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:

$$\begin{cases} \text{光的强度} \propto \text{光子密度} \\ \text{光的强度} \propto \text{电磁场强度的绝对值平方} \\ \text{波函数}\Psi\text{用以描述波的振幅，表示电磁场强度} \end{cases}$$

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$|\Psi|^2$）

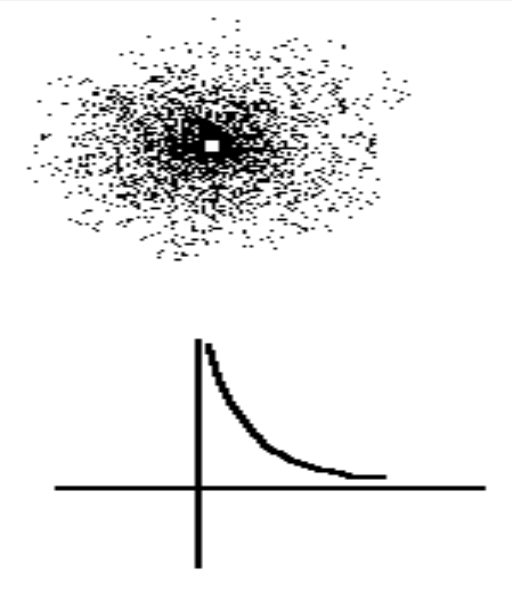
<u>概率密度</u>：电子在核外空间某单位体积内出现的概率

概率密度的形象化表示(小黑点的疏密)，即为电子云。

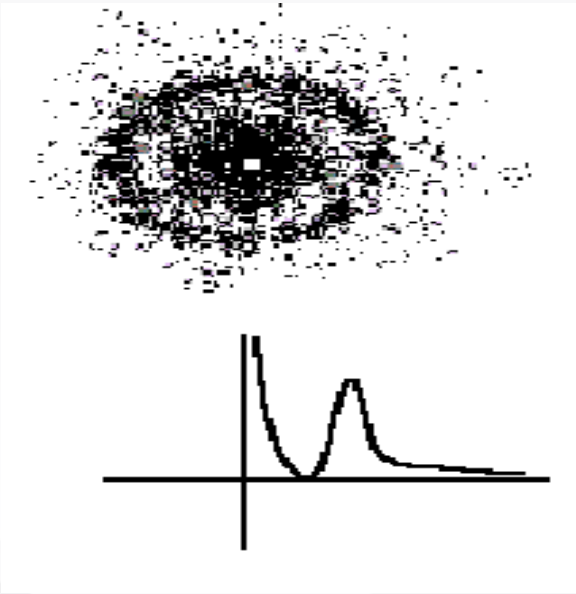
<u>概率</u>：电子在核外某空间出现的概率

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

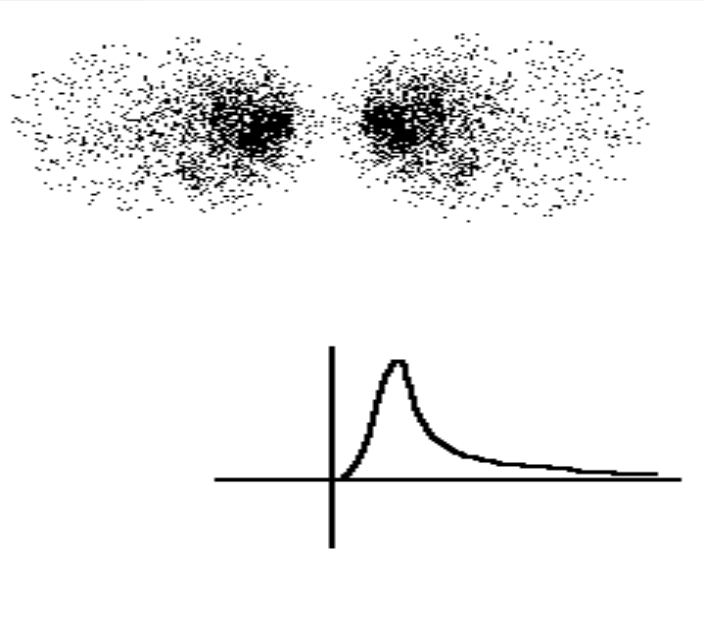
将核外一个电子每个瞬间的运动状态进行摄影。并将这样数百万张照片重叠，得到如下的统计效果图，形象地称为电子云图。



