Uvažujeme jen interakce s nejbližšími sousedy:
jen výměnný integrál β s nejbližším sousedem

($E\sim\alpha$, $t\sim\beta$, $S<<1$)

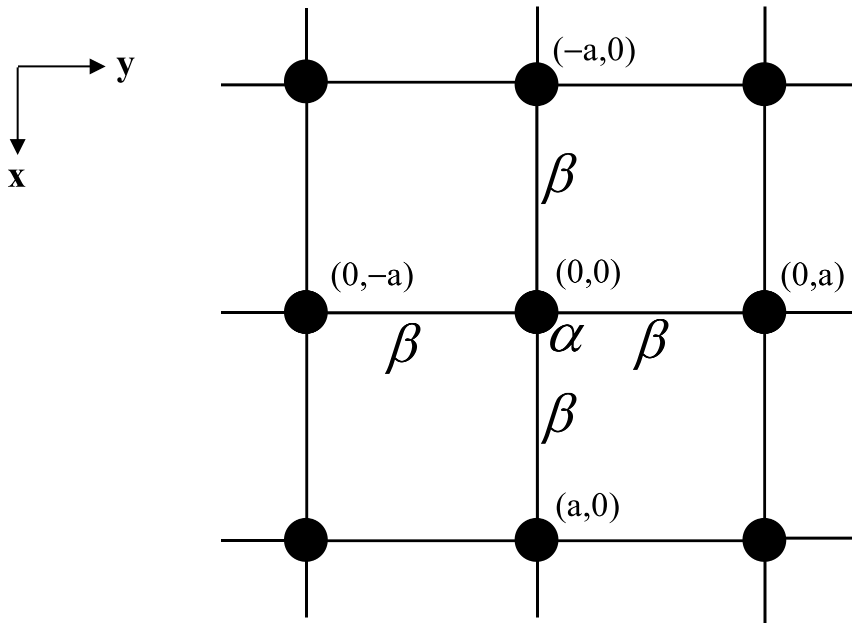
$$\beta e^{i\vec{k}\vec{a}} = \beta(\cos(\vec{k}\vec{a})+i\sin(\vec{k}\vec{a}))$$

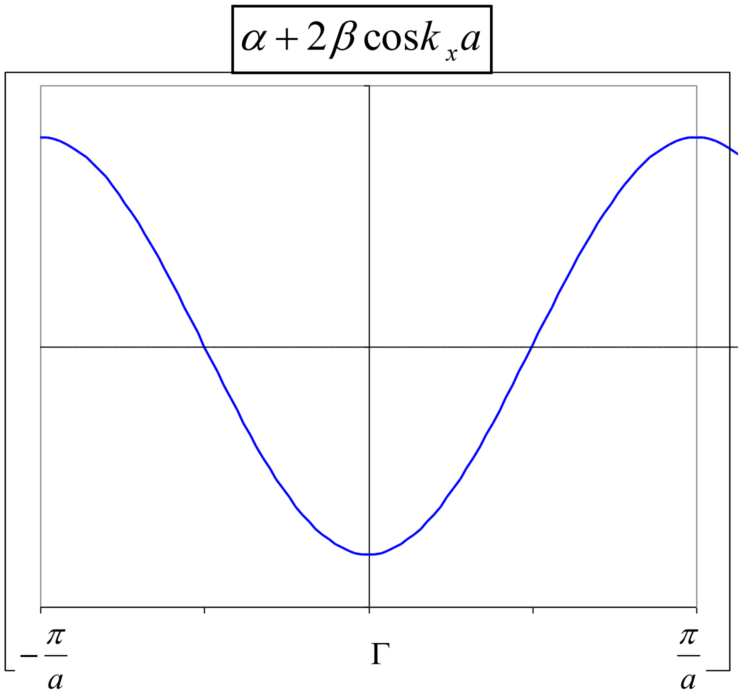
$$\beta e^{-i\vec{k}\vec{a}} = \beta(\cos(\vec{k}\vec{a})-i\sin(\vec{k}\vec{a}))$$

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

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

$$= \alpha + 2\beta(\cos k_x a + \cos k_y a + \cos k_z a)$$





$$+\beta e^{-i\vec{k}\vec{a}}+\beta e^{i\vec{k}\vec{a}} = +\beta(\cos(\vec{k}\vec{a})\text{-}i\sin(\vec{k}\vec{a}))+\beta(\cos(\vec{k}\vec{a})+i\sin(\vec{k}\vec{a})) \quad = 2\beta\cos(\vec{k}\vec{a})$$

$$-\beta e^{-i\vec{k}\vec{a}} - \beta e^{i\vec{k}\vec{a}} = -\beta(\cos(\vec{k}\vec{a})\text{-}i\sin(\vec{k}\vec{a}))-\beta(\cos(\vec{k}\vec{a})+i\sin(\vec{k}\vec{a})) \quad = -2\beta\cos(\vec{k}\vec{a})$$

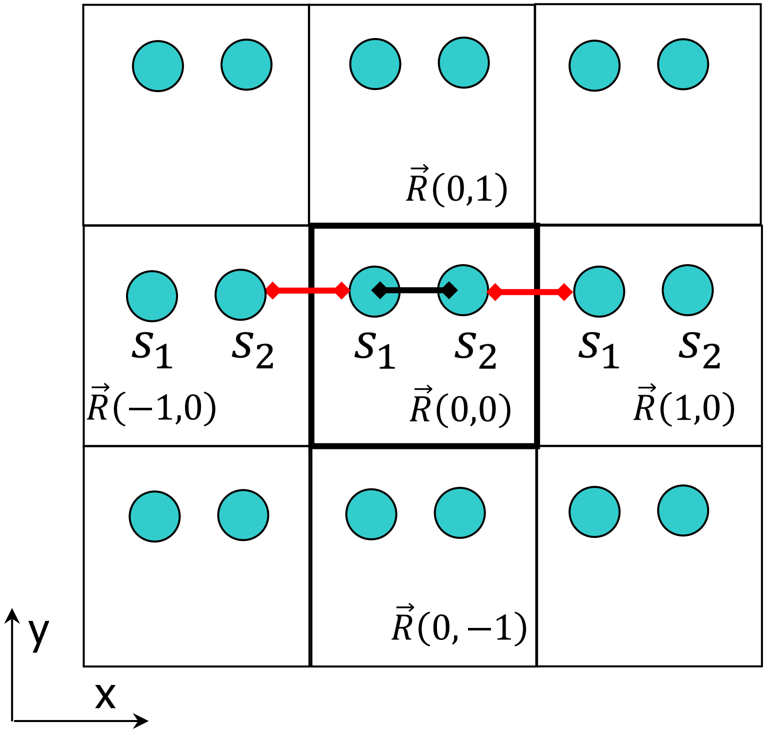
$$-\beta e^{-i\vec{k}\vec{a}}+\beta e^{i\vec{k}\vec{a}} = -\beta(\cos(\vec{k}\vec{a})\text{-}i\sin(\vec{k}\vec{a}))+\beta(\cos(\vec{k}\vec{a})+i\sin(\vec{k}\vec{a})) \quad = 2i\beta\sin(\vec{k}\vec{a})$$

$$+\beta e^{-i\vec{k}\vec{a}} - \beta e^{i\vec{k}\vec{a}} = +\beta(\cos(\vec{k}\vec{a})\text{-}i\sin(\vec{k}\vec{a}))-\beta(\cos(\vec{k}\vec{a})+i\sin(\vec{k}\vec{a})) \quad = -2i\beta\sin(\vec{k}\vec{a})$$

(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.

$$H[\vec{R}(0,0)] = \begin{matrix} & |s_1\rangle & |s_2\rangle \\ \langle s_1| & E_{s_1} & t \\ \langle s_2| & t & E_{s_2} \end{matrix} \qquad H[\vec{R}(1,0)] = \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} \qquad H[\vec{R}(-1,0)] = \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix}$$

$$H(\vec{k}) = \begin{bmatrix} E_{s_1} & t \\ t & E_{s_2} \end{bmatrix} e^{i\vec{k}(0,0)} + \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} e^{i\vec{k}(a,0)} + \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} e^{i\vec{k}(-a,0)}$$

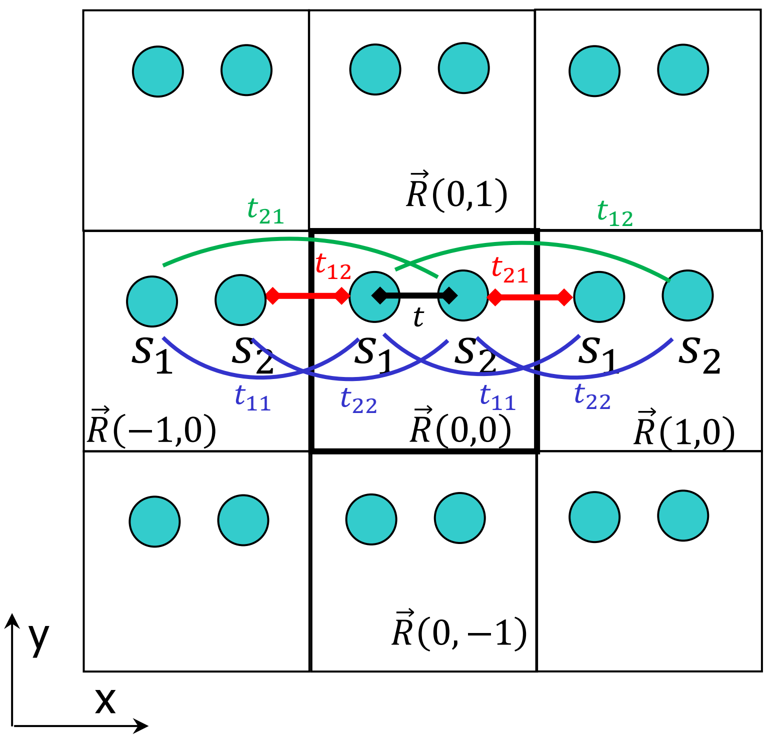


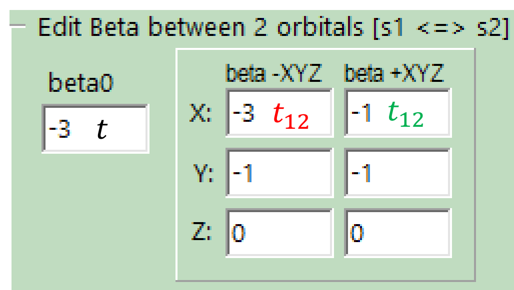
$$H(\vec{k}) = \begin{bmatrix} E_{s_1} & t + te^{i\vec{k}(a,0)} \\ t + te^{i\vec{k}(-a,0)} & E_{s_2} \end{bmatrix}$$

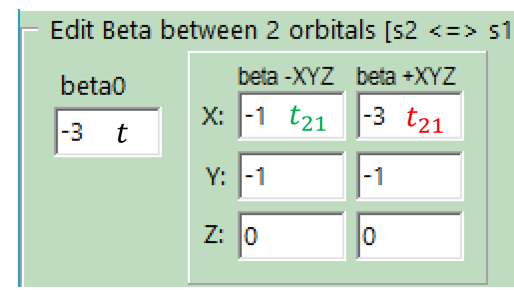
$$H[\vec{R}(0,0)] = \begin{matrix} & |s_1\rangle & |s_2\rangle \\ \langle s_1| & E_{s_1} & t \\ \langle s_2| & t & E_{s_2} \end{matrix} \qquad H[\vec{R}(1,0)] = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \qquad H[\vec{R}(-1,0)] = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix}$$

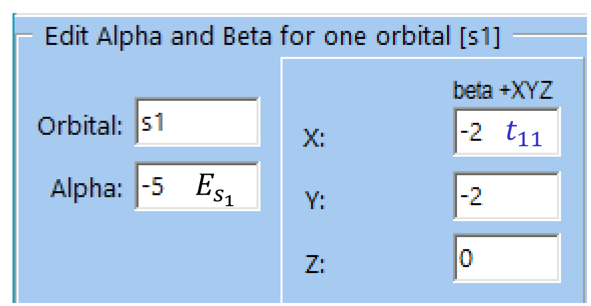
$$H(\vec{k}) = \begin{bmatrix} E_{s_1} & t \\ t & E_{s_2} \end{bmatrix} e^{i\vec{k}(0,0)} + \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} e^{i\vec{k}(a,0)} + \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} e^{i\vec{k}(-a,0)}$$

$$H(\vec{k}) = \begin{bmatrix} E_{s_1} + t_{11}e^{ik_x a_x} + t_{11}e^{-ik_x a_x} & t + t_{12}e^{ik_x a_x} + t_{12}e^{-ik_x a_x} \\ t + t_{21}e^{ik_x a_x} + t_{21}e^{-ik_x a_x} & E_{s_2} + t_{22}e^{ik_x a_x} + t_{22}e^{-ik_x a_x} \end{bmatrix}$$









$$H(\vec{k}) = \begin{bmatrix} E_{s_1} + t_{11}e^{i\vec{k}(a,0)} + t_{11}e^{i\vec{k}(-a,0)} & t + t_{12}e^{i\vec{k}(-a,0)} + t_{12}e^{i\vec{k}(a,0)} \\ t + t_{21}e^{i\vec{k}(a,0)} + t_{21}e^{i\vec{k}(-a,0)} & E_{s_2} + t_{22}e^{i\vec{k}(a,0)} + t_{22}e^{i\vec{k}(-a,0)} \end{bmatrix}$$

$$H(\vec{k}) = \begin{bmatrix} E_{s_1} + 2t_{11}\cos\vec{k}(a,0) & t + t_{12}e^{i\vec{k}(-a,0)} + t_{12}e^{i\vec{k}(a,0)} \\ t + t_{21}e^{i\vec{k}(a,0)} + t_{21}e^{i\vec{k}(-a,0)} & E_{s_2} + 2t_{22}\cos\vec{k}(a,0) \end{bmatrix}$$

