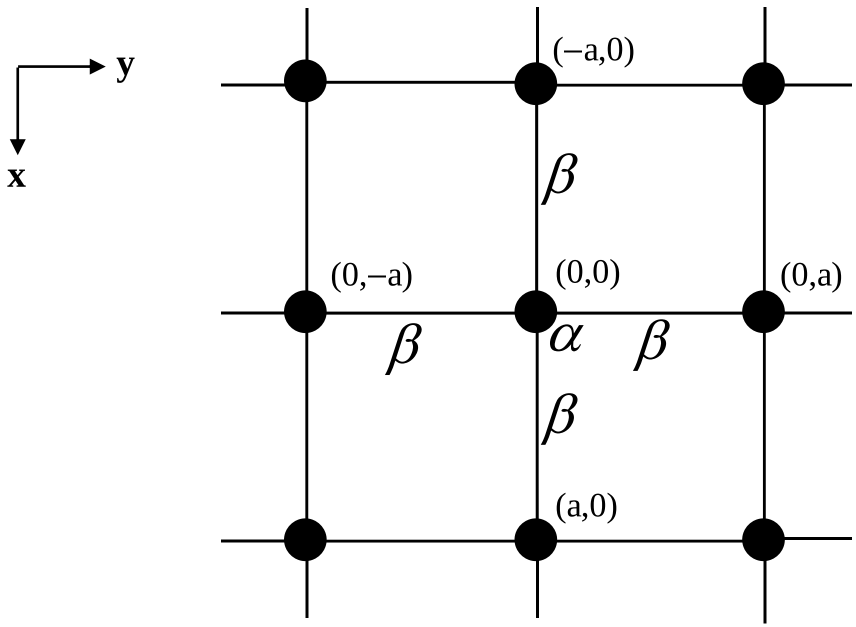
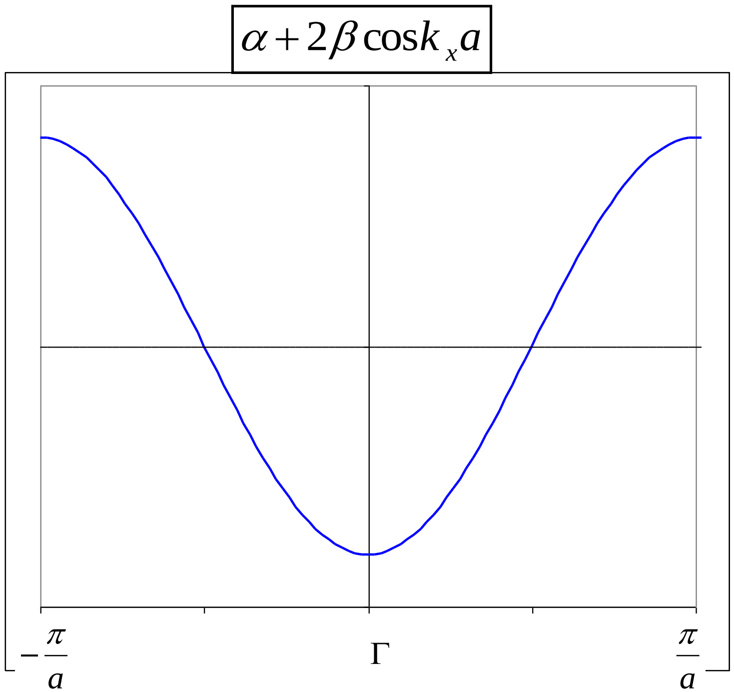
Only the interaction with the nearest neighbours are taken into account: only the exchange integral β with the nearest neighbour (*E*~α, *t*~β,*S*<<1)

$$H(\vec{k}) = \alpha + \beta e^{ik_x a} + \beta e^{-ik_x a} = \alpha + 2\beta \cos k_x a$$

$$H(\vec{k}) = \alpha + \beta e^{ik_x a} + \beta e^{-ik_x a} + \beta e^{ik_y a} + \beta e^{-ik_y a} + \beta e^{ik_z a} + \beta e^{-ik_z a} =$$
$$= \alpha + 2\beta(\cos k_x a + \cos k_y a + \cos k_z a)$$





$$+\beta e^{-ika/2}+\beta e^{ika/2}=\beta(\cos ka/2-i\sin ka/2)+\beta(\cos ka/2+i\sin ka/2)=$$
$$=\beta(\cos ka/2+\cos ka/2-i\sin ka/2+i\sin ka/2)=2\beta\cos ka/2$$

