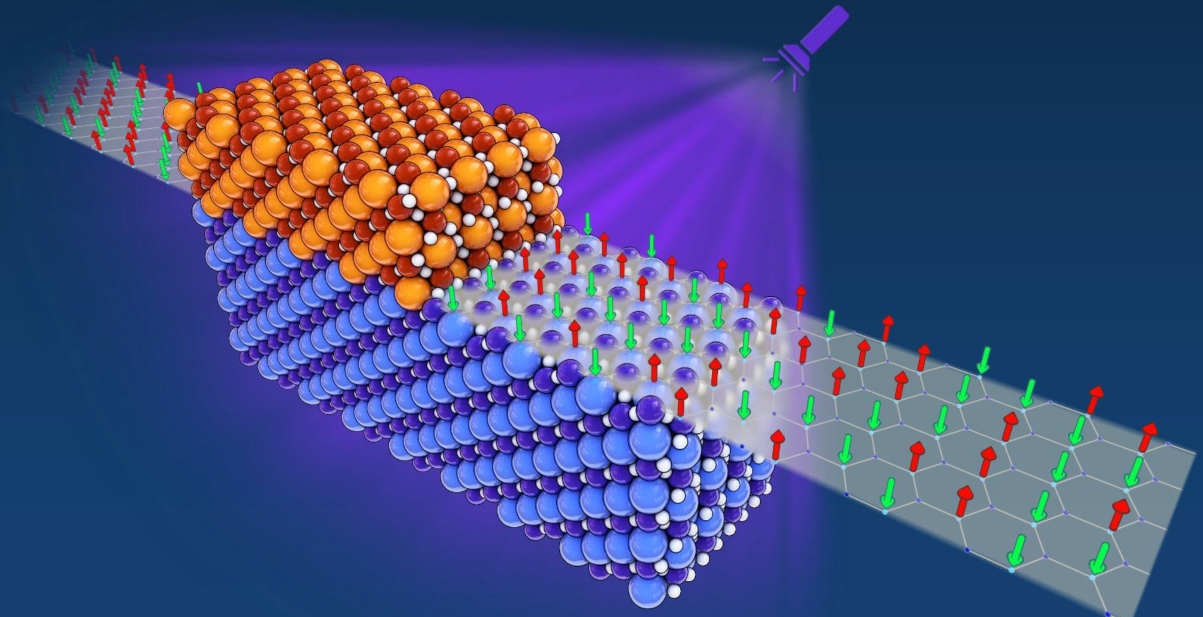
Berry phase engineering at oxide interfaces

Caviglia Lab

Department of Quantum Matter Physics

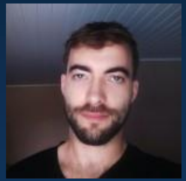
University of Geneva



Collaborators and funding

Thierry van Thiel, Yildiz Saglam, Edouard Lesne,
Ulderico Filippozzi, Patrick Blah, Graham Kimbell



Carmine Autieri,
Wojciech Brzezicki, **Mario Cuoco**
CNR Spin

Nicolas Gauquelin, J. Verbeeck
University of Antwerp

Marc Gabay
Uni Paris Sud

Raffaele Battilomo, **Carmine Ortix**
Uni Utrecht
Uni Salerno

European Research Council
Established by the European Commission

GORDON AND BETTY MOORE FOUNDATION

UNIVERSITÉ DE GENÈVE

Anomalous velocity and Berry phase

$$\gamma_n = \int_C \boldsymbol{A}_n(\boldsymbol{k}) \cdot d\boldsymbol{k}$$

$$\gamma_n = \oiint_\Omega \boldsymbol{B}_n(\boldsymbol{k}) \cdot d\boldsymbol{\Omega}$$

$$\boxed{\boldsymbol{A}_n(\boldsymbol{k}) = -i\langle u_n(\boldsymbol{k})|\nabla_{\boldsymbol{k}}|\, u_n(\boldsymbol{k})\rangle}$$

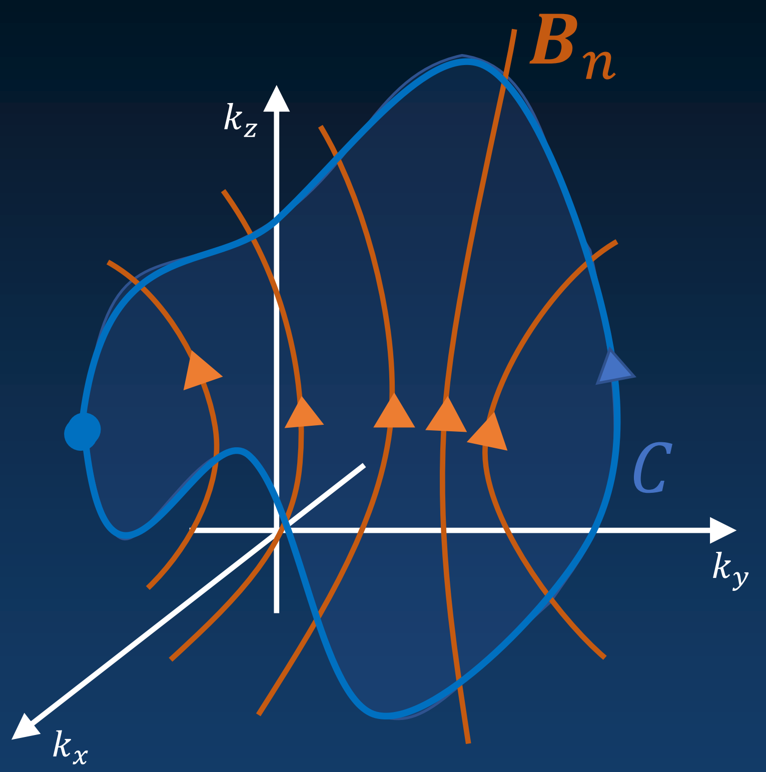
Berry Connection

$$\boxed{\boldsymbol{B}_n(\boldsymbol{k}) = \nabla_{\mathbf{k}} \times \boldsymbol{A}_n(\boldsymbol{k})}$$

Berry Curvature

Effective Vector Potential

Effective Magnetic Field



$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\epsilon_n(\boldsymbol{k}) - \frac{e}{\hbar}\, \boldsymbol{E} \times \boldsymbol{B}_n(\boldsymbol{k})$$

Karplus, Luttinger Phys. Rev. 95, 1154 (1954)
Berry Proc. R. Soc. London A 392, 45 (1984)
Chang, Niu PRL 75, 1348 (1995)

Sources of Berry curvature

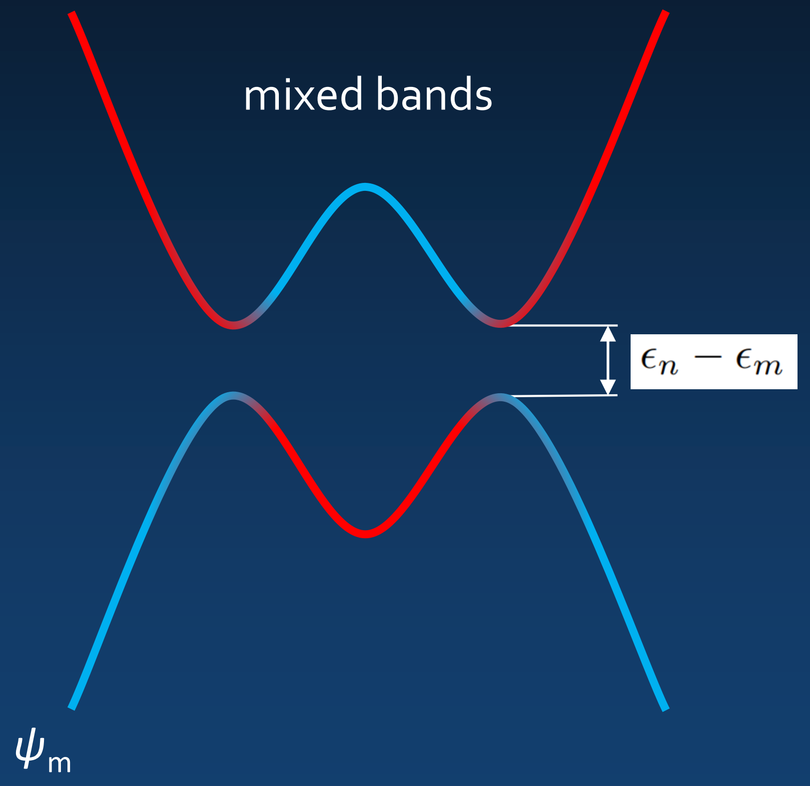
Zero for real wavefunctions

Zero for planar spin textures

$$\Omega_z^{\pm}(\mathbf{k}) = \pm\hat{\mathbf{d}}\cdot(\partial_{k_x}\hat{\mathbf{d}}\times\partial_{k_y}\hat{\mathbf{d}})/2$$

