Topological Phases Driven By Orbital Entanglement In Transition Metal Oxide Perovskite Interfaces

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Acknowledgments:
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cnrs dépasser les frontières

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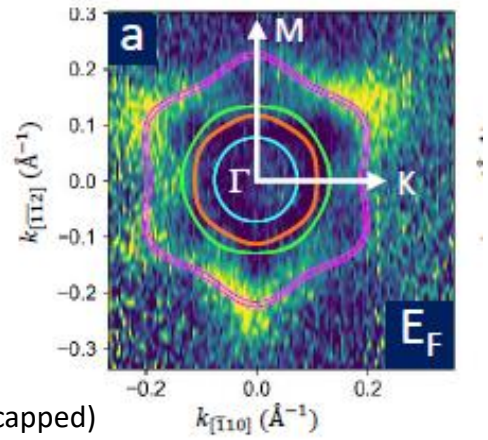
université Paris-Saclay | Faculté des Sciences d'Orsay

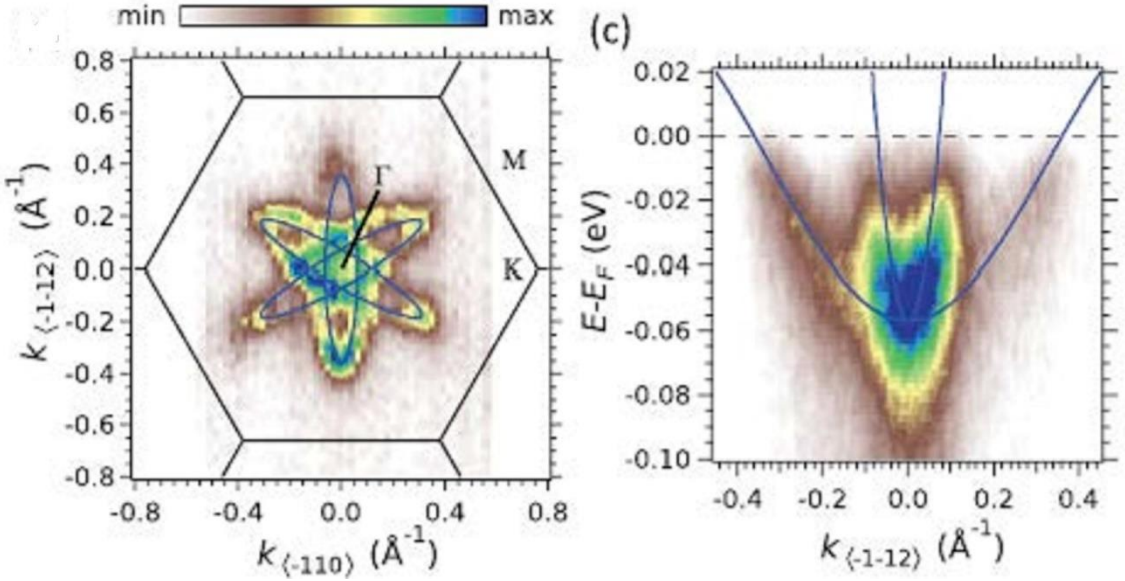
111-oriented surfaces or interfaces of transition metal oxide perovskites ABO_3

- Pure ABO_3 is insulating. Doping $\rightarrow$ metallic state where carriers hop from B to B via O ; B (Ti,Ta..) , A (Ba, Sr, Ca, K,..)
- Generic band spectrum derived from t_{2g} orbitals.
- Experimental spectrum is well captured by a tight-binding modeling (+ Poisson Schroedinger)
- **111-orientation gives rise to geometric contributions which promote orbital- and spin- tronic transport and lead to a non standard superconducting regime**



KTO 111 (Eu capped)

S. Mallik et al APL Mater. 11, 121108 (2023)

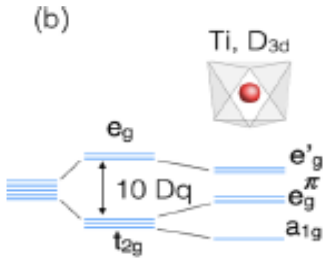


STO 111 (cleaved)

T.C Rödel et al. PR Applied Lett. 1, 051002 (2014)

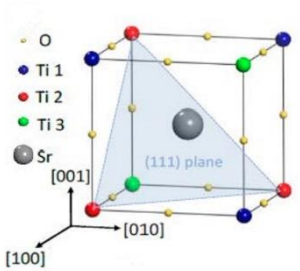
→ Modeling the electronic structure of 111-oriented 2DEG

- Trigonal crystal field



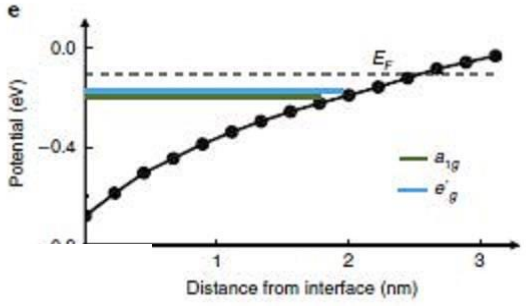
$3d = 10meV$ (LAO/STO)

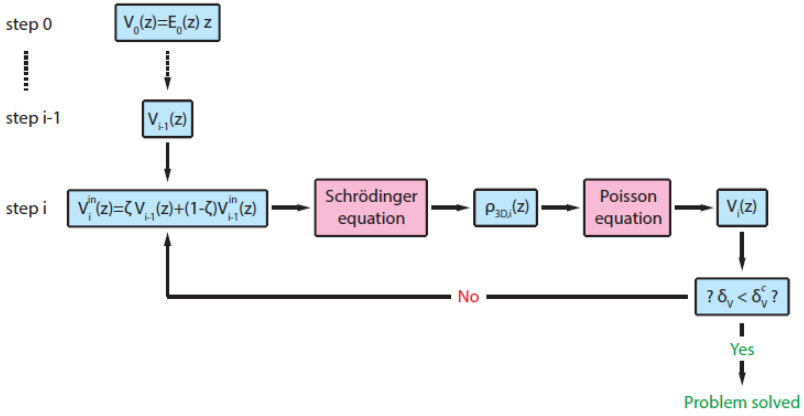
Salluzzo et al. Phys Rev B 98 115 143 (2018)



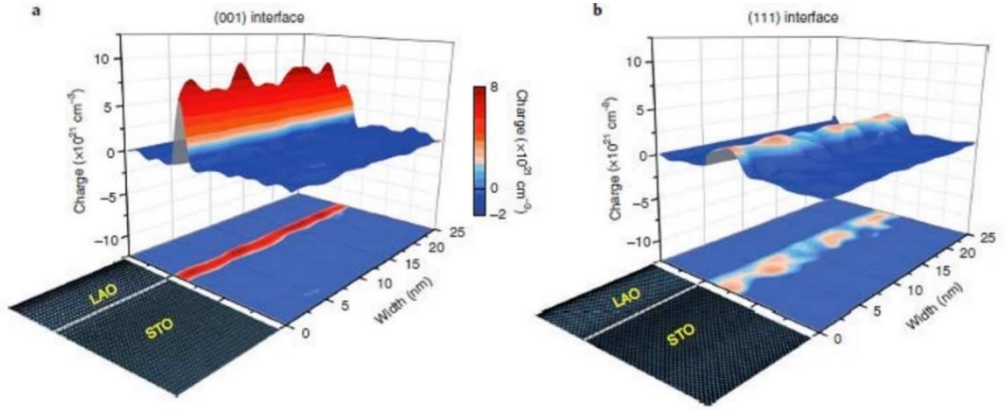
- Confinement near surface/interface (same for all orbitals) V~100meV

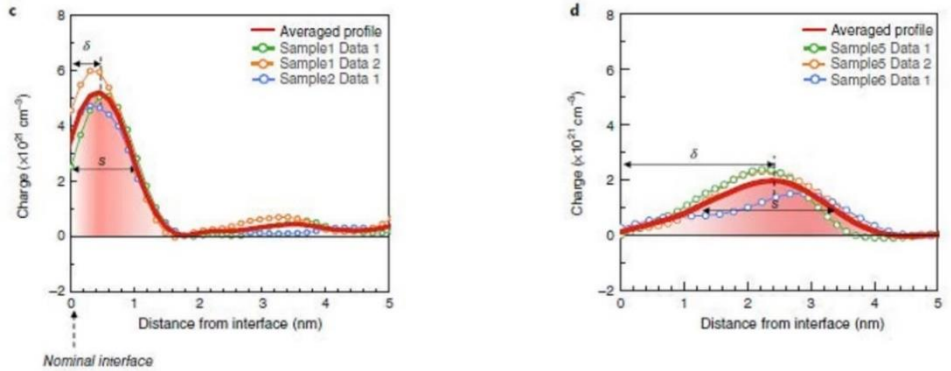
K. Song et al. Nat. Nanotechnology 13, 198 (2018)





