

波函数



波函数、电子云和概率分布（角度分布和径向分布）

Ψ ：描述原子核外电子运动方式的数学函数式

$|\Psi|^2$ ：原子核外发现电子的几率密度 ？

经典力学：

{ 光的强度 \propto 光子密度
光的强度 \propto 电磁场强度的绝对值平方
波函数 Ψ 用以描述波的振幅，表示电磁场强度

所以：： $|\Psi|^2 \propto$ 光子密度

电子与光子类似：

物质波强的区域是电子出现机会较多的区域

$|\Psi|^2 \propto$ 电子密度

1. 电子云：电子出现的概率密度 $|\Psi|^2$)

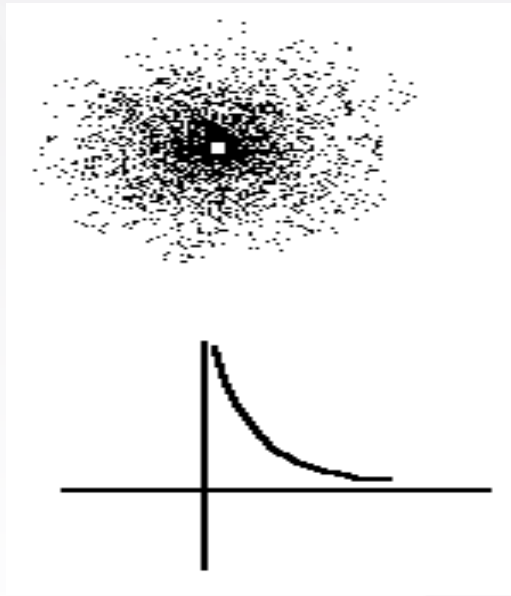
概率密度：电子在核外空间某单位体积内出现的概率

概率密度的形象化表示(小黑点的疏密)，即为电子云。

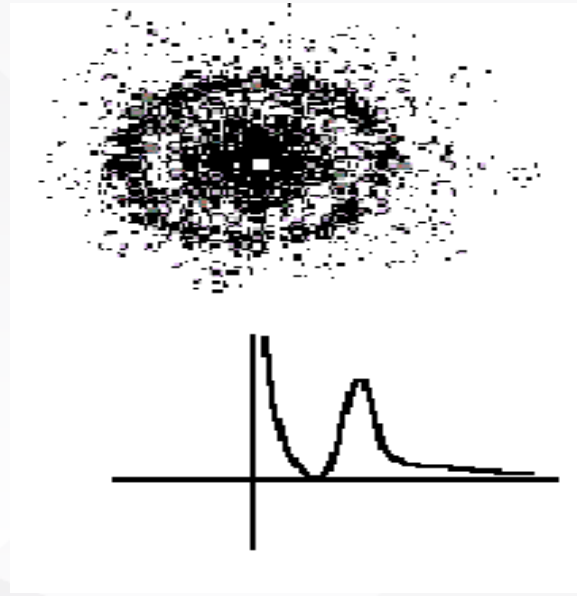
概率：电子在核外某空间出现的概率

$$= |\Psi|^2 \times dV$$

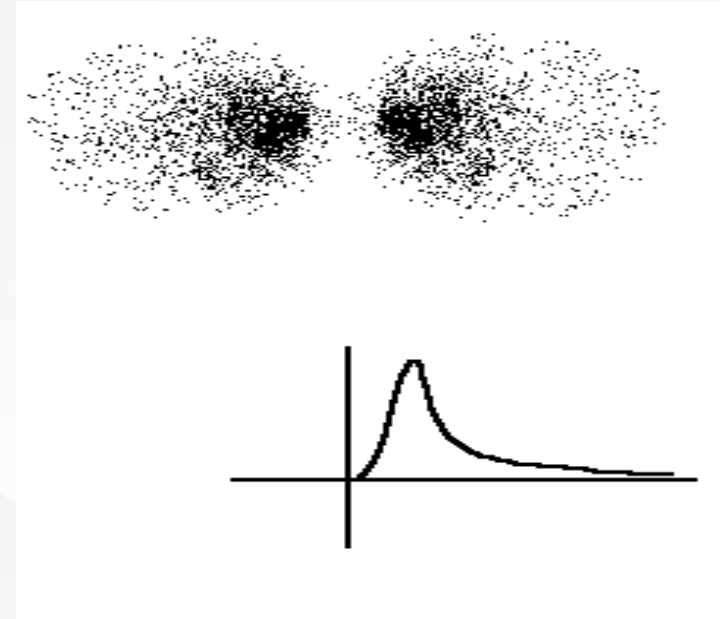
将核外一个电子每个瞬间的运动状态进行摄影。并将这样数百万张照片重叠，得到如下的统计效果图，形象地称为电子云图。