$t_{12}=t_{21}$ $t_{12}=t_{21}$

$$H(\vec{k}) = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix}$$

$$H_{11} = E_{s_1} + 2t_{11}\cos\vec{k}(a,0)$$

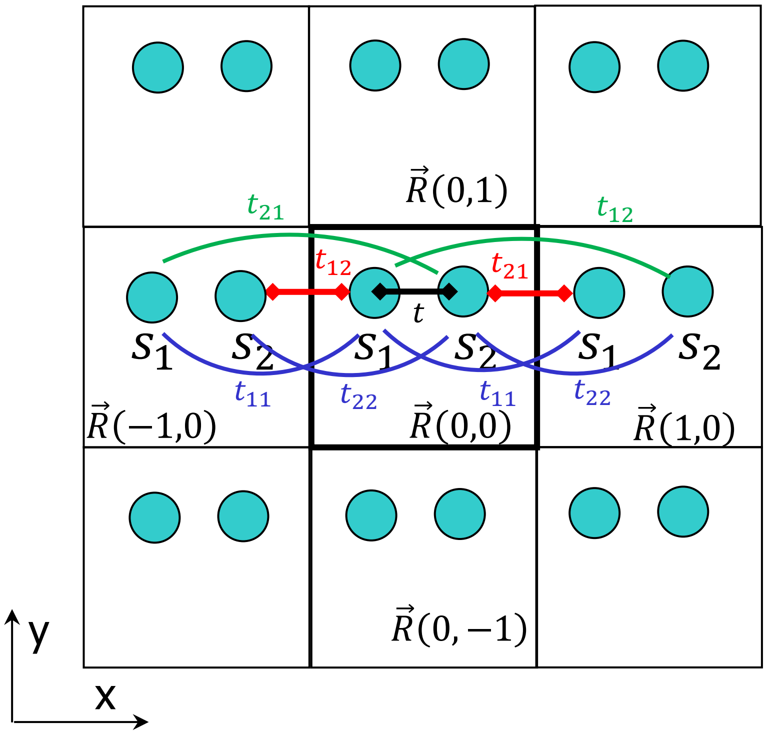
$$H_{22} = E_{s_2} + 2t_{22}\cos\vec{k}(a,0)$$

$$H_{12} = t + te^{i\vec{k}(a,0)} + te^{i\vec{k}(-a,0)} = H_{21}^*$$

$$H_{21} = t + te^{i\vec{k}(-a,0)} + te^{i\vec{k}(a,0)} = H_{12}^*$$

$H_{12} = H_{21}^*$, tj. $H_{12} = A + iB$, $H_{21} = A - iB$

Podmínka pro "Hermitovskou matici". Je-li splněna, je zaručené, že výsledná vlastní čísla (energie pásů) jsou reálná čísla.



$$\beta e^{i\vec{k}\vec{a}} = \beta(\cos(\vec{k}\vec{a}) + i\sin(\vec{k}\vec{a}))$$

$$\beta e^{-i\vec{k}\vec{a}} = \beta(\cos(\vec{k}\vec{a}) - i\sin(\vec{k}\vec{a}))$$

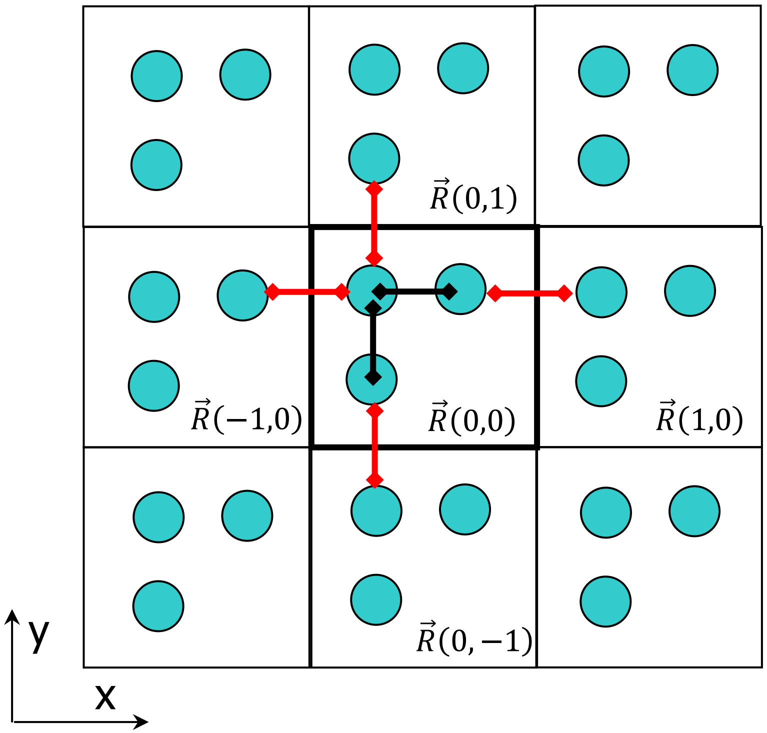
$$H[\vec{R}(0,0)] = \begin{matrix} & |s\rangle & |s_x\rangle & |s_y\rangle \\ \langle s| & E_s & t & t \\ \langle s_x| & t & E_{s_x} & 0 \\ \langle s_y| & t & 0 & E_{s_y} \end{matrix}$$

$$H[\vec{R}(1,0)] = \begin{bmatrix} 0 & t & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$H[\vec{R}(-1,0)] = \begin{bmatrix} 0 & 0 & 0 \\ t & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$H[\vec{R}(0,1)] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ t & 0 & 0 \end{bmatrix}$$

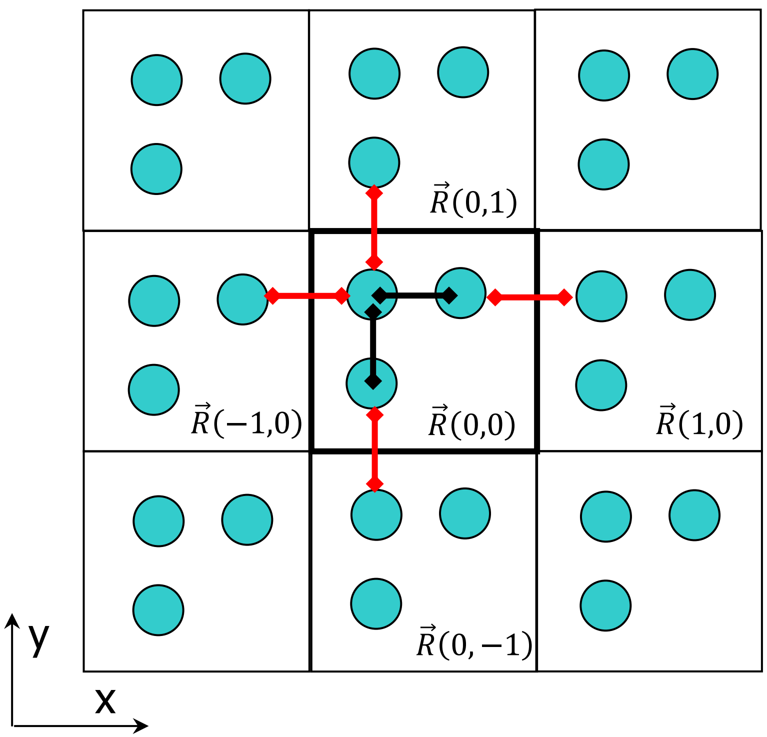
$$H[\vec{R}(0,-1)] = \begin{bmatrix} 0 & 0 & t \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



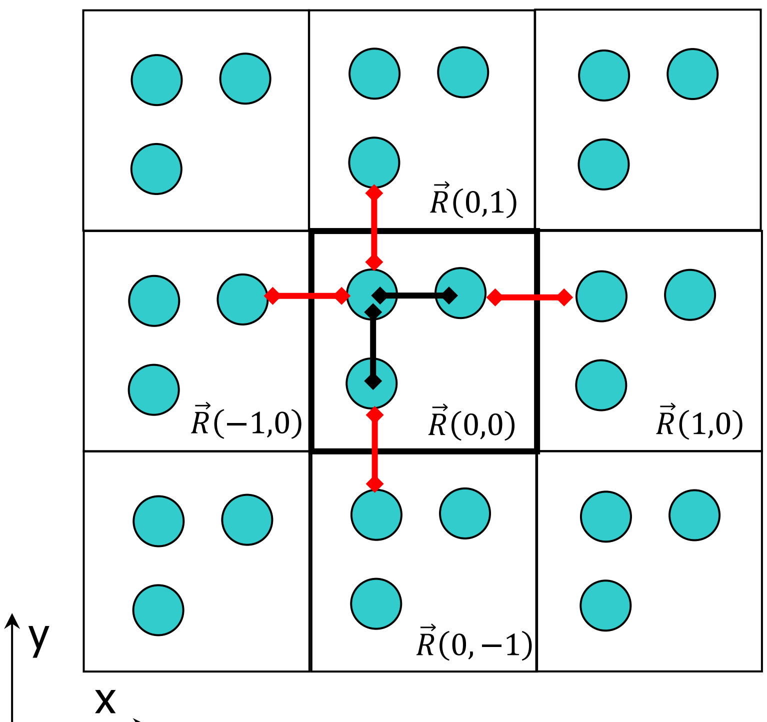
$$H(\vec{k}) = \sum_{\vec{R}} e^{i\vec{k}\vec{R}} H(\vec{R})$$

$$H(\vec{k}) = \begin{bmatrix} E_s & t & t \\ t & E_{s_x} & 0 \\ t & 0 & E_{s_y} \end{bmatrix} e^{i\vec{k}(0,0)} + \begin{bmatrix} 0 & t & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} e^{i\vec{k}(a,0)} + \begin{bmatrix} 0 & 0 & 0 \\ t & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} e^{i\vec{k}(-a,0)} +$$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ t & 0 & 0 \end{bmatrix} e^{i\vec{k}(0,a)} + \begin{bmatrix} 0 & 0 & t \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} e^{i\vec{k}(0,-a)}$$

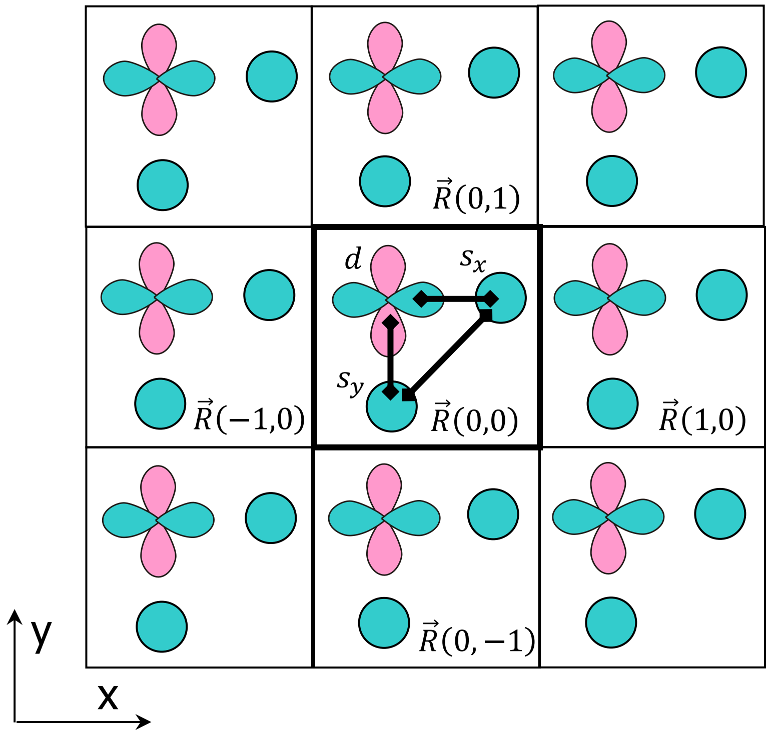


$$H(\vec{k}) = \begin{bmatrix} E_s & t + t e^{i\vec{k}(a,0)} & t + t e^{i\vec{k}(0,-a)} \\ t + t e^{i\vec{k}(-a,0)} & E_{s_x} & 0 \\ t + t e^{i\vec{k}(0,a)} & 0 & E_{s_y} \end{bmatrix}$$



(1) Interakce uvnitř buňky.