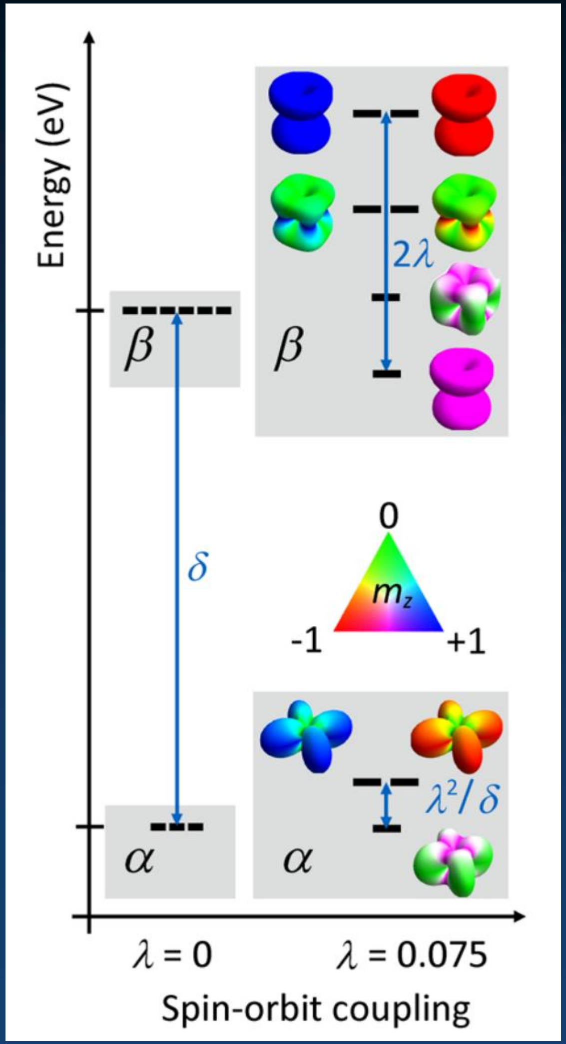
Large near avoided band crossings

$$\begin{aligned}\mathcal{B}_z &= \left[\langle\psi_m|\nabla\psi_n\rangle \times \langle\nabla\psi_n|\psi_m\rangle\right]_z \\ &= \frac{\left[\langle\psi_m|\nabla\hat{H}|\psi_n\rangle \times \langle\psi_n|\nabla\hat{H}|\psi_m\rangle\right]_z}{(\epsilon_m - \epsilon_n)^2}\end{aligned}$$



Band anticrossings

Ruthenates



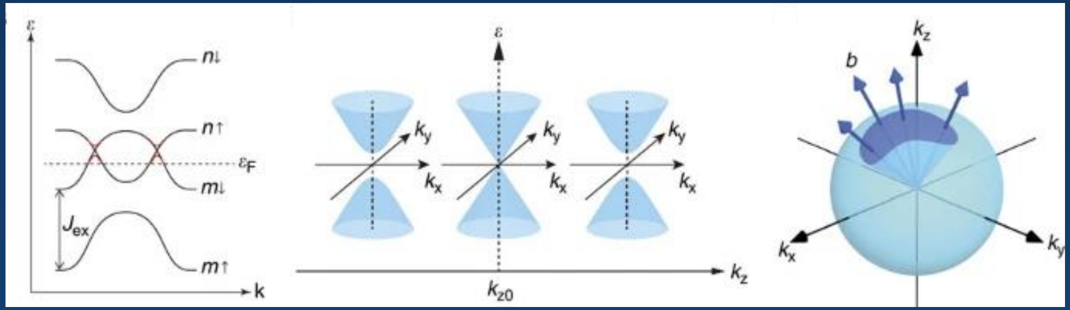
Das et al., Phys. Rev. X 8, 011048 (2018)

Ru^{4+} [Kr] 4d^4

Tetragonal crystal field splitting of t2g orbitals: δ.

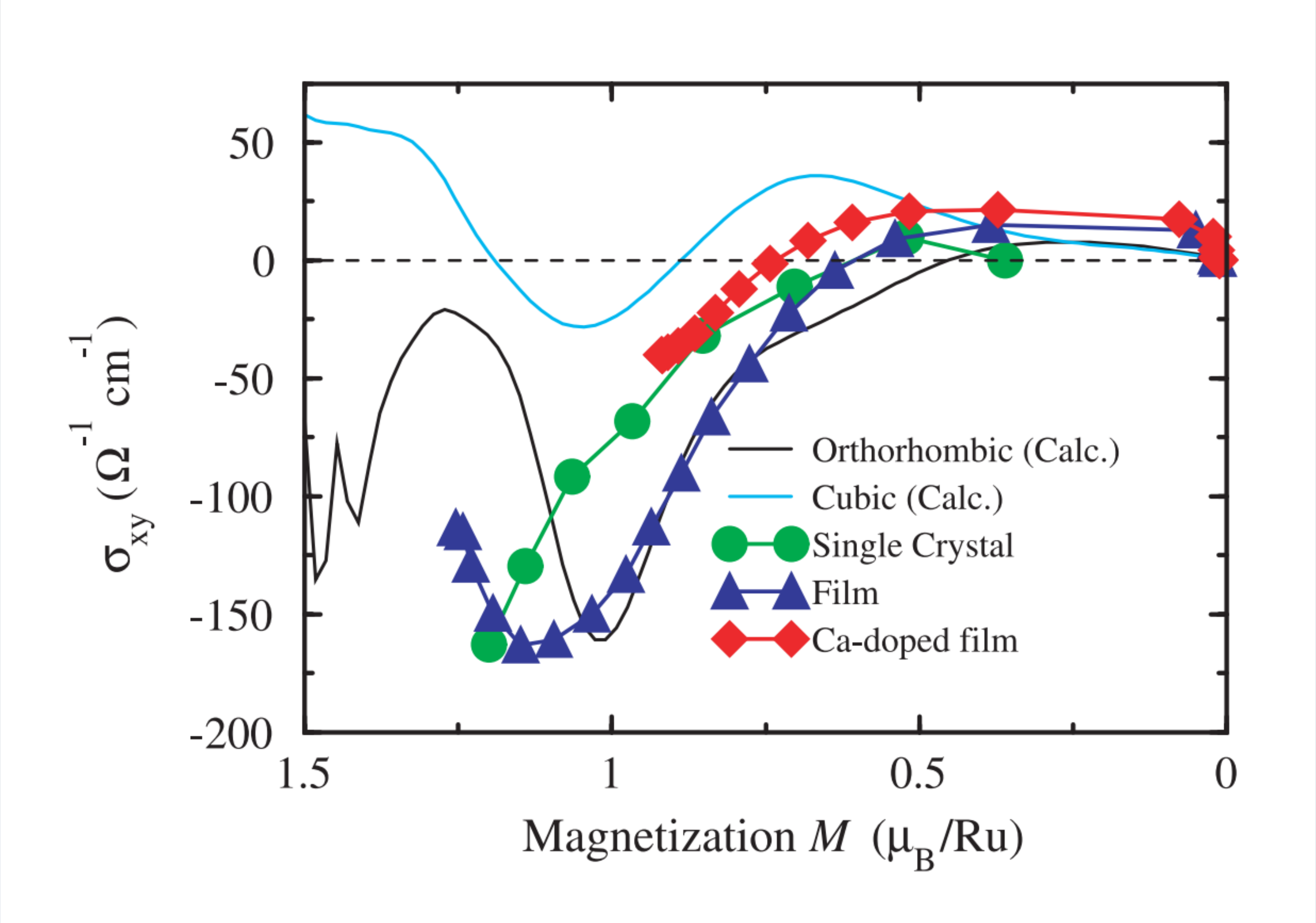
Spin-orbit driven mixing with inherent quantum phase.

Weyl points acting as sources of emergent magnetic fields, anomalous Hall conductivity, and unconventional spin dynamics.



