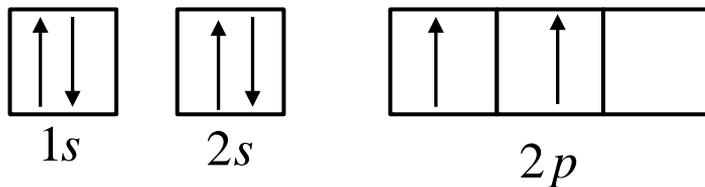
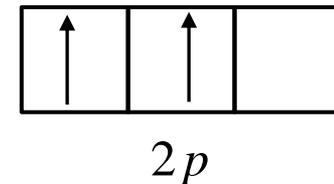
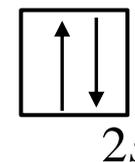


# Rappels sur l'hybridation du carbone

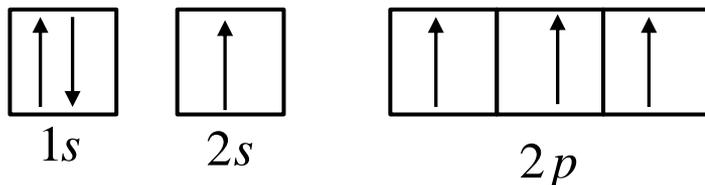
Etat fondamental du carbone atomique  $1s^2 2s^2 2p^2$



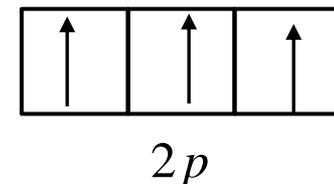
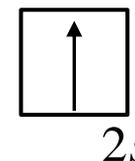
Carbone divalent: C=O



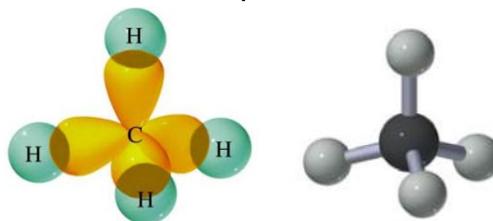
Promotion d'un électron 2s dans une orbitale p  $1s^2 2s^1 2p^3$



Carbone tétravalent: CO<sub>2</sub>: O=C=O  
CH<sub>4</sub>



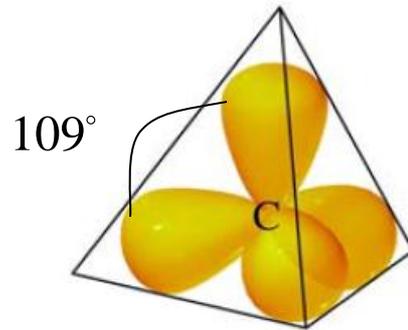
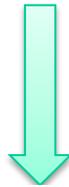
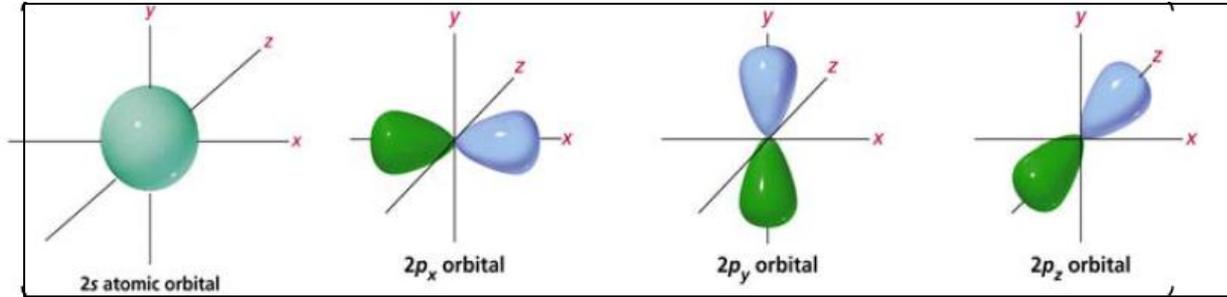
Liaison dirigée vers les 4 sommets d'un tétraèdre régulier



# Rappels sur l'hybridation du carbone

## Orbitales hybrides

$sp^3$



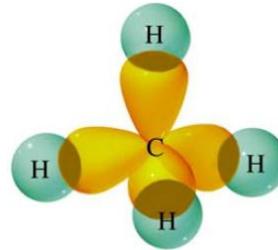
$$\begin{cases} h_1 = \frac{1}{2}(s + p_x + p_y + p_z) \\ h_2 = \frac{1}{2}(s + p_x - p_y - p_z) \\ h_3 = \frac{1}{2}(s - p_x + p_y - p_z) \\ h_4 = \frac{1}{2}(s - p_x - p_y + p_z) \end{cases}$$

