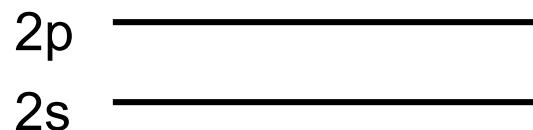


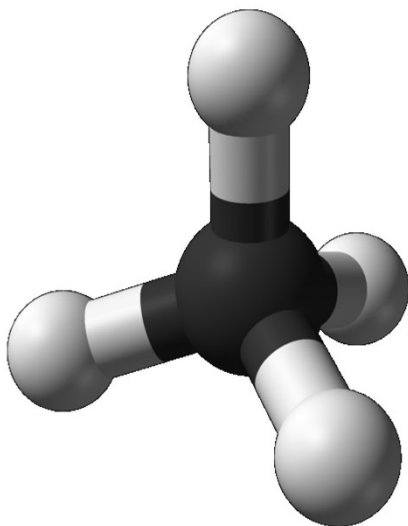
# Hybrid orbitals

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isolated carbon atom



In molecules, carbon forms  $sp$ ,  $sp^2$ , and  $sp^3$  orbitals.



$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{\frac{3}{2}} \left( 2 - \frac{r}{a_0} \right) e^{-\frac{r}{2a_0}}$$

$$\psi_{2p_x} = \frac{x}{\sqrt{32\pi a_0^5}} e^{-r/2a_0}$$

$$\psi_{2p_y} = \frac{y}{\sqrt{32\pi a_0^5}} e^{-r/2a_0}$$

$$\psi_{2p_z} = \frac{z}{\sqrt{32\pi a_0^5}} e^{-r/2a_0}$$

# $sp^3$ hybrid orbitals $109^\circ$

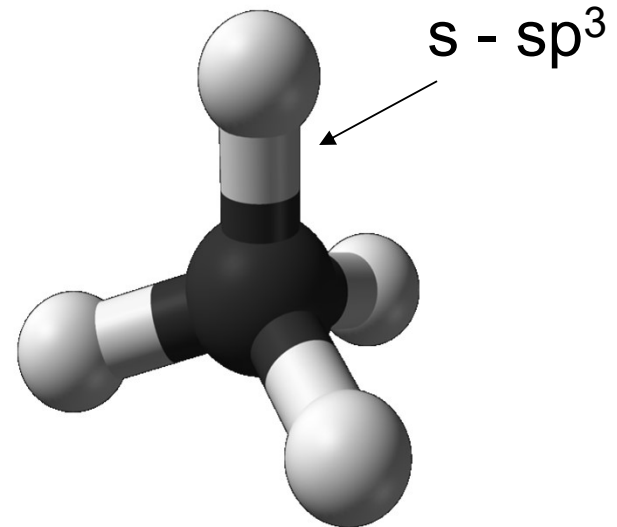
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$$\psi_1 = \frac{1}{2}(\phi_{2s} + \phi_{2p_x} + \phi_{2p_y} + \phi_{2p_z})$$

$$\psi_2 = \frac{1}{2}(\phi_{2s} + \phi_{2p_x} - \phi_{2p_y} - \phi_{2p_z})$$

$$\psi_3 = \frac{1}{2}(\phi_{2s} - \phi_{2p_x} + \phi_{2p_y} - \phi_{2p_z})$$

$$\psi_4 = \frac{1}{2}(\phi_{2s} - \phi_{2p_x} - \phi_{2p_y} + \phi_{2p_z})$$



In this molecular orbital, the coefficients of these 4 atomic orbitals are about  $c_{2s} = 1$ ,  $c_{2p_x} = -1$ ,  $c_{2p_y} = -1$ ,  $c_{2p_z} = 1$ .

# $sp^3$ hybrid orbitals

$$1/\sqrt{4} \phi_{2s} + 1/\sqrt{4} \phi_{2p_x} + 1/\sqrt{4} \phi_{2p_y} + 1/\sqrt{4} \phi_{2p_z}$$



$$1/\sqrt{4} \phi_{2s} + 1/\sqrt{4} \phi_{2p_x} - 1/\sqrt{4} \phi_{2p_y} - 1/\sqrt{4} \phi_{2p_z}$$



$$1/\sqrt{4} \phi_{2s} - 1/\sqrt{4} \phi_{2p_x} - 1/\sqrt{4} \phi_{2p_y} + 1/\sqrt{4} \phi_{2p_z}$$



$$1/\sqrt{4} \phi_{2s} - 1/\sqrt{4} \phi_{2p_x} + 1/\sqrt{4} \phi_{2p_y} - 1/\sqrt{4} \phi_{2p_z}$$