Itoh et al., Nature Comm 7: 11788 (2016)

Ruthenates



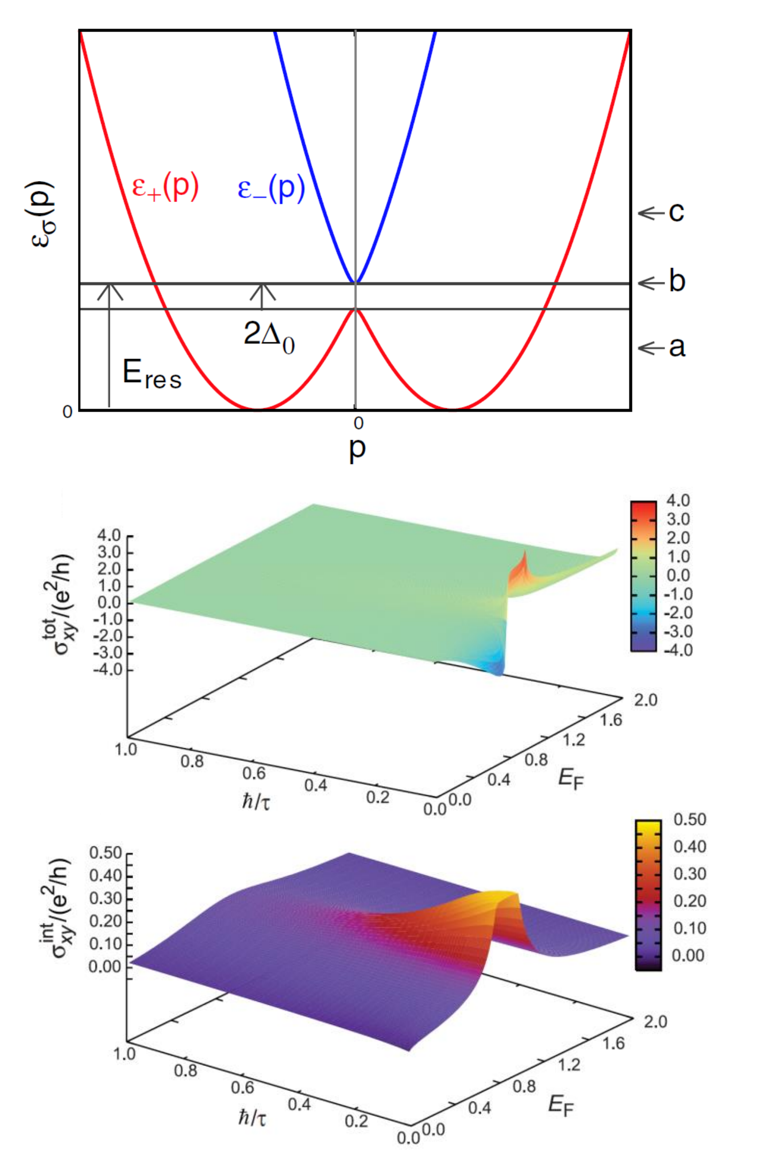
Fang et al. Science 302, 92 (2003)

Anomalous Hall effect from Berry phase

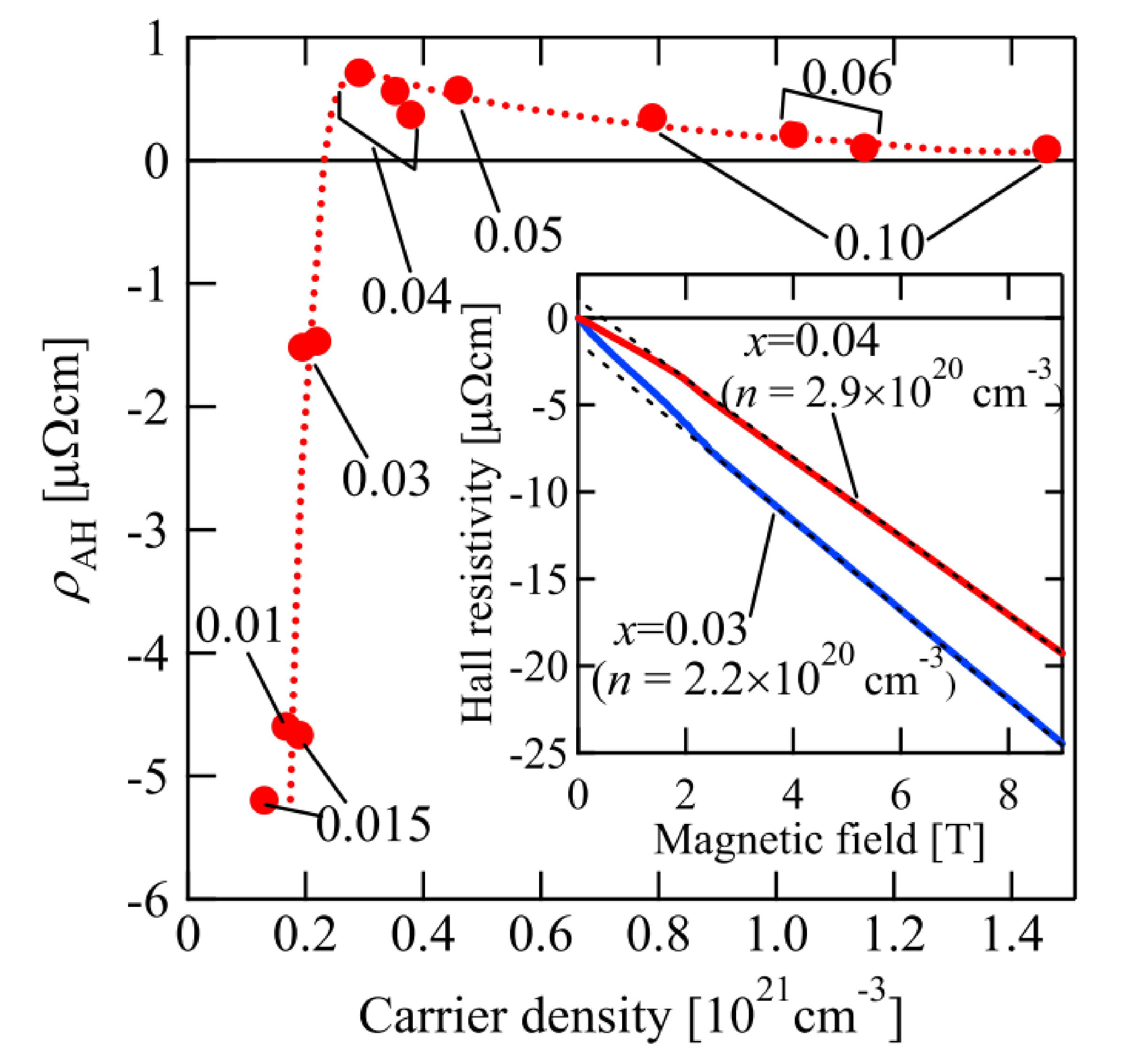
Berry curvature becomes sizable at the anticrossing of spin-orbit split bands with a Zeeman term.

Sign changes well described by theory that includes Berry phase and impurity scattering

Onoda et al. PRL 97, 126602 (2006)



Anomalous Hall effect from Berry phase



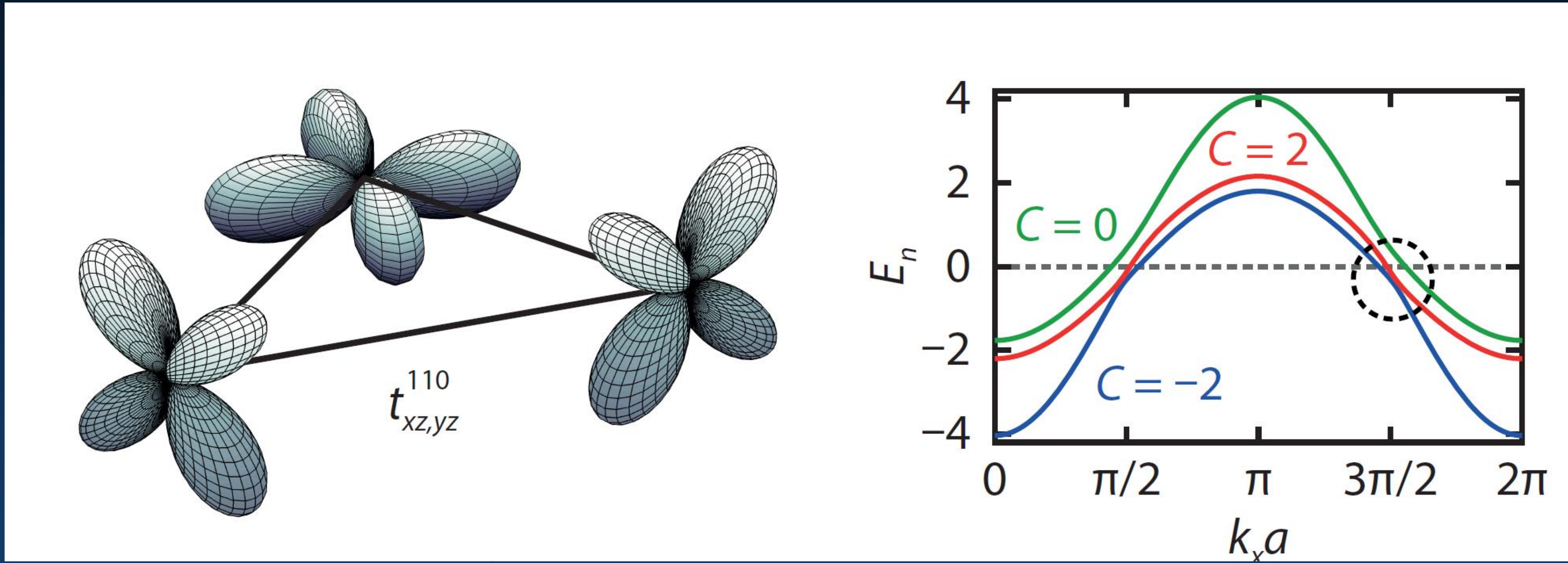
Controlling the AHE by band filling in EuTiO3