1s



2s



2 p

图片上部图形表示$|Y|^2$

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。

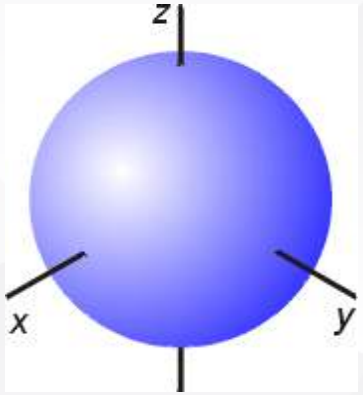
※ 将Ψ对θ,φ作图，所得图像称为原子轨道的角度分布图。

※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

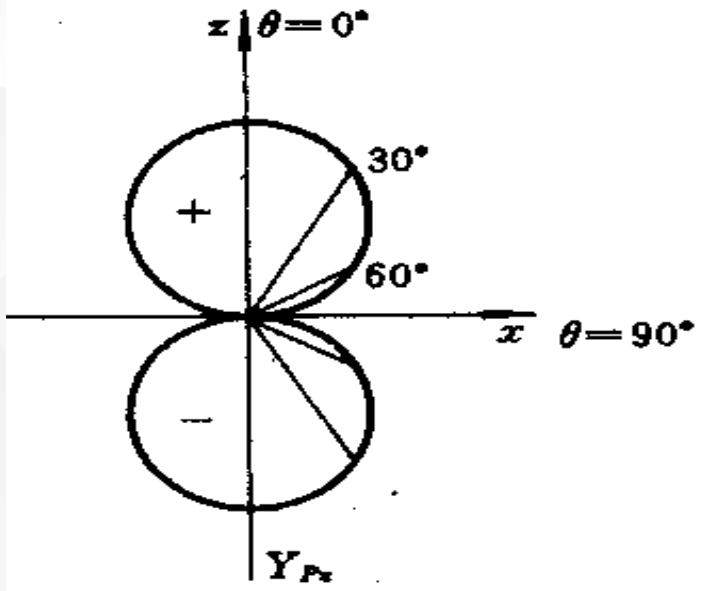
例2． $2p_z$的角度部分图

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

径向部分　　角度部分

波函数$2P_Z$角度部分为：

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

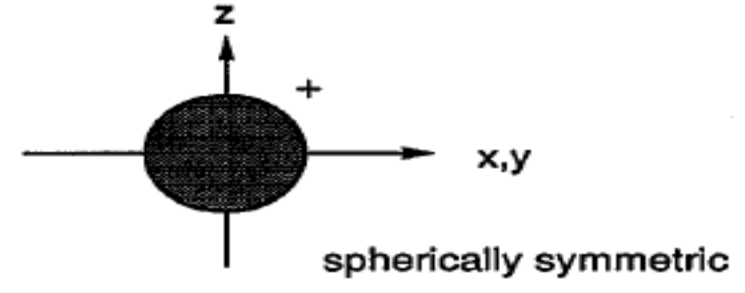


p_z 轨道角度分布图

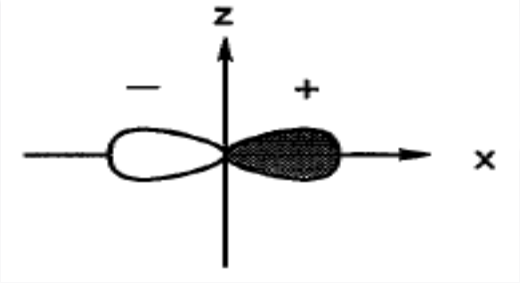
θ	0	30	45	60	90	120	135	150	180
Y= Rcosθ	1.0	0.87	0.71	0.50	0	-0.50	-0.71	-0.87	-1.0
Y^2= $R^2\cos^2\theta$	1.0	0.75	0.50	0.25	0	0.25	0.50	0.75	1.0