1s



2s



2p

图片上部图形表示 $|\Psi|^2$

图片下部的曲线为 $|R|^2$ ，横坐标为球半径 r

2.角度分布

波函数： $\Psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$

$R(r)$ ： Ψ 的径向波函数； $Y(\theta,\varphi)$ ： Ψ 的角度波函数。

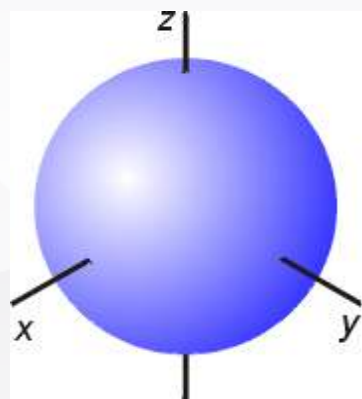
※ 将 Ψ 对 θ,φ 作图，所得图像称为原子轨道的角度分布图。

※ 若将 $|\Psi|^2$ 中的角度部分函数($|Y|^2$ 随 θ,φ 的变化)作图，即求出 $(|Y|^2)$ 值，则可得到电子云的角度分布图

例1. 1s轨道的角度部分图

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

$\Psi_{1s}(r, \theta, \varphi)$ 是一种球形对称分布



n=1

例2. $2p_z$ 的角度部分图

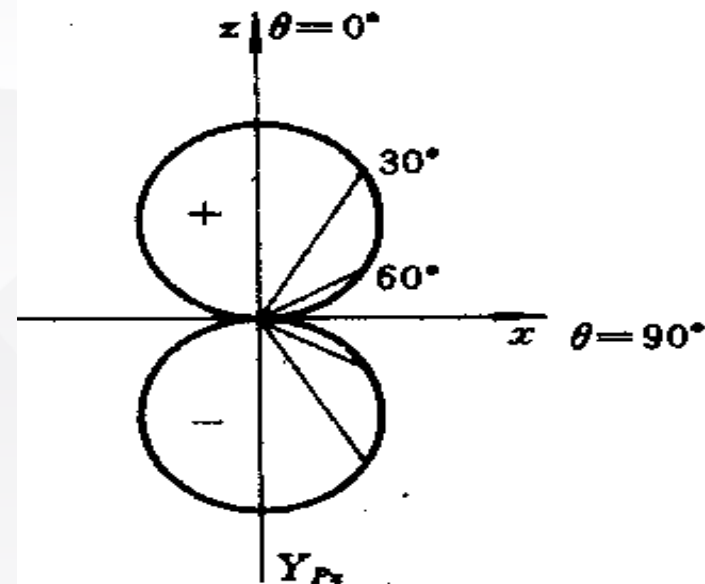
$$\psi_{2p_z} = \left[\sqrt{\frac{1}{24a_0^3}} \left(\frac{r}{a_0} \right) e^{-r/2a_0} \right] \times \left[\sqrt{\frac{3}{4\pi}} \cos \theta \right]$$

径向部分

角度部分

波函数 $2P_z$ 角度部分为:

$$Y_{2Pz} = \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos\theta$$

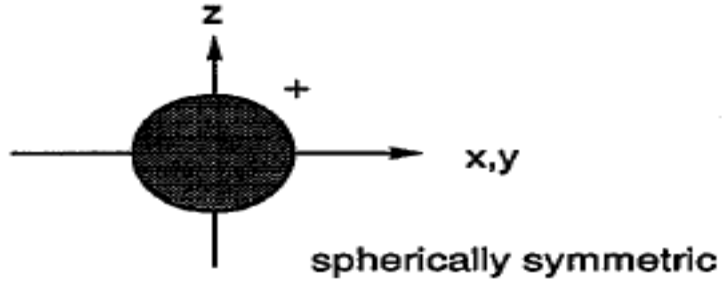


p_z 轨道角度分布图

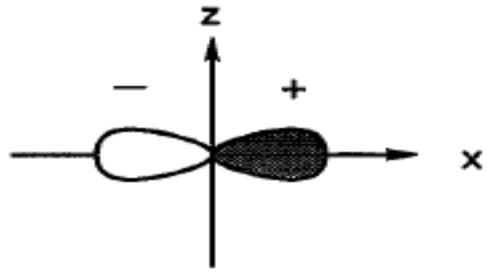
θ	0	30	45	60	90	120	135	150	180
$Y = R \cos\theta$	1.0	0.87	0.71	0.50	0	-0.50	-0.71	-0.87	-1.0
$Y^2 = R^2 \cos^2 \theta$	1.0	0.75	0.50	0.25	0	0.25	0.50	0.75	1.0