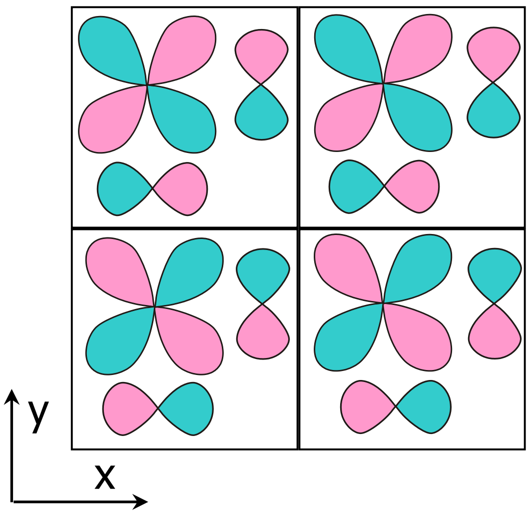
$$-\beta e^{-ika/2}-\beta e^{ika/2}=-\beta(\cos ka/2-i\sin ka/2)-\beta(\cos ka/2+i\sin ka/2)=$$
$$=-\beta(\cos ka/2+\cos ka/2-i\sin ka/2+i\sin ka/2)=-2\beta\cos ka/2$$

$$-\beta e^{-ika/2}+\beta e^{ika/2}=-\beta(\cos ka/2-i\sin ka/2)+\beta(\cos ka/2+i\sin ka/2)=$$
$$=\beta(-\cos ka/2+\cos ka/2+i\sin ka/2+i\sin ka/2)=2i\beta\sin ka/2$$

$$+\beta e^{-ika/2}-\beta e^{ika/2}=+\beta(\cos ka/2-i\sin ka/2)-\beta(\cos ka/2+i\sin ka/2)=$$
$$=\beta(\cos ka/2-\cos ka/2-i\sin ka/2-i\sin ka/2)=-2i\beta\sin ka/2$$

d_{xy}, p_x, p_y,

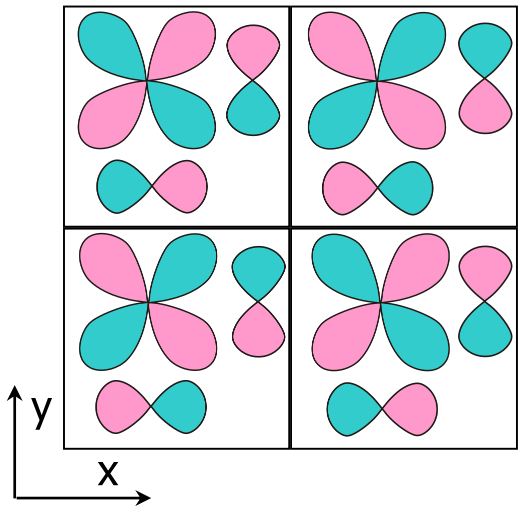
$$\begin{vmatrix} \alpha_{d_{xy}} & -i2\beta_{dp}\sin k_y a/2 & i2\beta_{dp}\sin k_x a/2 \\ H_{12}^* & \alpha_{p_x} & -i2\beta_{pp}\sin k_x a/2 - i2\beta_{pp}\sin k_y a/2 \\ H_{13}^* & H_{23}^* & \alpha_{p_y} \end{vmatrix}$$



Y

$$\begin{bmatrix} k_x & k_y \\ 0 & \frac{\pi}{a} \end{bmatrix}$$

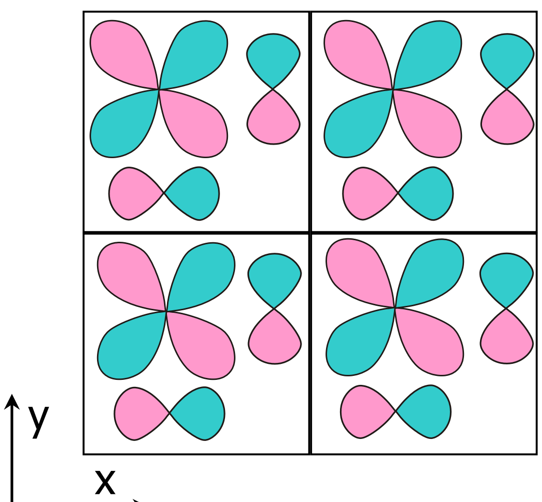
$$\begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$



S

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & \frac{\pi}{a} \end{bmatrix}$$

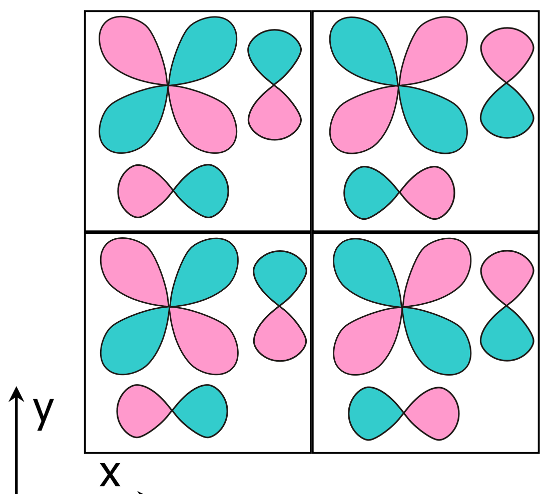
$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$



