Using *linear combination* to construct **p** and **d** orbitals

$$\Psi_{n,l,m}(x,y,z) \Rightarrow \Psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)Y_{l,m}(\theta,\varphi)$$

$$\text{Radial part } R_{n,l}(r) = N_{n,l}\left(\frac{\rho}{n}\right)^{l} L_{n,l}(r)\,\mathrm{e}^{-\rho/2n},\ \rho = \frac{2Zr}{a_0},\ a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$$

$$\text{Angular part } Y_{1,m}(\theta,\varphi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m!|)}{(l+|m!|)}}P_l^{|m|}(\cos\theta)\,\mathrm{e}^{im\varphi}$$

$$\Psi_{n,1,m} = R_{n,1}(r)Y_{1,m}(\theta,\varphi) \quad \text{for p orbitals, } m = 0,\pm 1$$

$$\Psi_{n,2,m} = R_{n,2}(r)Y_{2,m}(\theta,\varphi) \quad \text{for d orbitals, } m = 0,\pm 1,\pm 2$$

For s orbitals, l=0, m=0

$Y_{l,m}=Y_{0,0}=(4\pi)^{-1/2}$

The orbital shape of s orbitals is only related to the radial part, and is spherically symmetric.

$$p_0 \propto \cos\theta$$

$$p_{\pm 1} \propto \sin\theta \times \mathrm{e}^{\pm i\varphi}$$

$$p_z = p_0 \propto \cos\theta \propto z/r$$

$$p_x = \frac{p_{+1} + p_{-1}}{\sqrt{2}} \propto \sin\theta\cos\varphi \propto x/r$$

$$p_y = -i\frac{p_{+1} + p_{-1}}{\sqrt{2}} \propto \sin\theta\sin\varphi \propto y/r$$

$$d_0 \propto 3\cos^2\theta - 1$$

$$d_{\pm 1} \propto \cos\theta \sin\theta \times \mathrm{e}^{\pm i\varphi}$$

$$d_{\pm 2} \propto \sin^2\theta \times \mathrm{e}^{\pm 2i\varphi}$$

$$\boxed{d_{z^2} = d_0 \propto 3\cos^2\theta - 1 \propto 3(z-r)^2 - 1}$$

$$d_{xz} = \frac{d_{+1} + d_{-1}}{\sqrt{2}} \propto \sin\theta\cos\theta\cos\varphi \propto xz/r^2$$

$$d_{yz} = -i\frac{d_{+1} + d_{-1}}{\sqrt{2}} \propto \sin\theta\cos\theta\sin\varphi \propto yz/r^2$$

$$d_{x^2-y^2} = \frac{d_{+2} + d_{-2}}{\sqrt{2}} \propto \sin^2\theta\cos 2\varphi \propto (x^2 - y^2)/r^2$$

$$d_{xy} = -i\frac{d_{+2} + d_{-2}}{\sqrt{2}} \propto \sin^2\theta\sin 2\varphi \propto xy/r^2$$