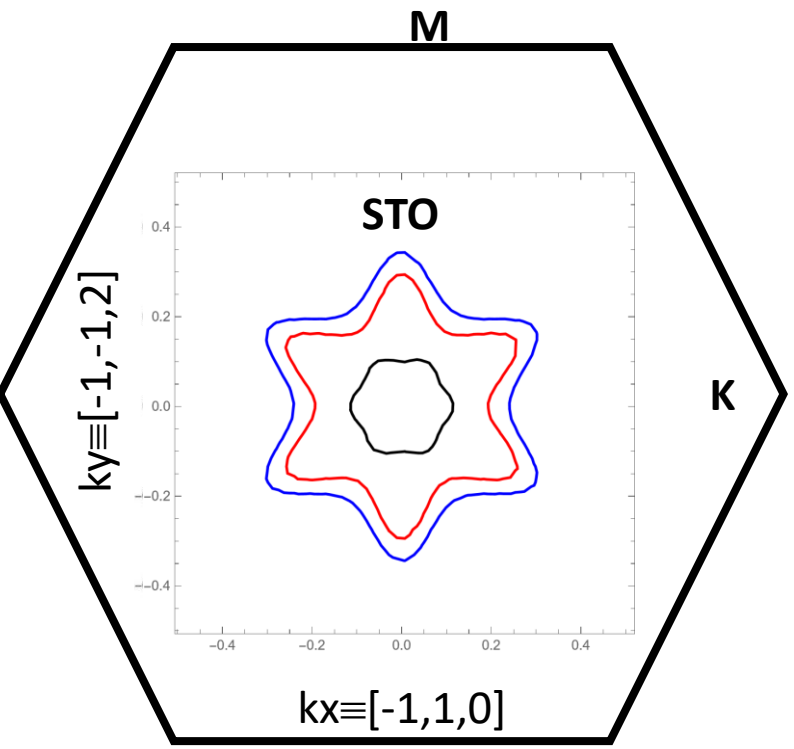
+ Hubbard U

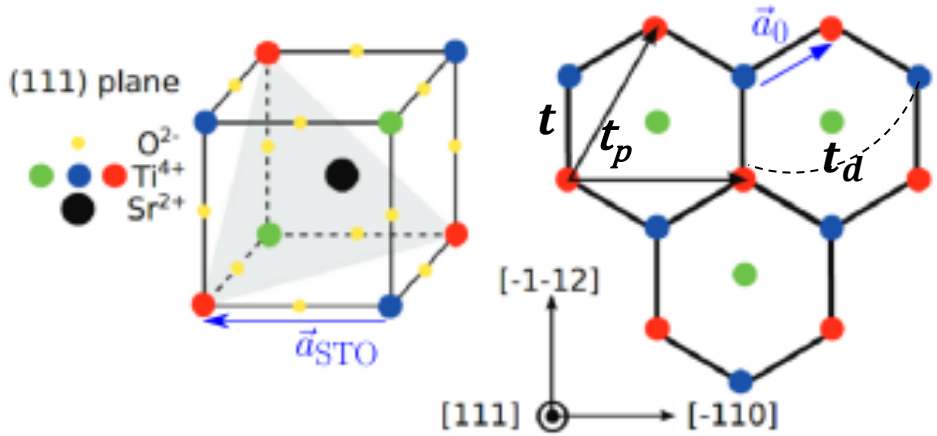


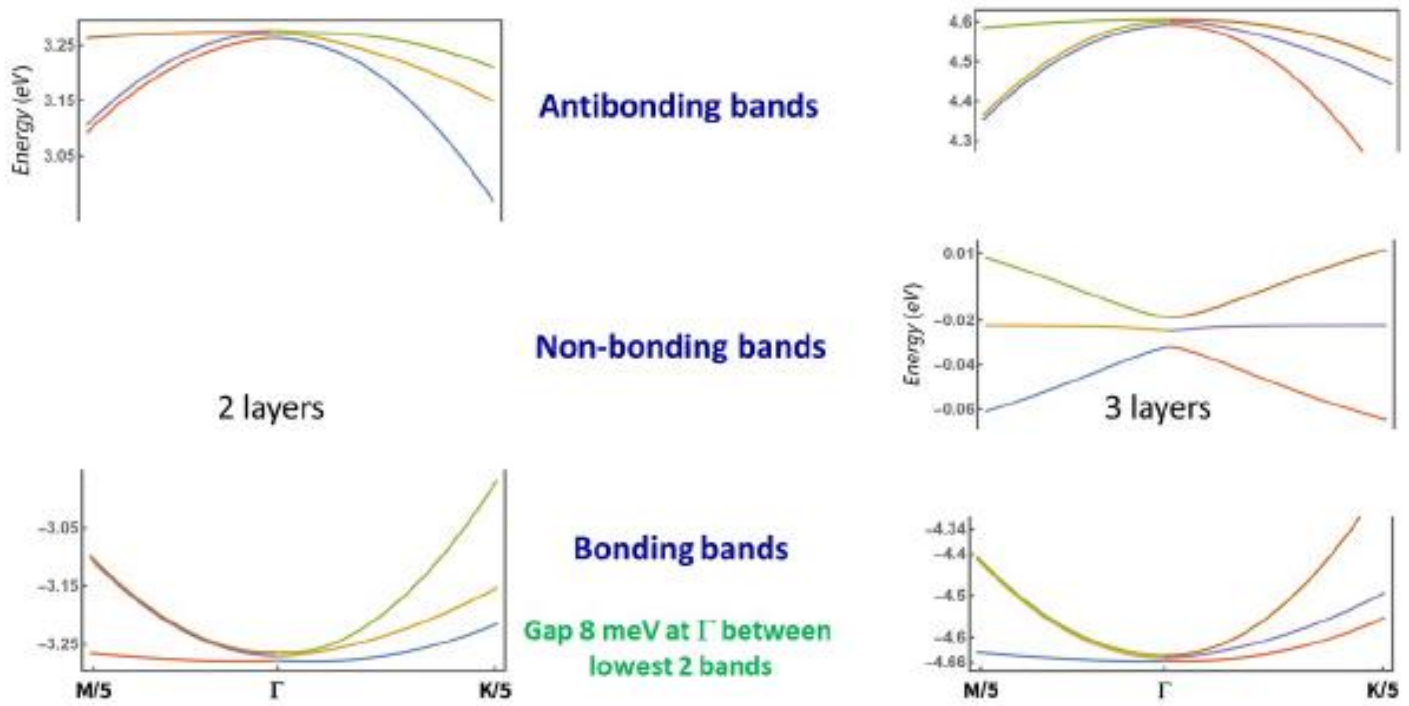


- 2D Kinetic energy (nearest neighbor hops are between layers)

Hopping amplitudes t=1.6 eV , t_d =70meV (STO)
t=1.8 eV , t_d =100meV, t_p=140meV (KTO)