Γ

$$\begin{bmatrix} k_x & k_y \\ 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

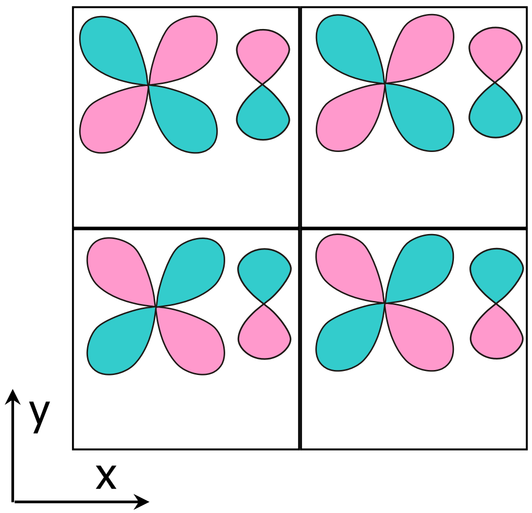


X

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$$

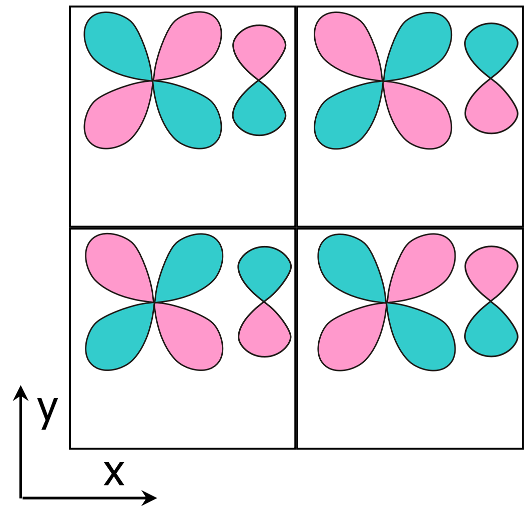
$$\Gamma: -\beta_{dp} e^{-ik_x a/2} + \beta_{dp} e^{ik_x a/2} = 2i\beta_{dp} \sin k_x a/2$$



Y

$$\begin{bmatrix} k_x & k_y \\ 0 & \dfrac{\pi}{a} \end{bmatrix}$$

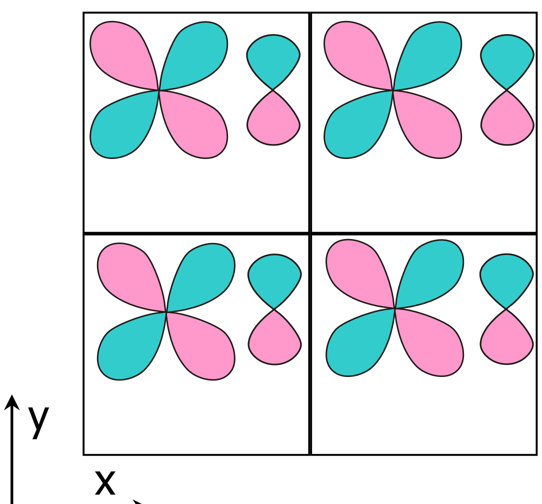
$$\begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$



S

$$\begin{bmatrix} k_x & k_y \\ \dfrac{\pi}{a} & \dfrac{\pi}{a} \end{bmatrix}$$

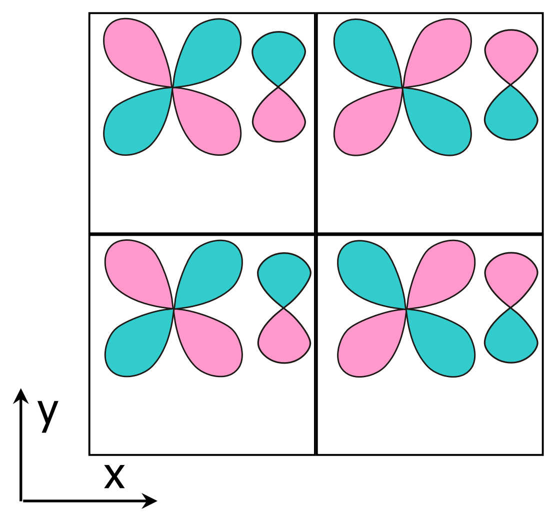
$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$



Γ

$$\begin{bmatrix} k_x & k_y \\ 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$