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

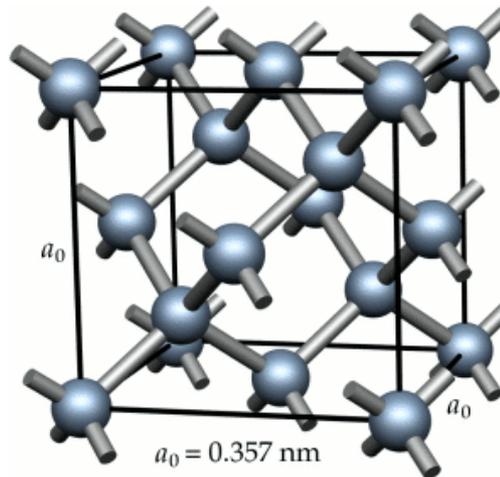
# Rappels sur l'hybridation du carbone

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Exemple: méthane



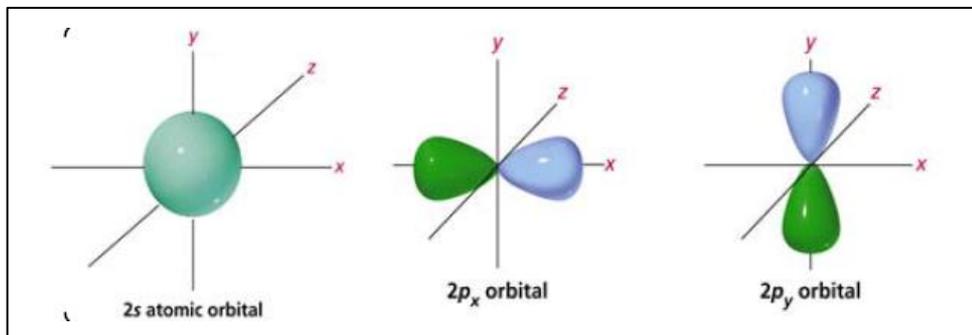
Exemple: diamant



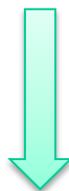
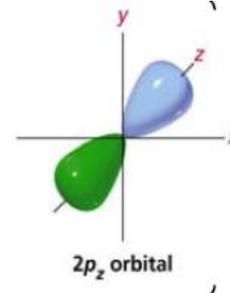
# Rappels sur l'hybridation du carbone

## Orbitales hybrides

$sp^2$



Orbitale non affectée par l'hybridation



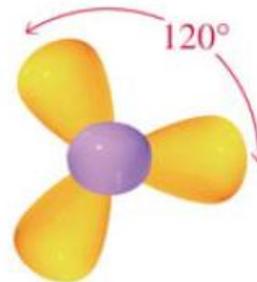
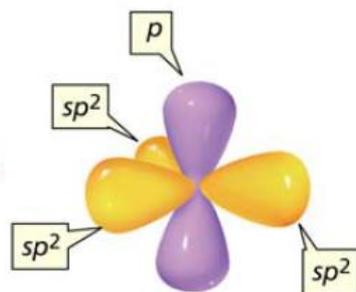
$$\begin{cases} h_1 = \frac{1}{\sqrt{3}}(s + \sqrt{2}p_x) \\ h_2 = \frac{1}{\sqrt{3}}(s - \frac{1}{\sqrt{2}}p_x + \frac{\sqrt{3}}{\sqrt{2}}p_y) \\ h_3 = \frac{1}{\sqrt{3}}(s - \frac{1}{\sqrt{2}}p_x - \frac{\sqrt{3}}{\sqrt{2}}p_y) \\ h_4 = p_z \end{cases}$$

$$p_z \perp sp^2$$

Vue de côté

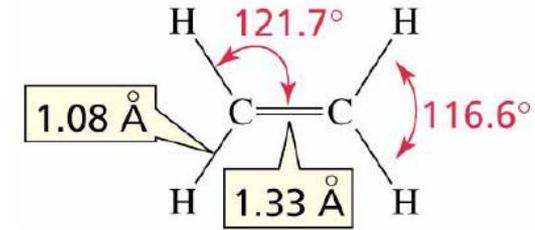
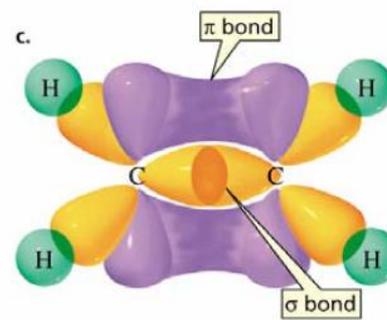
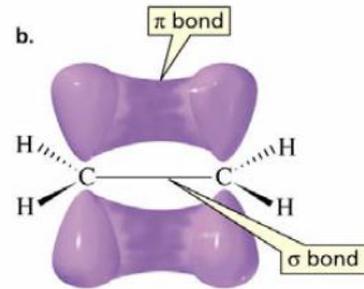
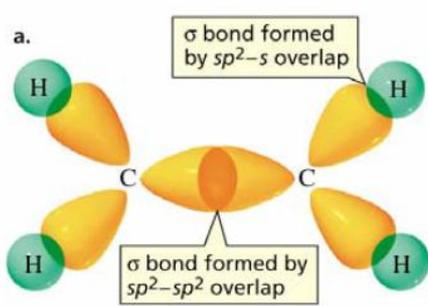
Vue de dessus

