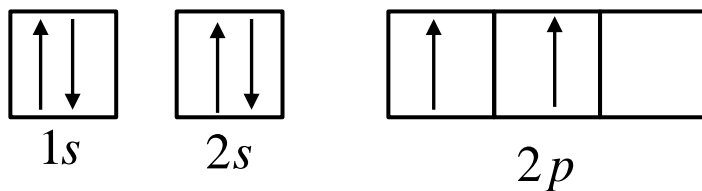
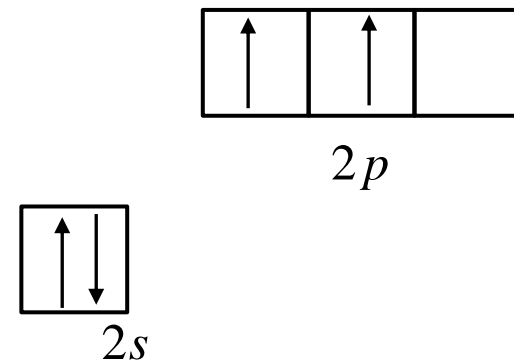


Rappels sur l'hybridation du carbone

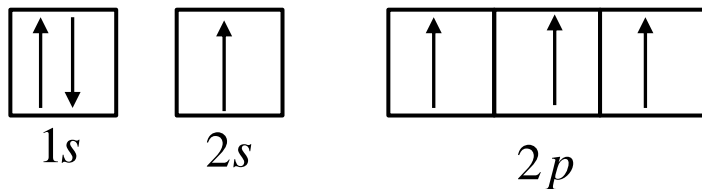
Etat fondamental du carbone atomique $1s^2 2s^2 2p^2$



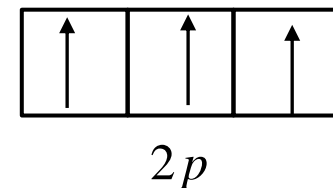
Carbone divalent: C=O



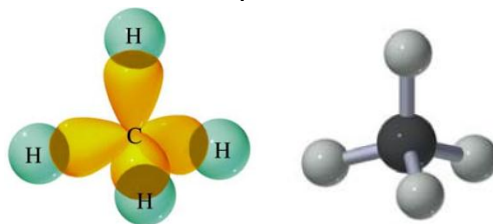
Promotion d'un électron 2s dans une orbitale p $1s^2 2s^1 2p^3$



Carbone tétravalent: CO₂: O=C=O
CH₄



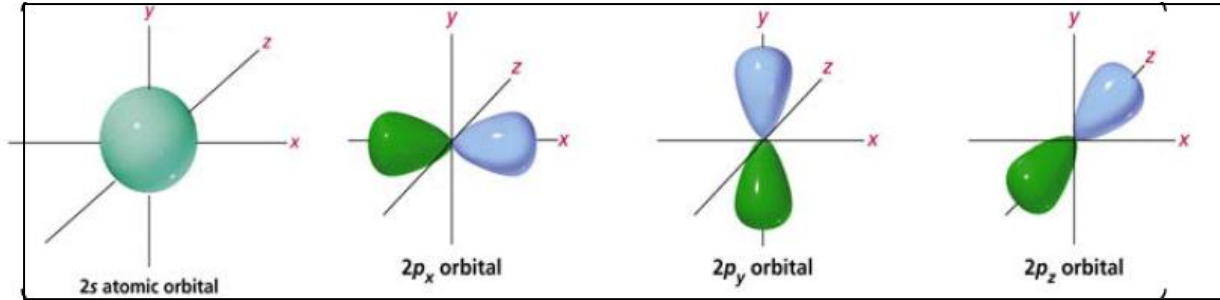
Liaison dirigée vers les 4 sommets d'un tétraèdre régulier



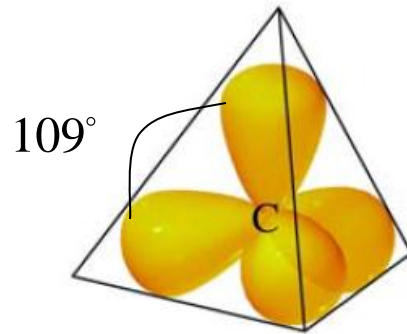
Rappels sur l'hybridation du carbone

Orbitales hybrides

sp^3



sp^3

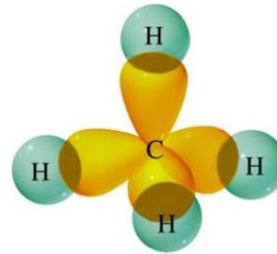


$$\begin{cases} h_1 = \frac{1}{2}(s + p_x + p_y + p_z) \\ h_2 = \frac{1}{2}(s + p_x - p_y - p_z) \\ h_3 = \frac{1}{2}(s - p_x + p_y - p_z) \\ h_4 = \frac{1}{2}(s - p_x - p_y + p_z) \end{cases}$$