原子轨道角度分布图

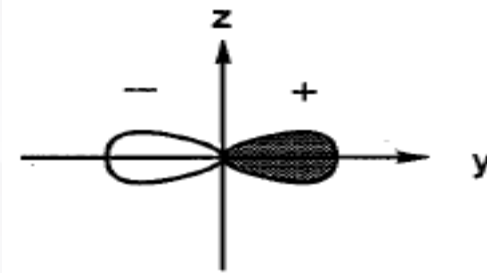
$$Y(\theta, \varphi)$$



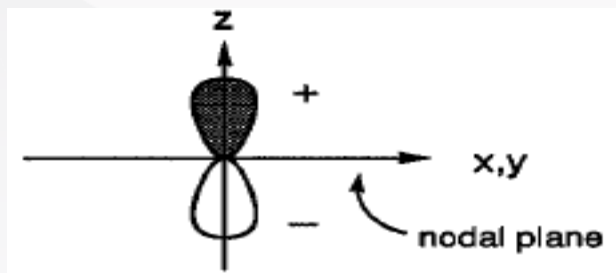
s-orbital



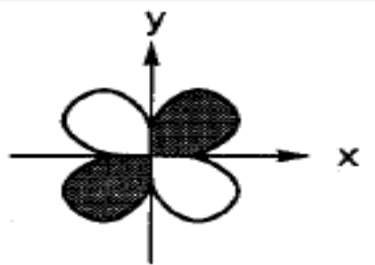
p_x



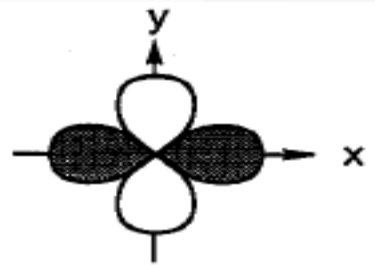
p_y



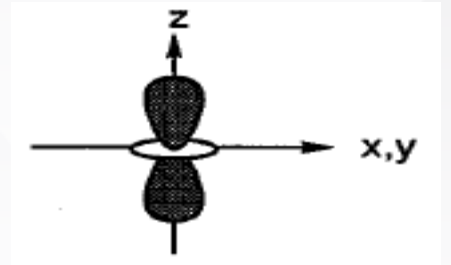
p_z



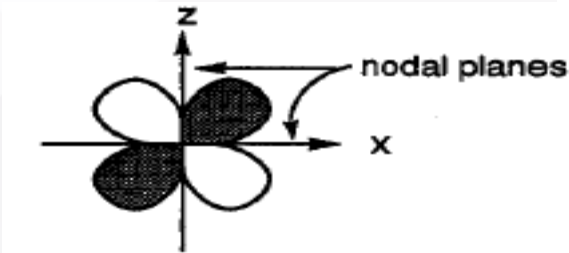
d_{xy}



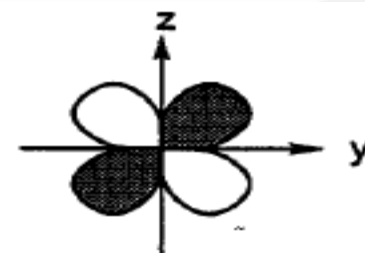
$d_{x^2-y^2}$



d_{z^2}



d_{xz}



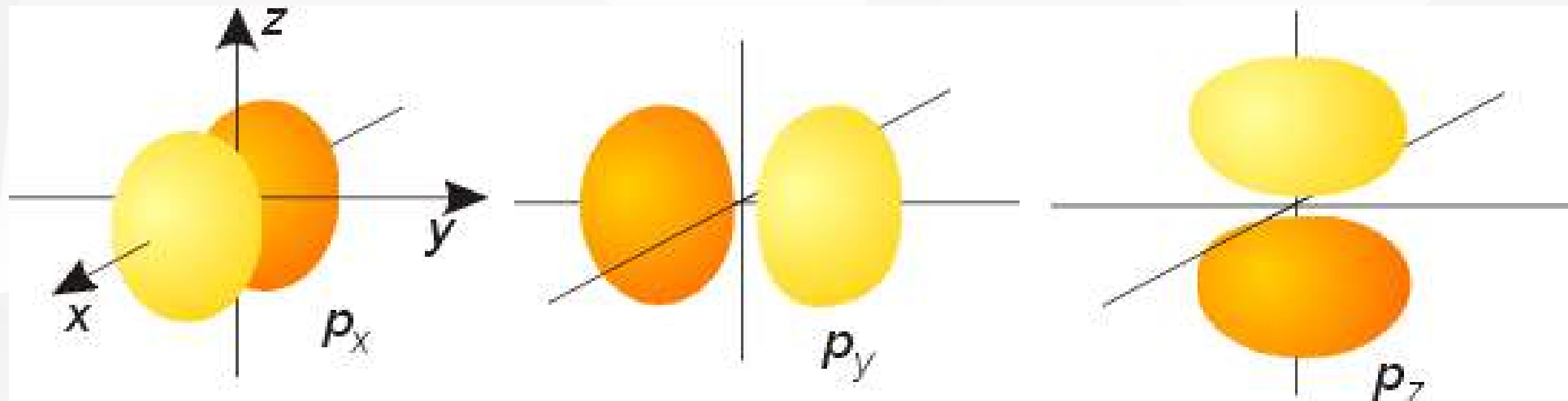
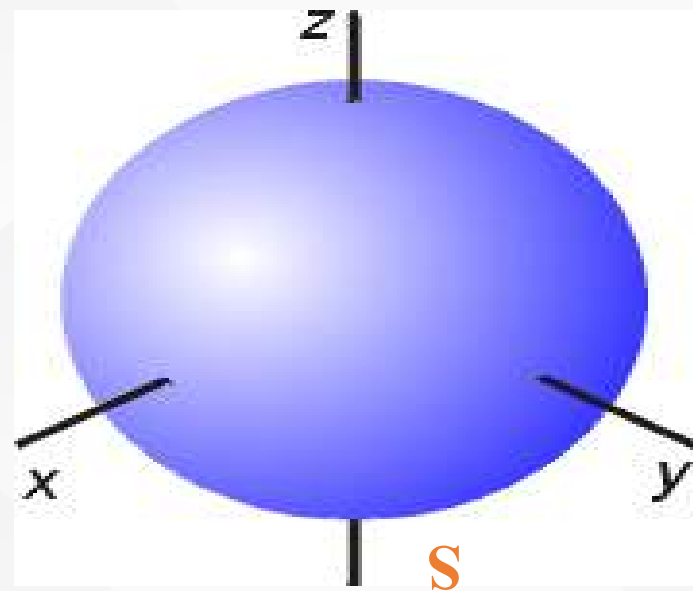
d_{yz}