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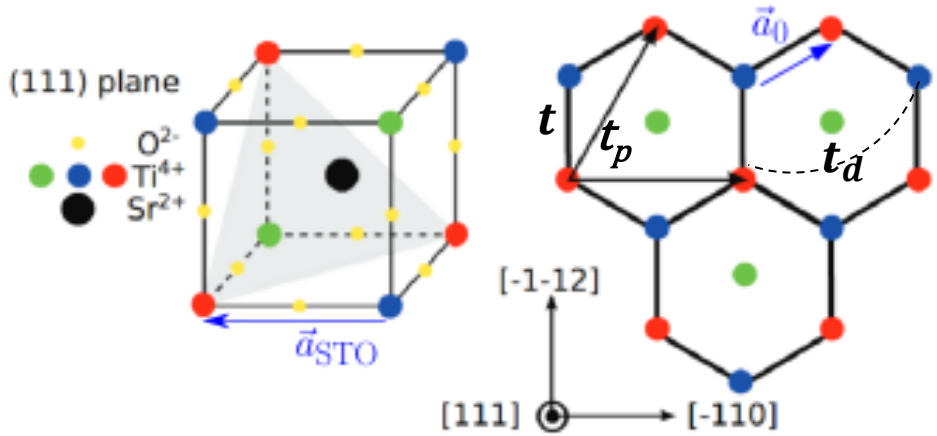
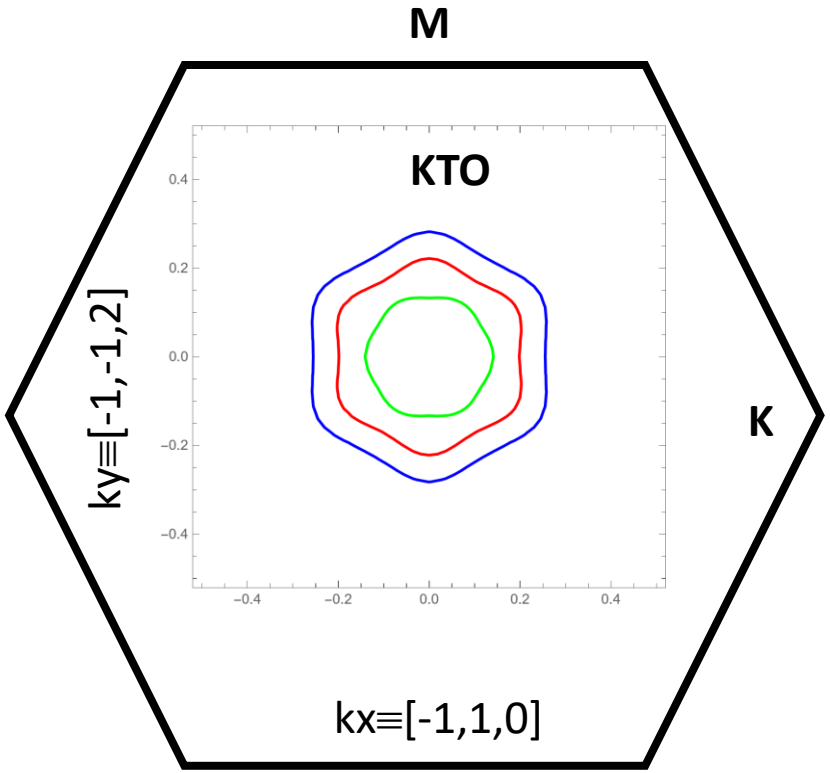
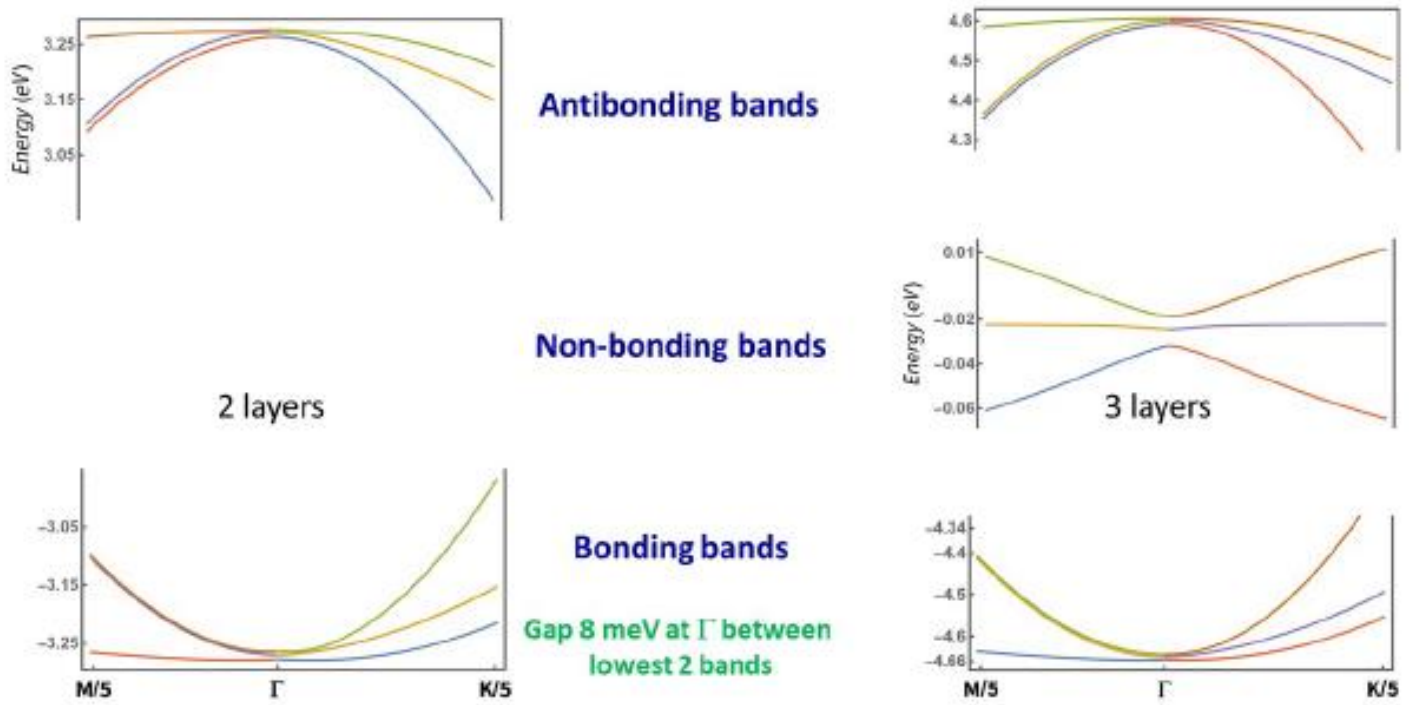




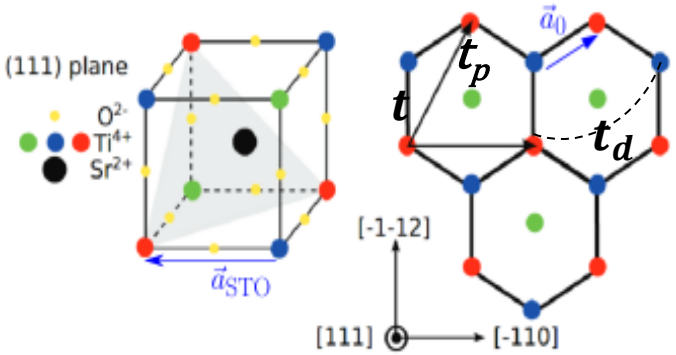


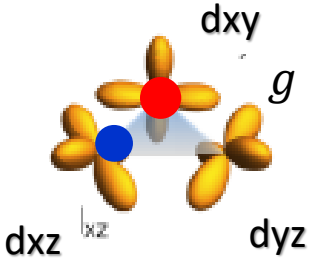
- Atomic spin-orbit

$E_{SO} \sim 25\ meV$ (STO), $E_{SO} \sim 400\ meV$ (KTO)

- Orbital mixing (at the surface/interface, bond distorsions → the orbital character can change after a hop)

Symmetries : rotation about (111) diagonal of cube and mirror plane [1,1,1]-[-1,-1,2] →





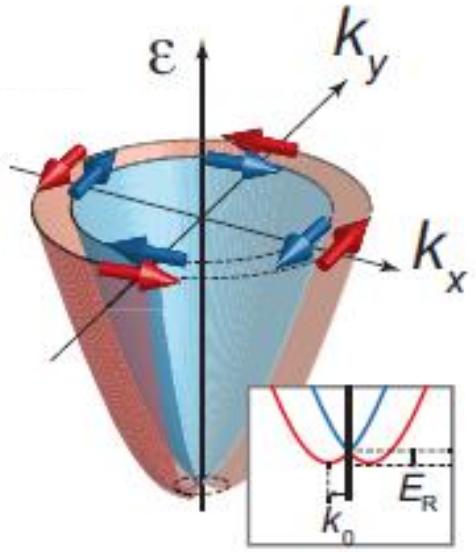
$g = 25 - 40\ meV$

$$H_{OM} = \boldsymbol{d}.\boldsymbol{L}$$

L=1 angular momentum operator in the t_{2g} Hilbert space (Gell-Mann matrices)

$$g\left(\sin(\frac{\sqrt{3}}{2}k_x a_0 - \frac{3}{2}k_y a_0), \sin(\frac{\sqrt{3}}{2}k_x a_0 + \frac{3}{2}k_y a_0), -\sin(\sqrt{3}\,k_x a_0)\right)$$

In the low energy (small k) limit, $H_{OM} = (\boldsymbol{g}\,\boldsymbol{a_0})\boldsymbol{L}.(\boldsymbol{k} \times \boldsymbol{u_z})$ Orbital Rashba Hamiltonian; cf spin Rashba $\sim \alpha_R \boldsymbol{\sigma}.(\boldsymbol{k} \times \boldsymbol{u_z})$



Y. A. Bychkov and E. I. Rashba, *JETP Lett.* **39,** 78–81 (1984)

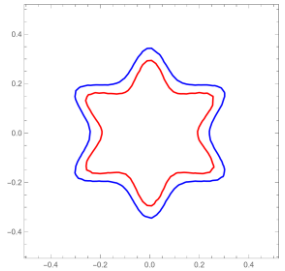
- Rotational symmetry breaking about (111) axis at low T (STO)