$$H[\vec{R}(0,0)] = \begin{bmatrix} E_d & t_{ds_x} & t_{ds_y} \\ t_{s_x d} & E_{s_x} & t_{s_x s_y} \\ t_{s_y d} & t_{s_y s_x} & E_{s_y} \end{bmatrix}$$



$$H[\vec{R}(1,0)] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

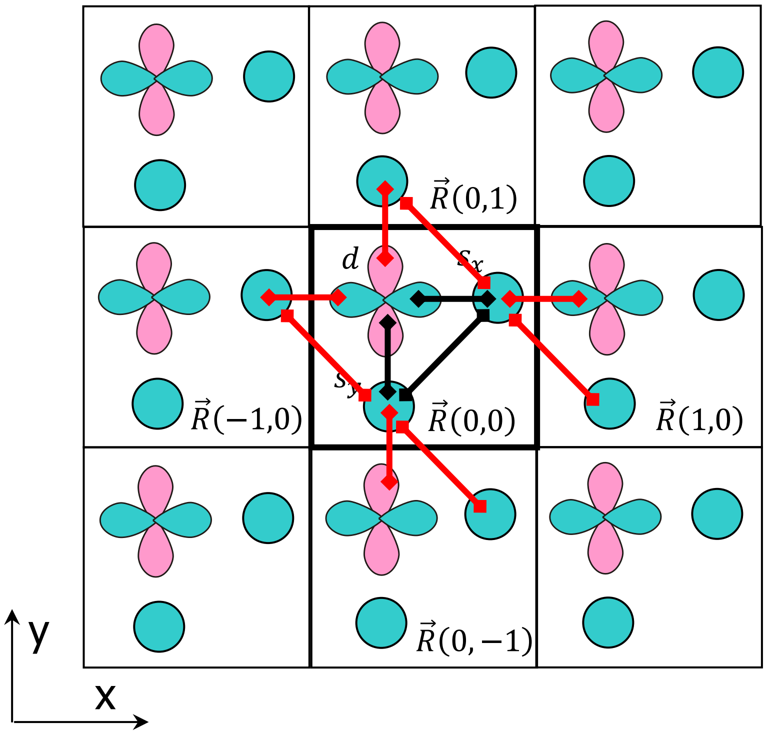
$$H[\vec{R}(-1,0)] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$H[\vec{R}(0,1)] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$H[\vec{R}(0,-1)] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.

$$H[\vec{R}(0{,}0)] = \begin{bmatrix} E_d & t_{ds_x} & t_{ds_y} \\ t_{s_x d} & E_{s_x} & t_{s_x s_y} \\ t_{s_y d} & t_{s_y s_x} & E_{s_y} \end{bmatrix}$$



$$H[\vec{R}(1{,}0)] = \begin{bmatrix} 0 & 0 & 0 \\ t_{s_x d} & 0 & t^x_{s_x s_y} \\ 0 & 0 & 0 \end{bmatrix}$$

$$H[\vec{R}(-1{,}0)] = \begin{bmatrix} 0 & t_{ds_x} & 0 \\ 0 & 0 & 0 \\ 0 & t^x_{s_y s_x} & 0 \end{bmatrix}$$

$$H[\vec{R}(0{,}1)] = \begin{bmatrix} 0 & 0 & t_{ds_y} \\ 0 & 0 & t^y_{s_x s_y} \\ 0 & 0 & 0 \end{bmatrix}$$

$$H[\vec{R}(0,-1)] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ t_{s_y d} & t^y_{s_y s_x} & 0 \end{bmatrix}$$

(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.
(2) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±x.

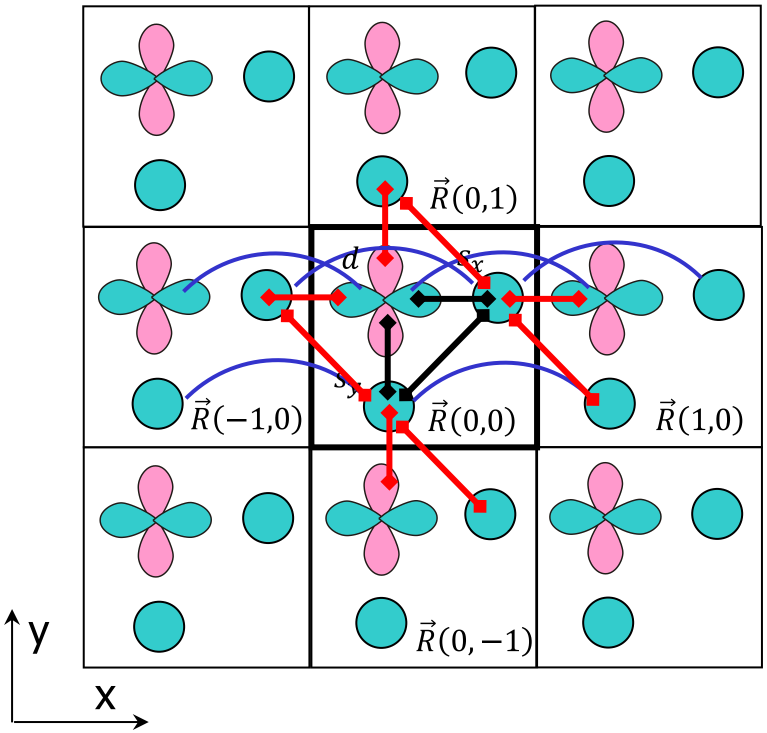
$$H[\vec{R}(0,0)] = \begin{bmatrix} E_d & t_{ds_x} & t_{ds_y} \\ t_{s_xd} & E_{s_x} & t_{s_xs_y} \\ t_{s_yd} & t_{s_ys_x} & E_{s_y} \end{bmatrix}$$

$$H[\vec{R}(1,0)] = \begin{bmatrix} t_{dd}^x & 0 & 0 \\ t_{s_xd} & t_{ss}^x & t_{s_xs_y}^x \\ 0 & 0 & t_{ss}^x \end{bmatrix}$$

$$H[\vec{R}(-1,0)] = \begin{bmatrix} t_{dd}^x & t_{ds_x} & 0 \\ 0 & t_{ss}^x & 0 \\ 0 & t_{s_ys_x}^x & t_{ss}^x \end{bmatrix}$$

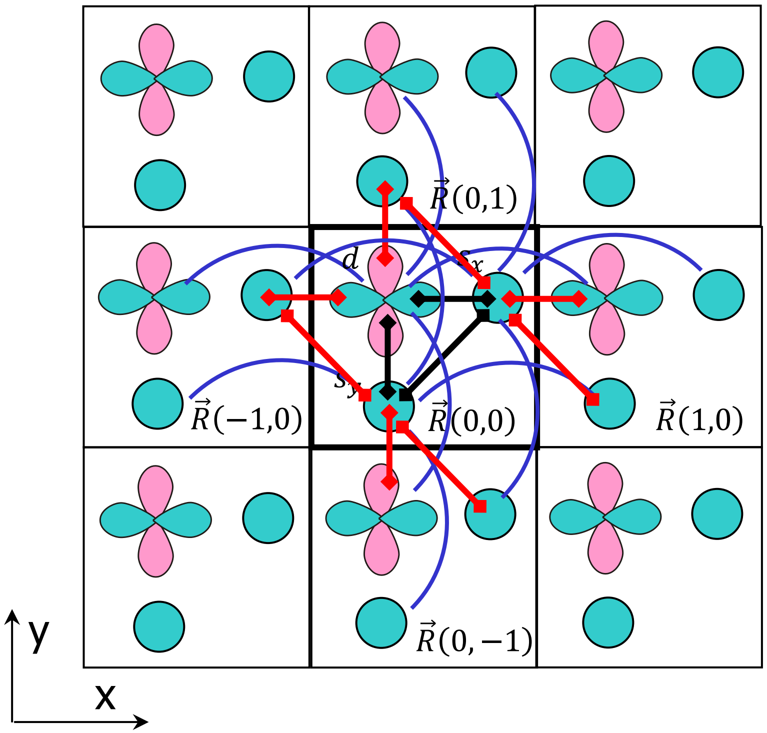
$$H[\vec{R}(0,1)] = \begin{bmatrix} 0 & 0 & t_{ds_y} \\ 0 & 0 & t_{s_xs_y}^y \\ 0 & 0 & 0 \end{bmatrix}$$

$$H[\vec{R}(0,-1)] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ t_{s_yd} & t_{s_ys_x}^y & 0 \end{bmatrix}$$



(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.
(2) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±x.
(3) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±y.

$$H[\vec{R}(0,0)] = \begin{bmatrix} E_d & t_{ds_x} & t_{ds_y} \\ t_{s_xd} & E_{s_x} & t_{s_xs_y} \\ t_{s_yd} & t_{s_ys_x} & E_{s_y} \end{bmatrix}$$



$$H[\vec{R}(1,0)] = \begin{bmatrix} t_{dd}^x & 0 & 0 \\ t_{s_xd} & t_{ss}^x & t_{s_xs_y}^x \\ 0 & 0 & t_{ss}^x \end{bmatrix}$$

$$H[\vec{R}(-1,0)] = \begin{bmatrix} t_{dd}^x & t_{ds_x} & 0 \\ 0 & t_{ss}^x & 0 \\ 0 & t_{s_ys_x}^x & t_{ss}^x \end{bmatrix}$$

$$H[\vec{R}(0,1)] = \begin{bmatrix} t_{dd}^y & 0 & t_{ds_y} \\ 0 & t_{ss}^y & t_{s_xs_y}^y \\ 0 & 0 & t_{ss}^y \end{bmatrix}$$

$$H[\vec{R}(0,-1)] = \begin{bmatrix} t_{dd}^y & 0 & 0 \\ 0 & t_{ss}^y & 0 \\ t_{s_yd} & t_{s_ys_x}^y & t_{ss}^y \end{bmatrix}$$

(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.
(2) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±x.
(3) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±y.
(4) Slabší interakce (vybrané) do sousedních buněk mezi různými orbitaly ve směru ±xy.

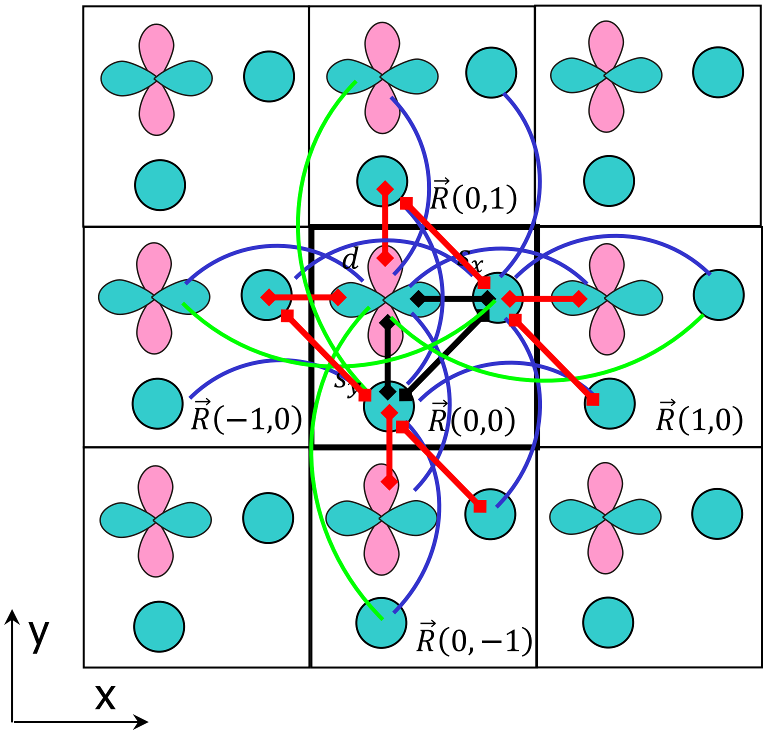
$$H[\vec{R}(0,0)] = \begin{bmatrix} E_d & t_{ds_x} & t_{ds_y} \\ t_{s_x d} & E_{s_x} & t_{s_x s_y} \\ t_{s_y d} & t_{s_y s_x} & E_{s_y} \end{bmatrix}$$

$$H[\vec{R}(1,0)] = \begin{bmatrix} t_{dd}^x & t_{ds_x} & 0 \\ t_{s_x d} & t_{ss}^x & t_{s_x s_y}^x \\ 0 & 0 & t_{ss}^x \end{bmatrix}$$

$$H[\vec{R}(-1,0)] = \begin{bmatrix} t_{dd}^x & t_{ds_x} & 0 \\ t_{s_x d} & t_{ss}^x & 0 \\ 0 & t_{s_y s_x}^x & t_{ss}^x \end{bmatrix}$$

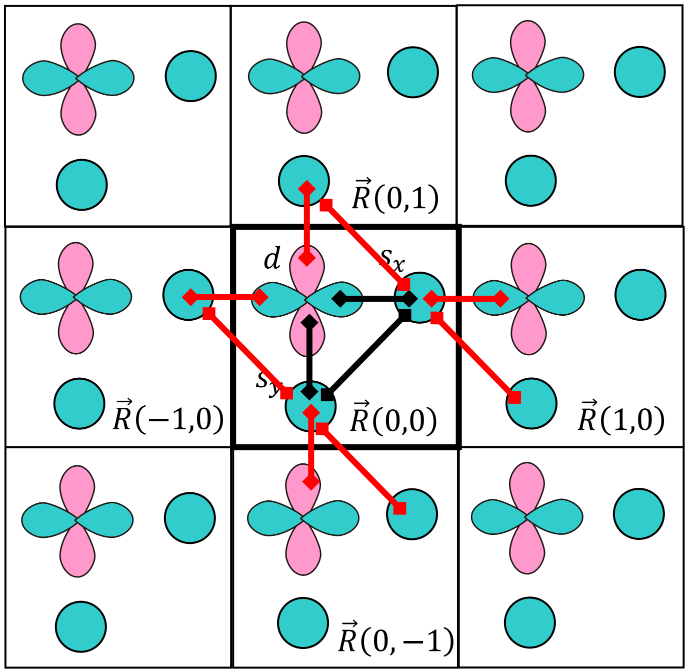
$$H[\vec{R}(0,1)] = \begin{bmatrix} t_{dd}^y & 0 & t_{ds_y} \\ 0 & t_{ss}^y & t_{s_x s_y}^y \\ t_{s_y d} & 0 & t_{ss}^y \end{bmatrix}$$