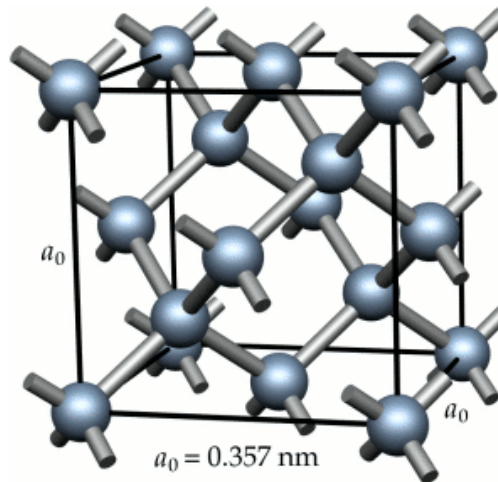
h_i Pointe dans la direction $(\pm 1, \pm 1, \pm 1)$

Rappels sur l'hybridation du carbone

Exemple: méthane



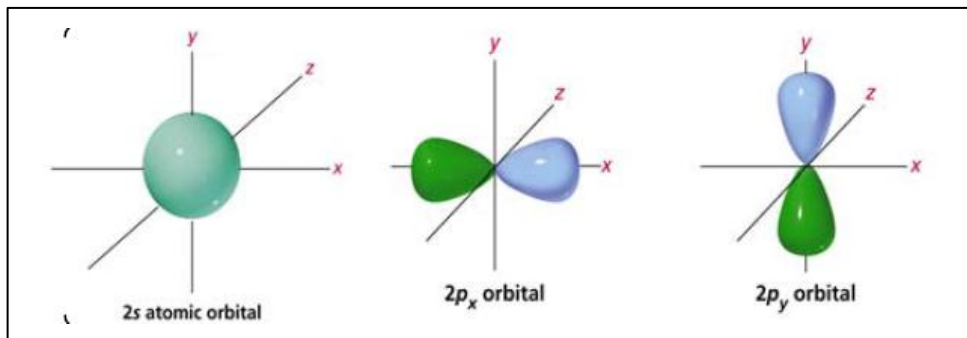
Exemple: diamant



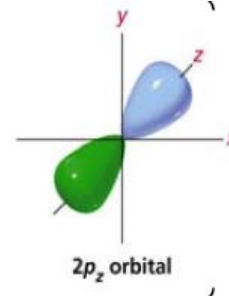
Rappels sur l'hybridation du carbone

Orbitales hybrides

sp^2



Orbitale non affectée par l'hybridation



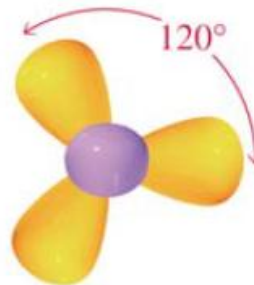
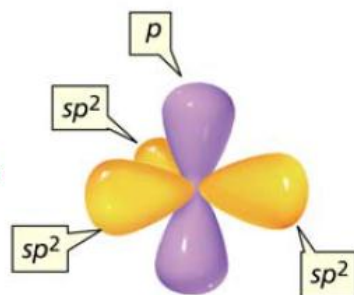
$$\begin{cases} h_1 = \frac{1}{\sqrt{3}}(s + \sqrt{2}p_x) \\ h_2 = \frac{1}{\sqrt{3}}(s - \frac{1}{\sqrt{2}}p_x + \frac{\sqrt{3}}{\sqrt{2}}p_y) \\ h_3 = \frac{1}{\sqrt{3}}(s - \frac{1}{\sqrt{2}}p_x - \frac{\sqrt{3}}{\sqrt{2}}p_y) \\ h_4 = p_z \end{cases}$$

$$p_z \perp sp^2$$

Vue de côté

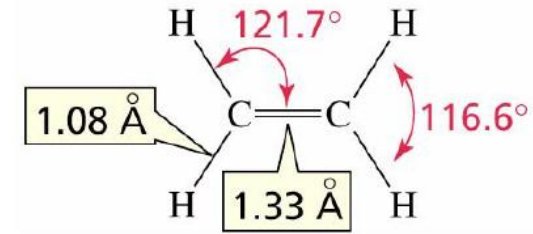
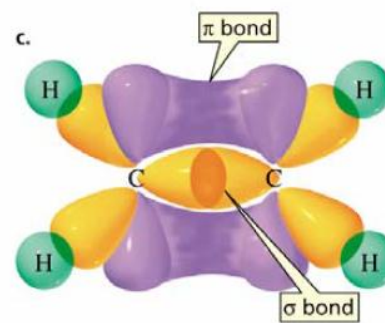
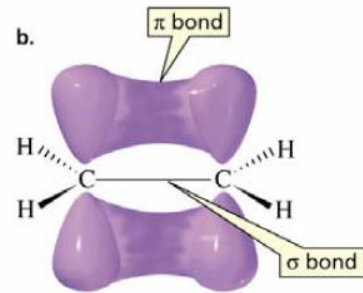
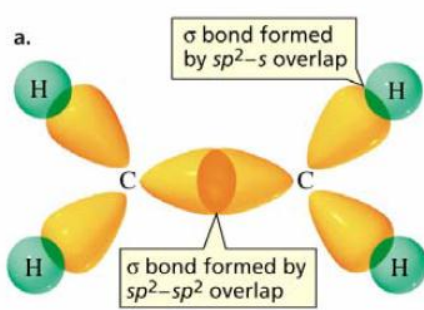
Vue de dessus