  E. Lesne et al. Nat. Materials 22, 576 (2023) M.T Mercaldo et al. NPJ Quantum Materials 8, art #12 (2023)

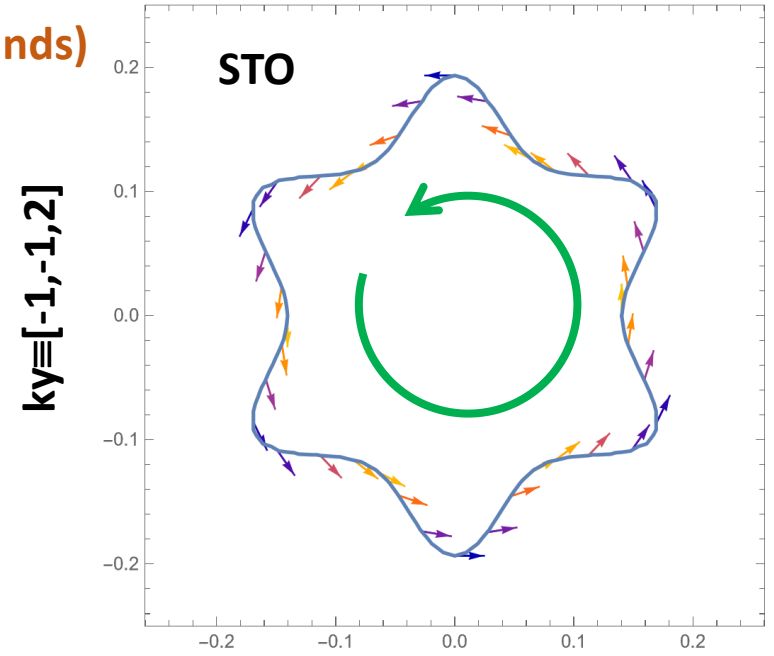
→ **Orbital winding**

Berry contributions are driven by orbital textures : $E_{SO}=0$

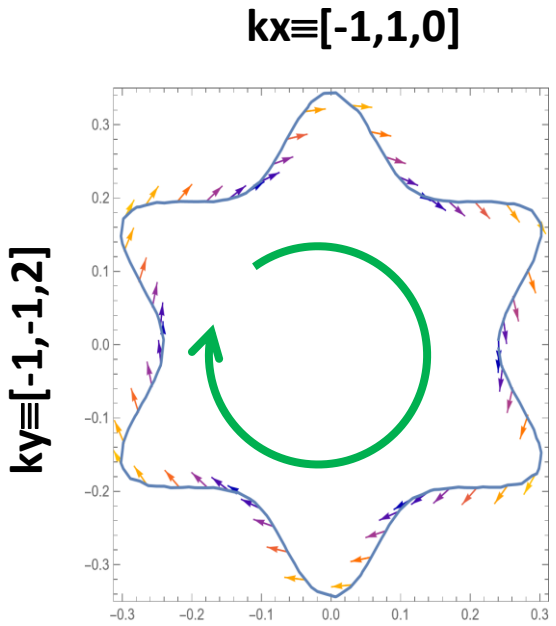
In-plane (Lx, Ly) textures (lowest 2 bands)

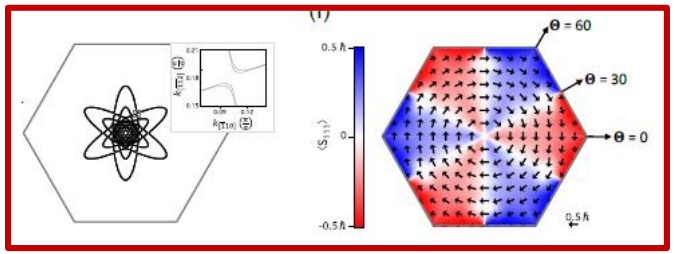


kx≡[-1,1,0]

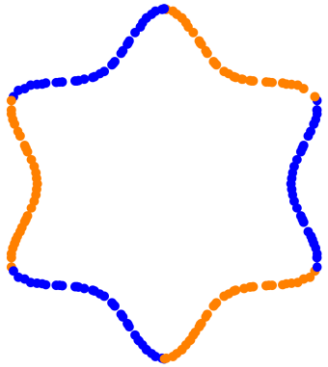


kx≡[-1,1,0]

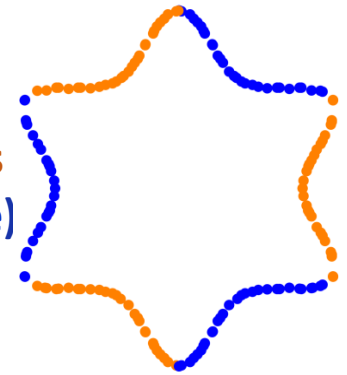




Arpes **STO111** Pan He et al.
Phys. Rev. Lett 2018



Out-of-plane (Lz)
textures lowest 2 bands
(sign only; blue=positive)



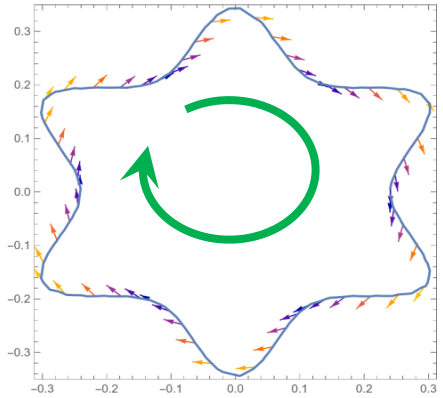
→ **Spin winding**

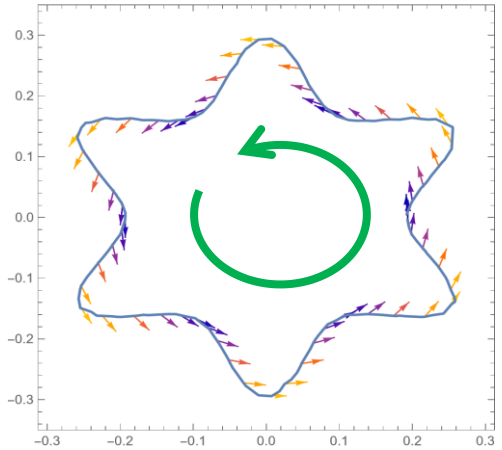
Spin effect : spin textures and additional BC contributions→ We "turn spin-orbit **on**" ($E_{SO} \neq 0$)

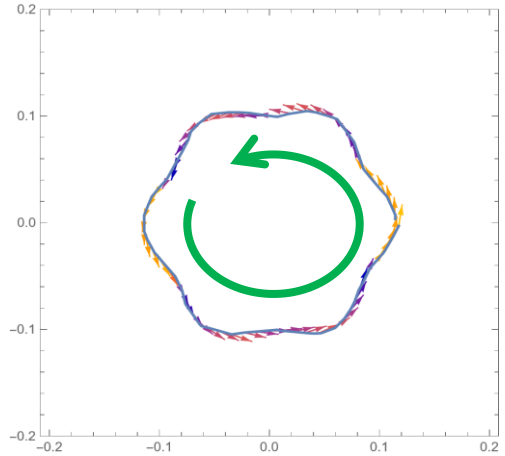
kx≡[-1,1,0]

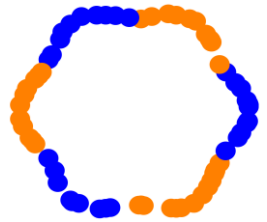
ky≡[-1,-1,2]

In-plane (Sx, Sy) textures







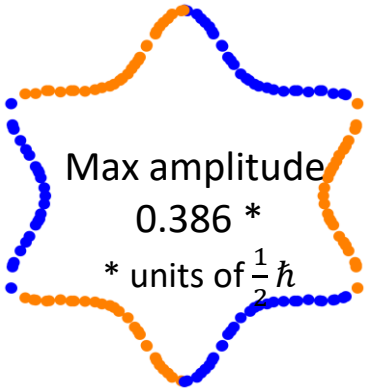


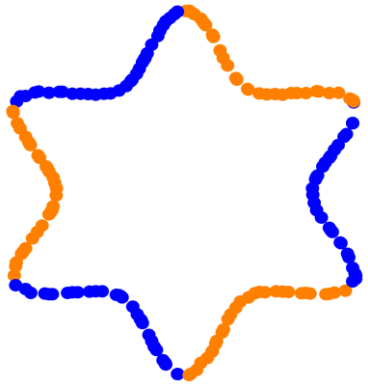
"Blue band"

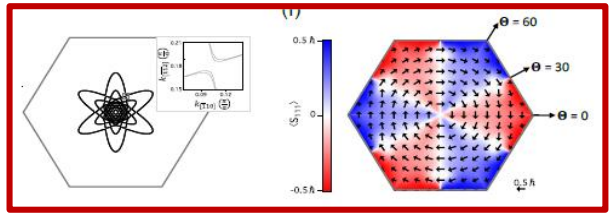
"Red band"