# $sp^2$ hybrid orbitals $120^\circ$

The four orbitals are  $sp^2, sp^2, sp^2, p$

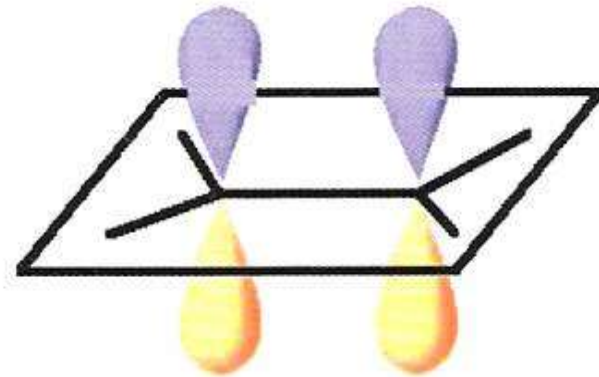
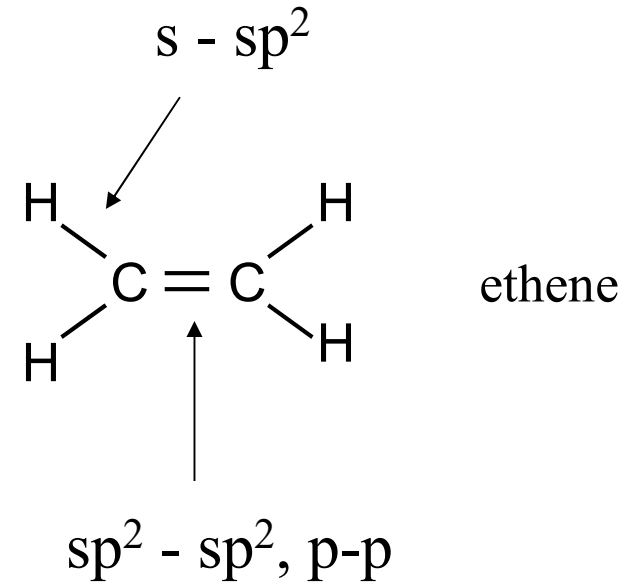
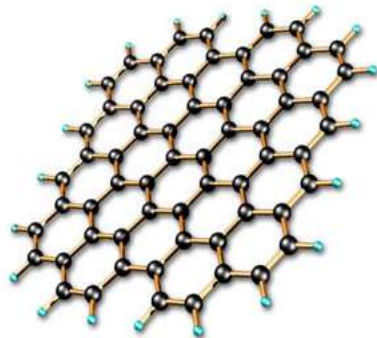
$$\psi_1 = \frac{1}{\sqrt{3}} (\phi_{2s} + \sqrt{2}\phi_{2p_x})$$

$$\psi_2 = \frac{1}{\sqrt{3}} \phi_{2s} - \frac{1}{\sqrt{6}} \phi_{2p_x} + \frac{1}{\sqrt{2}} \phi_{2p_y}$$

$$\psi_3 = \frac{1}{\sqrt{3}} \phi_{2s} - \frac{1}{\sqrt{6}} \phi_{2p_x} - \frac{1}{\sqrt{2}} \phi_{2p_y}$$

$$\psi_4 = \phi_{2p_z}$$

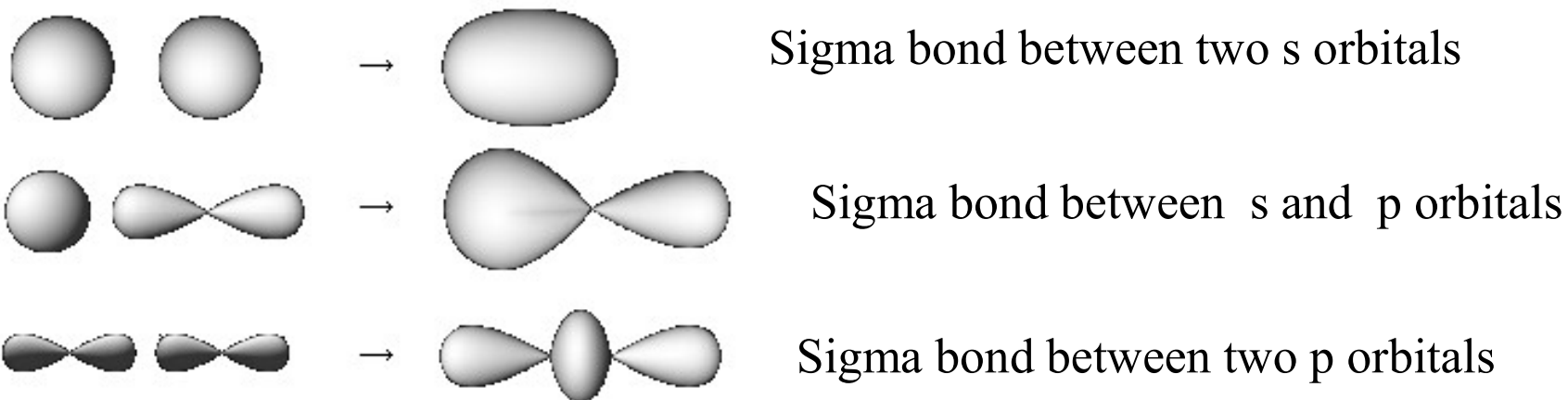
Graphene





# Sigma bonds

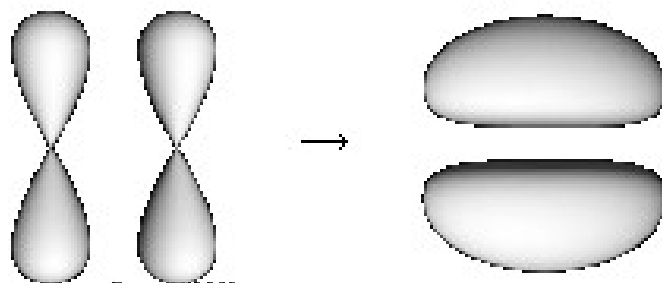
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The angular momentum of a sigma orbital around the interatomic axis is zero. A molecule can twist around a sigma bond.

# Pi bonds

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Pi bond between two p orbitals

There is an energy barrier for rotation around a Pi bond.

# Single bond / double bond / triple bonds

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Single bond : Two electrons are shared, sigma bond

Double bond : Four electrons are shared, sigma bond + pi bond

Triple bond : Six electrons are shared, sigma bond + 2 pi bonds



# Examples of bonds

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