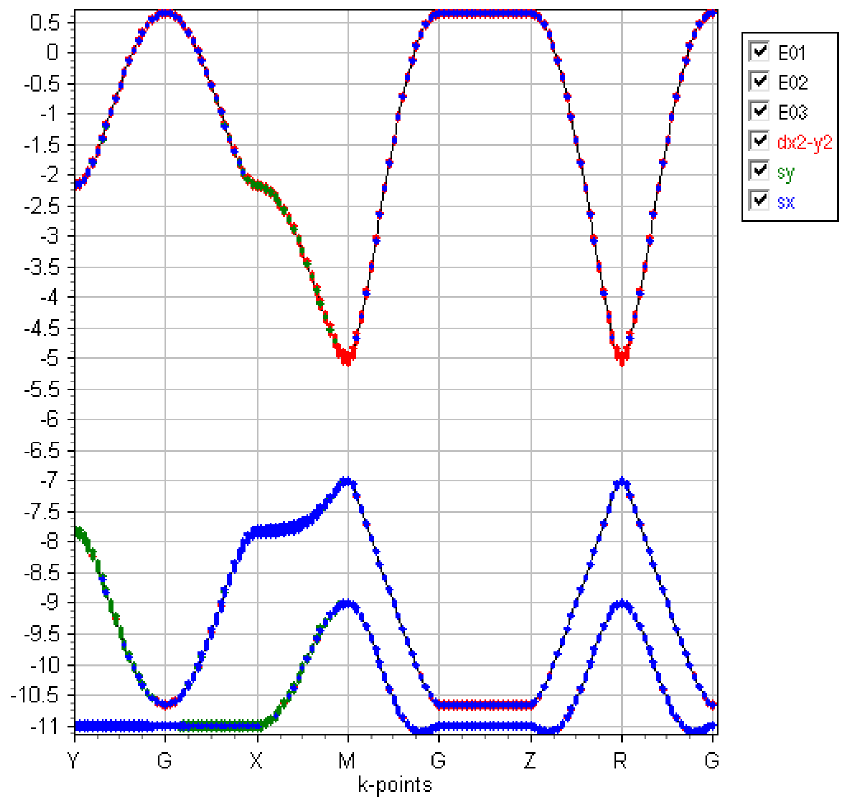
$$H[\vec{R}(0,-1)] = \begin{bmatrix} t_{dd}^y & 0 & t_{ds_y} \\ 0 & t_{ss}^y & 0 \\ t_{s_y d} & t_{s_y s_x}^y & t_{ss}^y \end{bmatrix}$$

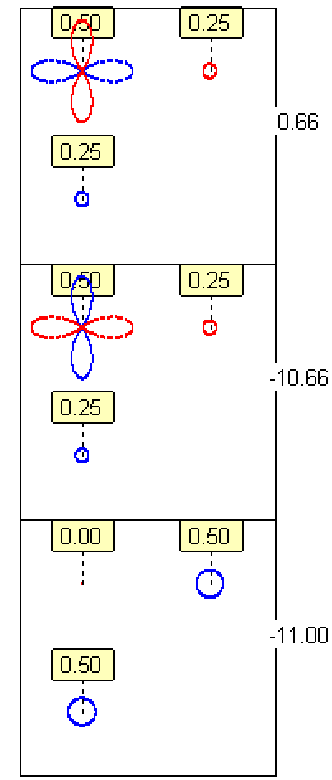


(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.

dx2y2_sx_sy (1).tba

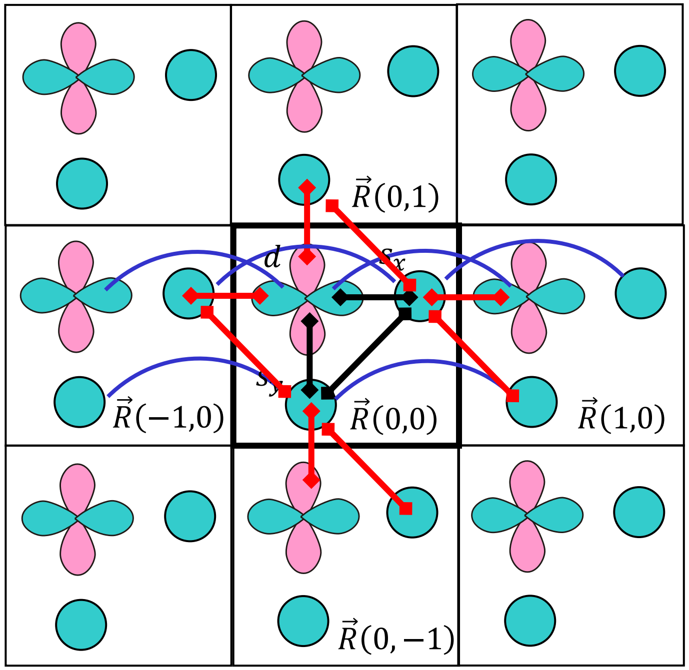


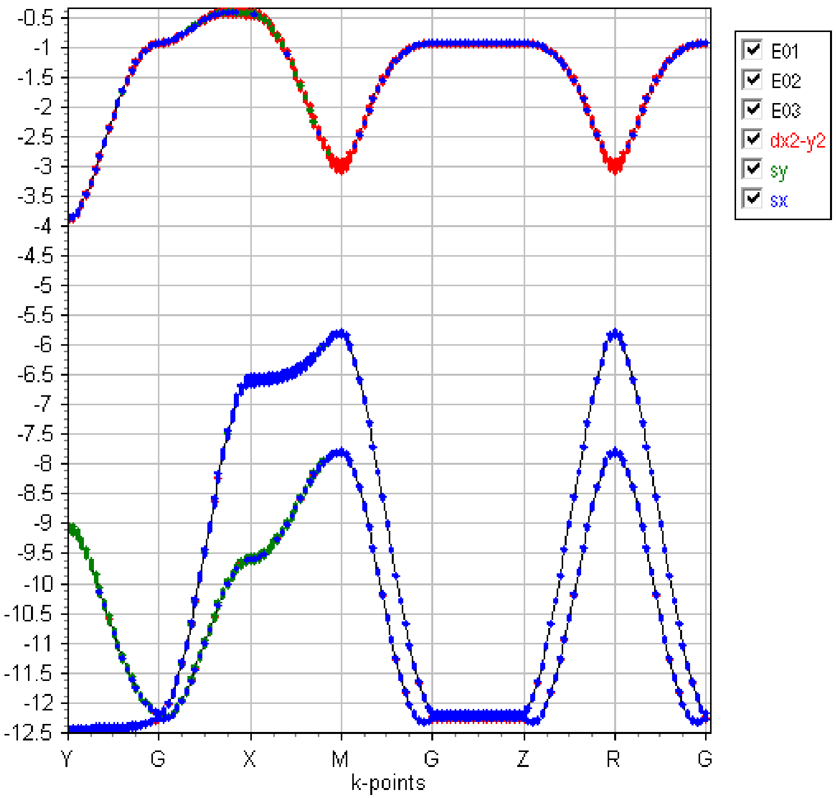


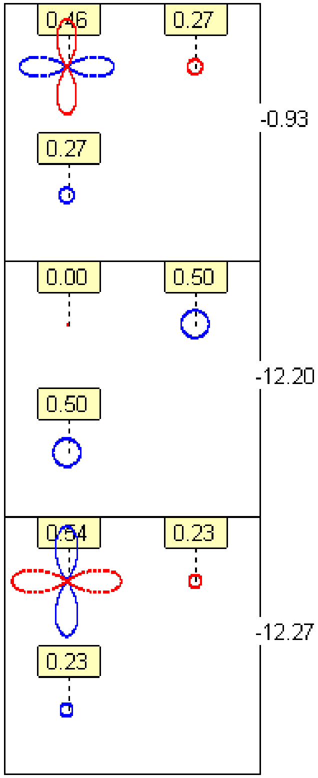


(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.
(2) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±x.

dx2y2_sx_sy (2).tba

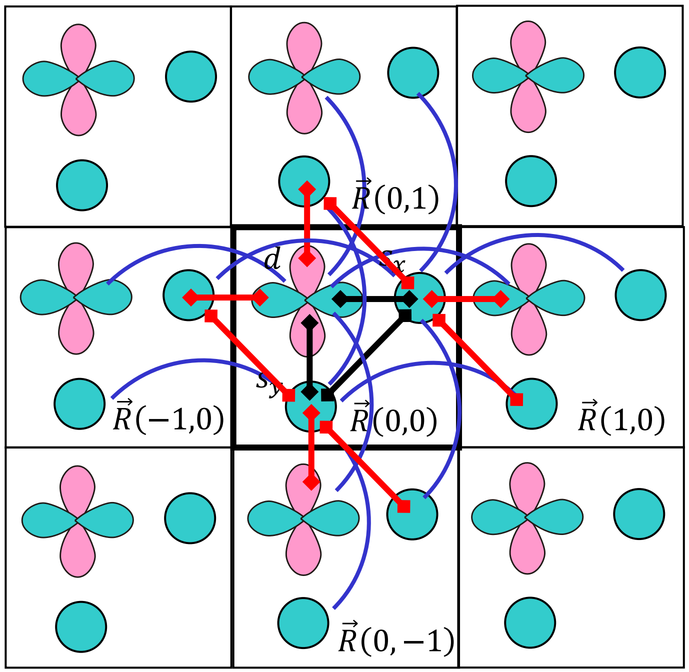


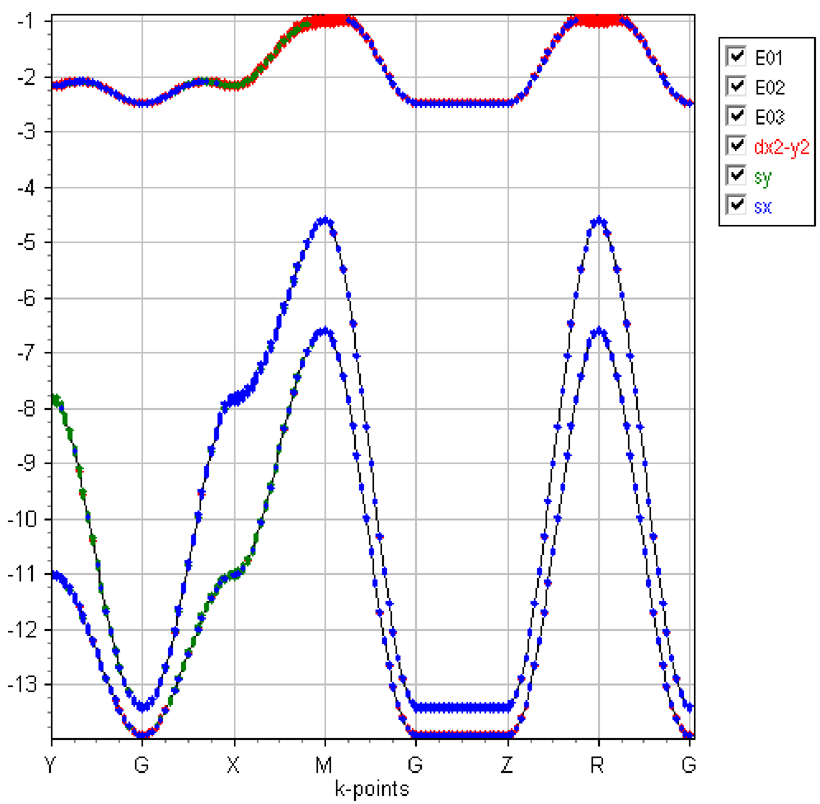


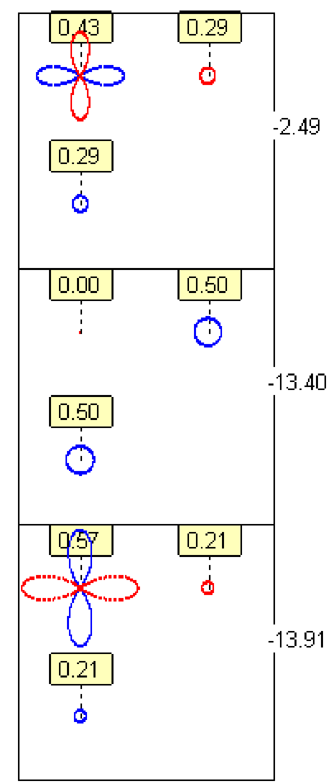


(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.
(2) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±x.
(3) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±y.