Third band

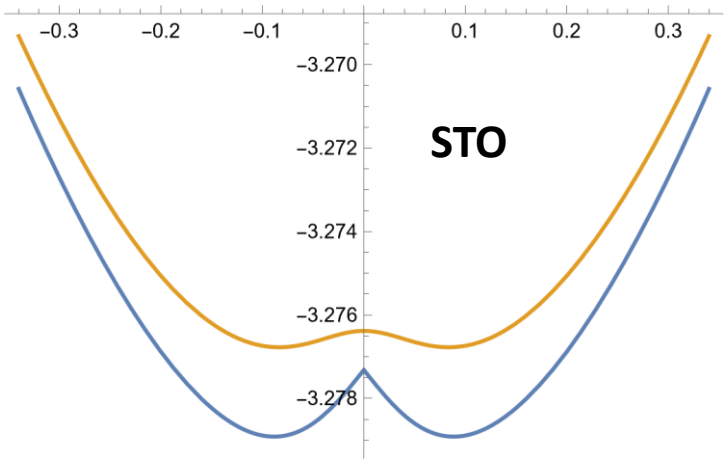
Out-of-plane (Sz) textures (sign only; blue=positive)







Arpes **STO111** Pan He et al.
Phys. Rev. Lett. 120, 266802 (2018)



$$k_R a_0 = \frac{t_R}{t} \rightarrow \Delta k_R a_0 = \frac{t_{RST}}{t}$$

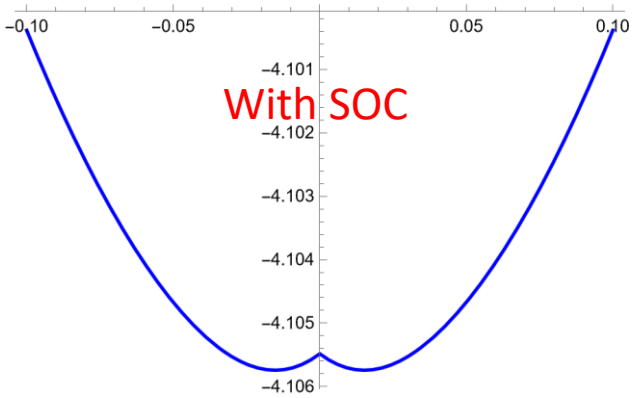
t_{RST} : spin texture part of t_R

$$t_{RST} = 4.8\, meV$$

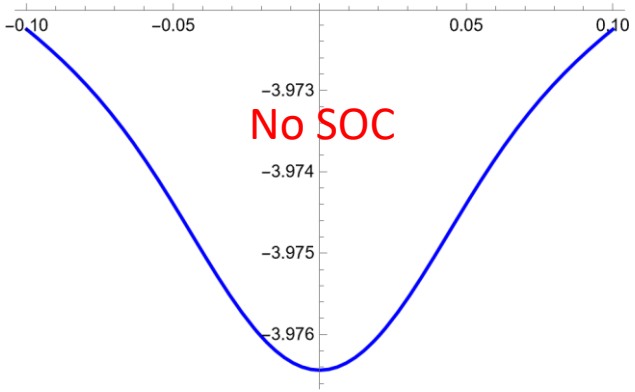
Dispersion along the (-1,-1,2) direction

- with orbital mixing and spin-orbit (blue)
- with orbital mixing but no spin-orbit (orange)

At Γ we get an estimate of the effective spin-orbit energy. β_{SO}~ 1meV



KTO



At Γ we get an estimate of the effective spin-orbit energy. β_{SO}~ 129meV

$$k_R a_0 = \frac{t_R}{t} \rightarrow \Delta k_R a_0 = \frac{t_{RST}}{t}$$

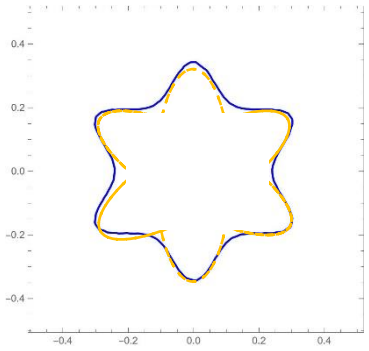
$$t_{RST} = 21\ meV$$

t_{RST} : spin texture part of t_R

→ Berry curvature (BC), Berry dipole (BCD)

Pure orbital contributions give rise to a BC near Γ → We "turn spin-orbit off" ($E_{SO} = 0$)

$$H_{TOT} = H_{KIN} + H_{TRIG} + H_{CONFIN} + H_{OM} \qquad \text{(6x6)}$$

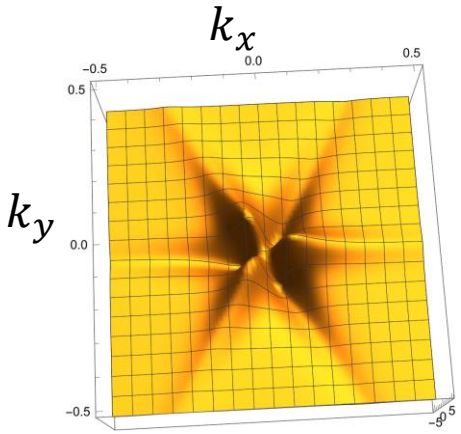


anisotropy of the band structure
+ mixing of bonding and antibonding components of the eigenfunctions (e.g <bonding|v|antibonding>).

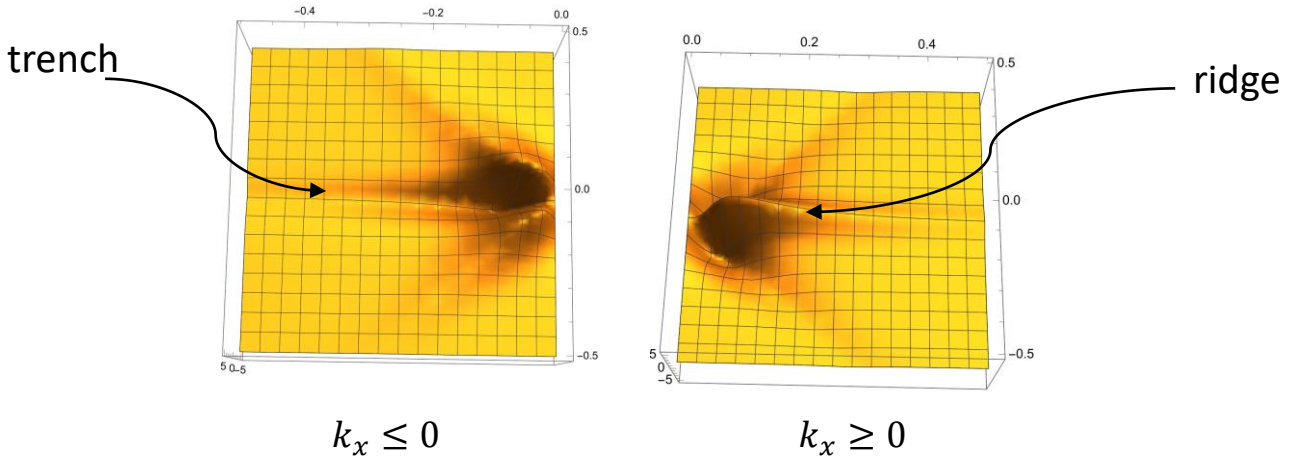
For L=1 one can generalize the expression found for 2-band case (A. Graf and F. Piechon Phys. Rev. B 104, 085114 (2021)). But for all practical purposes it is easier to use the generic form

$$\Omega_{\alpha}^{z} = -2\, Im \sum_{\beta \neq \alpha} \left[\frac{< u_{k\alpha} | \frac{\partial H_{TOT}}{\partial kx} | u_{k\beta} >< u_{k\beta} | \frac{\partial H_{TOT}}{\partial ky} | u_{k\alpha} >}{(E_{\alpha} - E_{\beta})^2} \right]$$

$|u_{k\lambda}>$ (E_{λ}) eigen-vectors (values) of H_{TOT}



$\Omega^z(k_x, k_y)$



$k_x \leq 0$ $\quad$ $k_x \geq 0$

Shows that the Berry curvature is even in ky and odd in kx → Berry curvature dipole

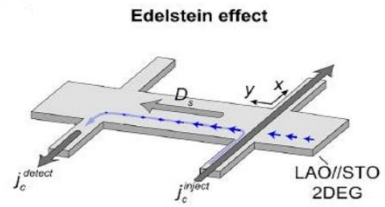
$$D_x = \frac{1}{(2\pi)^2}\int d_2k\,\frac{\partial\Omega^z}{\partial k_x} f_0$$ $\quad$ f_0 Fermi factor;

$D_x = 0.02$ (0.06) a_0 for STO (KTO) . When filling such that higher levels (8meV higher) get populated, $D_x \nearrow 80$ then drops

- Non linear second harmonic Hall current → $\boldsymbol{j}_{2\omega} = \frac{1}{\hbar^2}\frac{e^3\tau}{2(1+i\omega\tau)}\hat{z}\times\boldsymbol{\mathcal{E}}(\boldsymbol{D}.\boldsymbol{\mathcal{E}})$ $\quad$ ($\boldsymbol{\mathcal{E}}//\hat{x}$)