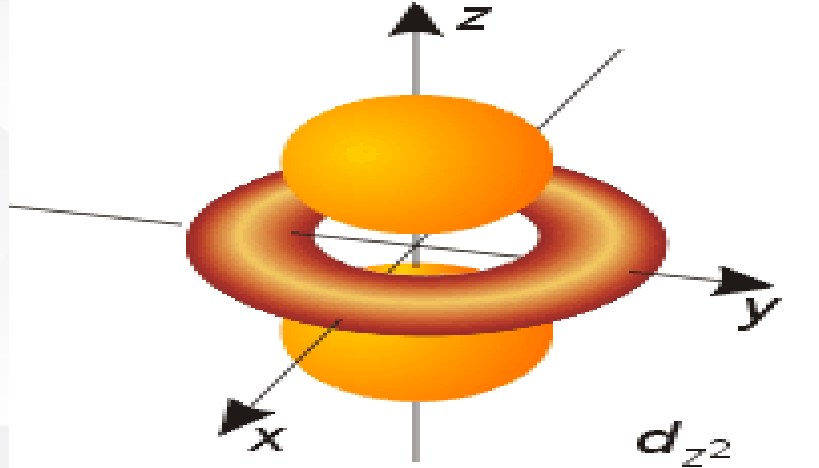
s, d 轨道中心对称

p, f 轨道中心反对称

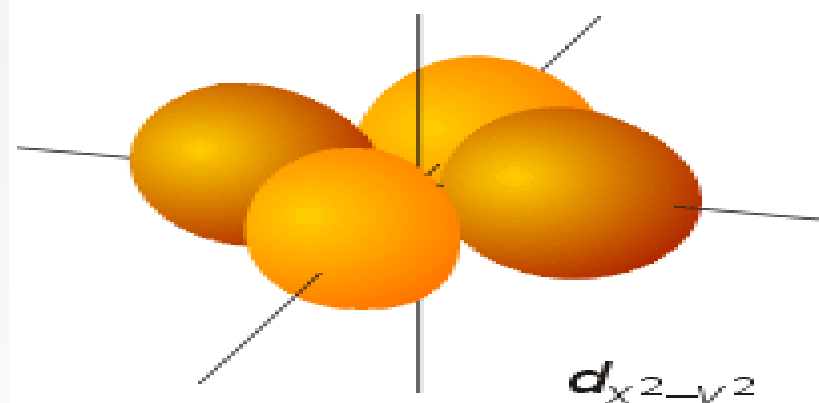
有正负之分
黑—正
白—负

模型1

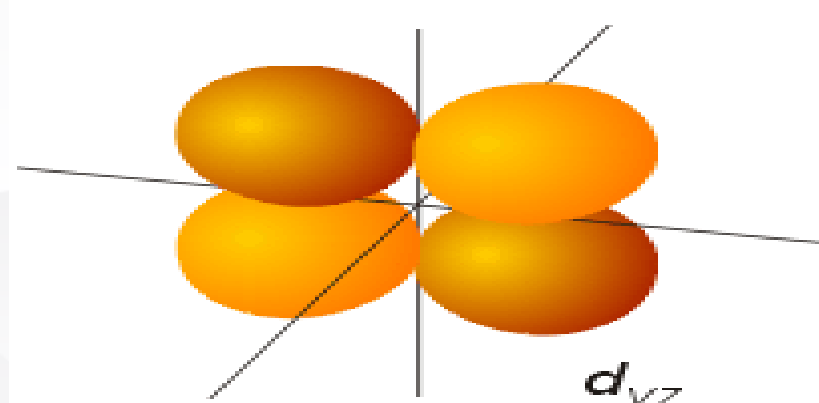




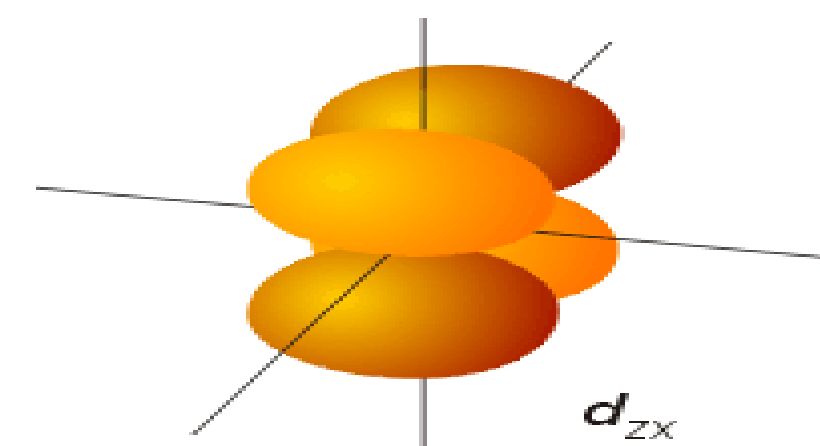
d_{z^2}



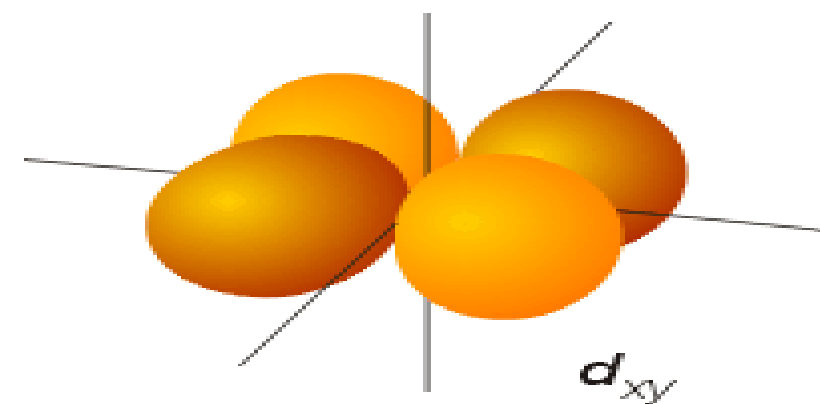