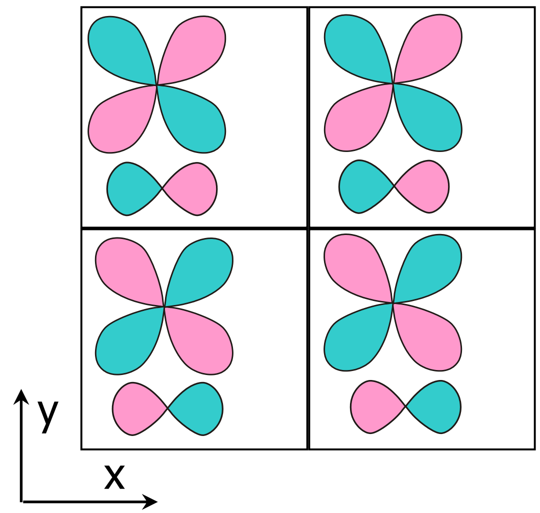
X

$$\begin{bmatrix} k_x & k_y \\ \dfrac{\pi}{a} & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$$

d_{xy}, p_x, p_y : d_{xy}- p_x

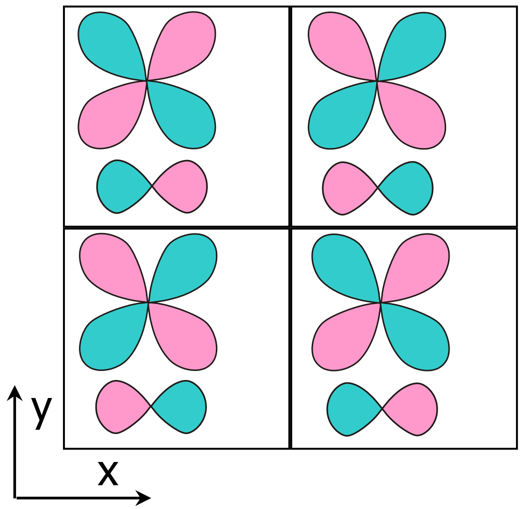
$$\Gamma: \ \beta_{dp} e^{-ik_y a/2} - \beta_{dp} e^{ik_y a/2} = -2i\beta_{dp} \sin k_y a/2$$



Y

$$\begin{bmatrix} k_x & k_y \\ 0 & \frac{\pi}{a} \end{bmatrix}$$

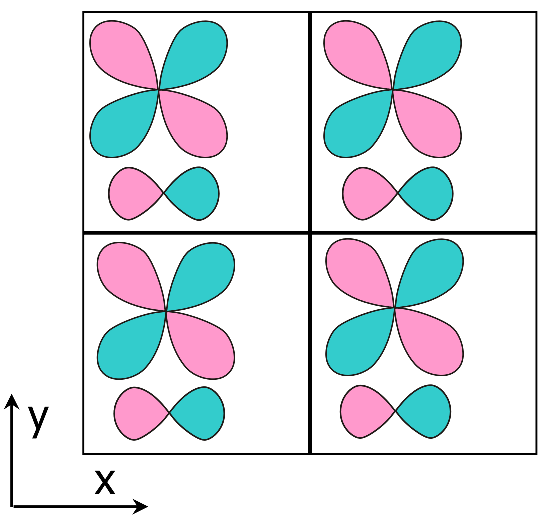
$$\begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$



S

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & \frac{\pi}{a} \end{bmatrix}$$

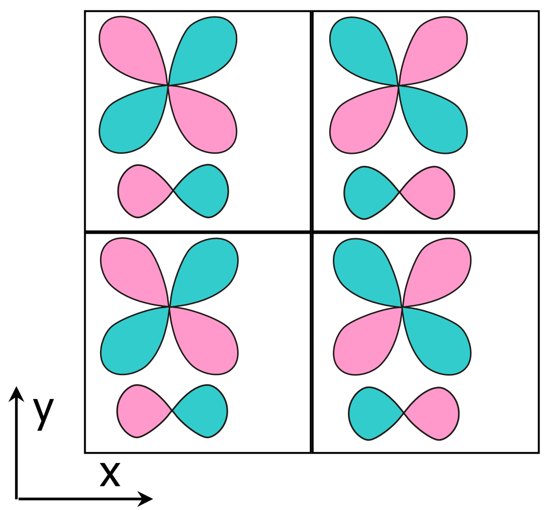
$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$



Γ

$$\begin{bmatrix} k_x & k_y \\ 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