dx2y2_sx_sy (3).tba

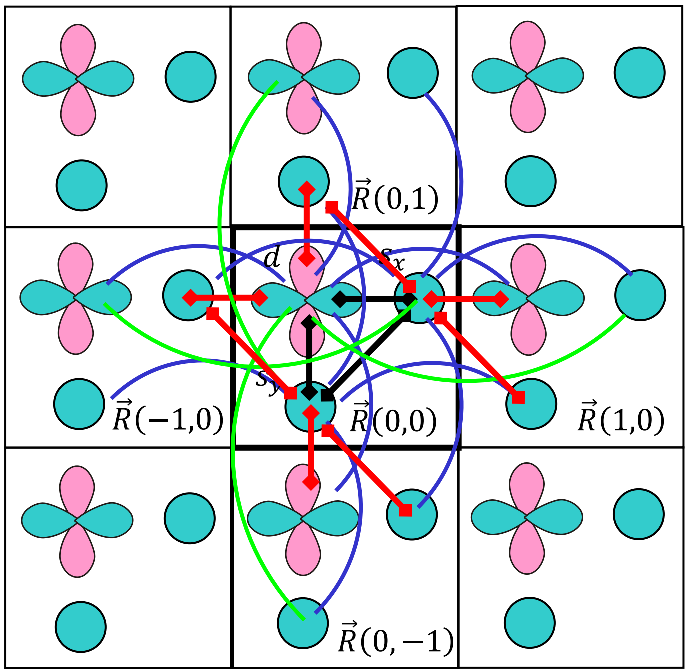


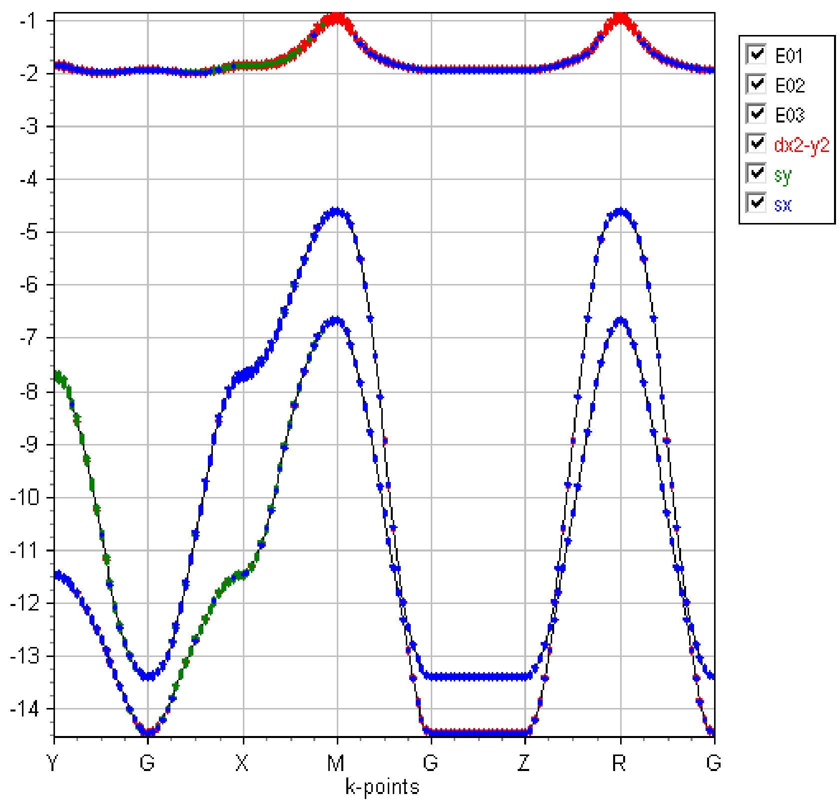


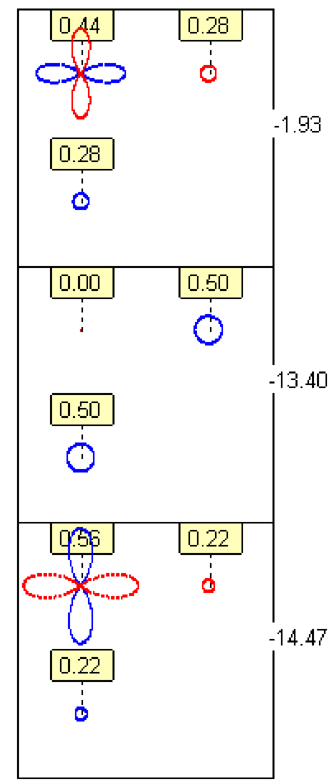


(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.
(2) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±x.
(3) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±y.
(4) Slabší interakce (vybrané) do sousedních buněk mezi různými orbitaly ve směru ±xy.

dx2y2_sx_sy (4).tba

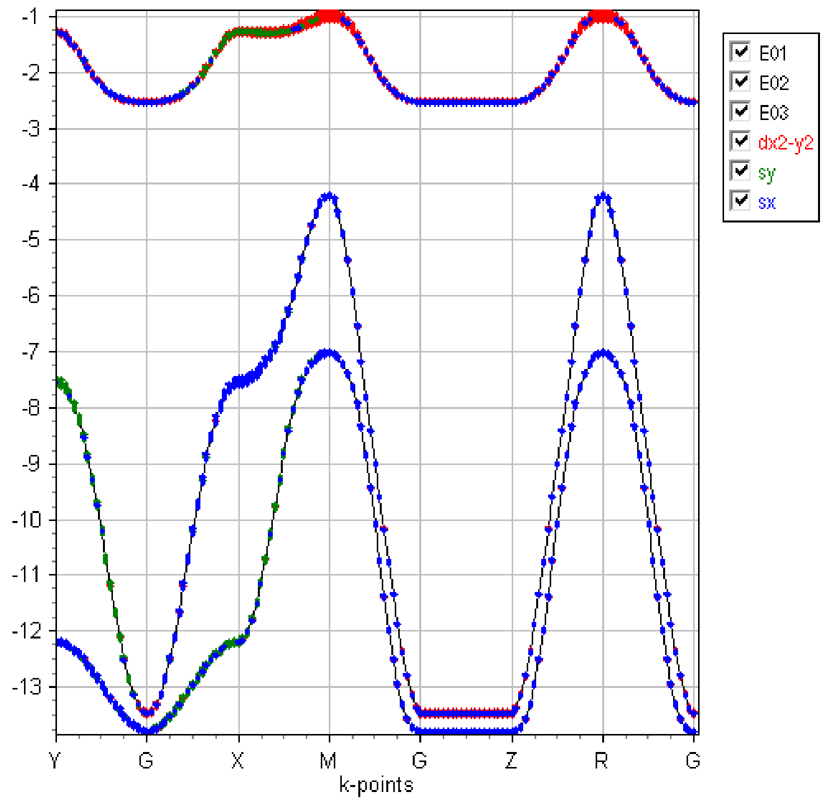


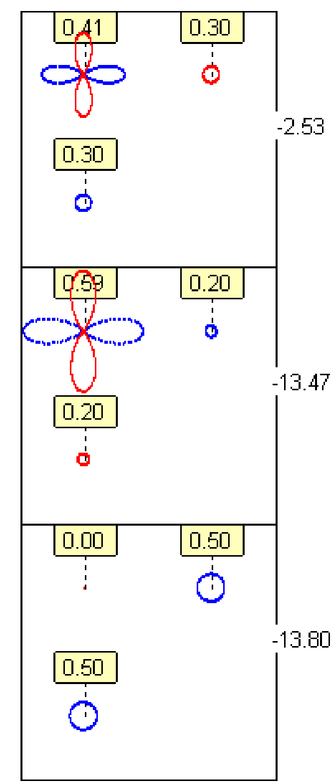




(1) Interakce uvnitř buňky, nejsilnější interakce mezi různými orbitaly do sousedních buněk.
(2) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±x.
(3) Interakce do sousedních buněk mezi stejnými orbitaly ve směru ±y.
(4) Slabší interakce (všechny) do sousedních buněk mezi různými orbitaly ve směru ±xy.

dx2y2_sx_sy (5).tba

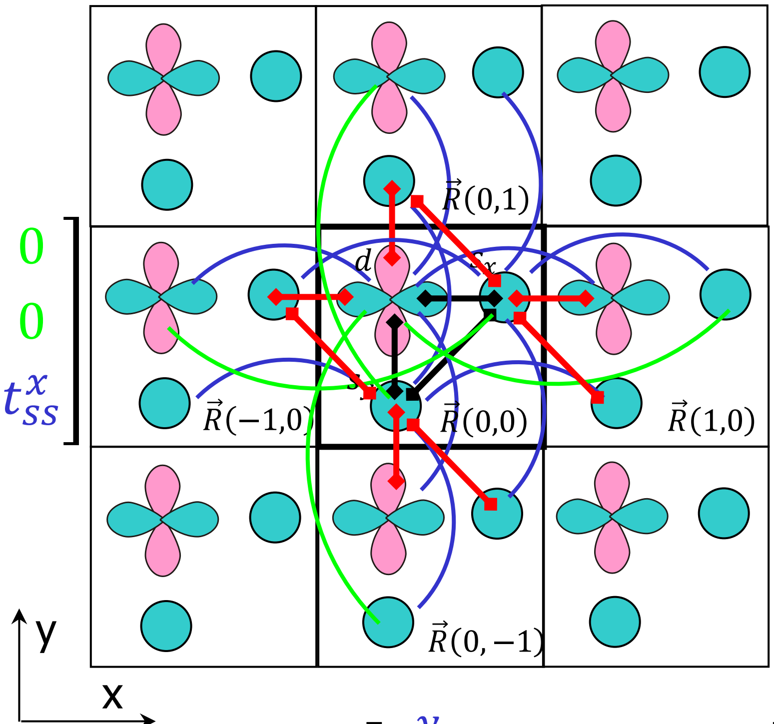




$$H[\vec{R}(0,0)] = \begin{bmatrix} E_d & t_{ds_x} & t_{ds_y} \\ t_{s_xd} & E_{s_x} & t_{s_xs_y} \\ t_{s_yd} & t_{s_ys_x} & E_{s_y} \end{bmatrix}$$

$$H[\vec{R}(0,1)] = \begin{bmatrix} t_{dd}^y & 0 & t_{ds_y} \\ 0 & t_{ss}^y & t_{s_xs_y}^y \\ t_{s_yd} & 0 & t_{ss}^y \end{bmatrix}$$

$$H[\vec{R}(-1,0)] = \begin{bmatrix} t_{dd}^x & t_{ds_x} & 0 \\ t_{s_xd} & t_{ss}^x & 0 \\ 0 & t_{s_ys_x}^x & t_{ss}^x \end{bmatrix}$$



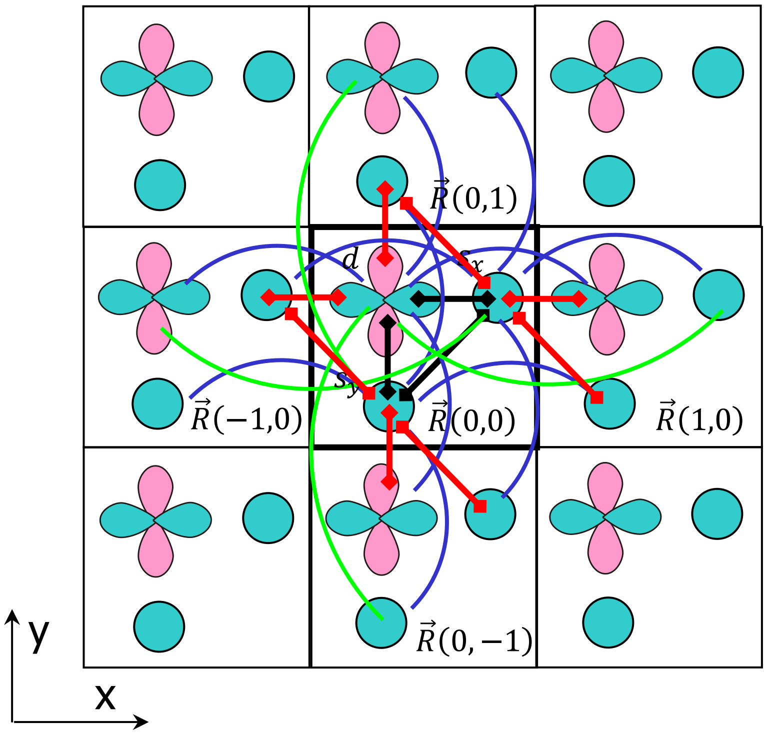
$$H[\vec{R}(1,0)] = \begin{bmatrix} t_{dd}^x & t_{ds_x} & 0 \\ t_{s_xd} & t_{ss}^x & t_{s_xs_y}^x \\ 0 & 0 & t_{ss}^x \end{bmatrix}$$

$$H[\vec{R}(0,-1)] = \begin{bmatrix} t_{dd}^y & 0 & t_{ds_y} \\ 0 & t_{ss}^y & 0 \\ t_{s_yd} & t_{s_ys_x}^y & t_{ss}^y \end{bmatrix}7$$

$$H(\vec{k}) = \sum_{\vec{R}} e^{i\vec{k}\vec{R}} H(\vec{R})$$

$$H(\vec{k}) = \begin{bmatrix} E_d + t_{dd}2(cos\vec{k}(a,0) + cos\vec{k}(0,a)) & t_{ds_x} + t_{ds_x}e^{i\vec{k}(-a,0)} + t_{ds_x}e^{i\vec{k}(a,0)} & t_{ds_y} + t_{ds_y}e^{i\vec{k}(0,a)} + t_{ds_y}e^{i\vec{k}(0,-a)} \\ t_{s_xd} + t_{s_xd}e^{i\vec{k}(a,0)} + t_{s_xd}e^{i\vec{k}(-a,0)} & E_{s_x} + t_{ss}2(cos\vec{k}(a,0) + cos\vec{k}(0,a)) & t_{s_xs_y} + t^x_{s_xs_y}e^{i\vec{k}(a,0)} + t^y_{s_xs_y}e^{i\vec{k}(0,a)} \\ t_{s_yd} + t_{s_yd}e^{i\vec{k}(0,-a)} + t_{s_yd}e^{i\vec{k}(0,a)} & t_{s_ys_x} + t^x_{s_ys_x}e^{i\vec{k}(-a,0)} + t^y_{s_ys_x}e^{i\vec{k}(0,-a)} & E_{s_y} + t_{ss}2(cos\vec{k}(a,0) + cos\vec{k}(0,a)) \end{bmatrix}$$

$$2t^x cos\vec{k}(a,0) + 2t^y cos\vec{k}(0,a) = t^x e^{i\vec{k}(-a,0)} + t^x e^{i\vec{k}(a,0)} + t^y e^{i\vec{k}(0,-a)} + t^y e^{i\vec{k}(0,a)}$$