$d_{x^2-y^2}$



d_{yz}

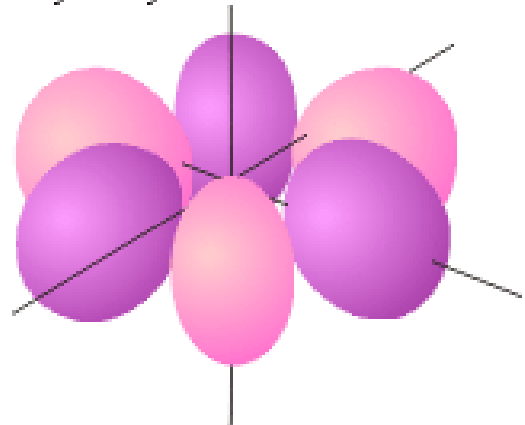


d_{zx}

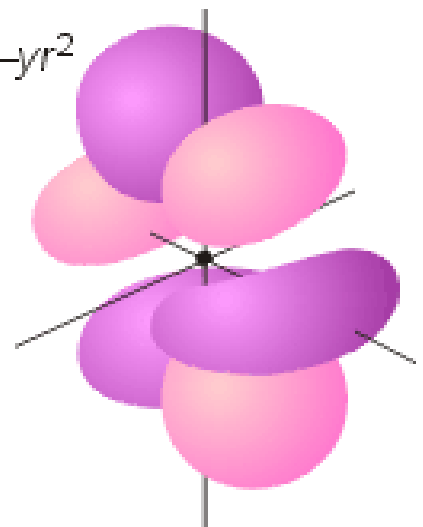


d_{xy}

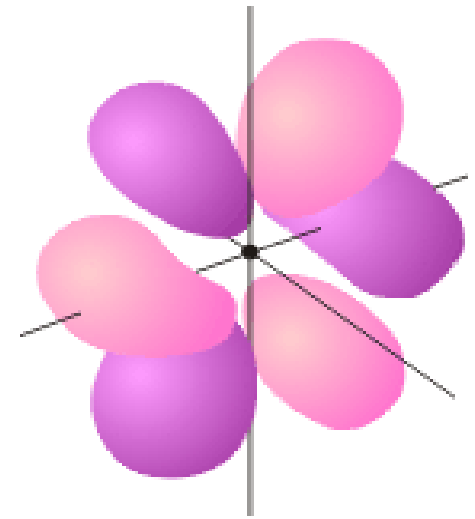
$$4f_{y^3-3yx^2}$$



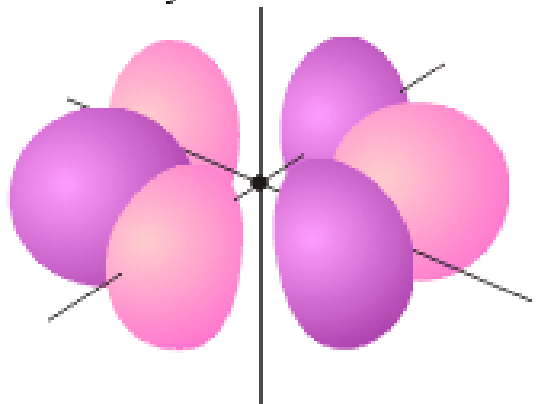
$$4f_{5yz^2-yr^2}$$