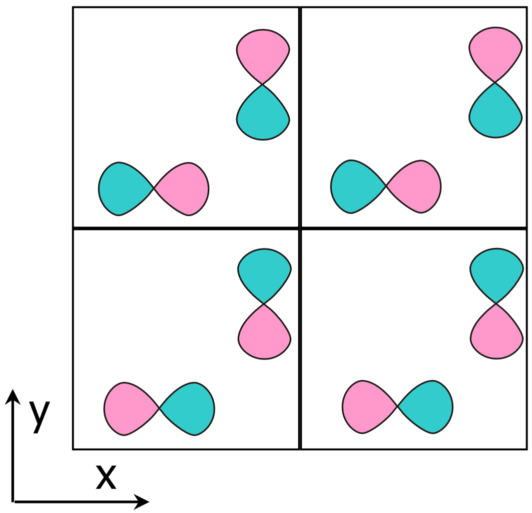


X

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & 0 \end{bmatrix}$$

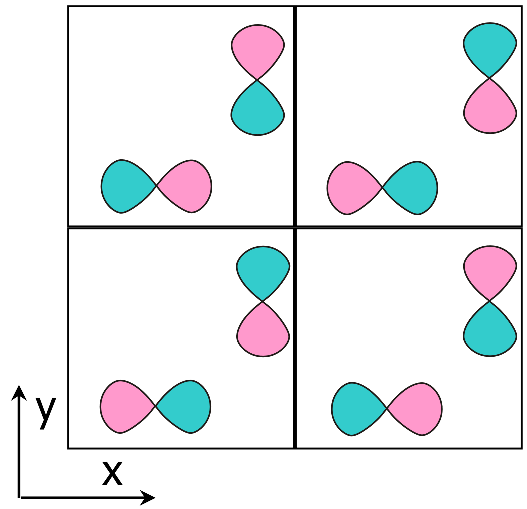
$$\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$$

$$\Gamma:\ \beta_{pp}e^{-ik_xa/2}-\beta_{pp}e^{ik_xa/2}+\beta_{pp}e^{-ik_ya/2}-\beta_{pp}e^{ik_ya/2}=$$
$$-2i\beta_{pp}\sin k_xa/2-2i\beta_{pp}\sin k_ya/2$$



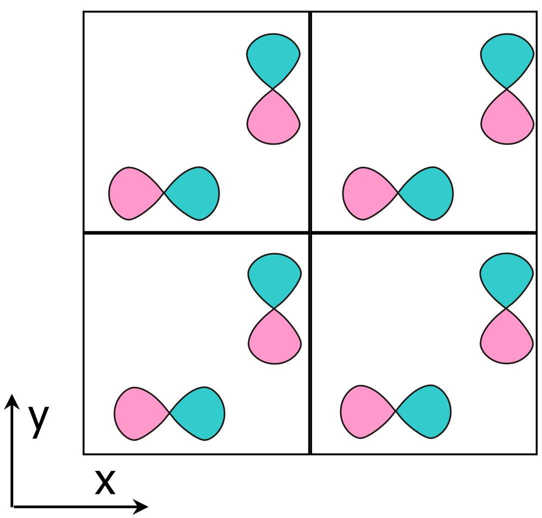
Y

$$\begin{bmatrix} k_x & k_y \\ 0 & \dfrac{\pi}{a} \end{bmatrix}$$
$$\begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$



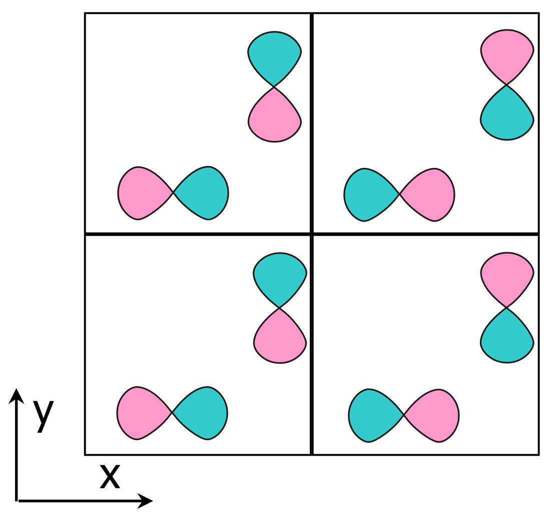
S

$$\begin{bmatrix} k_x & k_y \\ \dfrac{\pi}{a} & \dfrac{\pi}{a} \end{bmatrix}$$
$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$



Γ

$$\begin{bmatrix} k_x & k_y \\ 0 & 0 \end{bmatrix}$$
$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