原子轨道角度分布图

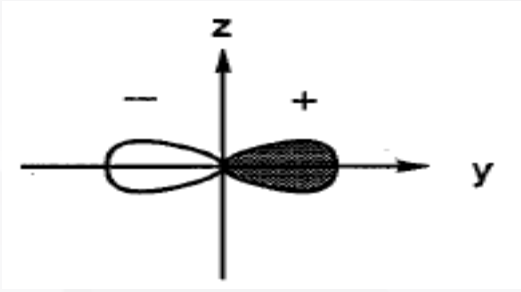
$Y(\theta,\varphi)$



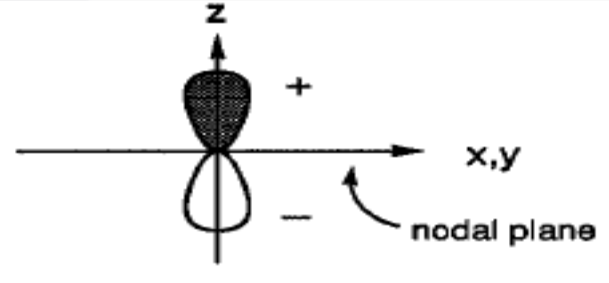
s-orbital



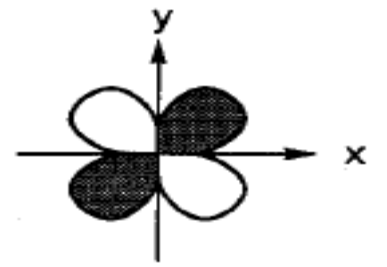
p_x



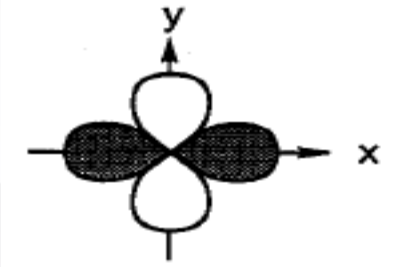