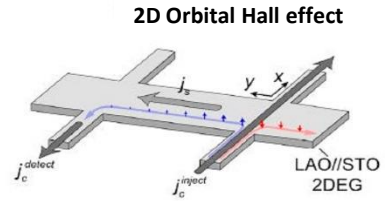
Sodemann, Fu PRL 115 , 216806 (2015), Lesne et al. (2023)

- Orbital Edelstein effect → orbital moment accumulation (Kerr)



- Orbital Berry Hall current transverse to current flow → $\sigma_{xy} \sim \sum_\alpha \iint \frac{d2k}{(4\pi^2)} f_{0\alpha}\omega_{xy}^{\alpha z}$

$$\omega_{xy}^{\alpha z} = -2\,Im\sum_{\beta\neq\alpha}\left[\frac{<u_{k\alpha}|\mathcal{J}_{xz}|u_{k\beta}><u_{k\beta}|\frac{\partial H_{TOT}}{\partial ky}|u_{k\alpha}>}{(E_\alpha - E_\beta)^2}\right]$$ where $\mathcal{J}_{xz} = \left\{\frac{\partial H_{TOT}}{\partial kx}, L_z\right\}$



→ Quantum geometry and superconductivity

The quantum geometric tensor characterizes the k-space metric of the Hamiltonian eigenstates n.

$$Q^n_{\alpha\beta} = \left[< \frac{\partial n}{\partial k_\alpha} | (1 - |n><n|) | \frac{\partial n}{\partial k_\beta} > \right] = g^n_{\alpha\beta} - \frac{i}{2}\Omega^n_{\alpha\beta}$$

$g^n_{\alpha\beta}$ is a real symmetric tensor ("distance" between quantum states in k-space) (*)

$\Omega^n_{\alpha\beta}$ is an antisymmetric tensor (Berry curvature in k-space)

* See Sala et al. arXiv:2407.06659

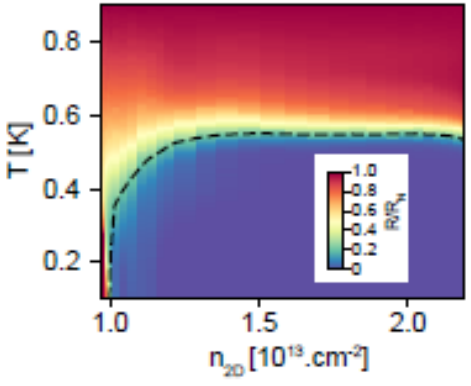
$\boldsymbol{j}(\boldsymbol{q},\omega) = \boldsymbol{K}(\boldsymbol{q},\omega)\mathbf{A}(\boldsymbol{q},\omega)$; the superfluid weight $D \propto K(\boldsymbol{q} \to \mathbf{0}, \omega = 0)$

The superfluid weight $D = \frac{\hbar^2}{\mu_0 e^2}\frac{1}{\Lambda_{2D}}$ Λ_{2D} is the Pearl length. D∝ superfluid density/m*

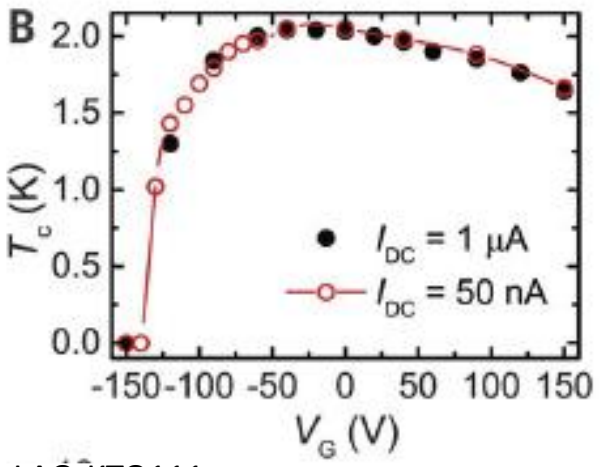
In 2D, for an isotropic case, $T_{BKT} = \frac{\pi}{8k_B}\mathrm{D}(T_{BKT})$

$D = D_{conv} + D_{geom} \to \propto \iint d_2\, k\, f(k) g^n_{\alpha\beta}(k)$

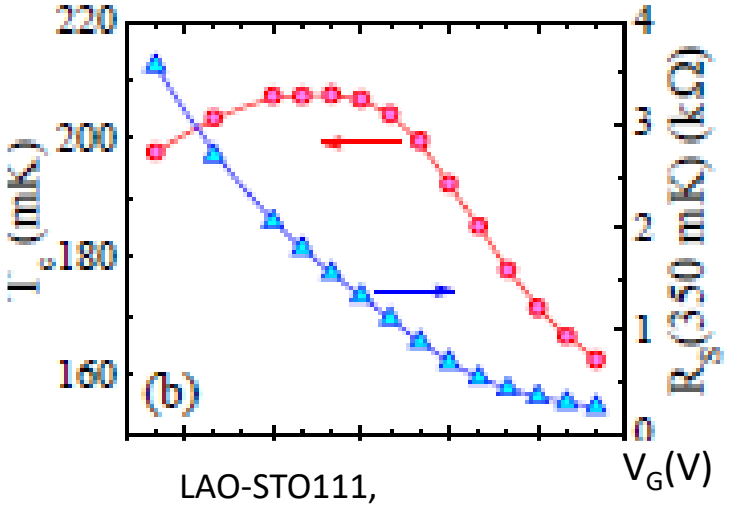
See e.g Bernevig et al. *Nat. Rev. Phys.*, 528–542 (2022)



Superfluid density KTO111,
Mallik et al. Nat. Comm. 13, 4625 (2022)



LAO-KTO111,
Chen et al. Science 372, 721 (2021)



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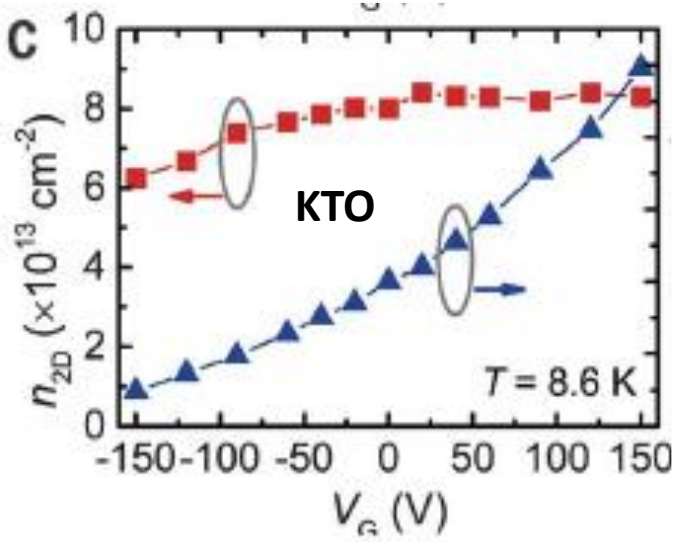

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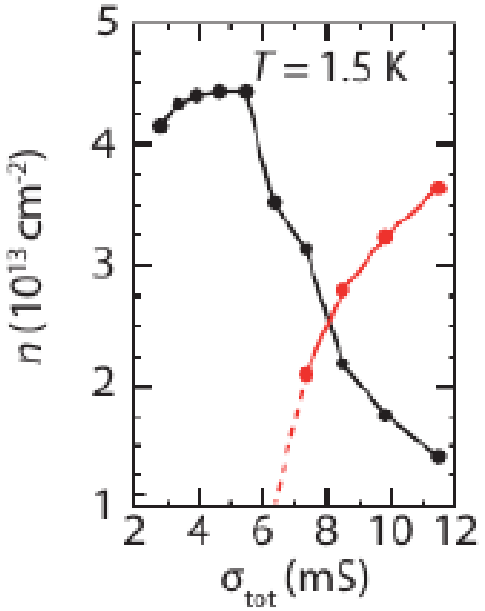