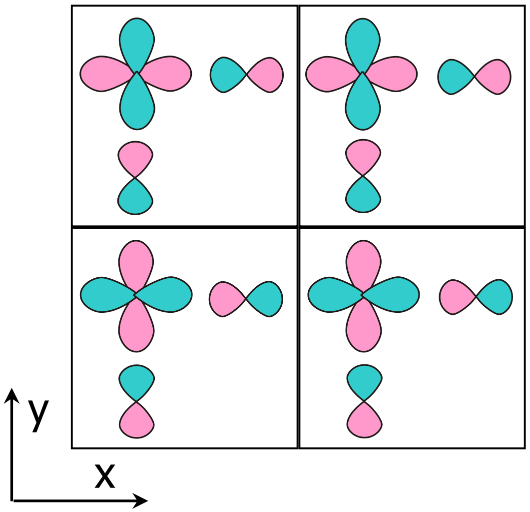


X

$$\begin{bmatrix} k_x & k_y \\ \dfrac{\pi}{a} & 0 \end{bmatrix}$$
$$\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$$

d_{x2-y2}, p_x, p_y,
$\beta_{pp}^{\pi} > \beta_{pp}^{\sigma}$
α

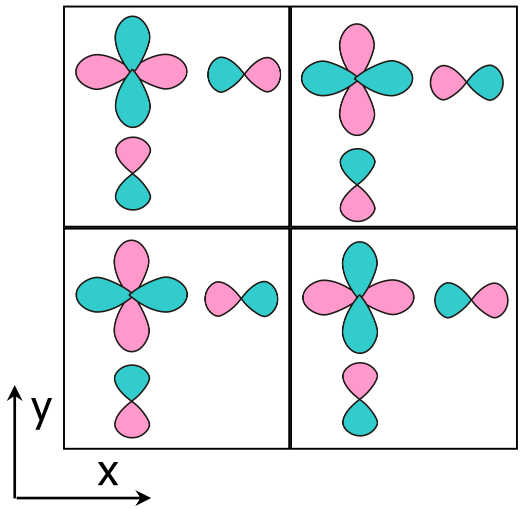
$$\begin{vmatrix} \alpha_{d_{x^2-y^2}} & -i2\beta_{dp}\sin k_y a/2 & i2\beta_{dp}\sin k_x a/2 \\ H_{12}^* & \alpha_{p_x} & -i2\beta_{pp}\sin k_x a/2 - i2\beta_{pp}\sin k_y a/2 \\ H_{13}^* & H_{23}^* & \alpha_{p_y} \end{vmatrix}$$



Y

$$\begin{bmatrix} k_x & k_y \\ 0 & \frac{\pi}{a} \end{bmatrix}$$

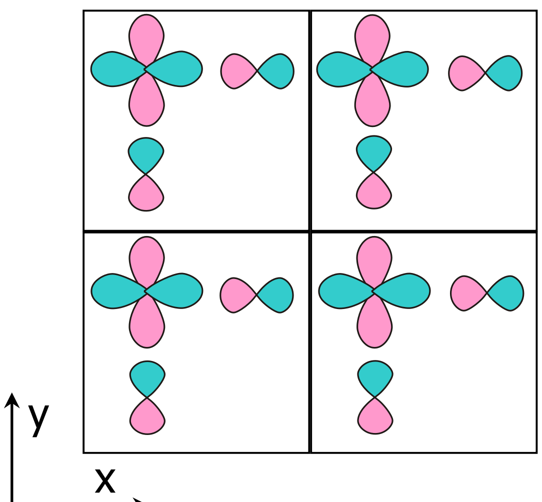
$$\begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$



S

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & \frac{\pi}{a} \end{bmatrix}$$

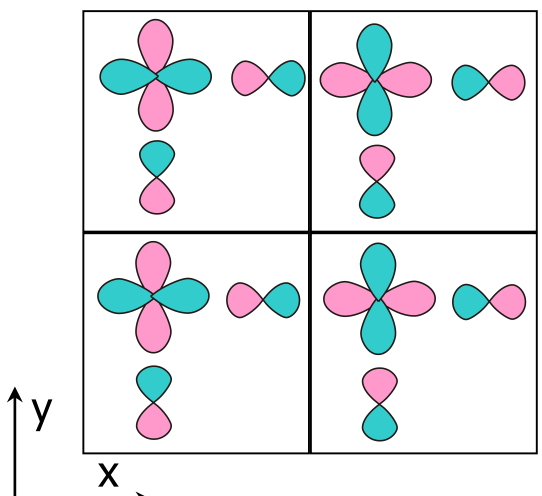
$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$



Γ

$$\begin{bmatrix} k_x & k_y \\ 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$



X

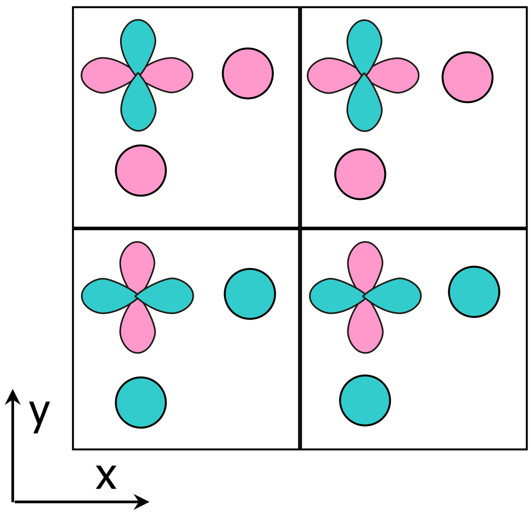
$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$$