Takahashi et al.
PRL 103, 057204 (2009)

What is the electronic band topology of the 3D Weyl system $SrRuO_3$ in the two-dimensional limit?

Model system calculations

How do the Weyl points evolve in the two-dimensional limit?



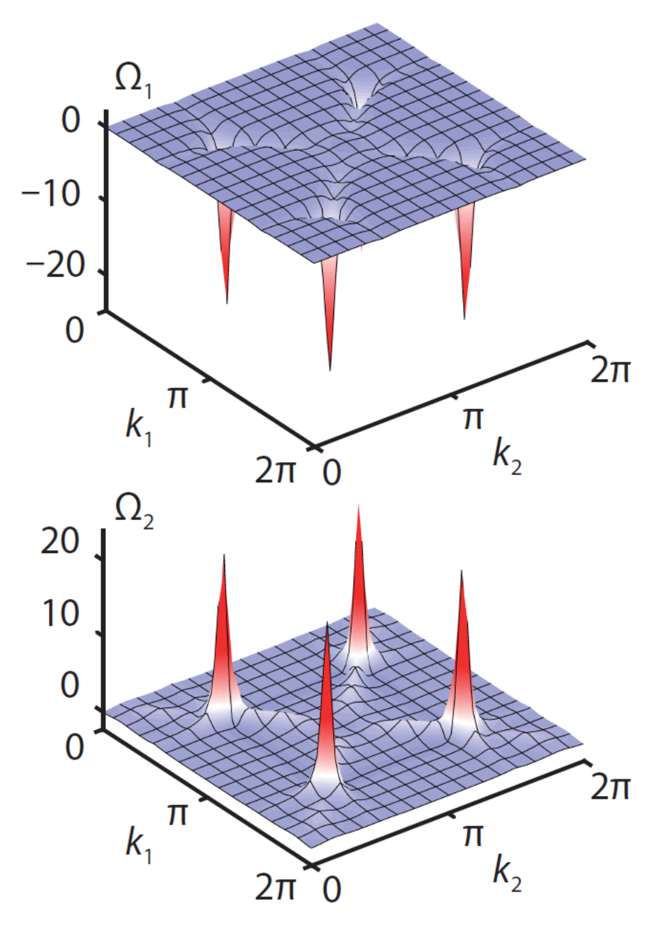
Effective Hamiltonian with spin-orbit coupling and next-nearest neighbours interorbital hopping

Mario Cuoco (CNR Spin)

Physical Review Research 2, 023404 (2020)

2 groups of 3 bands with different spin-orbital parity.
Within each sector, 2 topologically non-trivial bands with Chern numbers +2 and -2 and a single trivial band.
Avoided level crossing at finite k

Model system calculations



Physical Review Research 2, 023404 (2020)

Berry curvature of the topologically non-trivial bands.

Sharp peaks with opposite sign located at the avoided level crossings.

Since the bands have non-trivial Chern number their contribution to the Berry curvature cannot vanish and is robust against variations in electron occupation.

The splitting and relative occupation of the two non-trivial bands determine a competition between positive and negative Berry curvature.

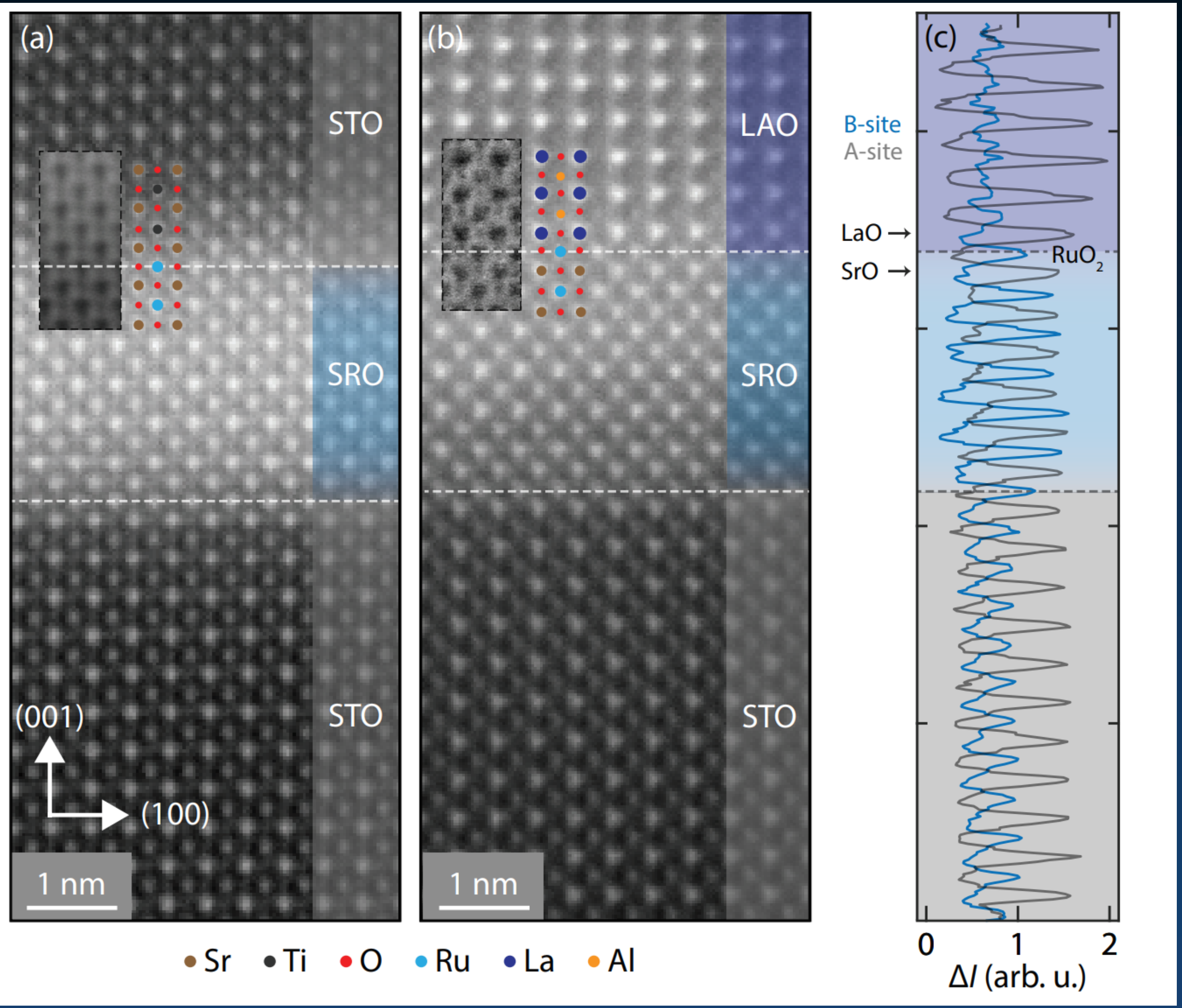
Intermediate summary

- Curved momentum-space leads to an emergent magnetic field, anomalous velocity and Hall effect
- The curvature appears for complex wavefunctions
- Band anticrossings are sources of Berry curvature
- Ultrathin $SrRuO_3$ hosts topological bands (two-dimensional vortex-like objects sources of Berry curvature)

Question: How to manipulate these charges?