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

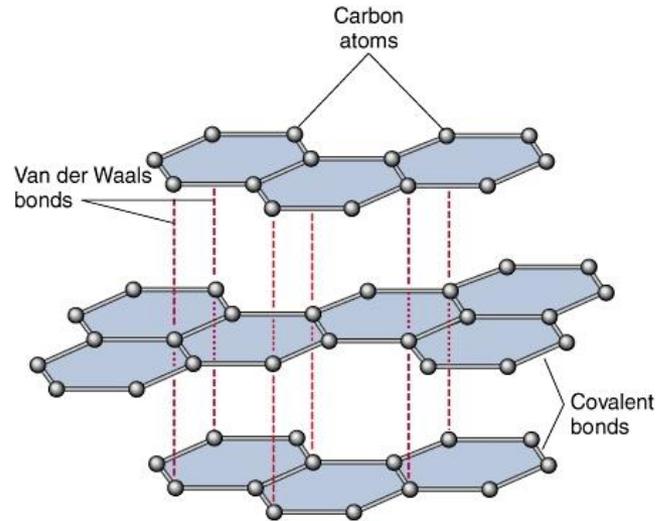


# Rappels sur l'hybridation du carbone

Exemple: éthylène:  $C_2H_4$



Exemple: graphite ou graphène

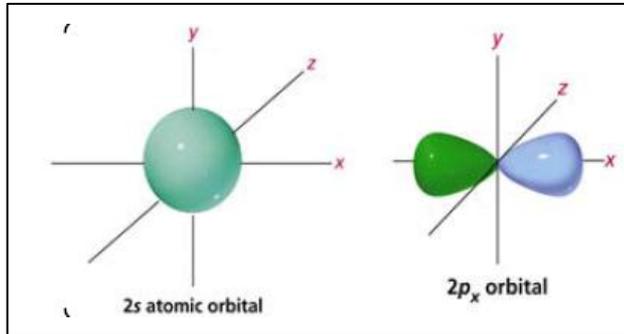


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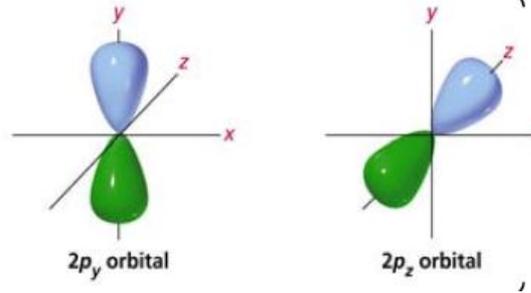
# Rappels sur l'hybridation du carbone