d_{x2-y2}, s

s + d_{x2-y2}

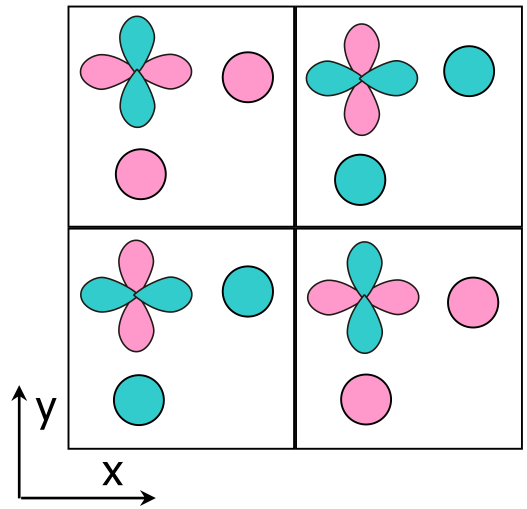
$$\begin{vmatrix} \alpha_{d_{x^2-y^2}} & 2\beta\cos k_x a/2 & -2\beta\cos k_y a/2 \\ H_{12}^* & \alpha_s & 0 \\ H_{13}^* & H_{23}^* & \alpha_s \end{vmatrix}$$



Y

$$\begin{bmatrix} k_x & k_y \\ 0 & \frac{\pi}{a} \end{bmatrix}$$

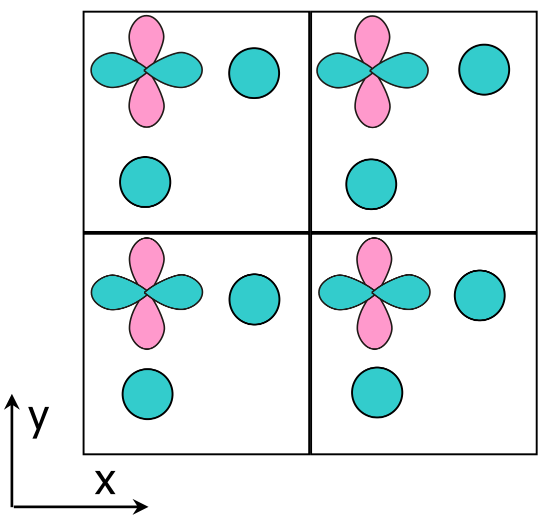
$$\begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$



S

$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & \frac{\pi}{a} \end{bmatrix}$$

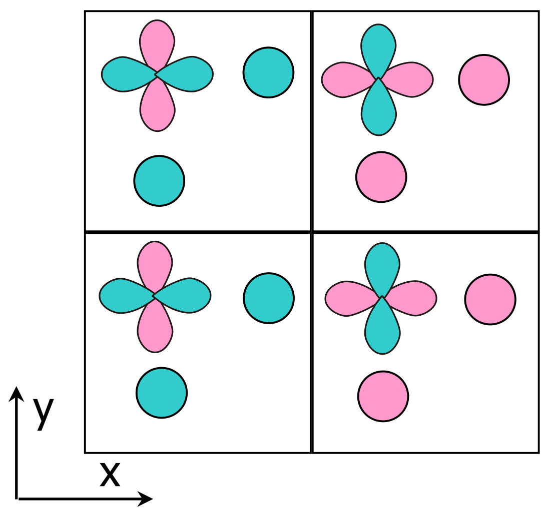
$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$



Γ

$$\begin{bmatrix} k_x & k_y \\ 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