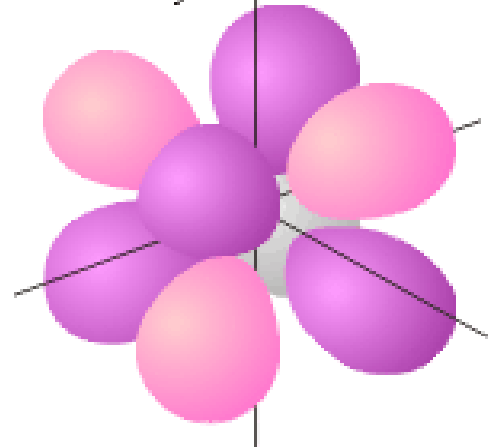
$$4f_{5xz^2-3xr^2}$$



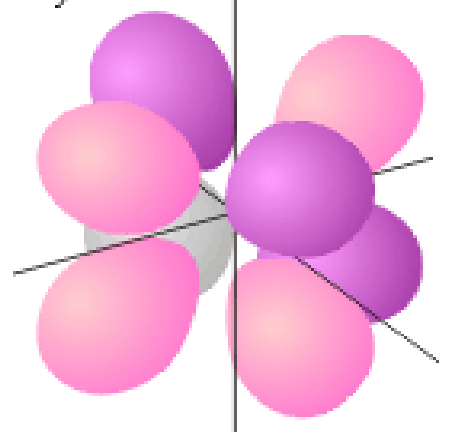
$$4f_{x^3-3xy^2}$$



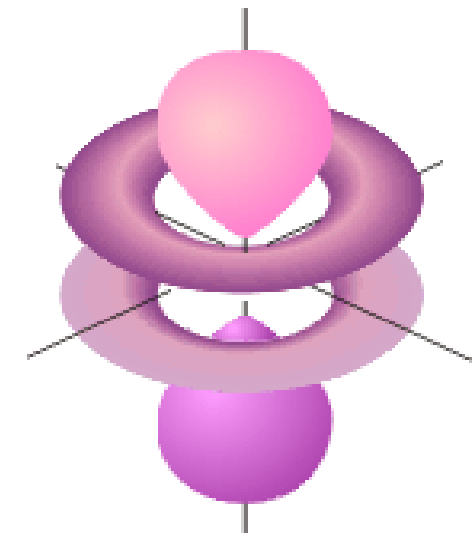
$$4f_{zx^2-zy^2}$$



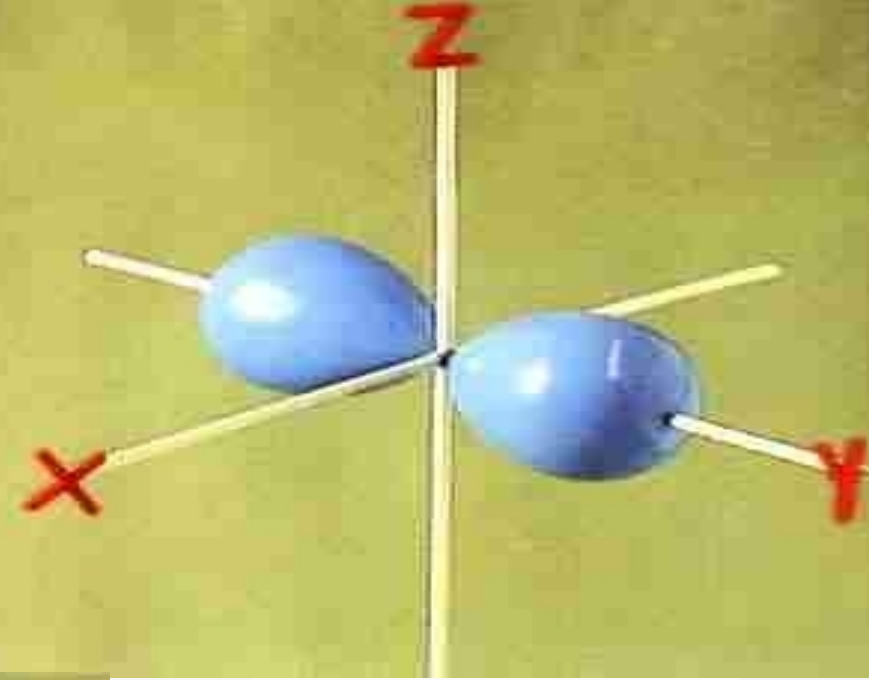
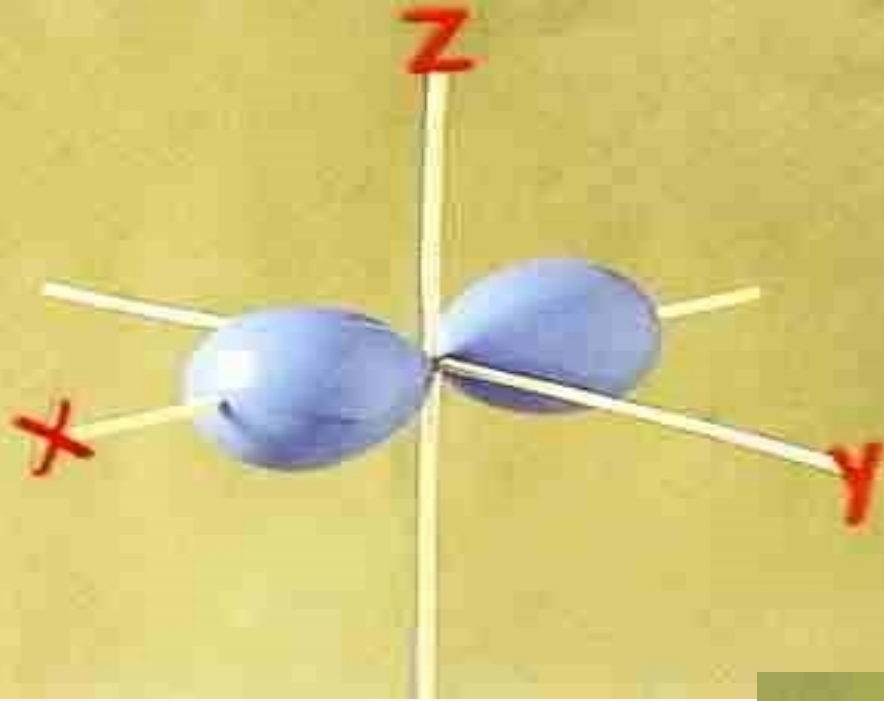
$$4f_{xyz}$$



