Atomic orbitals & hybridization:

$\underline{Y_{l,m}}$

$$Y_{0,0}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,1}(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}}\,\sin\theta\,(\cos\varphi + i\sin\varphi)$$

$$= -\sqrt{\frac{3}{8\pi}}\,\left(\frac{x+iy}{r}\right)$$

$$\left.Y_{1,0}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\,\cos\theta = \sqrt{\frac{3}{4\pi}}\,\frac{z}{r}\right\} p_z$$

$$Y_{1,-1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}}\,\frac{(x-iy)}{r}$$

$$\left.\frac{1}{\sqrt{2}}\left(Y_{1,-1} - Y_{1,1}\right) = \frac{1}{\sqrt{2}}\sqrt{\frac{3}{8\pi}}\,\frac{2x}{r} = \sqrt{\frac{3}{4\pi}}\,\frac{x}{r}\right\} p_x$$

$$\left.\frac{i}{\sqrt{2}}\left(Y_{1,-1} + Y_{1,1}\right) = \sqrt{\frac{3}{4\pi}}\,\frac{y}{r}\right\} p_y$$

$$Y_{2,2}(\theta,\varphi) = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta \,(\underbrace{\cos 2\varphi}_{\cos^2\varphi - \sin^2\varphi} + i\underbrace{\sin 2\varphi}_{2\cos\varphi\sin\varphi})$$

$$Y_{2,2} = \left(\frac{15}{32\pi}\right)^{1/2} \frac{x^2 - y^2 + 2ixy}{r^2}$$

$$Y_{2,-2} = \left(\frac{15}{32\pi}\right)^{1/2} \frac{x^2 - y^2 - 2ixy}{r^2}$$

$$Y_{2,1} = -\left(\frac{15}{8\pi}\right)^{1/2} \frac{z(x+iy)}{r^2}$$

$$Y_{2,-1} = \left(\frac{15}{8\pi}\right)^{1/2} \frac{z(x-iy)}{r^2}$$

$$Y_{2,0} = \left(\frac{5}{16\pi}\right)^{1/2} \frac{3z^2 - r^2}{r^2} \leftarrow \frac{2z^2 - x^2 - y^2}{r^2}$$

The are 6 combinations: $x^2, y^2, z^2, xy, yz, zx$, but because $x^2 + y^2 + z^2 = r^2$, there are only 5 independent combinations.

Hybridization example: sp^2

$$R_{20}(r) = \frac{1}{\sqrt{2}}\frac{1}{a^{3/2}}\left(1-\frac{r}{2a}\right)e^{-r/2a}$$

$$R_{21}(r) = \frac{1}{\sqrt{24}}\frac{1}{a^{3/2}}\frac{r}{a}\,e^{-r/2a}$$

Four $n=2$ wavefunctions:

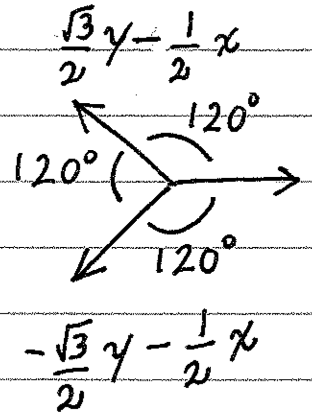
ψ_1 ψ_2

$$R_{20}(r)\cdot\frac{1}{\sqrt{4\pi}},\; R_{21}(r)\sqrt{\frac{3}{4\pi}}\,\frac{x}{r},\; R_{21}(r)\sqrt{\frac{3}{4\pi}}\,\frac{y}{r}$$

ψ_0

$$R_{21}(r)\sqrt{\frac{3}{4\pi}}\,\frac{z}{r}$$

ψ_3



Leave ψ_3 the same, but combine the other 3 to create new hybridized wave functions.

$$f_0 = \sqrt{\frac{2}{3}}\left(\psi_1 + \frac{1}{\sqrt{2}}\psi_0\right)$$

$$f_1 = \sqrt{\frac{2}{3}}\left(\frac{\sqrt{3}}{2}\psi_2 - \frac{1}{2}\psi_1 + \frac{1}{\sqrt{2}}\psi_0\right)$$

$$f_2 = \sqrt{\frac{2}{3}}\left(-\frac{\sqrt{3}}{2}\psi_2 - \frac{1}{2}\psi_1 + \frac{1}{\sqrt{2}}\psi_0\right)$$

$$\rightarrow \quad f_0 = \sqrt{\frac{2}{3}}\psi_1 + \frac{1}{\sqrt{3}}\psi_0$$

$$f_1 = \frac{1}{\sqrt{2}}\psi_2 - \frac{1}{\sqrt{6}}\psi_1 + \frac{1}{\sqrt{3}}\psi_0$$

$$f_2 = -\frac{1}{\sqrt{2}}\psi_2 - \frac{1}{\sqrt{6}}\psi_1 + \frac{1}{\sqrt{3}}\psi_0$$

These are orthonormal:

$$\int f_0^* f_0\, d^3r = \frac{2}{3} + \frac{1}{3} = 1$$
$$\int f_1^* f_1\, d^3r = \frac{1}{2} + \frac{1}{6} + \frac{1}{3} = 1$$
$$\int f_2^* f_2\, d^3r = \frac{1}{2} + \frac{1}{6} + \frac{1}{3} = 1$$

$$\int f_0^* f_1\, d^3r = -\sqrt{\frac{2}{3}}\frac{1}{\sqrt{6}} + \frac{1}{3} = 0$$
$$\int f_1^* f_2\, d^3r = \frac{2}{3}\left(-\frac{3}{4} + \frac{1}{4} + \frac{1}{2}\right) = 0$$
$$\int f_0^* f_2\, d^3r = -\sqrt{\frac{2}{3}}\frac{1}{\sqrt{6}} + \frac{1}{3} = 0.$$

See pdf's of contour plots.