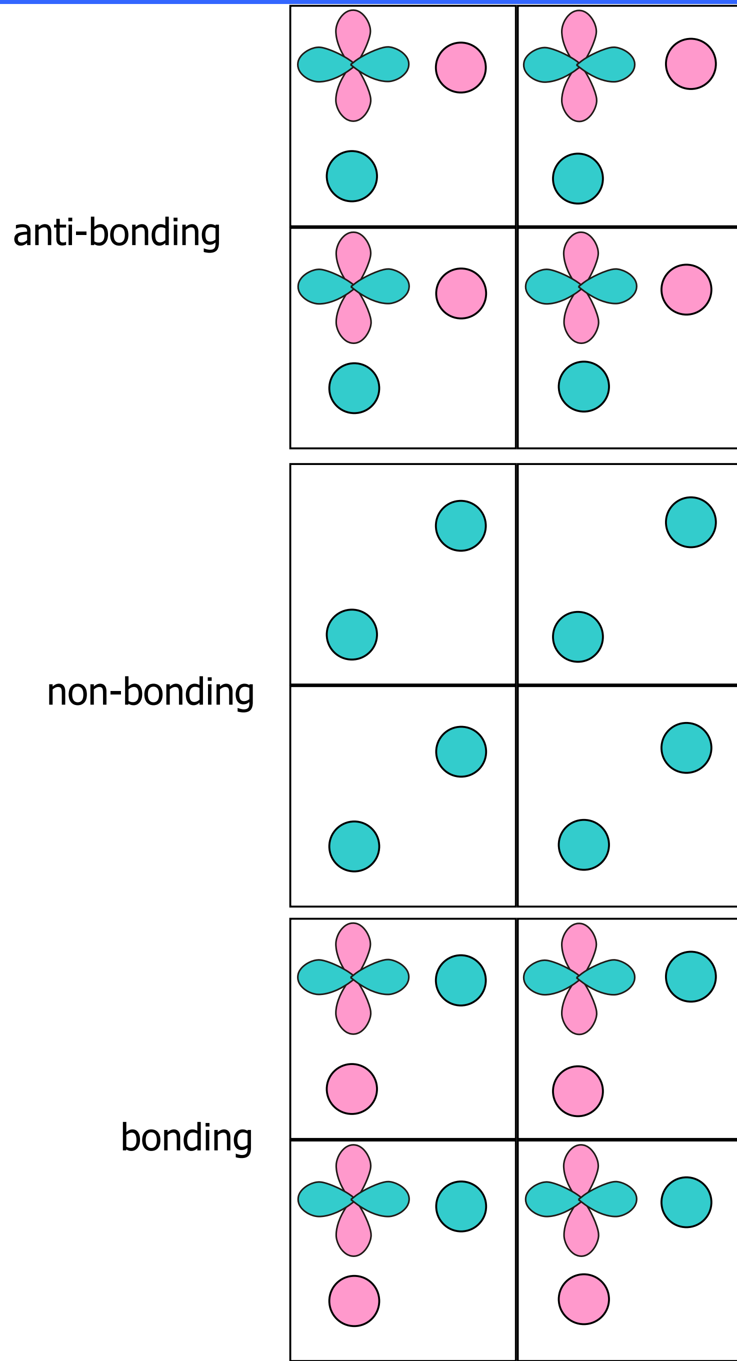


X

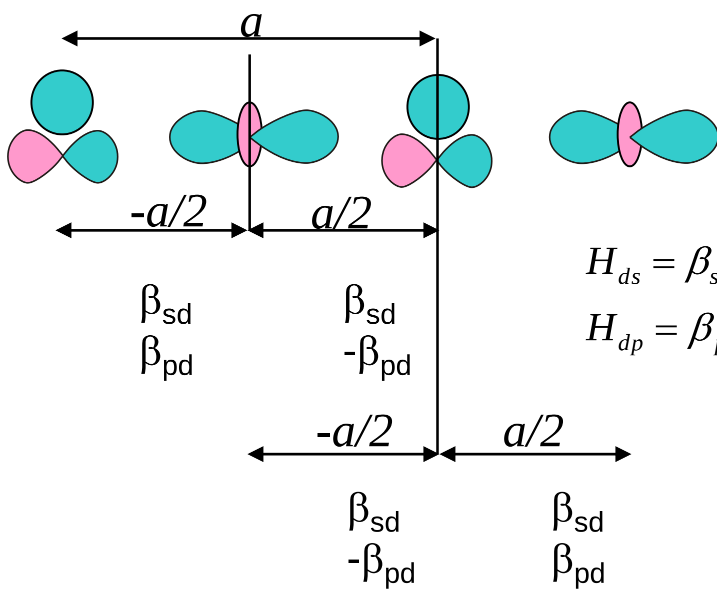
$$\begin{bmatrix} k_x & k_y \\ \frac{\pi}{a} & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$$

d_{x2-y2}, s – MO in Γ point



Linear chain in the *z*-direction, site A: s, p_z; site B: d_{z2};



$$H_{ds} = \beta_{sd} e^{-ik_x a/2} + \beta_{sd} e^{ik_z a/2} = 2\beta \cos k_x a/2$$

$$H_{dp} = \beta_{pd} e^{-ik_x a/2} - \beta_{pd} e^{ik_z a/2} = -i2\beta \sin k_x a/2$$

$$H_{sd} = \beta_{sd} e^{-ik_x a/2} + \beta_{sd} e^{ik_z a/2} = 2\beta \cos k_x a/2$$

$$H_{pd} = -\beta_{pd} e^{-ik_x a/2} + \beta_{pd} e^{ik_z a/2} = i2\beta \sin k_x a/2$$

$$\begin{vmatrix} \alpha_s & 0 & 2\beta \cos k_x a/2 \\ 0 & \alpha_p & i2\beta \sin k_x a/2 \\ 2\beta \cos k_x a/2 & -i2\beta \sin k_x a/2 & \alpha_d \end{vmatrix}$$