$$4f_{5z^3-3zr^2}$$

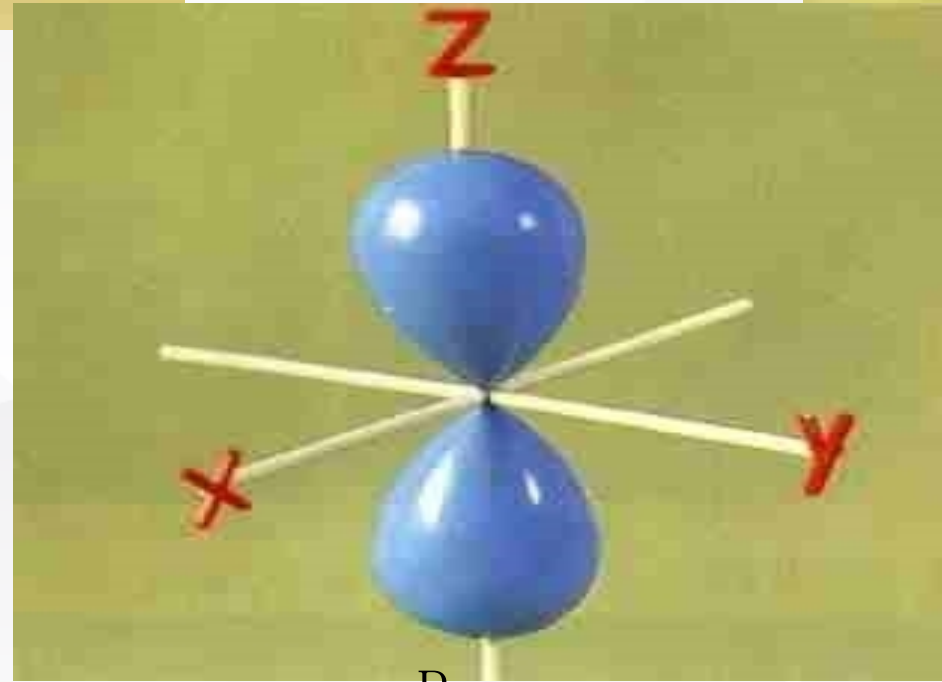


模型2

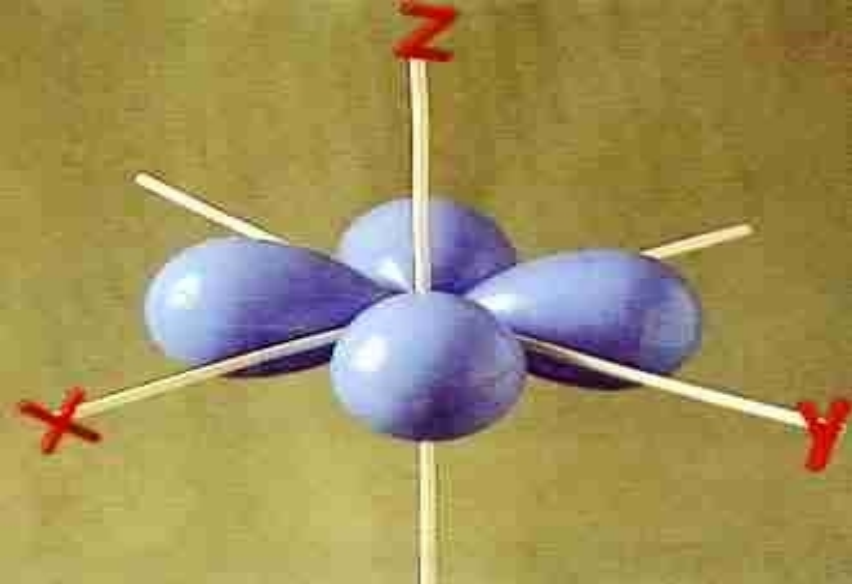


P_x

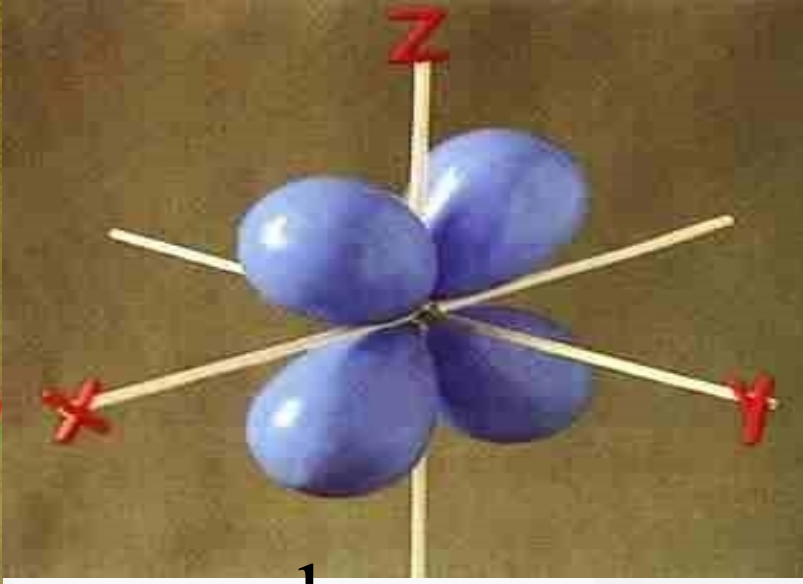
P_y



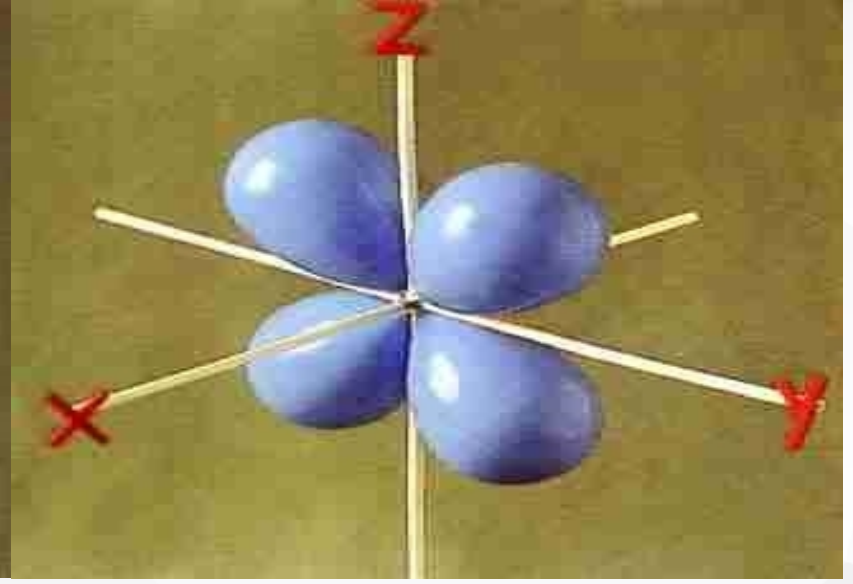