Let's open up the complex oxide toolbox…

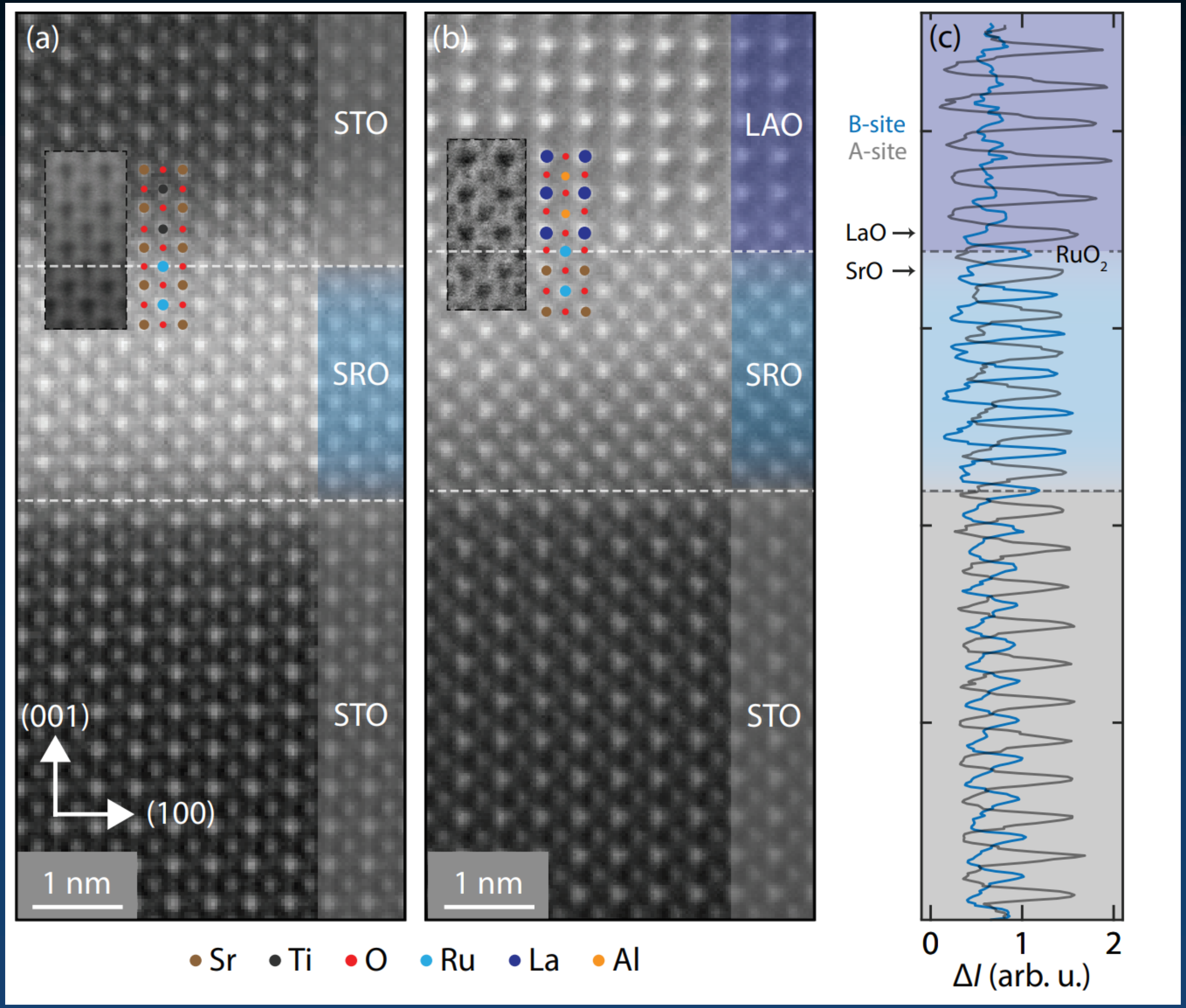
RuO_2/LaO interface

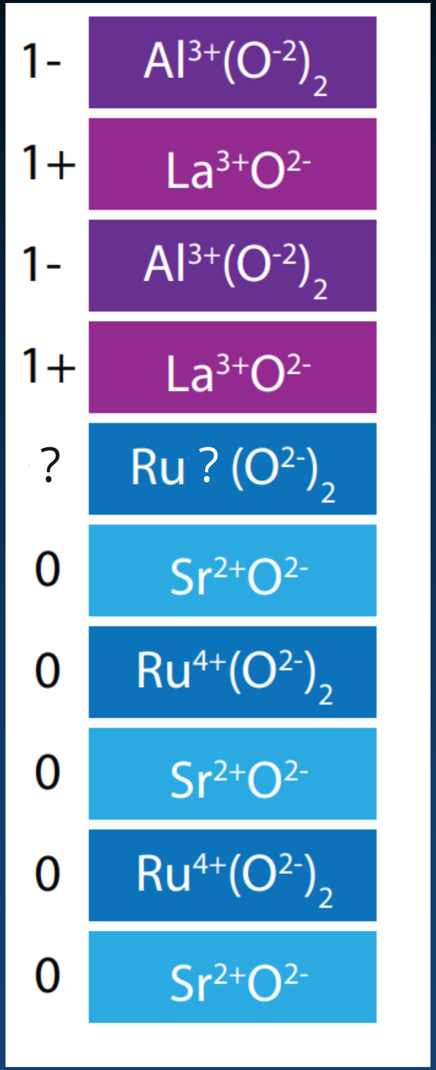


Thierry van Thiel