## Orbitales hybrides

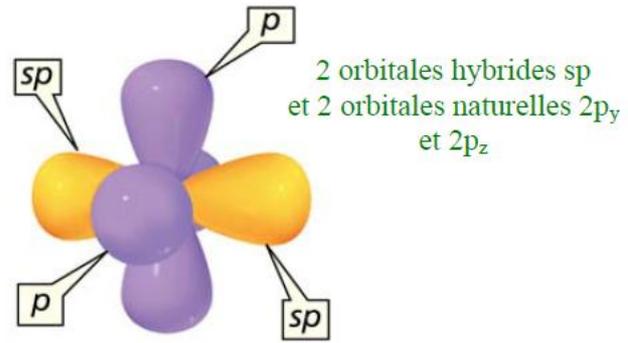
sp



Orbitales non affectées par l'hybridation

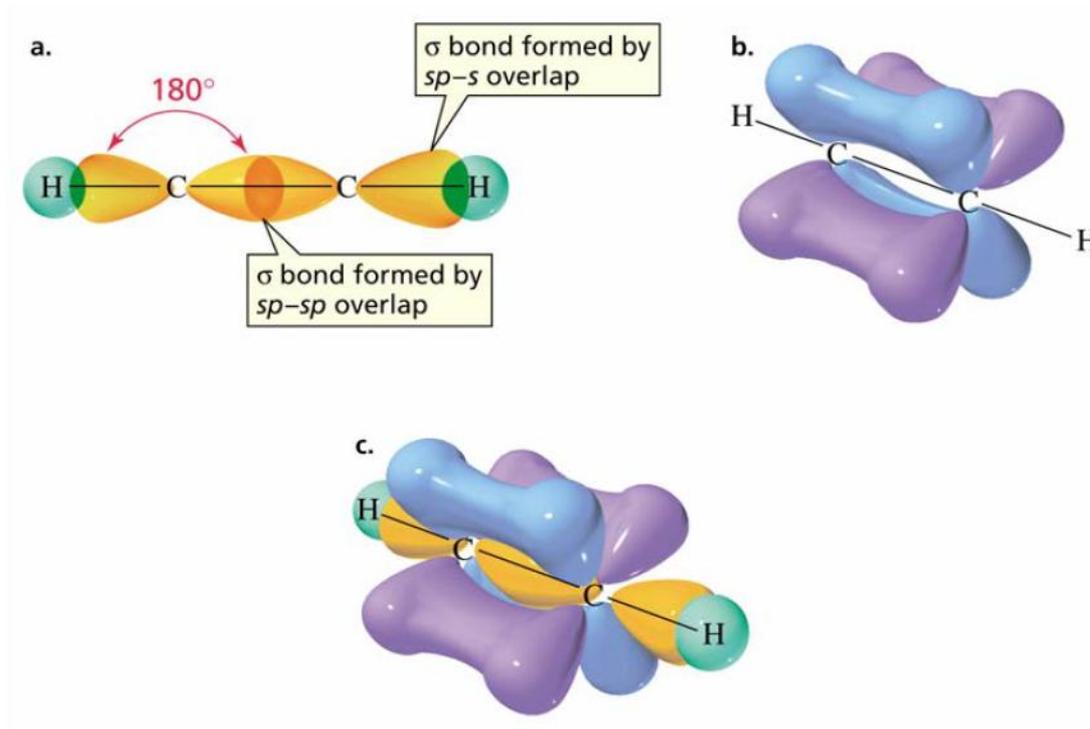


$$\begin{cases} h_1 = \frac{1}{\sqrt{2}}(s + p_x) \\ h_2 = \frac{1}{\sqrt{2}}(s - p_x) \\ h_3 = p_y \\ h_4 = p_z \end{cases} \quad p_y, p_z \perp sp$$



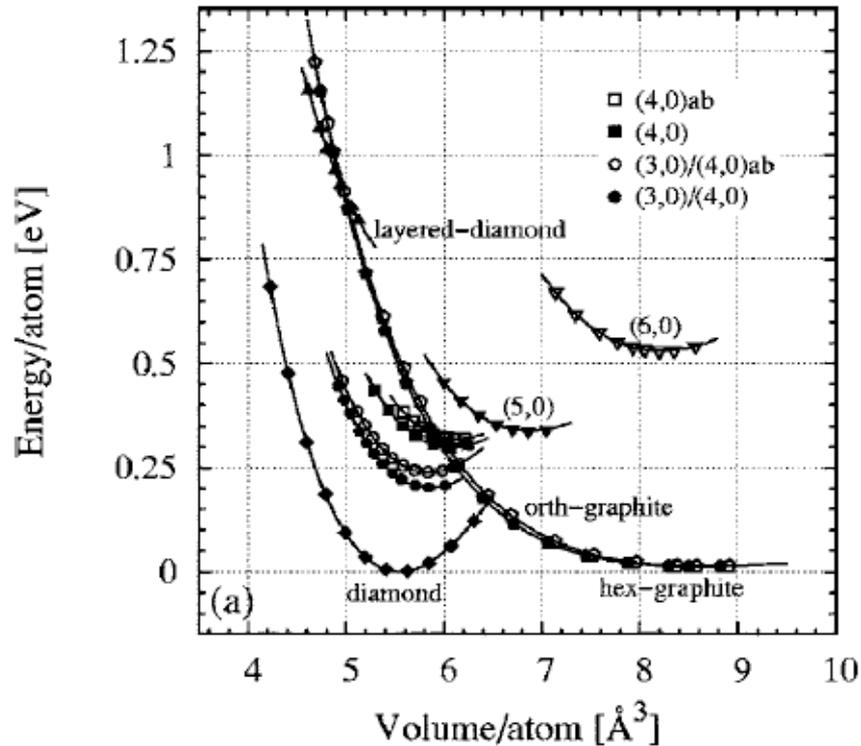
# Rappels sur l'hybridation du carbone

Exemple: acétylène  $C_2H_2$



# Rappels sur l'hybridation du carbone

## Stabilité relative des différents phases du carbone



PRB 72, 214109 (2005)