p_y



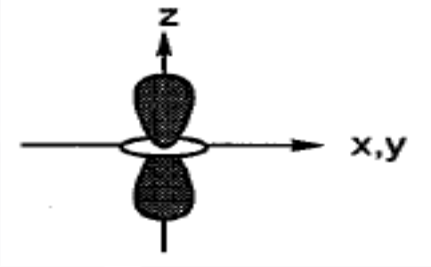
p_z



d_{xy}



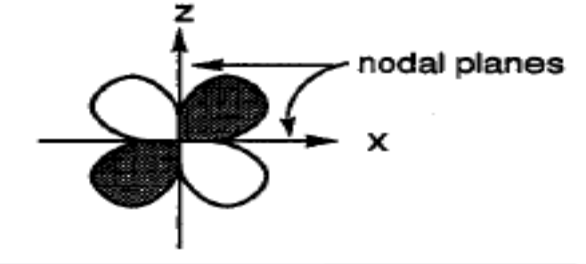
$d_{x^2-y^2}$



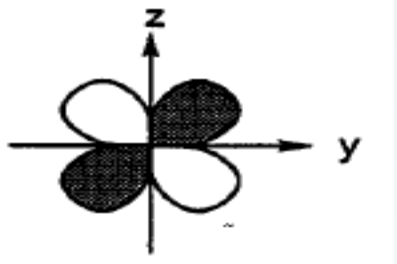
d_{z^2}

s, d 轨道中心对称

p, f 轨道中心反对称



d_{xz}