Physical Review Letters (2021) arXiv:2107.03359

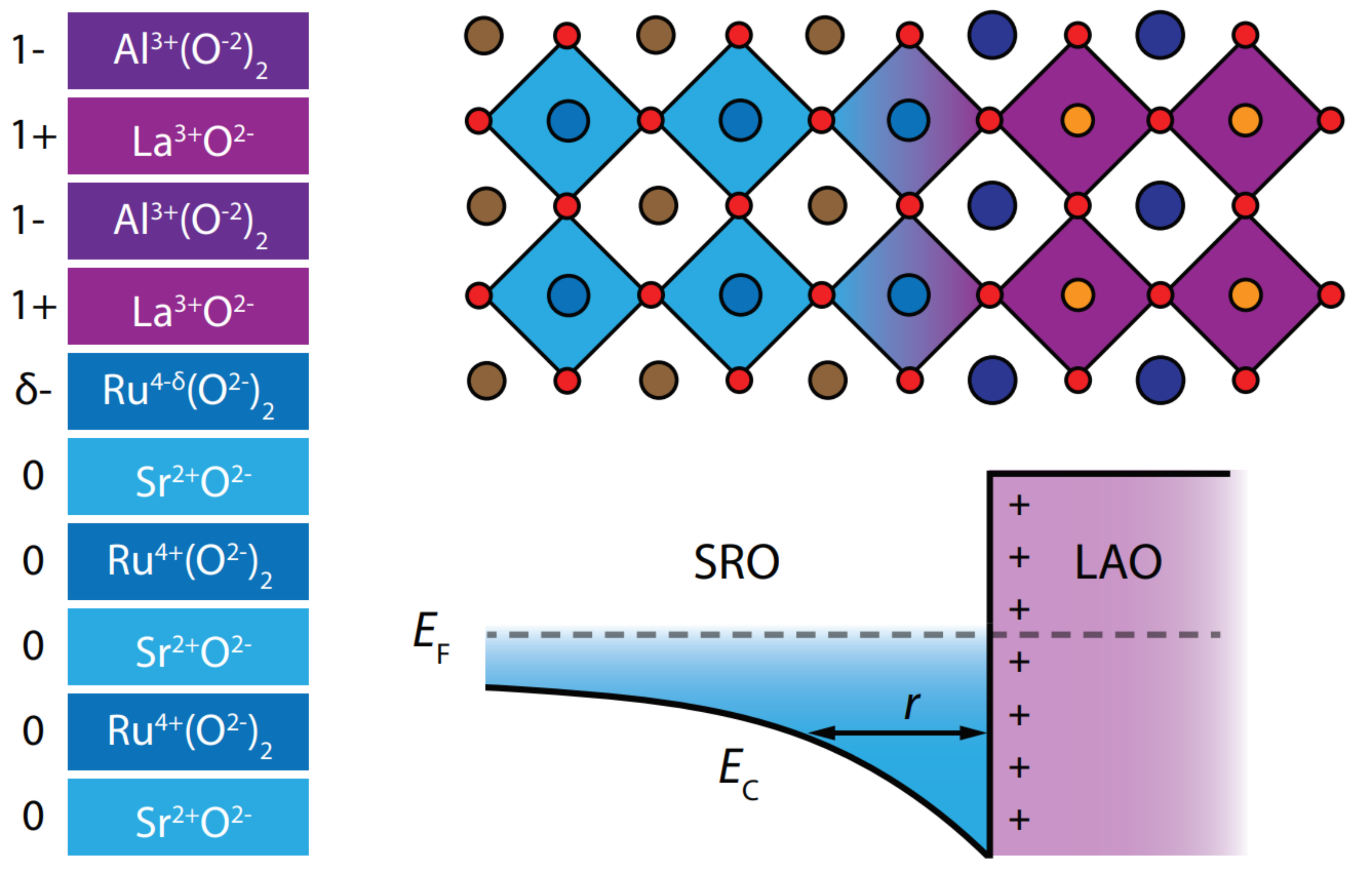
Charge reconstruction



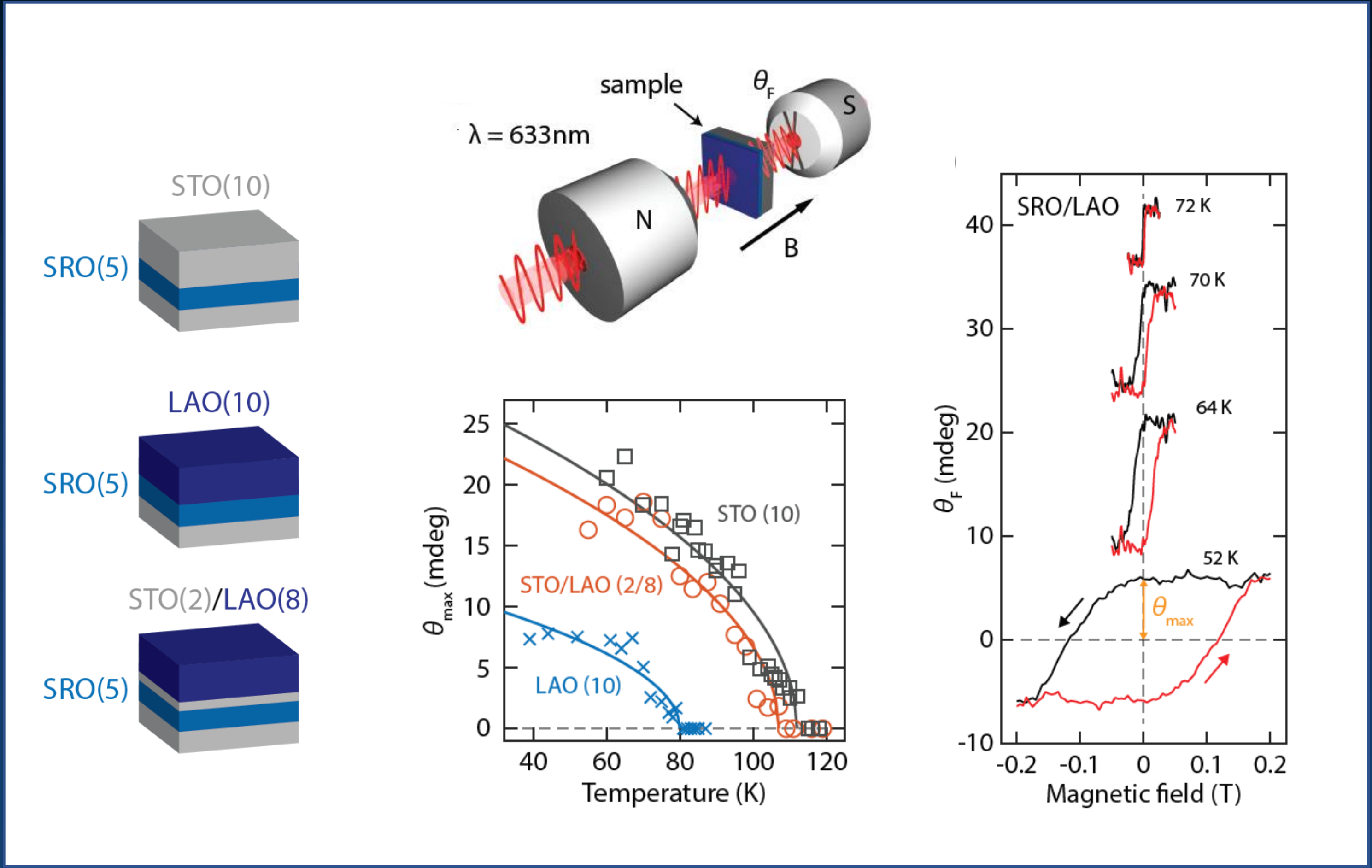


Physical Review Letters 127, 127202 (2021)