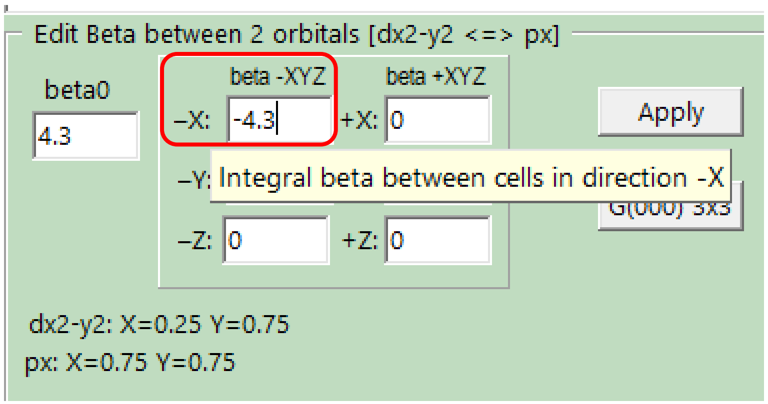


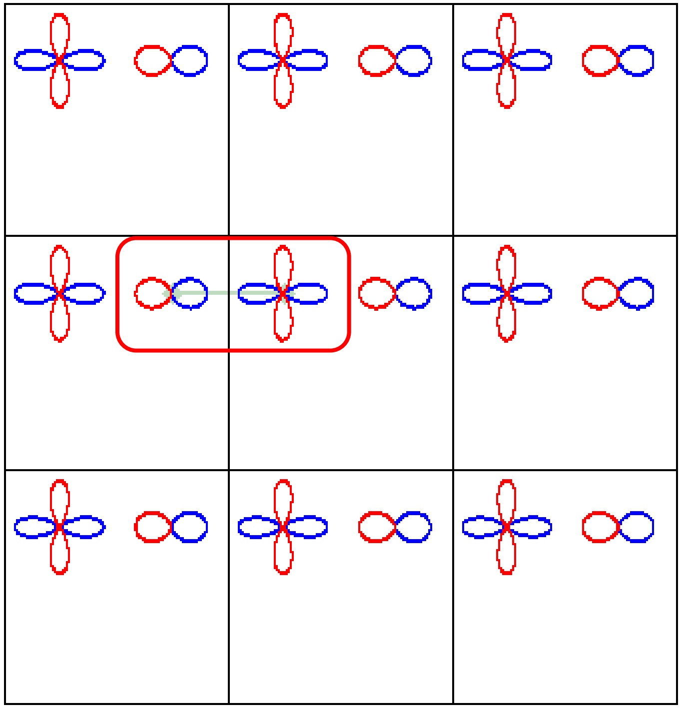
$$H[\vec{R}(0,0)] = \begin{bmatrix} E_d & t_{ds_x} & t_{ds_y} \\ t_{s_xd} & E_{s_x} & t_{s_xs_y} \\ t_{s_yd} & t_{s_ys_x} & E_{s_y} \end{bmatrix}$$

$$H[\vec{R}(-1,0)] = \begin{bmatrix} t^x_{dd} & t_{ds_x} & 0 \\ t_{s_xd} & t^x_{ss} & 0 \\ 0 & t^x_{s_ys_x} & t^x_{ss} \end{bmatrix} \quad H[\vec{R}(1,0)] = \begin{bmatrix} t^x_{dd} & t_{ds_x} & 0 \\ t_{s_xd} & t^x_{ss} & t^x_{s_xs_y} \\ 0 & 0 & t^x_{ss} \end{bmatrix}$$

$$H[\vec{R}(0,-1)] = \begin{bmatrix} t^y_{dd} & 0 & t_{ds_y} \\ 0 & t^y_{ss} & 0 \\ t_{s_yd} & t^y_{s_ys_x} & t^y_{ss} \end{bmatrix} \quad H[\vec{R}(0,1)] = \begin{bmatrix} t^y_{dd} & 0 & t_{ds_y} \\ 0 & t^y_{ss} & t^y_{s_xs_y} \\ t_{s_yd} & 0 & t^y_{ss} \end{bmatrix}$$

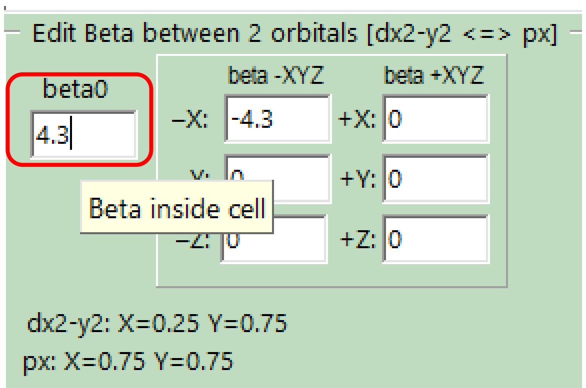
Překryv orbitalů se stejným znaménkem – záporný integrál beta.
Výhodný překryv snižuje energii systému.

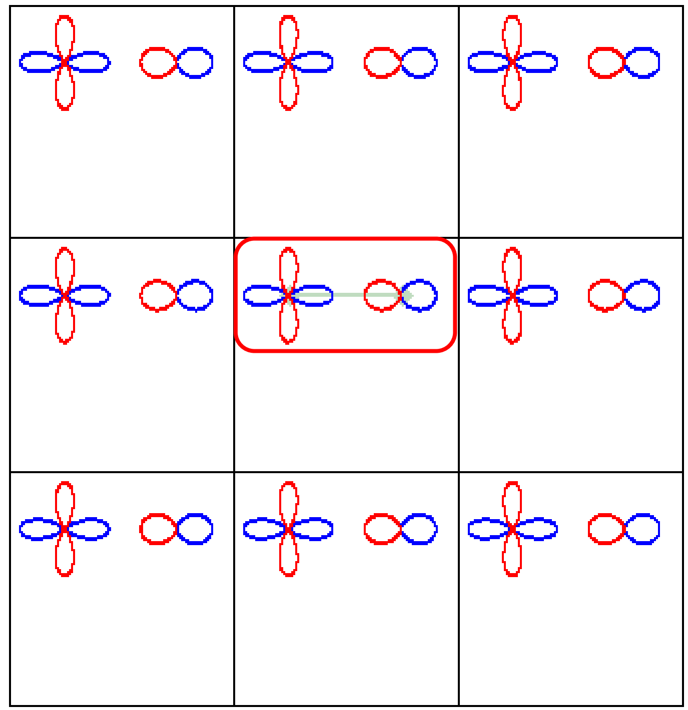




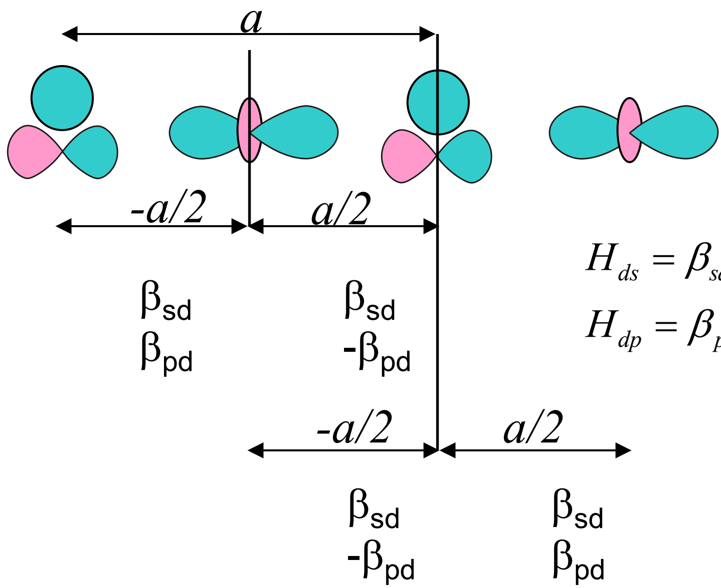
Metoda těsné vazby – znaménko integrálu

Překryv orbitalů s opačným znaménkem – kladný integrál beta.
Nevýhodný překryv zvyšuje energii systému.





Lineární řetěz ve směru *z*, poloha A: s, p_z; poloha B: d_{z2};



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

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

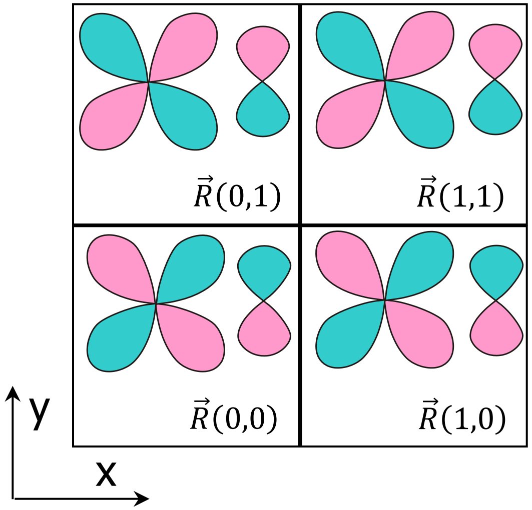
$$H_{sd} = \beta_{sd} e^{-ik_x a/2} + \beta_{sd} e^{ik_z a/2} = 2\beta \cos k_x a/2$$

