

Hybridization

Bonds form in the direction of maximum overlap.

(L. Pauling)

Mix n AOs to get n hybrids:

Orthonormal set of Atomic Orbitals

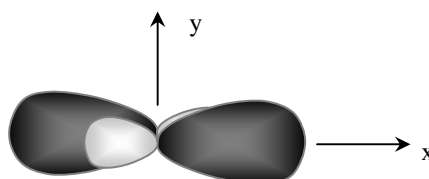
equivalent in extent, shape, and energy

differ in orientation: to maximize overlap

50% p-character

$$sp \quad \Psi_a = \frac{1}{\sqrt{2}} (s + p_x)$$

$$\Psi_b = \frac{1}{\sqrt{2}} (s - p_x)$$



$$\int \Psi_a^2 d\tau = \frac{1}{2} \int s^2 + 2 s p_x + p_x^2 d\tau = 1$$

$$\int \Psi_a \Psi_b d\tau = \frac{1}{2} \int (s + p_x)(s - p_x) d\tau = \frac{1}{2} \int s^2 - p_x^2 d\tau = 0$$

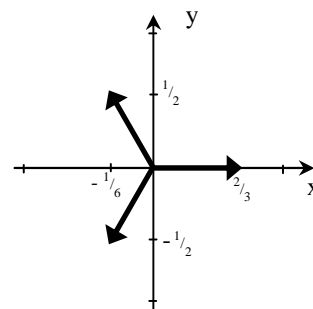
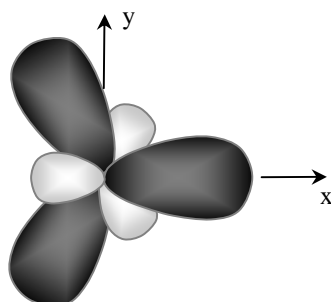
$$\int s^2 d\tau = \int p_x^2 d\tau = 1 \quad \text{atomic normalization} \quad \int s p_x d\tau = 0 \quad \text{orthogonality}$$

66% p-character

$$sp^2 \quad \Psi_a = \frac{1}{\sqrt{3}} s + \frac{\sqrt{2}}{\sqrt{3}} p_x$$

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

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



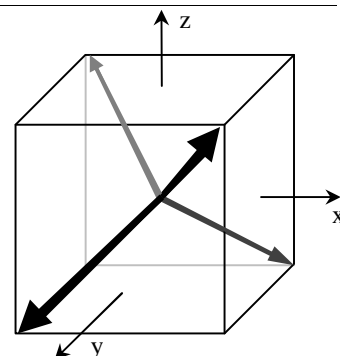
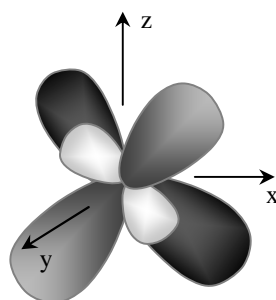
75% p-character

$$sp^3 \quad \Psi_a = \frac{1}{2} (s + p_x + p_y + p_z)$$

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

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

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



bond angle:	90°	109.5°	120°	180°
hybridization:	p^3	sp^3	sp^2	sp
examples:	PH ₃ (93°) H ₂ S (92°)	CH ₄ (109.5°) NH ₃ (107°) H ₂ O (104.5°)	BF ₃ (120°) CO ₃ ²⁻ (120°) :CH ₂ (137.8°)	BeH ₂ (180°) HC≡CH