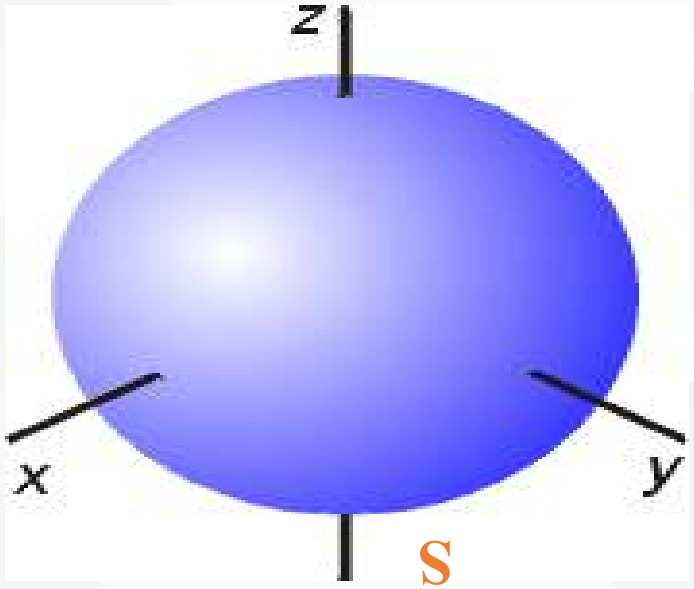
d_{yz}

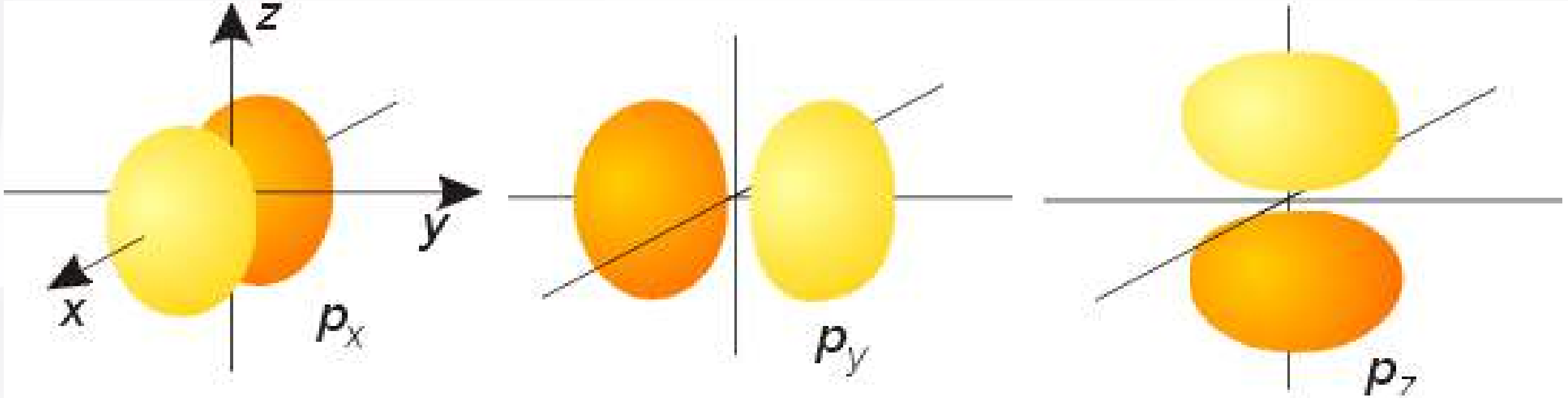
有正负之分

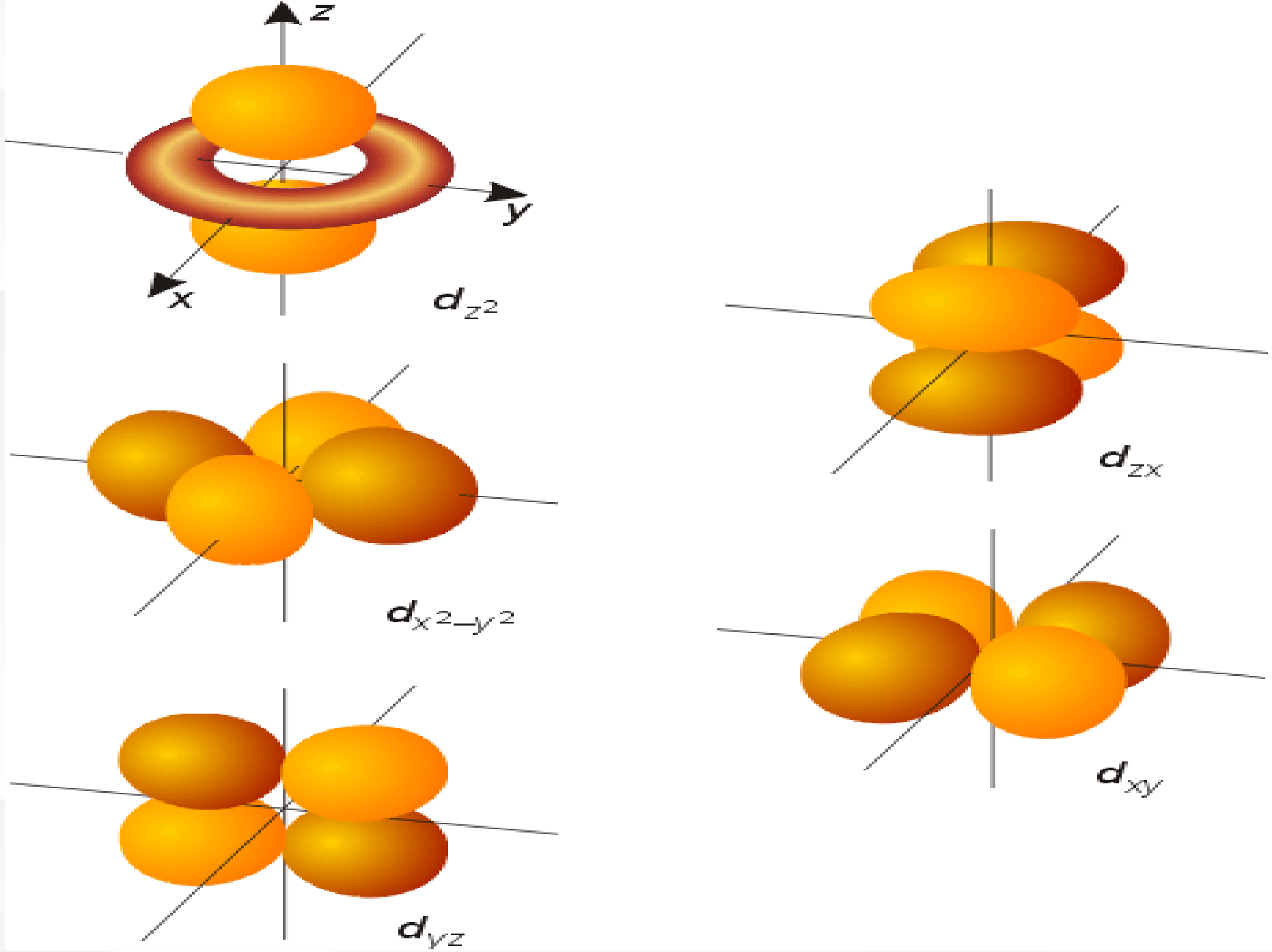
黑—正

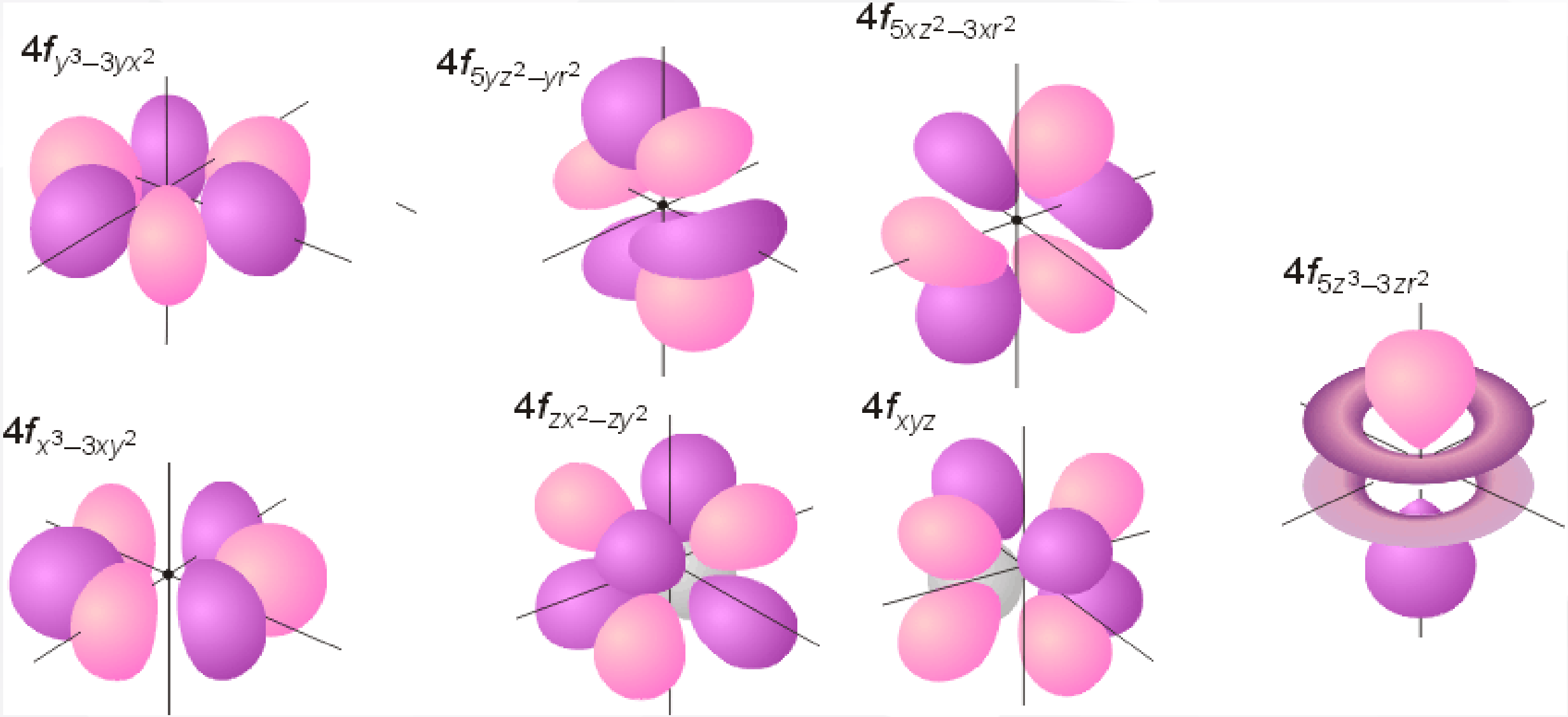
白—负

模型1

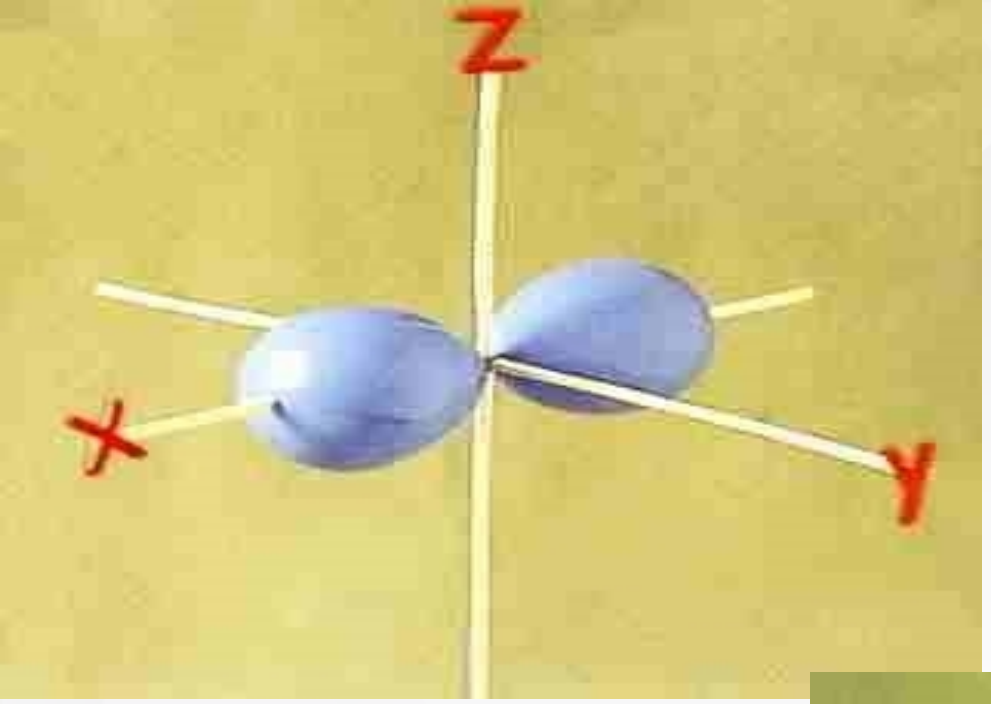




