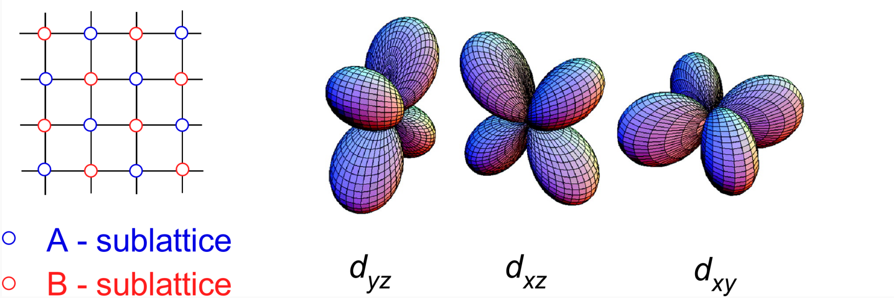
Example from current research in our group

Tight binding model of $Ca_{1.8}Sr_{0.2}RuO_4$

May 24, 2017

d-orbitals on two sublattices



Tight binding for two sublattices and d-orbitals

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$\hat{h}(\mathbf{k}) =$

$$\begin{pmatrix} -\mu & i\lambda + \epsilon^{\mathrm{off}}_{\mathbf{k}} & -\lambda & \epsilon^{\mathrm{yz}}_{\mathbf{k}} & 0 & 0 \\ -i\lambda + \epsilon^{\mathrm{off}}_{\mathbf{k}} & -\mu & i\lambda & 0 & \epsilon^{\mathrm{xz}}_{\mathbf{k}} & 0 \\ -\lambda & -i\lambda & -\mu + \epsilon^{\mathrm{xy}'}_{\mathbf{k}} & 0 & 0 & \epsilon^{\mathrm{xy}}_{\mathbf{k}} \\ \epsilon^{\mathrm{yz}}_{\mathbf{k}} & 0 & 0 & -\mu & i\lambda + \epsilon^{\mathrm{off}}_{\mathbf{k}} & -\lambda \\ 0 & \epsilon^{\mathrm{xz}}_{\mathbf{k}} & 0 & -i\lambda + \epsilon^{\mathrm{off}}_{\mathbf{k}} & -\mu & i\lambda \\ 0 & 0 & \epsilon^{\mathrm{xy}}_{\mathbf{k}} & -\lambda & -i\lambda & -\mu + \epsilon^{\mathrm{xy}'}_{\mathbf{k}} \end{pmatrix}$$

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$$\epsilon^{\mathrm{yz}}_{\mathbf{k}} = -2t_2 \cos\left(\frac{k_{\mathrm{x}} + k_{\mathrm{y}}}{2} a\right) - 2t_1 \cos\left(\frac{k_{\mathrm{x}} - k_{\mathrm{y}}}{2} a\right) \tag{2}$$

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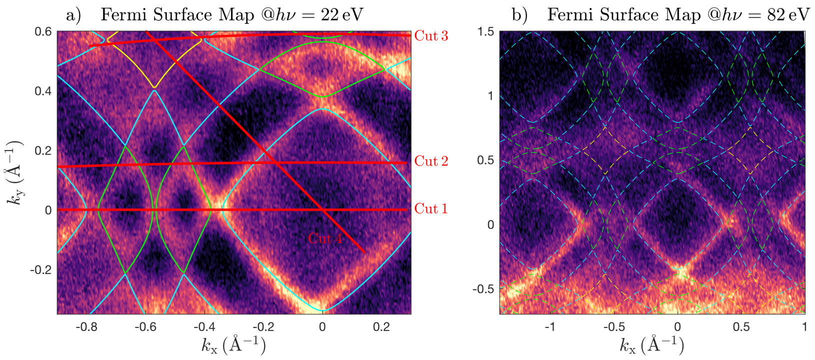
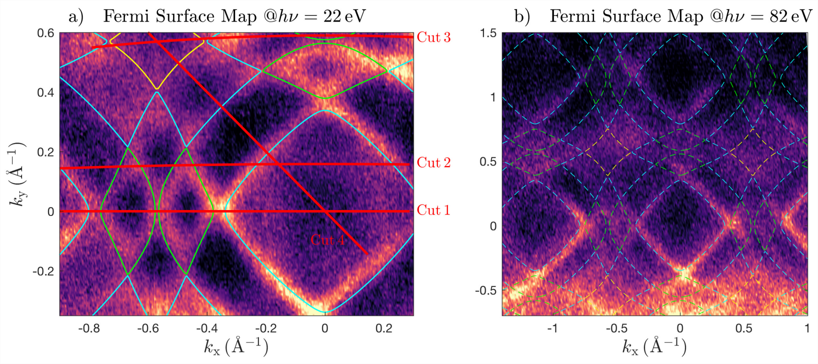
$$\epsilon^{\mathrm{xy}}_{\mathbf{k}} = -2t_3 \left[\cos\left(\frac{k_{\mathrm{x}} + k_{\mathrm{y}}}{2} a\right) + \cos\left(\frac{k_{\mathrm{x}} - k_{\mathrm{y}}}{2} a\right)\right] \tag{4}$$

$$\epsilon^{\mathrm{xy}\prime}_{\mathbf{k}} = -2t_4 \left[\cos(k_{\mathrm{x}} a) + \cos(k_{\mathrm{y}} a)\right] - 2t_5 \left[\cos((k_{\mathrm{x}} + k_{\mathrm{y}})a) + \cos((k_{\mathrm{x}} - k_{\mathrm{y}})a)\right] \tag{5}$$

$$\epsilon^{\mathrm{off}}_{\mathbf{k}} = -2t_6 \left[\cos(k_{\mathrm{x}} a) \cos(k_{\mathrm{y}} a)\right] \tag{6}$$


a) Fermi Surface Map @$h\nu = 22\,\mathrm{eV}$
b) Fermi Surface Map @$h\nu = 82\,\mathrm{eV}$
Cut 1
Cut 2
Cut 3
Cut 4
$k_y\ (\mathrm{\AA}^{-1})$
$k_x\ (\mathrm{\AA}^{-1})$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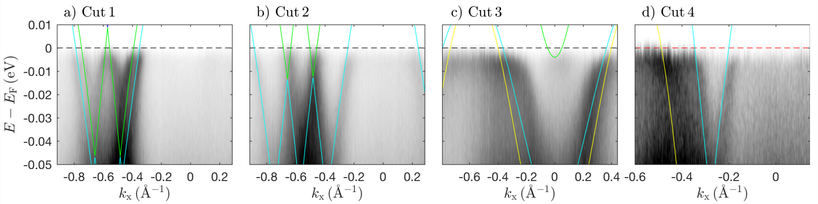
a) Cut 1
b) Cut 2
c) Cut 3
d) Cut 4
$E - E_F$ (eV)
k_x (Å^{-1})