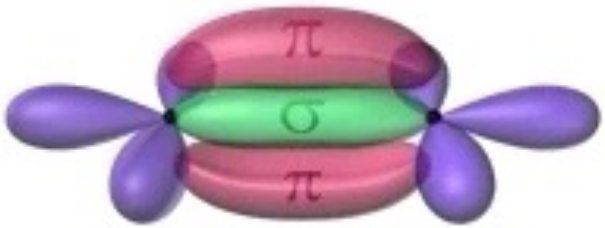


p-p Sigma (σ) bond



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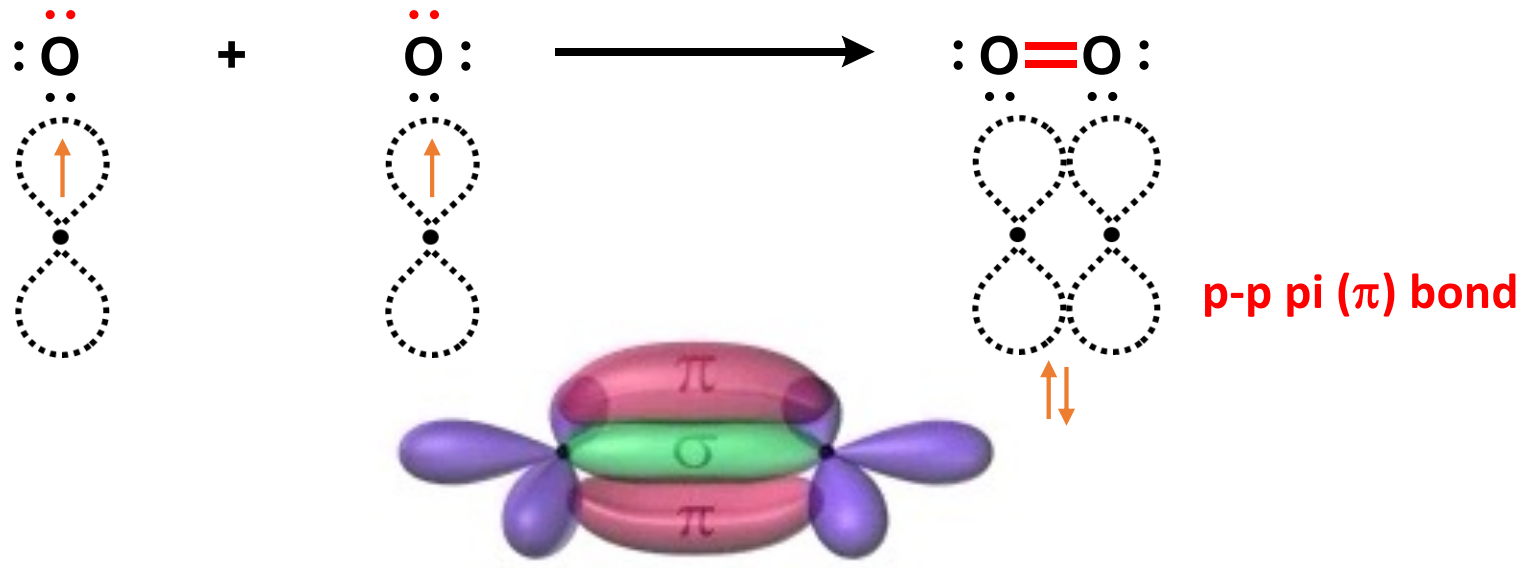
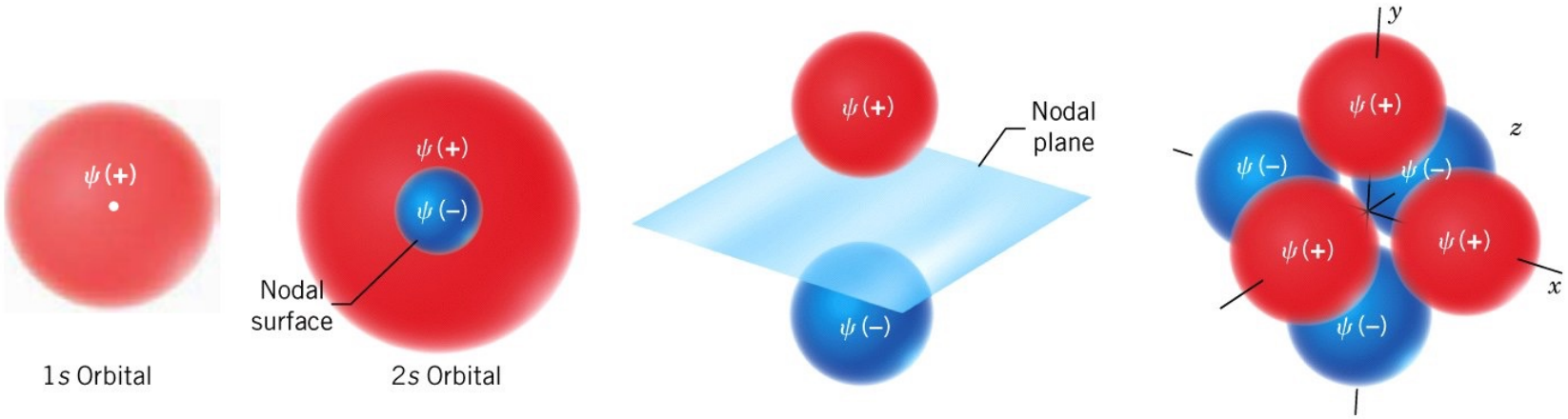
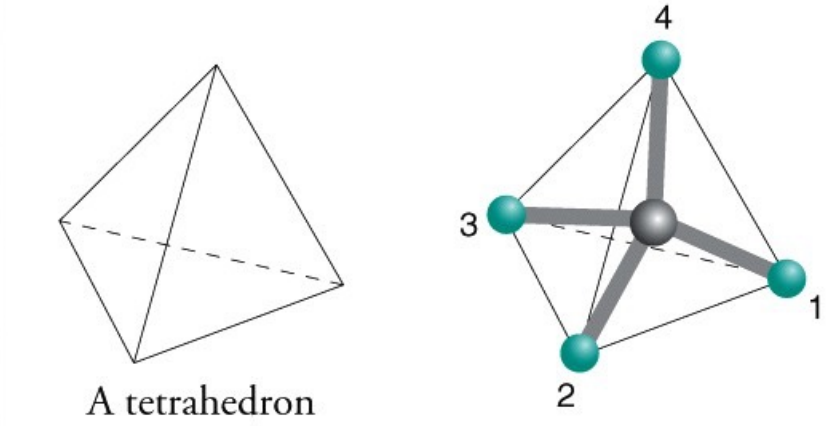


<u>π-bond</u> – formed from overlap of two orbitals. Is not symmetrical around bond axis. Side to side overlap

- The two electrons move over to the new **<u>π -bonding</u>** orbital
- The two electrons in the bonding orbital have opposite spin (Pauli's exclusion principle still followed)

Limitations of Valence Bond Theory





How can valence bond theory predict bond angles?

Valence bond theory cannot predict the geometry for all molecules