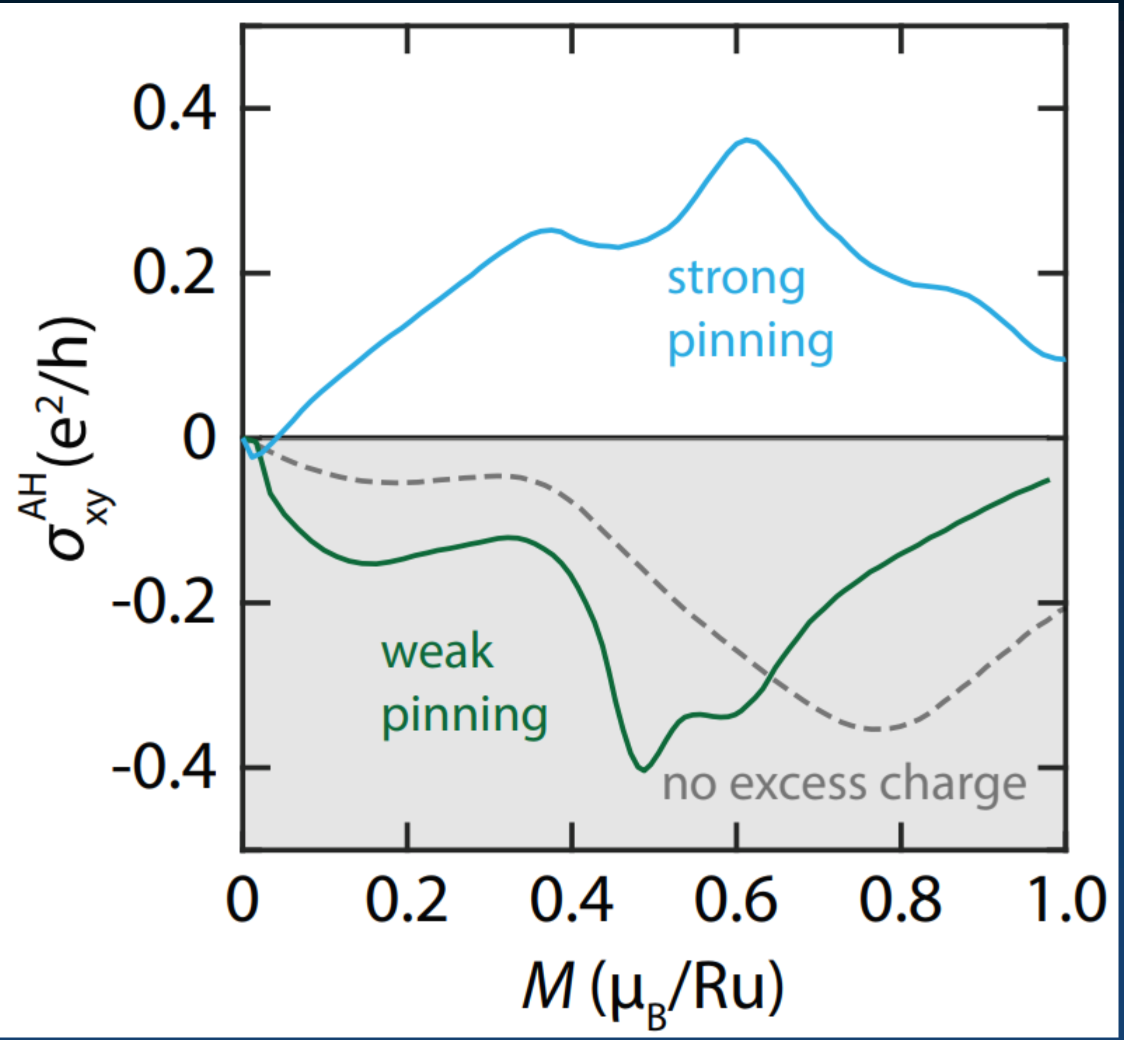
Charge reconstruction

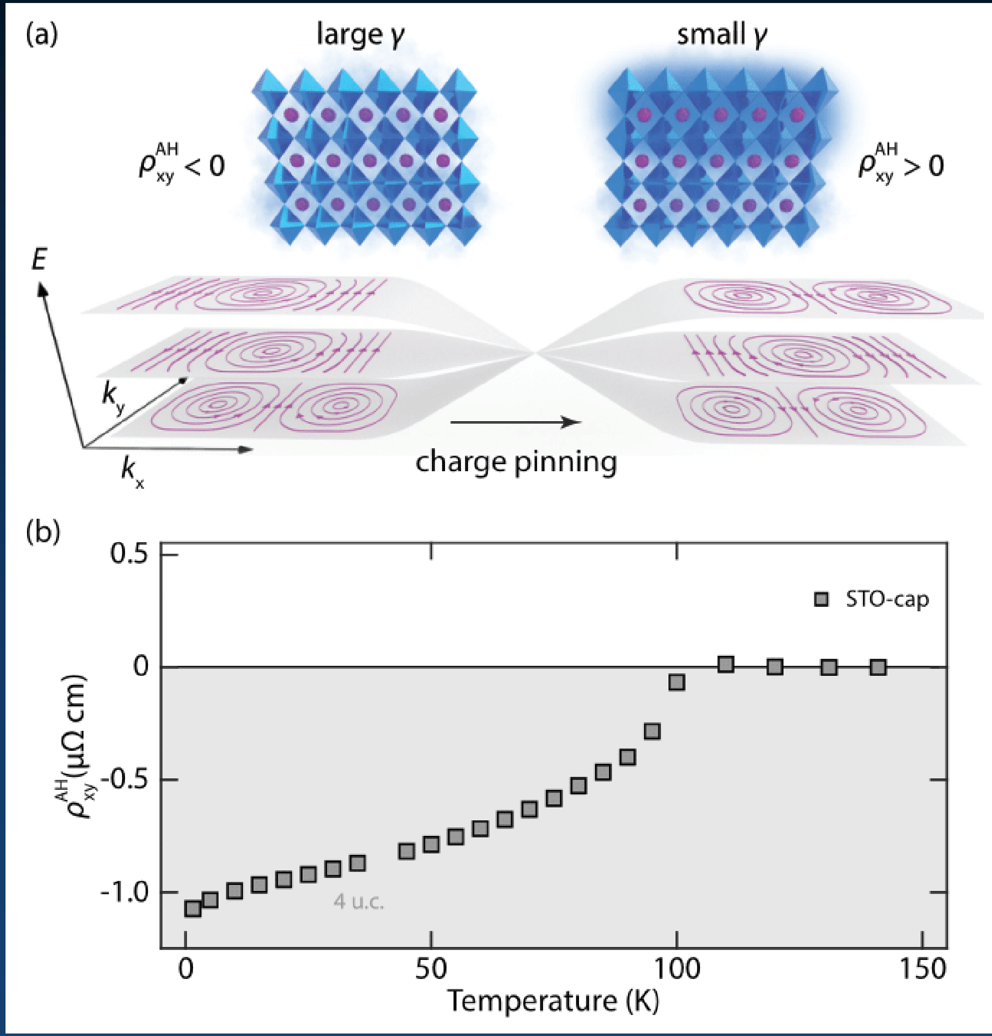


Magnetic reconstruction

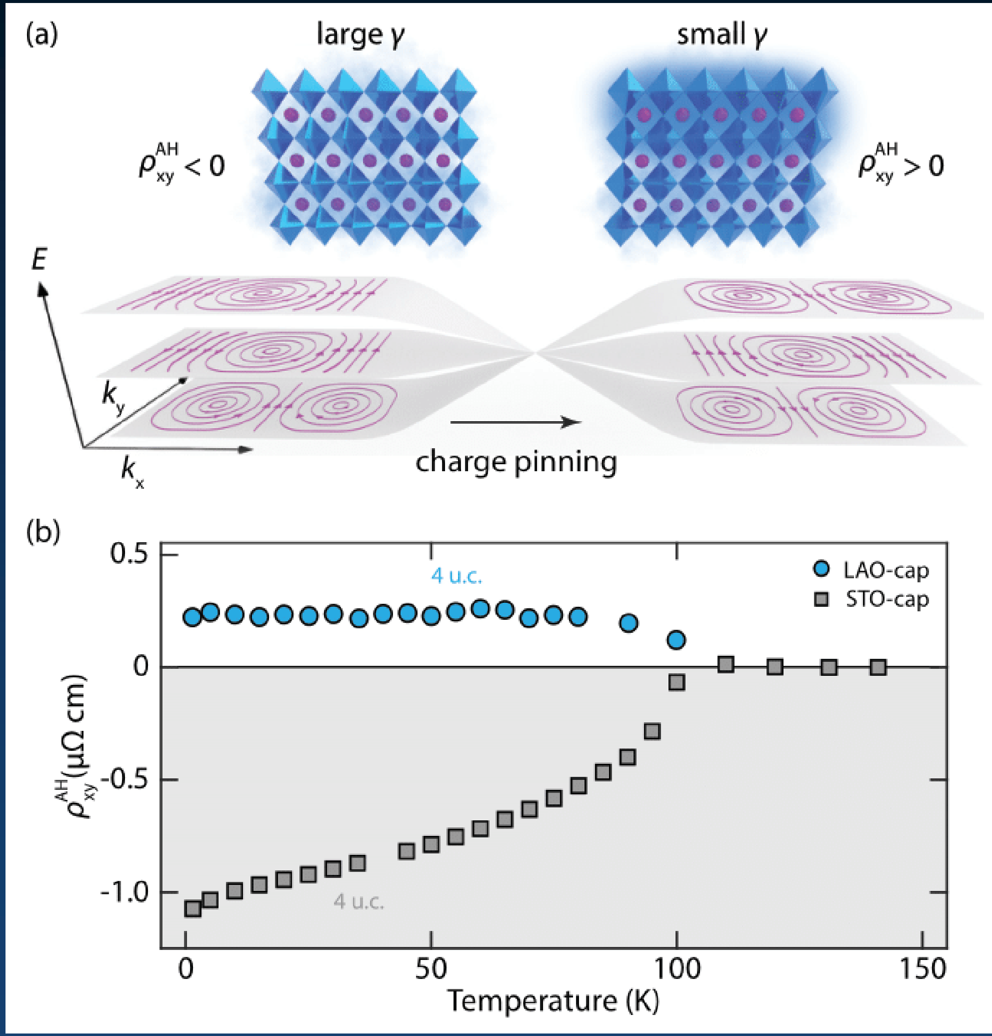


Berry curvature reconstruction in bilayer SRO

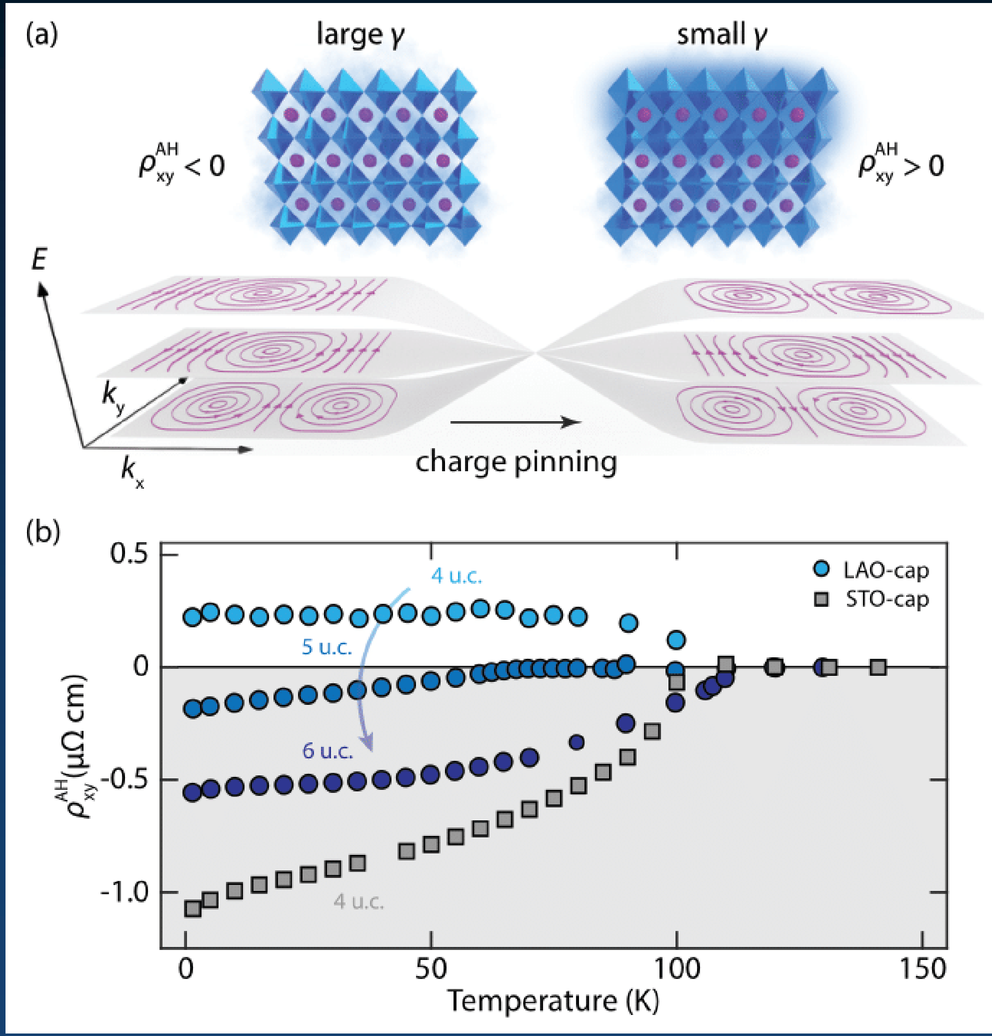




Physical Review Letters 127, 127202 (2021)