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

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

Silnější interakce ve směru x – energie: M = X < Y = Γ

Slabší interakce ve směru y – energie: M < X < Y < Γ

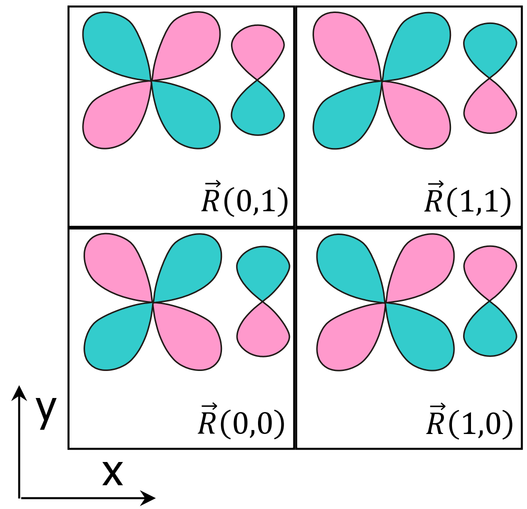


Y

$k_x = 0$

$k_y = \pi/a$

-1	-1
1	1

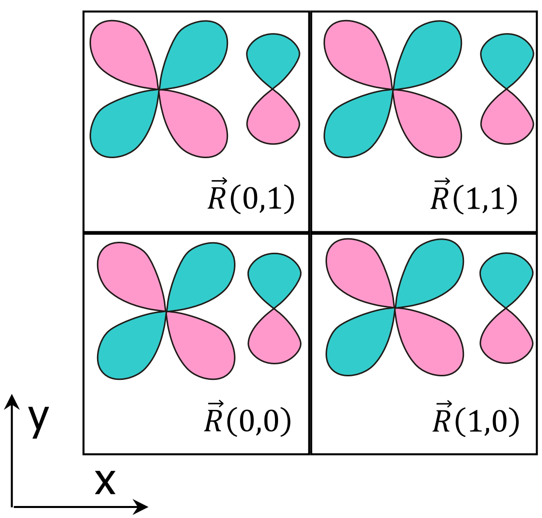


M

$k_x = \pi/a$

$k_y = \pi/a$

-1	1
1	-1

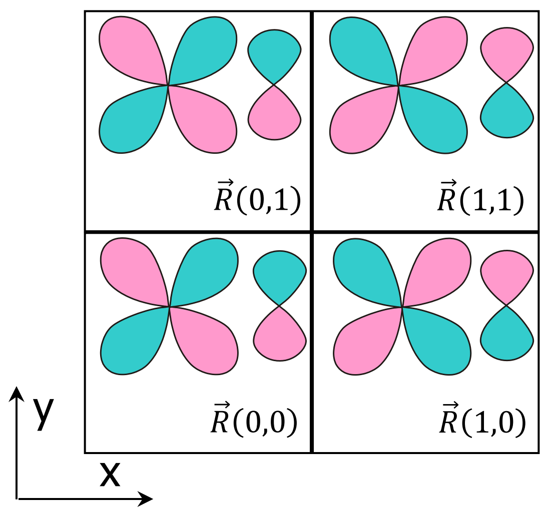


Γ

$k_x = 0$

$k_y = 0$

1	1
1	1



X

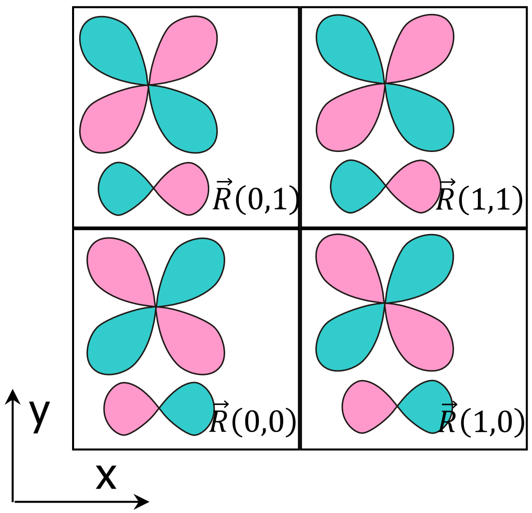
$k_x = \pi/a$

$k_y = 0$

1	-1
1	-1

Silnější interakce ve směru y – energie: M = Y < X = Γ

Slabší interakce ve směru x – energie: M < Y < X < Γ

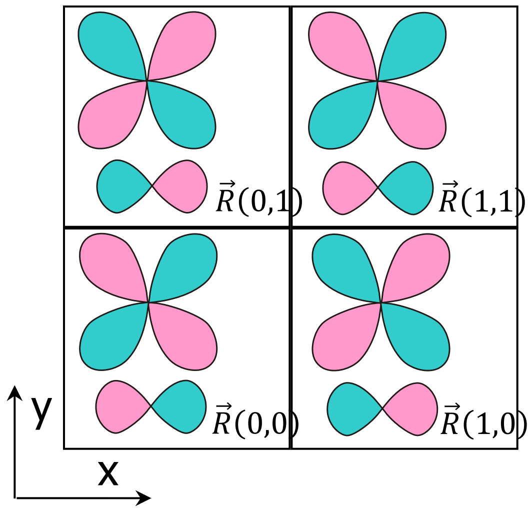


Y

$k_x = 0$

$k_y = {}^{\pi}/_{a}$

-1	-1
1	1

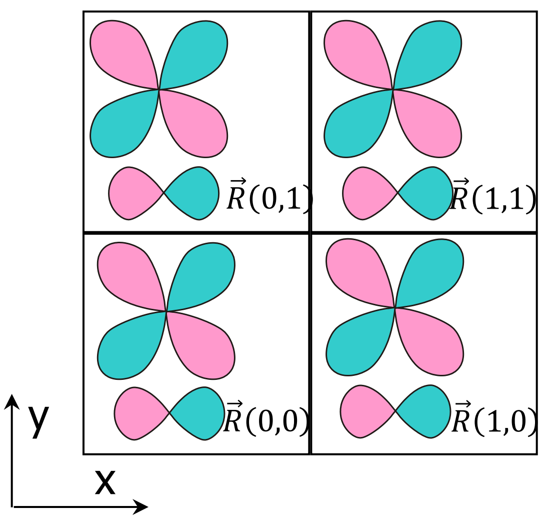


M

$k_x = {}^{\pi}/_{a}$

$k_y = {}^{\pi}/_{a}$

-1	1
1	-1

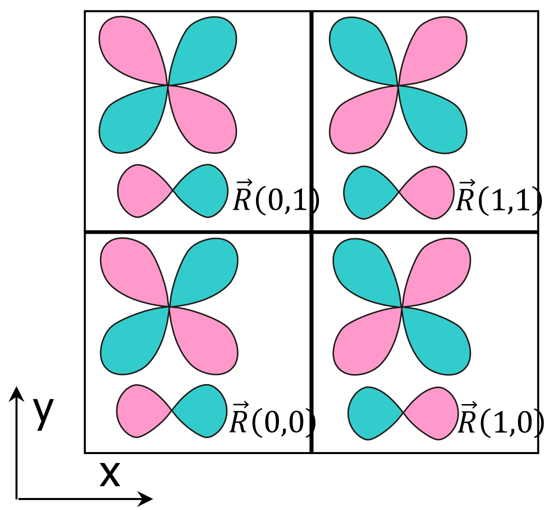


Γ

$k_x = 0$

$k_y = 0$

1	1
1	1



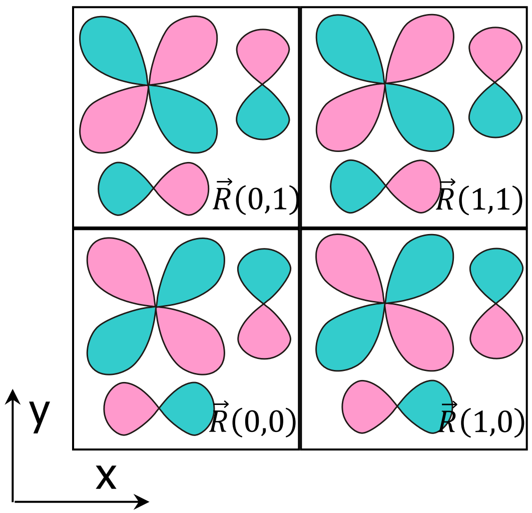
X

$k_x = {}^{\pi}/_{a}$

$k_y = 0$

1	-1
1	-1

Energie: M < X = Y < Γ

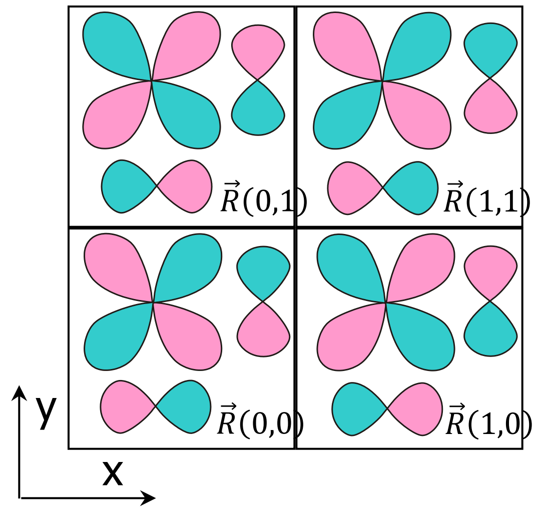


Y

$k_x = 0$

$k_y = {}^{\pi}/_{a}$

-1	-1
1	1

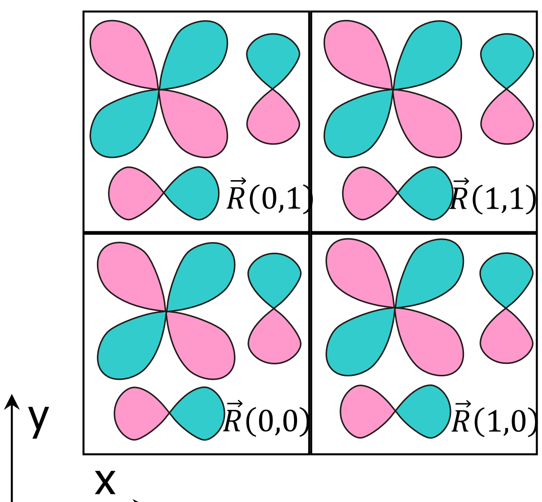


M

$k_x = {}^{\pi}/_{a}$

$k_y = {}^{\pi}/_{a}$

-1	1
1	-1

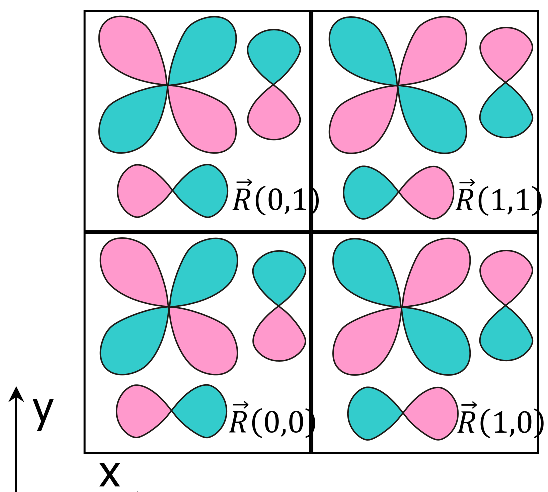


Γ

$k_x = 0$

$k_y = 0$

1	1
1	1



X

$k_x = {}^{\pi}/_{a}$

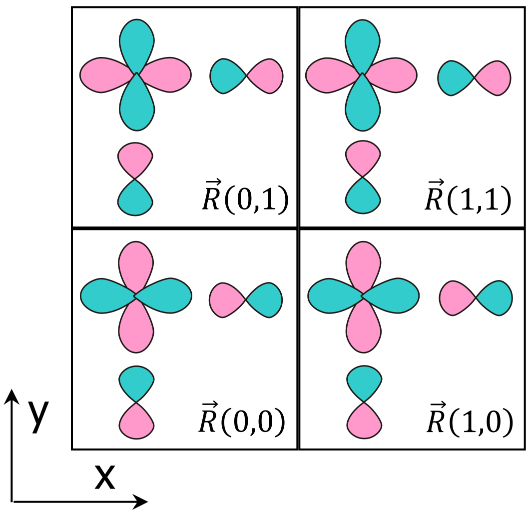
$k_y = 0$

1	-1
1	-1