3 orbitales hybrides sp^2
et une orbitale naturelle $2p_z$

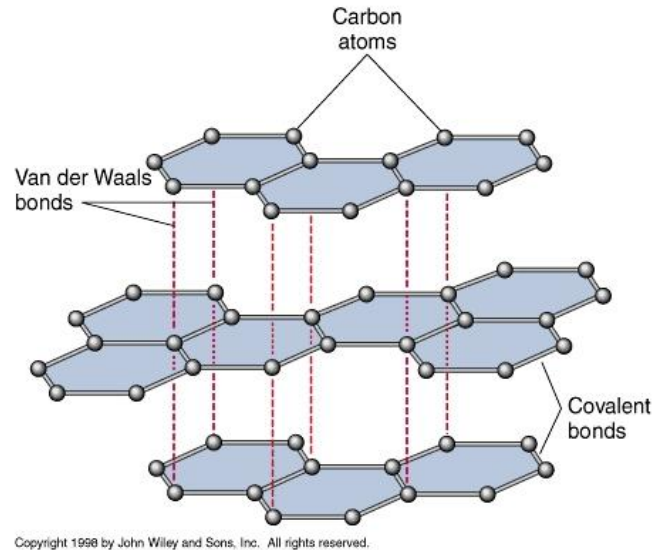


Rappels sur l'hybridation du carbone

Exemple: éthylène: C_2H_4



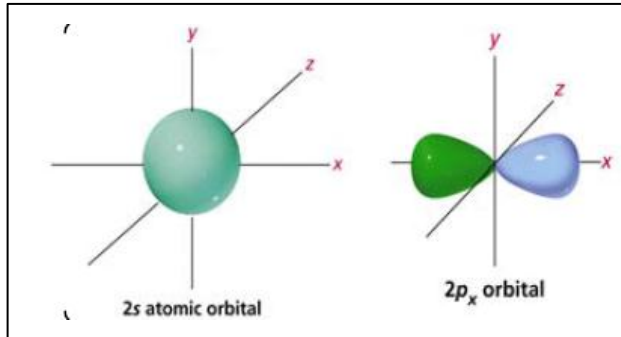
Exemple: graphite ou graphène



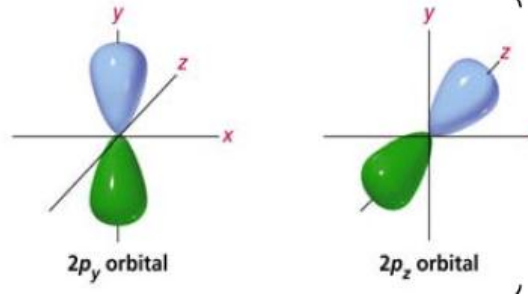
Rappels sur l'hybridation du carbone

Orbitales hybrides

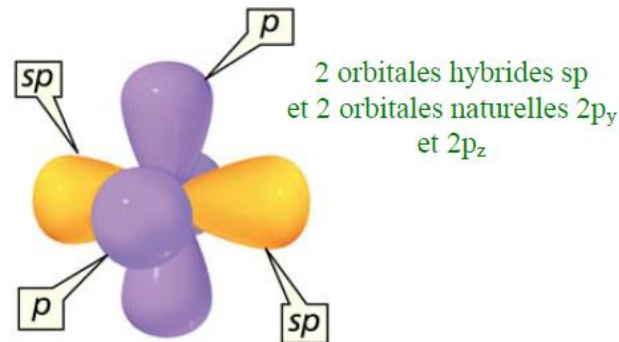
sp



Orbitales non affectées par l'hybridation