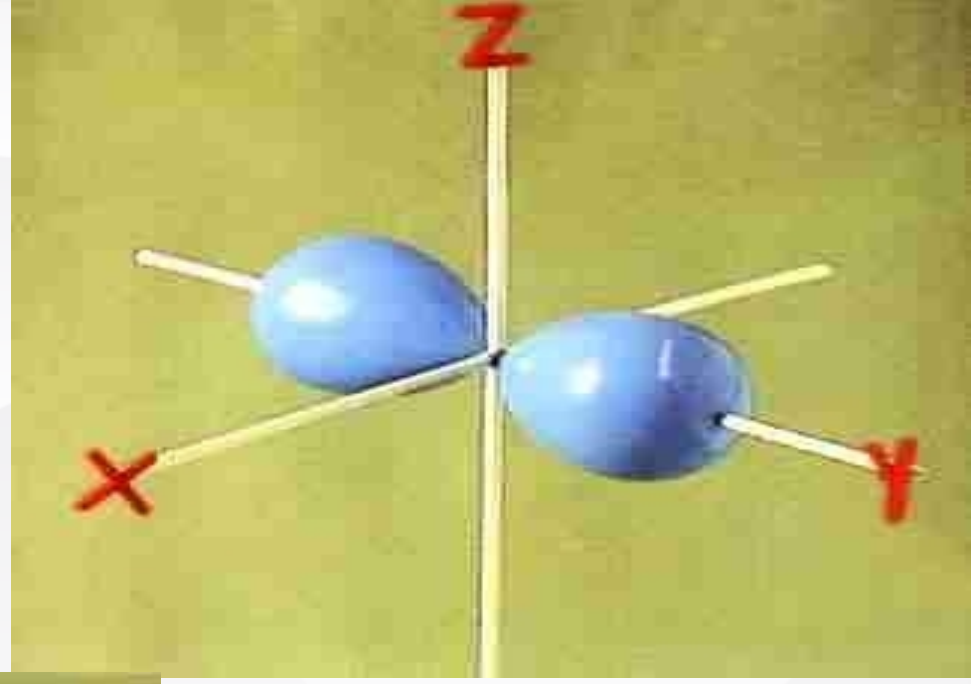

z
y
x
d_{z^2}
d_{zx}
$d_{x^2-y^2}$
d_{xy}
d_{yz}


$4f_{y^3-3yx^2}$
$4f_{5yz^2-yr^2}$
$4f_{5xz^2-3xr^2}$
$4f_{5z^3-3zr^2}$
$4f_{x^3-3xy^2}$
$4f_{zx^2-zy^2}$
$4f_{xyz}$