LAO/STO

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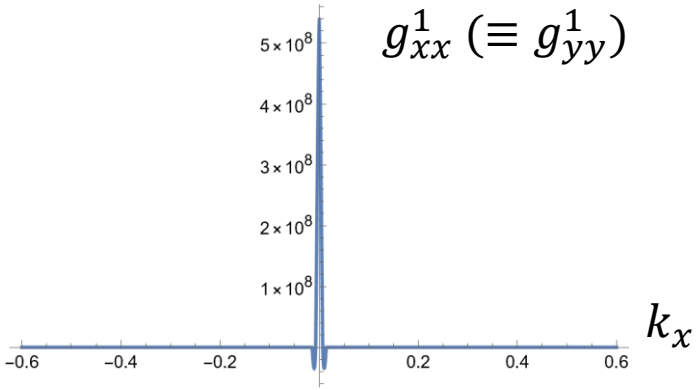
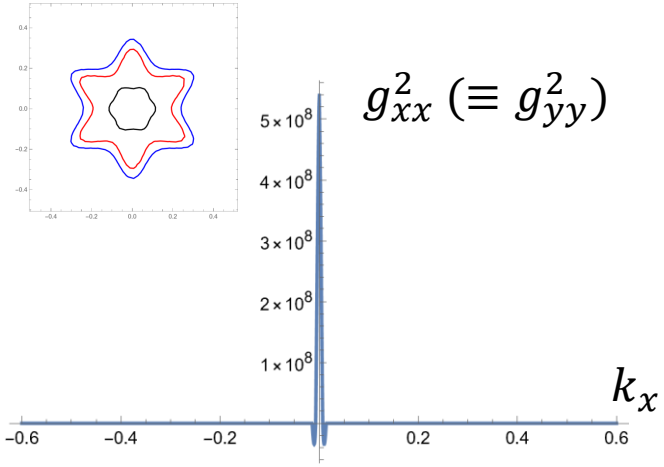
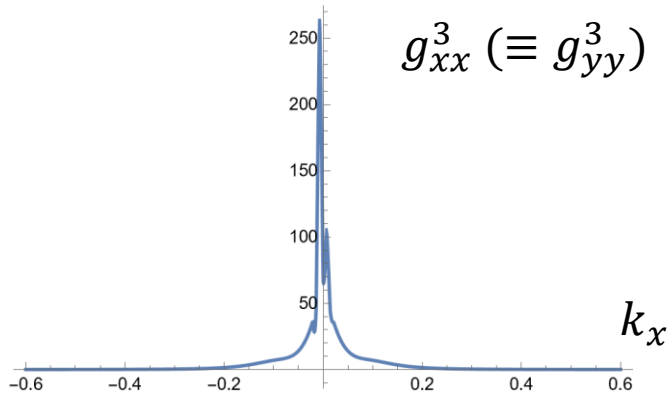
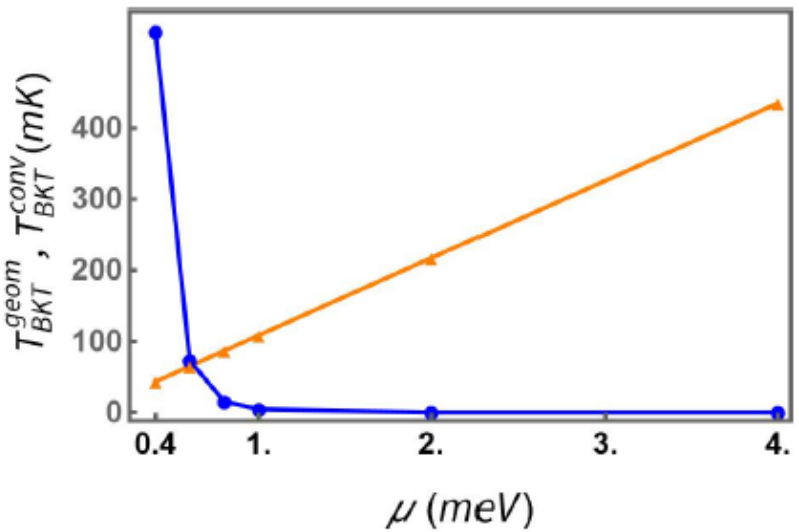
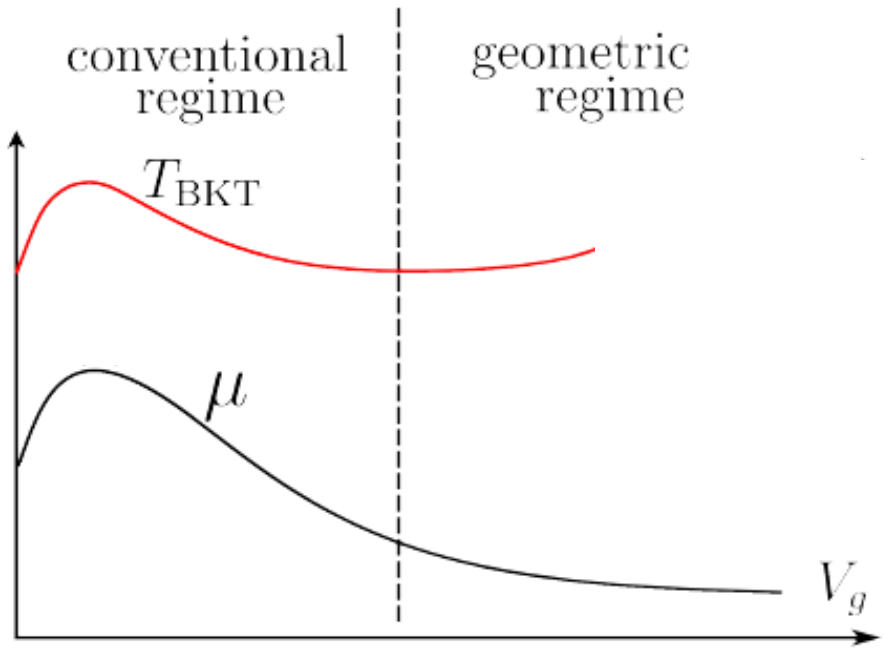








F. Simon et al. arXiv:2307.13993



→ Symmetry of the superconducting gap

The prominent role played by the effective interfacial spin-orbit interaction (mediated by the orbital-mixing, OM) allows for the possibility of spin-triplet superconductivity.

$$H(k) = \sum(\varepsilon(k) - \mu) c^{\dagger}_{k\sigma}\, c_{k\sigma} + \frac{1}{2}\sum \Delta_{\sigma\sigma'}(k) c^{\dagger}_{k\sigma} c^{\dagger}_{-k\sigma'} + \frac{1}{2}\sum \Delta^{*}_{\sigma'\sigma} c_{-k\sigma'} c_{k\sigma} + \alpha \sum \boldsymbol{g}(k) \cdot \boldsymbol{\sigma}_{\sigma\sigma'} c^{\dagger}_{k\sigma}\, c_{k\sigma'}$$

$\varepsilon(k)$ dispersion of the energy bands of the tight-binding Hamiltonian *without* the "Rashba-spin" contribution due to the OM term.

α **g**(k) fits the tight-binding energy bands *with* OM.

$$\Delta(k) = \underbrace{i\Delta_S \sigma_y}_{\text{s-wave}} + \underbrace{i\boldsymbol{d}(k) \cdot \boldsymbol{\sigma}}_{\text{p-wave}} \sigma_y$$

Large interfacial SOI $\rightarrow \boldsymbol{d}(k) = \Delta_T \boldsymbol{g}(k)$

Gap equation near Tc $\rightarrow$ $[1 - V_s A(T_c)][1 - V_P A(T_c)] = V_S\, V_P B^2(T_c)$ $\qquad B \ll A$

V_s , V_P attractive potentials for s- , p- wave pairing respectively

→ Topological superconductivity

$$H(k) = \sum(\varepsilon(k) - \mu) c_{k\sigma}^{\dagger} c_{k\sigma} + \frac{1}{2}\sum \Delta_{\sigma\sigma'}(k) c_{k\sigma}^{\dagger} c_{-k\sigma'}^{\dagger} + \frac{1}{2}\sum \Delta_{\sigma'\sigma}^{*} c_{-k\sigma'} c_{k\sigma} + \alpha \sum \boldsymbol{g}(k) \cdot \boldsymbol{\sigma}_{\sigma\sigma'} c_{k\sigma}^{\dagger} c_{k\sigma'}$$

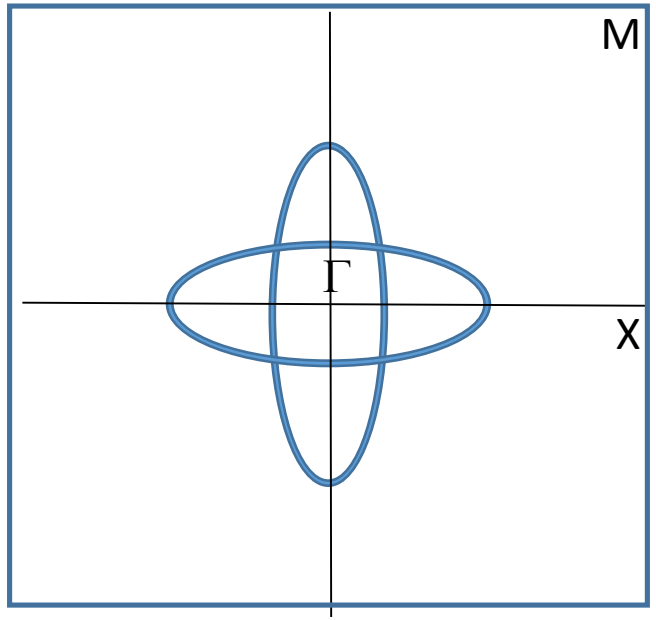
$$\Delta(k) = \underbrace{i\Delta_S \sigma_y}_{\text{s-wave}} + \underbrace{i\boldsymbol{d}(k) \cdot \boldsymbol{\sigma}}_{\text{p-wave}} \sigma_y$$