P_z



d_{xy}

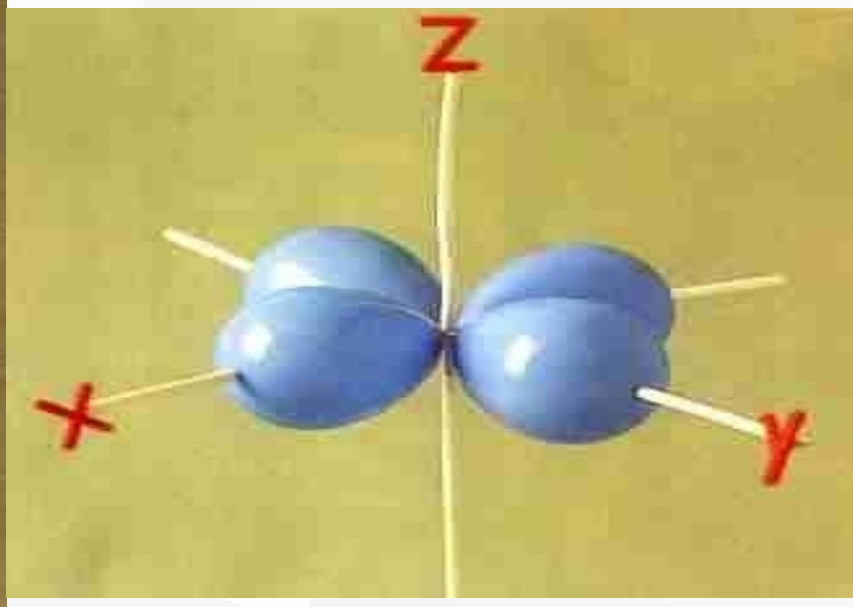
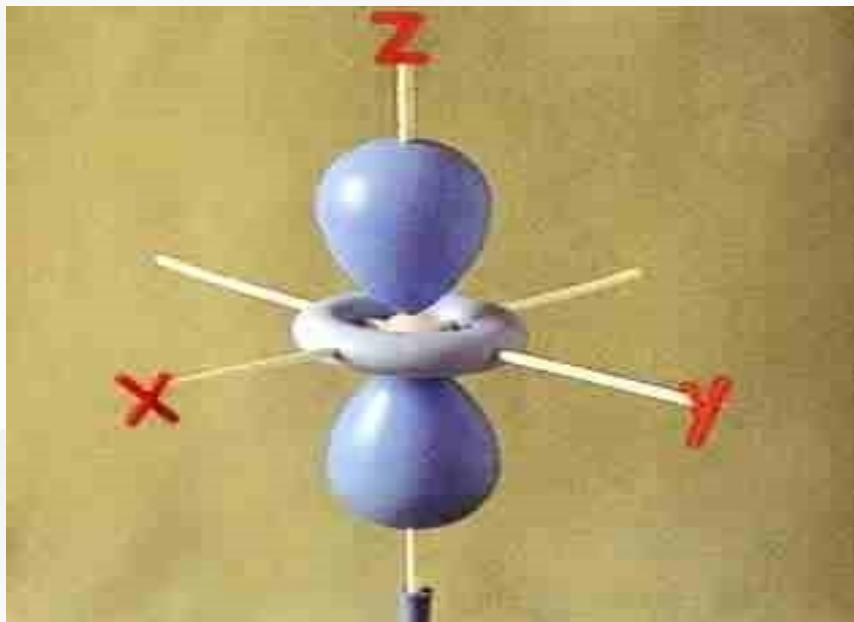


d_{xz}



d_{yz}

d_z^2



$d_{x^2-y^2}$

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