

Hydrogen Atomic Orbitals

$$\Psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$$

$$\Psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \left(2 - \frac{Zr}{a_0} \right) e^{-Zr/2a_0}$$

$$\Psi_{2pz} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/2a_0} \frac{Zr}{a_0} \cos\theta$$

$$\Psi_{211} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/2a_0} \frac{Zr}{a_0} \sin\theta e^{i\phi} \quad l_z = \hbar$$

$$\Psi_{21-1} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/2a_0} \frac{Zr}{a_0} \sin\theta e^{-i\phi} \quad l_z = -\hbar$$

$$\frac{e^{i\phi} + e^{-i\phi}}{2} = \frac{(\cos\phi + i\sin\phi) + (\cos\phi - i\sin\phi)}{2} = \cos\phi$$

$$\frac{e^{i\phi} - e^{-i\phi}}{2i} = \frac{(\cos\phi + i\sin\phi) - (\cos\phi - i\sin\phi)}{2i} = \sin\phi$$

$$\Psi_{2px} = \frac{\Psi_{211} + \Psi_{21-1}}{2} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/2a_0} \frac{Zr}{a_0} \sin\theta \cos\phi$$

$$\Psi_{2py} = \frac{\Psi_{211} - \Psi_{21-1}}{2i} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/2a_0} \frac{Zr}{a_0} \sin\theta \sin\phi$$

Angular portion of the d-orbitals

Notice that:

$$2p_z \Rightarrow r \cos\theta = z$$

$$2p_x \Rightarrow r \sin\theta \cos\phi = x$$

$$2p_y \Rightarrow r \sin\theta \sin\phi = y$$

$$d_{xz} \Rightarrow xz = \sin\theta \cos\phi \cos\theta$$

$$d_{yz} \Rightarrow yz = \sin\theta \sin\phi \cos\theta$$

$$d_{xy} \Rightarrow xy = \sin\theta \cos\phi \sin\theta \sin\phi = \sin^2\theta \cos\phi \sin\phi$$

$$d_{x^2-y^2} \Rightarrow x^2 - y^2 = \sin^2\theta \cos^2\phi - \sin^2\theta \sin^2\phi$$

$$d_{z^2} = d_{z^2-1} \Rightarrow 3 \cos^2\theta - 1$$

needed to make a sphere from superposition of all d orbitals