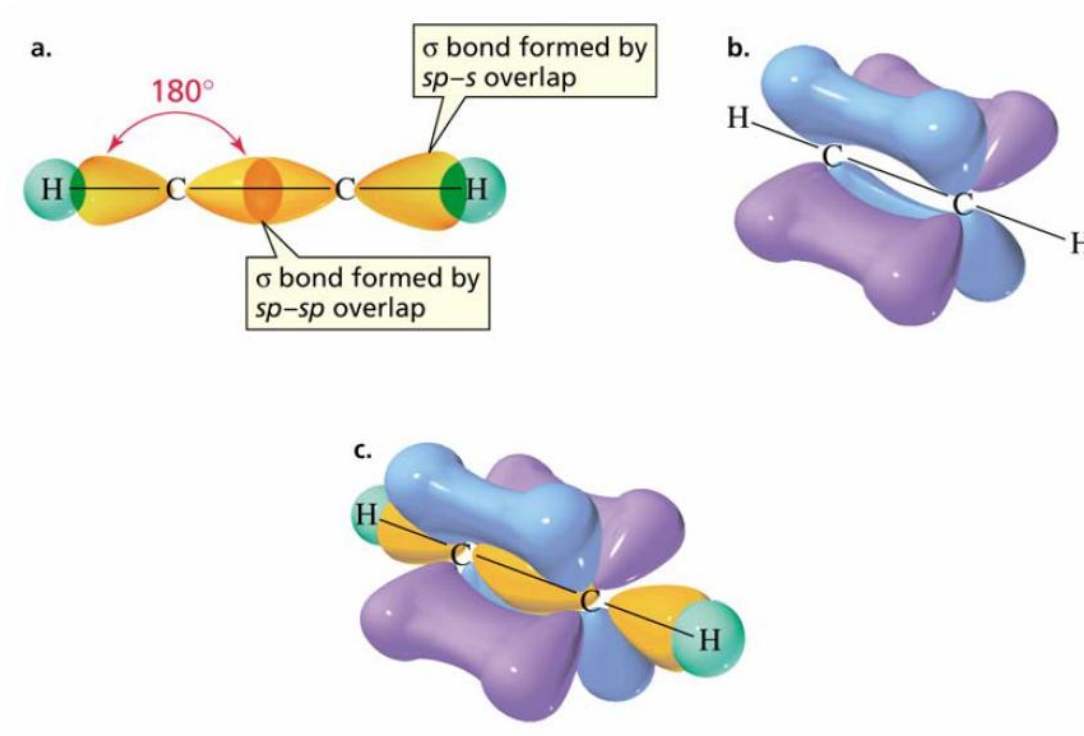


$$\begin{cases} h_1 = \frac{1}{\sqrt{2}}(s + p_x) \\ h_2 = \frac{1}{\sqrt{2}}(s - p_x) \\ h_3 = p_y \\ h_4 = p_z \end{cases} \quad p_y, p_z \perp sp$$



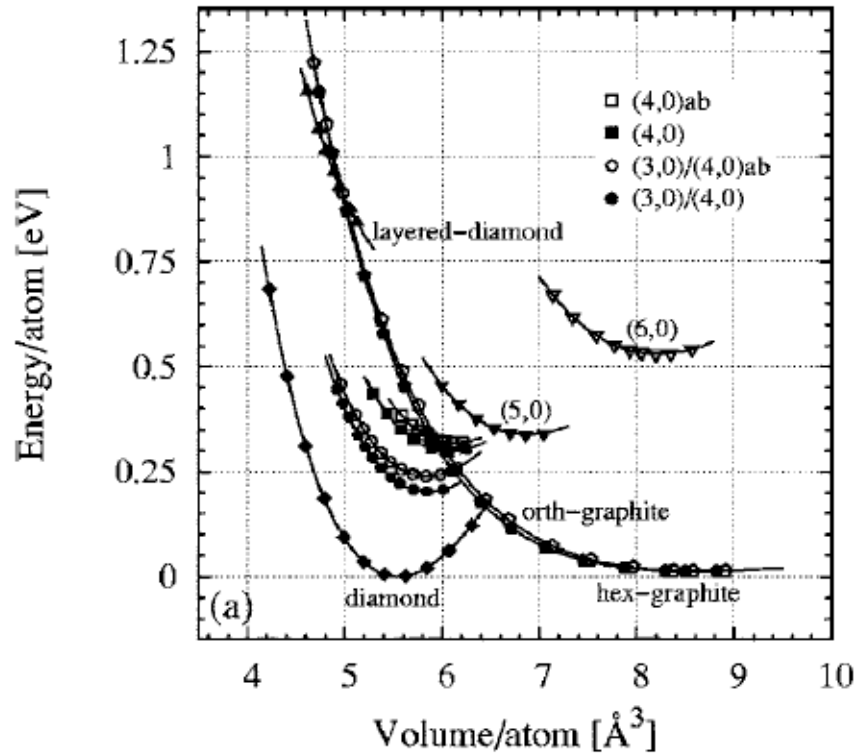
Rappels sur l'hybridation du carbone

Exemple: acétylène C_2H_2



Rappels sur l'hybridation du carbone

Stabilité relative des différents phases du carbone



PRB 72, 214109 (2005)