Ibridazione sp^2

$$\begin{cases} \psi_1 = a_1 \psi_{2s} + b_1 \psi_{2px} + c_1 \psi_{2py} \\ \psi_2 = a_2 \psi_{2s} + b_2 \psi_{2px} + c_2 \psi_{2py} \\ \psi_3 = a_3 \psi_{2s} + b_3 \psi_{2px} + c_3 \psi_{2py} \end{cases}$$

$c_1 = 0$ perché ibrido giace direzione x

Normalizzazione

$$\int \psi_1^* \psi_1 \, d\tau = 1 \qquad \int \psi_2^* \psi_2 \, d\tau = 1 \qquad \int \psi_3^* \psi_3 \, d\tau = 1$$

$$\langle 1|1 \rangle = 1 \qquad \langle 2|2 \rangle = 1 \qquad \langle 3|3 \rangle = 1$$

$$\begin{cases} a_1^2 + b_1^2 = 1 \\ a_2^2 + b_2^2 + c_2^2 = 1 \\ a_3^2 + b_3^2 + c_3^2 = 1 \end{cases}$$

Ortogonalità

$$\int \psi_1 \psi_2 \, d\tau = 0 \qquad \int \psi_1 \psi_3 \, d\tau = 0 \qquad \int \psi_2 \psi_3 \, d\tau = 0$$

$$\langle 1|2 \rangle = 0 \qquad \langle 1|3 \rangle = 0 \qquad \langle 2|3 \rangle = 0$$
$$\langle 2|1 \rangle = 0 \qquad \langle 3|1 \rangle = 0 \qquad \langle 3|2 \rangle = 0$$

$$\begin{cases} a_1 a_2 + b_1 b_2 + 0 = 0 \\ a_1 a_3 + b_1 b_3 + 0 = 0 \\ a_2 a_3 + b_2 b_3 + c_2 c_3 = 0 \end{cases}$$

S uguale contributo quindi $a_1 = a_2 = a_3 = a$

Ortogonalité

$$\begin{cases} a^2 + b_1 b_2 = 0 \\ a^2 + b_1 b_3 = 0 \\ a^2 + b_2 b_3 + c_2 c_3 = 0 \end{cases}$$

$\rightarrow b_1 b_2 = b_1 b_3 \Rightarrow b_2 = b_3$

Normalisation

$$\begin{cases} a^2 + b_1^2 = 1 \\ a^2 + b_2^2 + c_2^2 = 1 \\ a^2 + b_3^2 + c_3^2 = 1 \end{cases}$$

$\rightarrow b_2^2 + c_2^2 = b_3^2 + c_3^2$

$\rightarrow c_2^2 = c_3^2$

$c_2 = \pm c_3$

$c_2 = c_3$ impos.

$c_2 = -c_3$

$$\leftarrow \begin{cases} a^2 + b_1^2 = 1 \\ a^2 + b_2^2 + c_2^2 = 1 \\ a^2 + b_1 b_2 = 0 \\ a^2 + b_2 b_3 - c_2^2 = 0 \end{cases} \longrightarrow \begin{cases} a^2 + b_2^2 + c_2^2 = 1 \\ a^2 + b_2 b_3 - c_2^2 = 0 \end{cases}$$

$$\begin{cases} a^2 + b_2^2 + c_2^2 = 1 \\ a^2 + b_2^2 - c_2^2 = 0 \end{cases} \Rightarrow c_2^2 = 1 - c_2^2$$

$$c_2^2 + c_2^2 = 1$$

$$2c_2^2 = 1 \quad c_2 = \frac{1}{\sqrt{2}} \quad c_3 = -\frac{1}{\sqrt{2}}$$

$\rightarrow a^2 = -b_1 b_2$

$$\rightarrow \begin{cases} a^2 + b_1^2 = 1 \\ a^2 + b_2 b_3 - c_2^2 = 0 \end{cases} \rightarrow \begin{cases} -b_1 b_2 + b_1^2 = 1 \\ -b_1 b_2 + b_2^2 = \frac{1}{2} \end{cases}$$

$$\begin{cases} b_1 (b_1 - b_2) = 1 \\ b_2 (b_2 - b_1) = \frac{1}{2} \end{cases}$$

$$\begin{cases} (b_1 - b_2) = 1/b_1 \\ (b_1 - b_2) = -1/2\, b_2 \end{cases} \Rightarrow 1/b_1 = -1/2\, b_2$$

$$b_2 = -\frac{1}{2} b_1$$

$$a^2 = -b_1 b_2 = -b_1 \cdot \left(-\frac{1}{2} b_1\right) = \frac{1}{2} b_1^2$$

$$\begin{cases} a = \frac{1}{\sqrt{2}} b_1 \\ a^2 + b_1^2 = 1 \end{cases} \qquad \begin{cases} a = \frac{1}{\sqrt{2}} b_1 \\ \frac{1}{2} b_1^2 + b_1^2 = 1 \end{cases}$$

$$\begin{cases} a = \frac{1}{\sqrt{2}} b_1 \\ \frac{3}{2} b_1^2 = 1 \end{cases} \rightarrow \quad a = \frac{1}{\sqrt{2}} \cdot \frac{\sqrt{2}}{\sqrt{3}} = \frac{1}{\sqrt{3}}$$

$$\rightarrow \quad b_1 = \frac{\sqrt{2}}{\sqrt{3}}$$

$$b_2 = -\frac{1}{2} b_1 = -\frac{1}{2} \frac{\sqrt{2}}{\sqrt{3}} = -\frac{1}{2} \frac{\sqrt{2}}{\sqrt{3}} \frac{\sqrt{2}}{\sqrt{2}} = -\frac{1}{\sqrt{6}}$$

$$b_2 = b_3 = -\frac{1}{\sqrt{6}}$$

$$a_1 = a_2 = a_3 = \frac{1}{\sqrt{3}}$$

$$b_1 = \frac{\sqrt{2}}{\sqrt{3}} \qquad b_2 = -\frac{1}{\sqrt{6}} \qquad b_3 = -\frac{1}{\sqrt{6}}$$

$$c_1 = 0 \qquad c_2 = \frac{1}{\sqrt{2}} \qquad c_3 = -\frac{1}{\sqrt{2}}$$