d_{x2-y2}, p_x, p_y,

$\beta_{pp}^{\pi} > \beta_{pp}^{\sigma}$

α

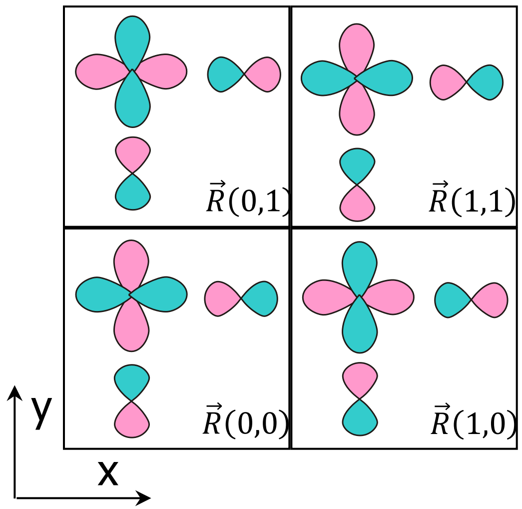


Y

$k_x = 0$

$k_y = \pi/a$

-1	-1
1	1

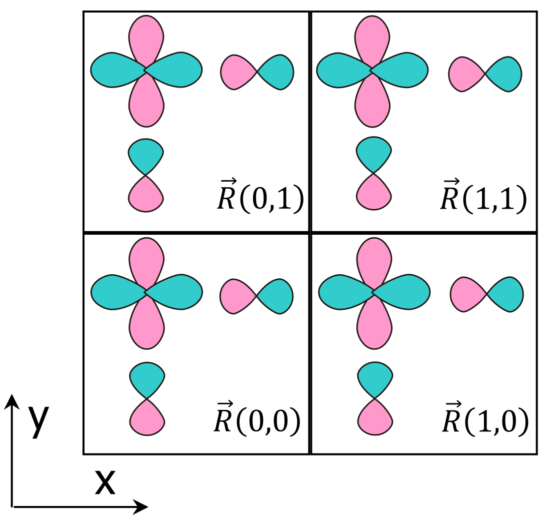


M

$k_x = \pi/a$

$k_y = \pi/a$

-1	1
1	-1

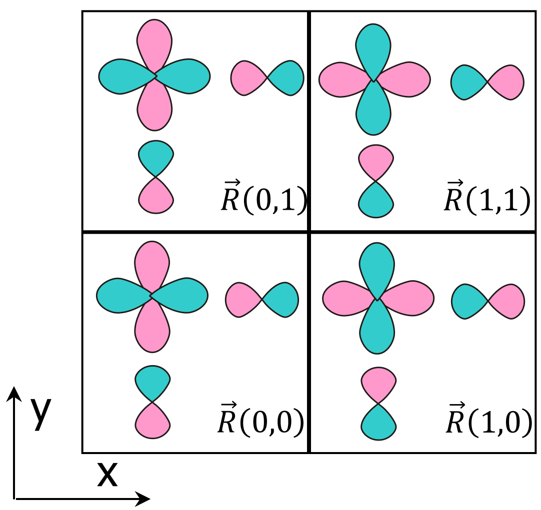


Γ

$k_x = 0$

$k_y = 0$

1	1
1	1

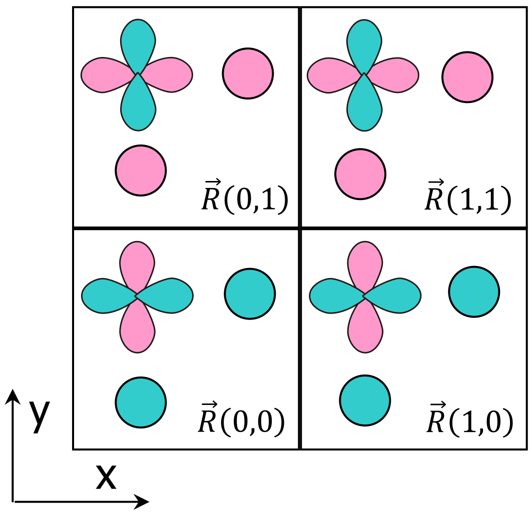


X

$k_x = \pi/a$

$k_y = 0$

1	-1
1	-1

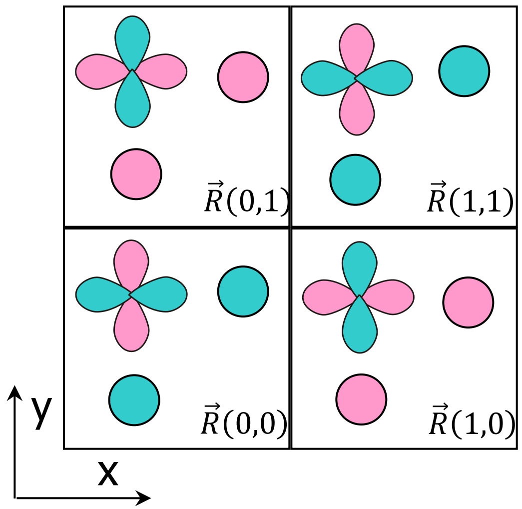


Y

$k_x = 0$

$k_y = {}^{\pi}/_{a}$

-1	-1
1	1

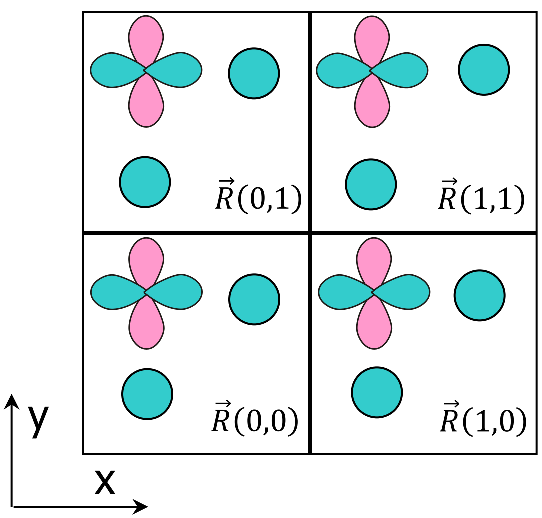


M

$k_x = {}^{\pi}/_{a}$

$k_y = {}^{\pi}/_{a}$

-1	1
1	-1

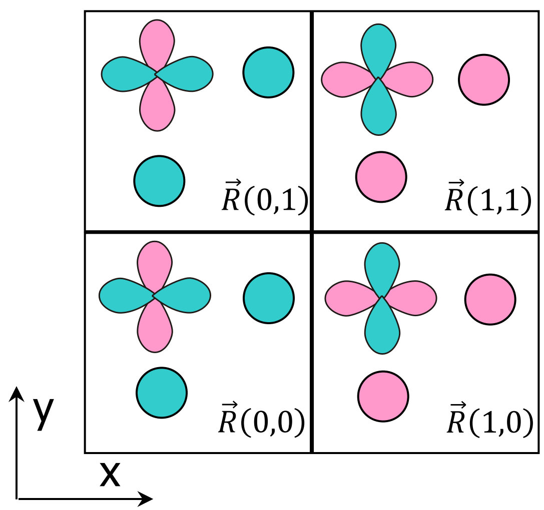


Γ

$k_x = 0$

$k_y = 0$

1	1
1	1

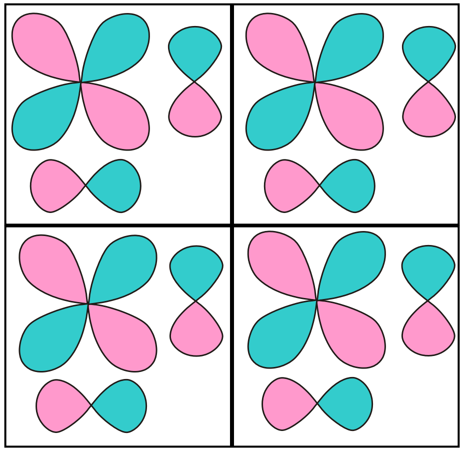


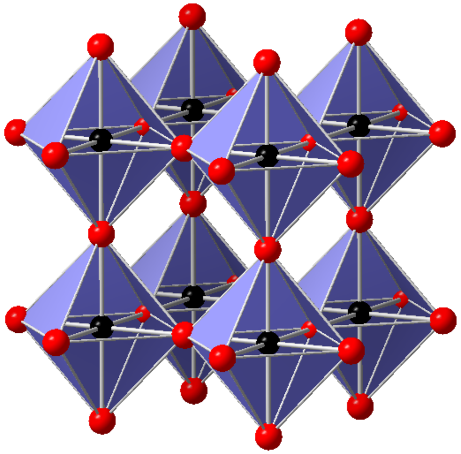
X

$k_x = {}^{\pi}/_{a}$

$k_y = 0$

1	-1
1	-1





ReO_3:

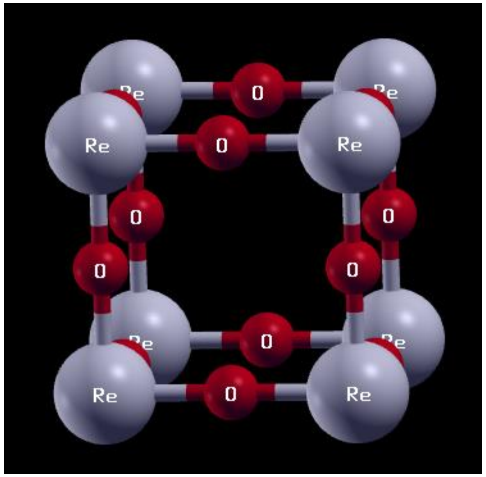
Re6+ d1

π-vazby t_{2g} - p

d_{xy} – $p_x(y)$, $p_y(x)$

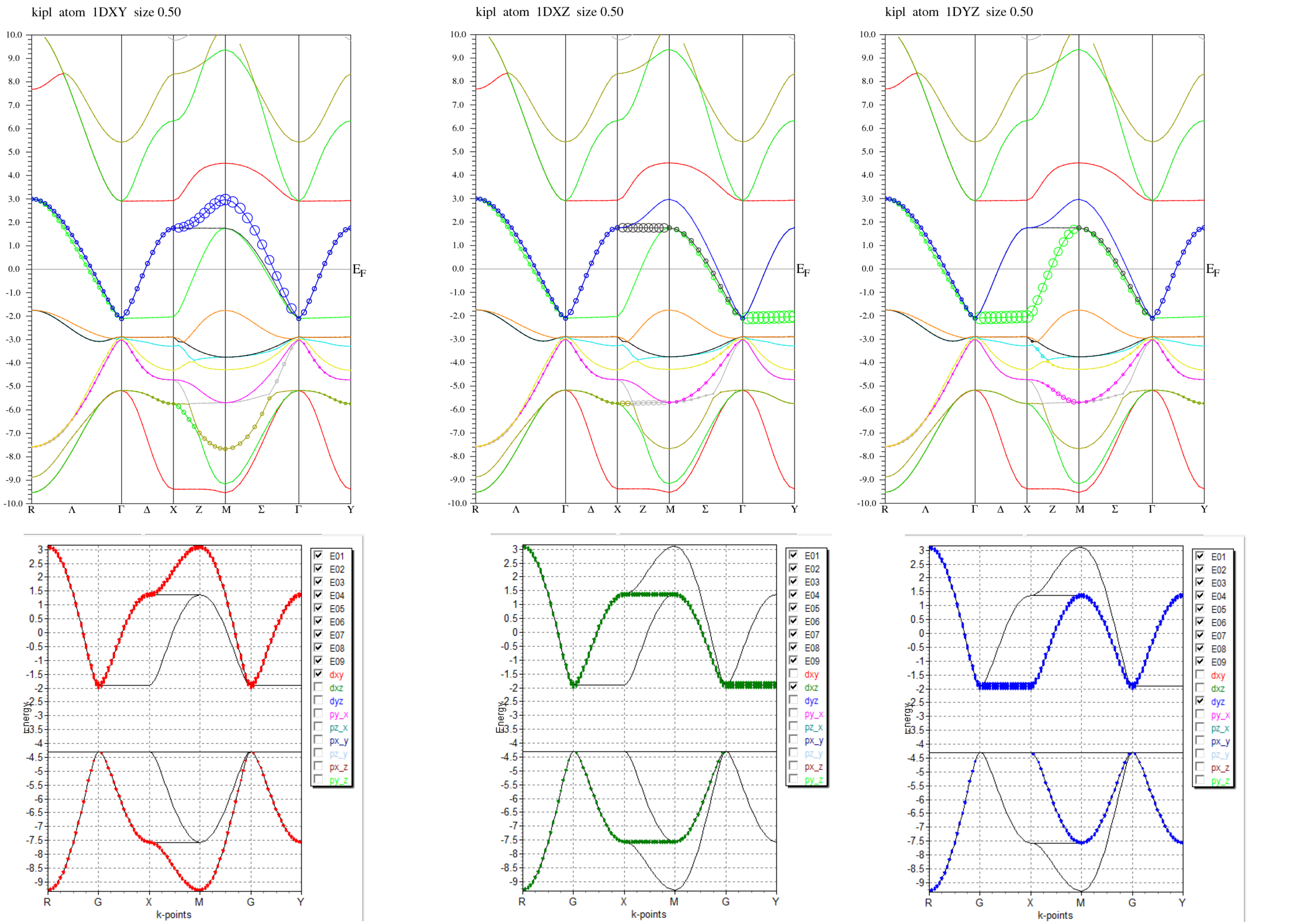
d_{xz} – $p_x(z)$, $p_z(x)$

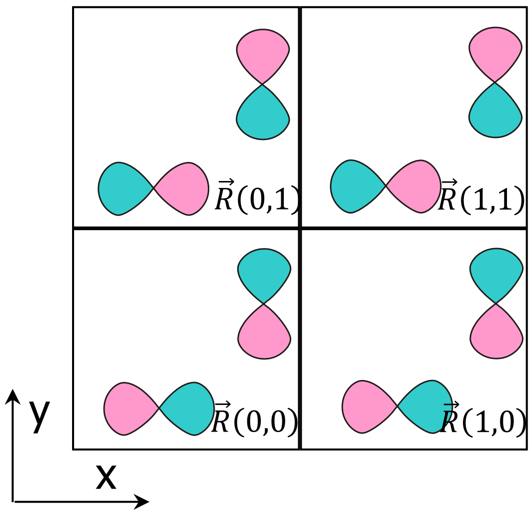
d_{yz} – $p_y(z)$, $p_z(y)$



Pásová struktura ReO_3 – srovnání DFT a TB (t2g_p_ReO3.tba)

DFT



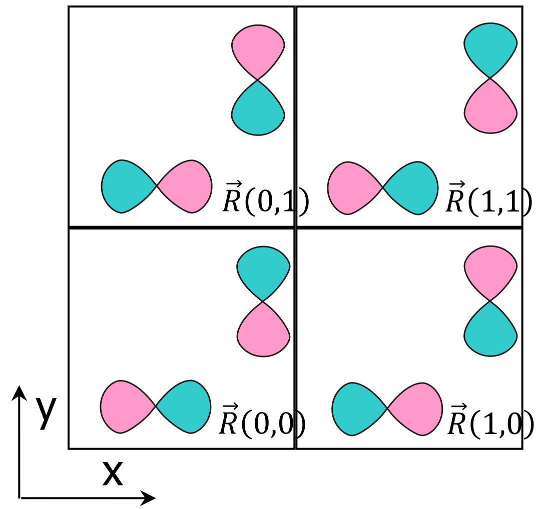


Y

$k_x = 0$

$k_y = \pi/a$

-1	-1
1	1

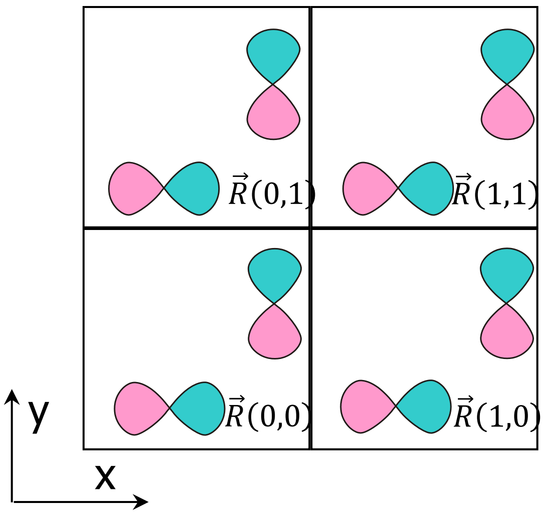


M

$k_x = \pi/a$

$k_y = \pi/a$

-1	1
1	-1

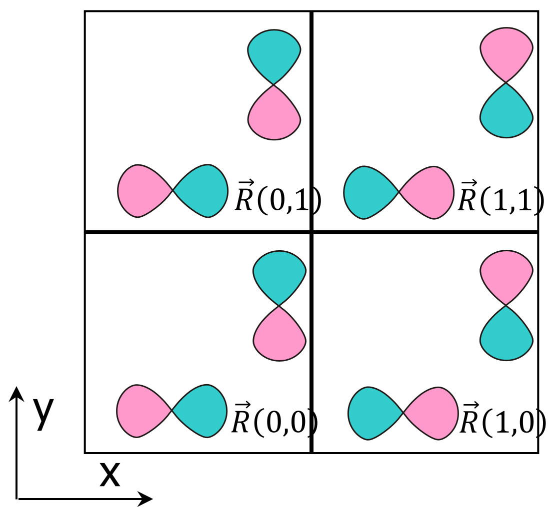


Γ

$k_x = 0$

$k_y = 0$

1	1
1	1



X

$k_x = \pi/a$

$k_y = 0$

1	-1
1	-1