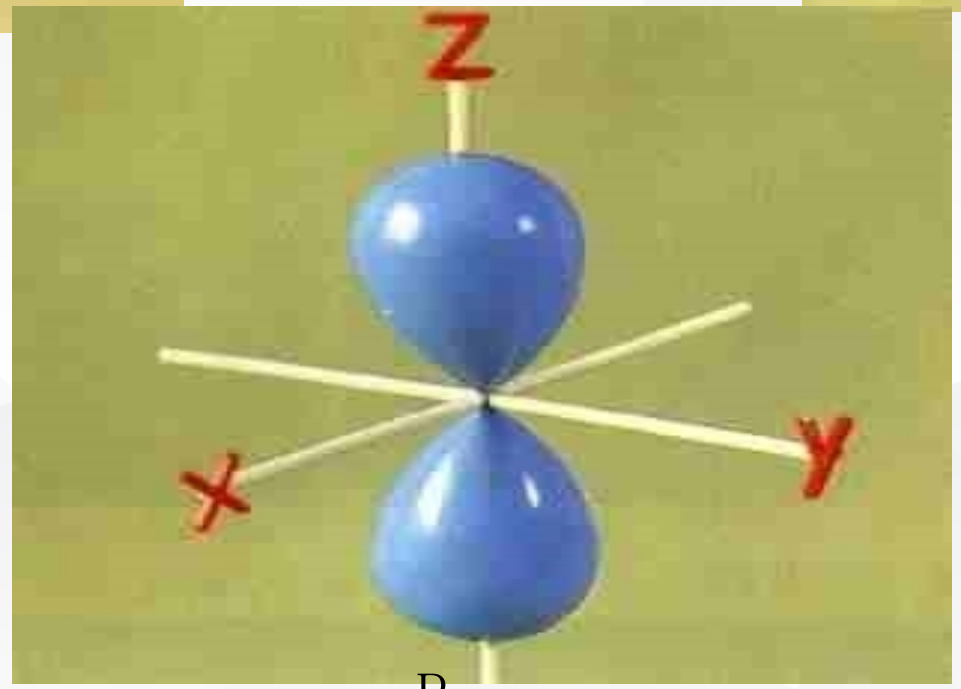
模型2



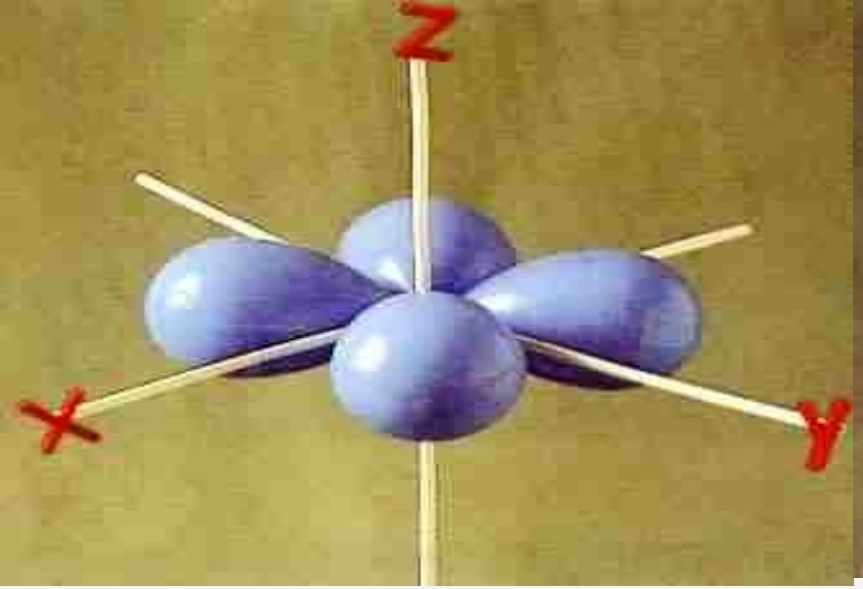
P_x



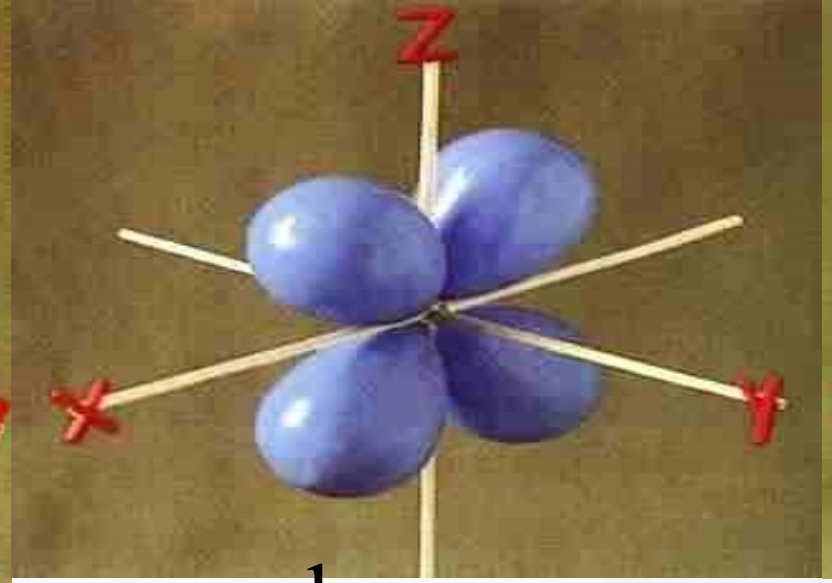
P_y



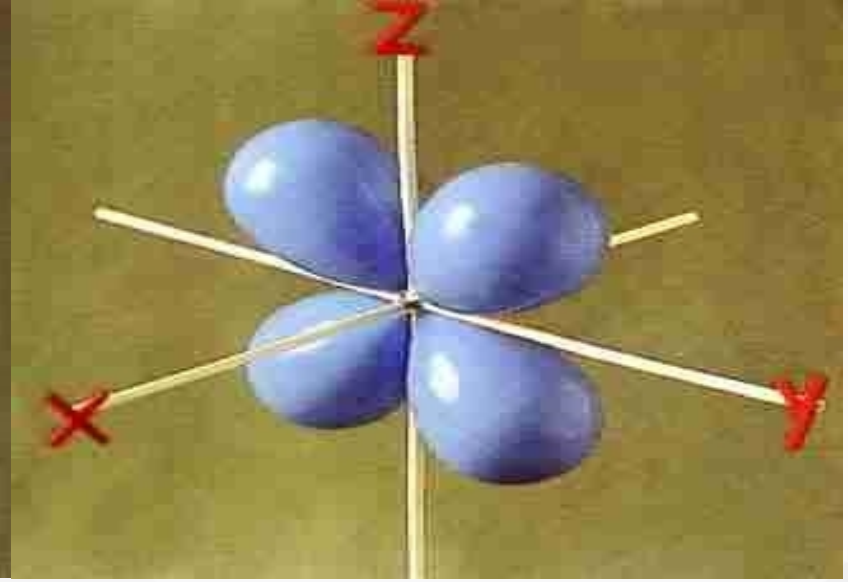