Large interfacial SOI $\rightarrow \boldsymbol{d}(k) = \Delta_T \boldsymbol{g}(k)$

$$E(k) = \pm\sqrt{(\varepsilon(k) - \mu)^2 + {\Delta_S}^2 + \boldsymbol{g}(k)^2\left(\alpha^2 + {\Delta_T}^2\right) \pm 2[(\varepsilon(k) - \mu)\alpha + \Delta_S \Delta_T]\|\boldsymbol{g}(k)\|}$$

→ Gap closing and topological regime if $\left(\Delta_T \boldsymbol{g}(k)\right)^2 = (\Delta_S)^2$; $(\varepsilon(k) - \mu)^2 = \alpha^2 \boldsymbol{g}(k)^2$

BUT!! even when d_3=0, we may get a Berry curvature due to the band anisotropy



$$H = \begin{pmatrix} ak_x{}^2 + bk_y{}^2 & -i\alpha_R k_- \\ i\alpha_R k_+ & bk_x{}^2 + ak_y{}^2 \end{pmatrix}$$

$$\varepsilon_0 = \frac{1}{2}(a+b)(k_x{}^2 + k_y{}^2) \qquad \Delta' = \frac{1}{2}(a-b)(k_x{}^2 - k_y{}^2) \rightarrow$$

$$H = \varepsilon_0(\boldsymbol{k})\boldsymbol{\sigma_0} + \begin{pmatrix} +\Delta' & -i\alpha_R k_- \\ i\alpha_R k_+ & -\Delta' \end{pmatrix} \quad \mathbf{d.\sigma}$$

$$\Omega^z \mp \frac{1}{2}\hat{\boldsymbol{d}}.(\partial_{kx}\hat{\boldsymbol{d}} \times \partial_{ky}\hat{\boldsymbol{d}})$$

$$\Omega^z = \mp\frac{1}{2}\alpha_R^2 \frac{\Delta'(\boldsymbol{k})}{(\Delta'^2 + \alpha_R^2 k^2)^{3/2}}$$

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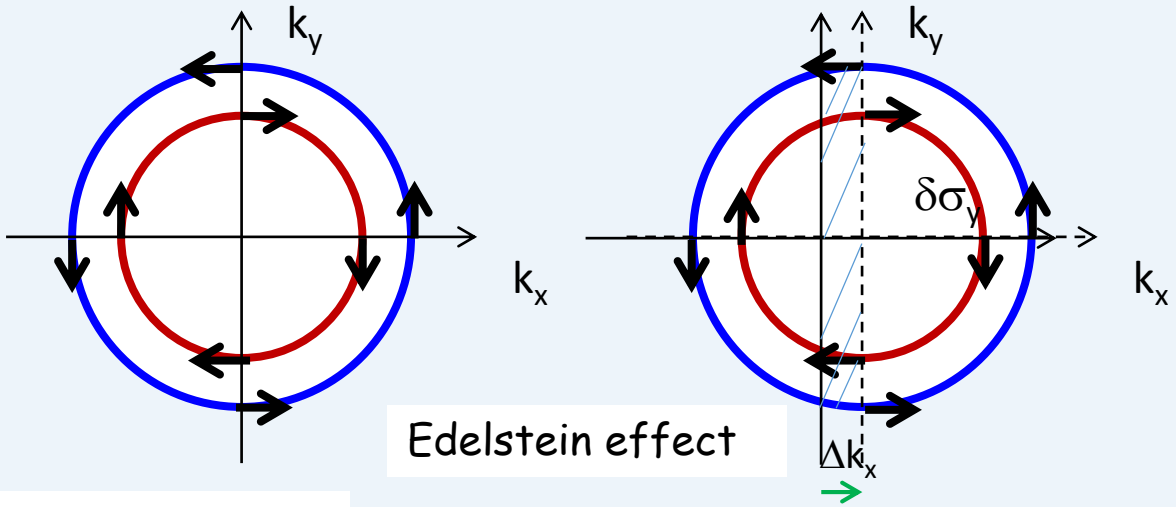
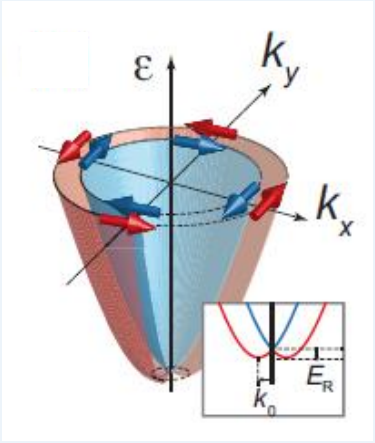


Edelstein effect

$\kappa \equiv$ conversion efficiency of EE (*spin or orbital*)

$$\kappa(\mu) = \frac{e\tau_0}{2\pi h}\sum_{\nu}\int_0^{2\pi} d\varphi k_F(\varphi) < S >_{\nu}^{T}(\varphi)$$

$$\kappa(\mu) = \frac{e\tau_0}{2\pi\hbar}\sum_{\nu}\iint_{BZ} d_2k f_{\nu k}(\mu)\left(\vec{\nabla}_k \times \langle\vec{S}\rangle_{\nu}\right)\cdot\vec{z}$$



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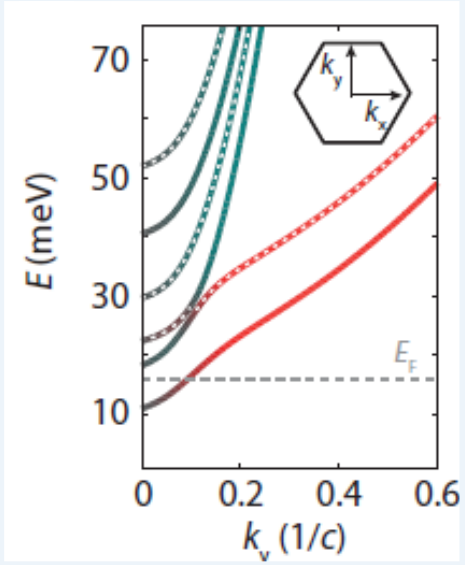
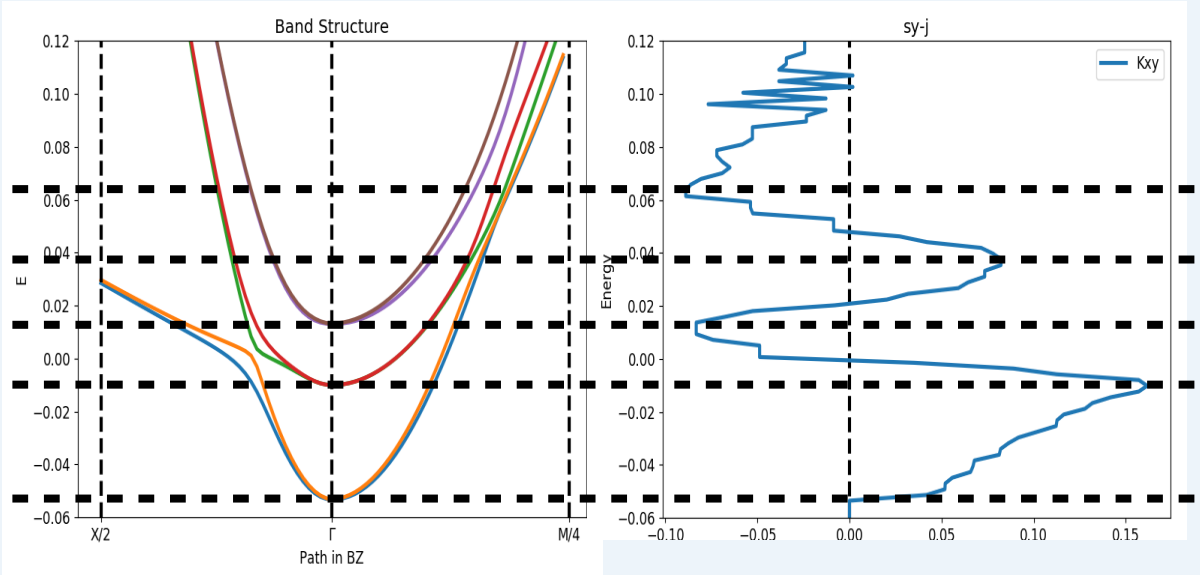


LAO/STO (111)



LAO/STO (001)

Edelstein coefficient

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