P_z



d_{xy}

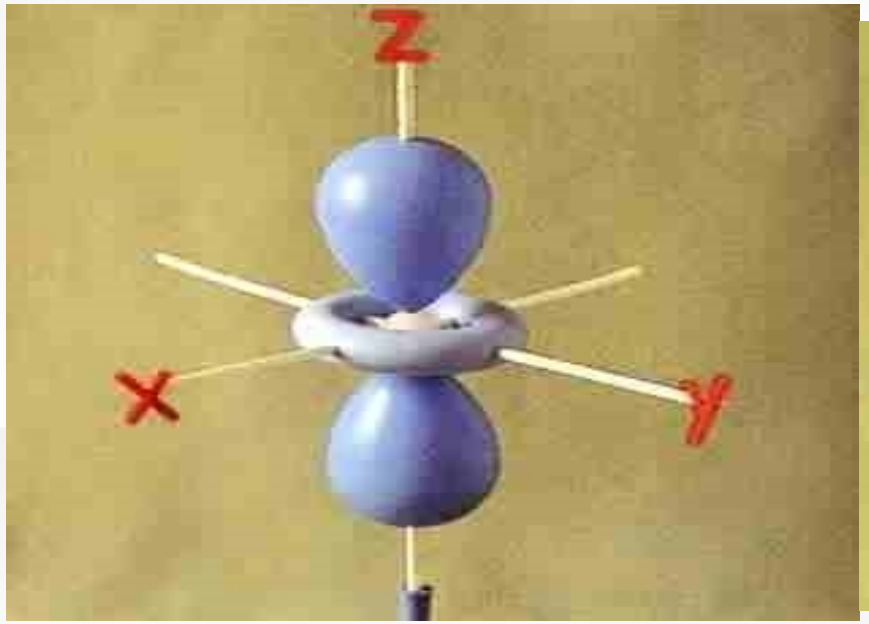


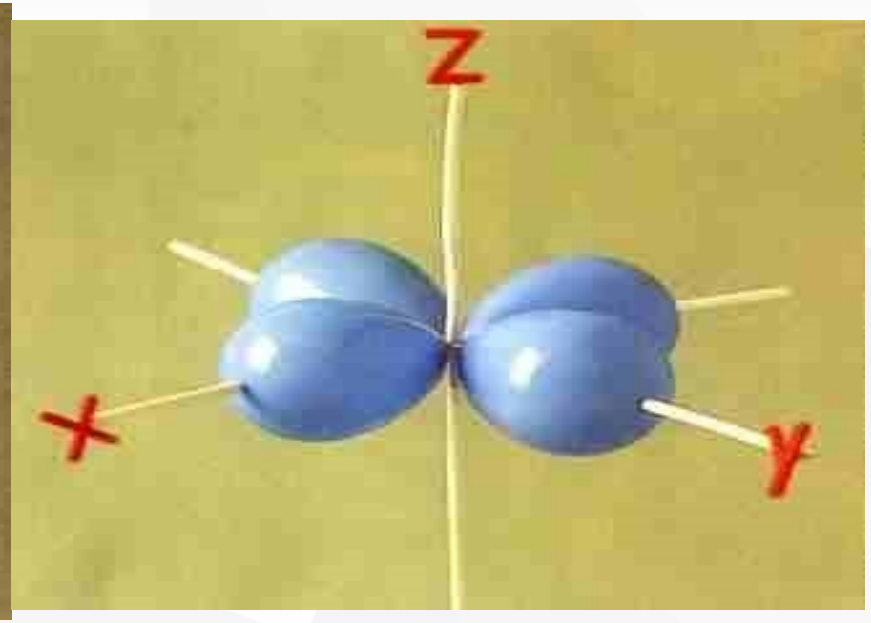
d_{xz}



d_{yz}

d_z^2





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