Physical Review Letters 127, 127202 (2021)

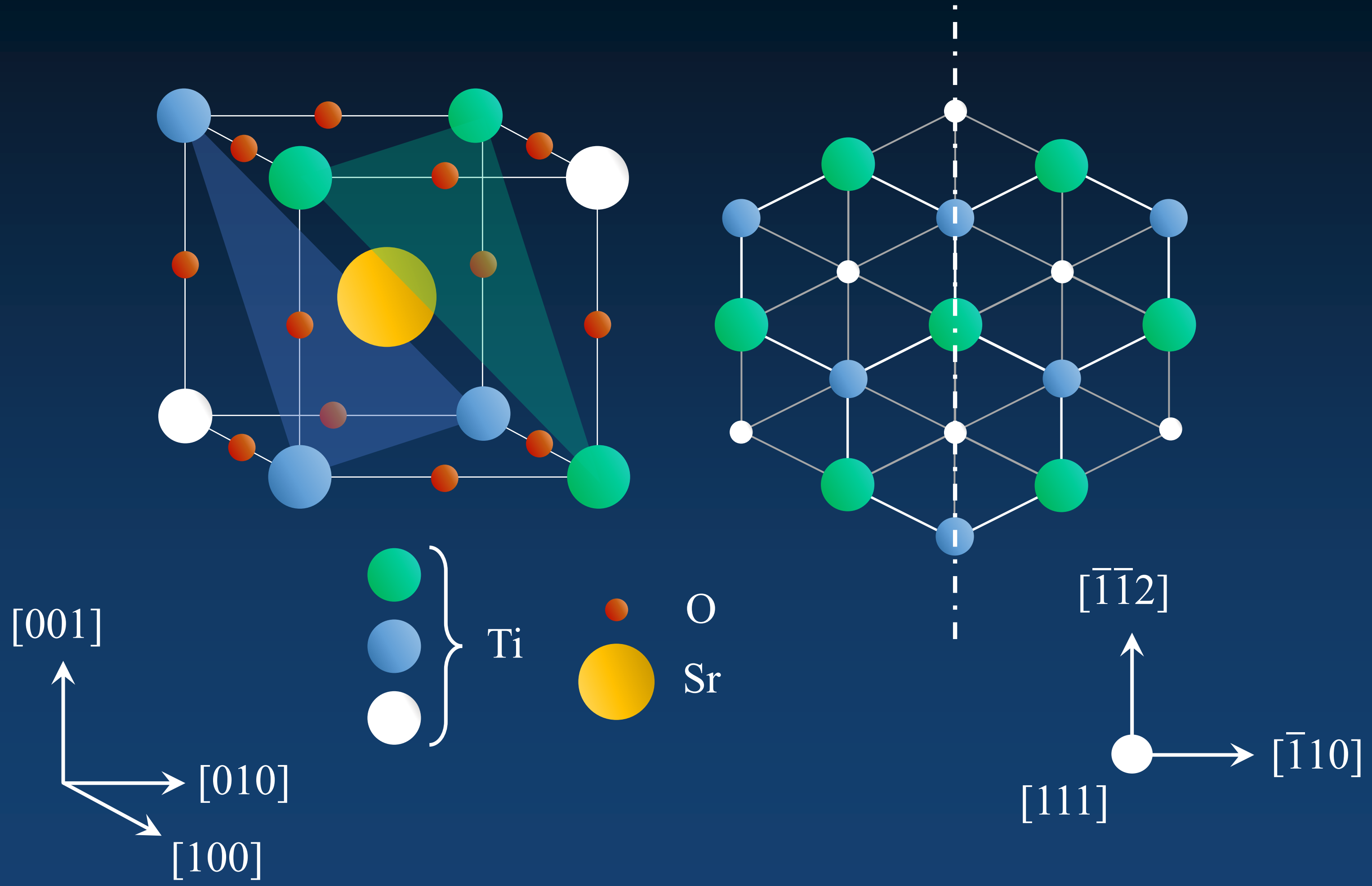


Physical Review Letters 127, 127202 (2021)

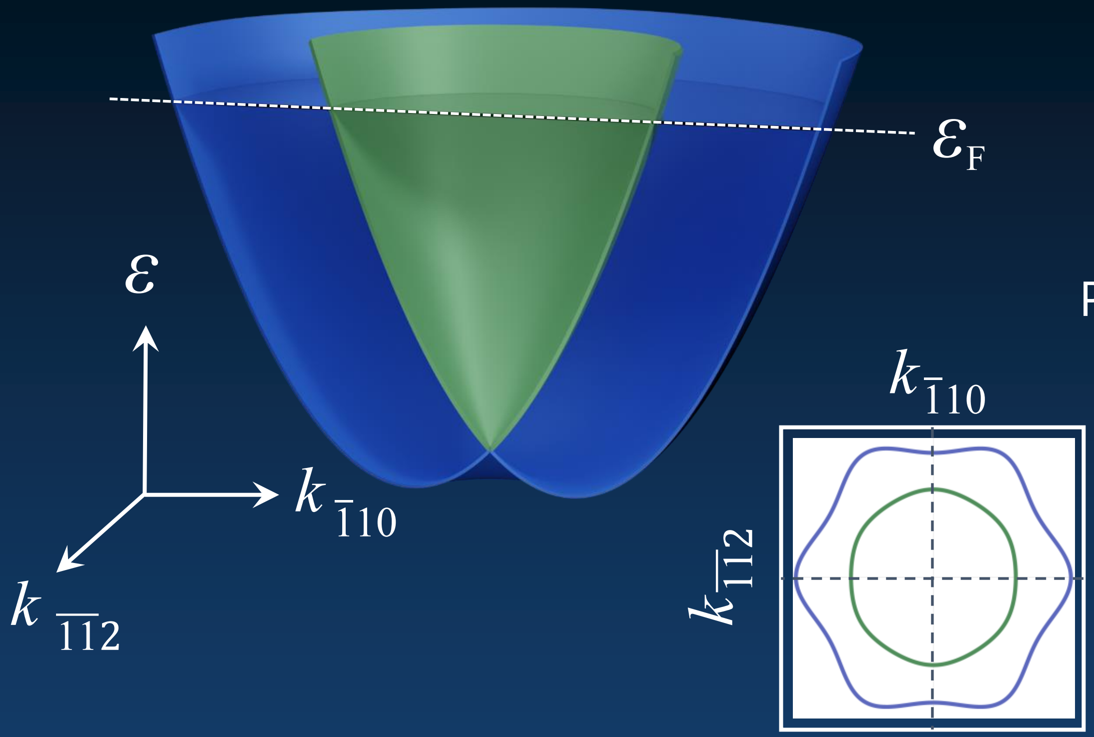
Research question

Can we engineer Berry curvature
at time-reversal invariant (non-magnetic) oxide interfaces?

Exploring hexagonal symmetry



Trigonal warping

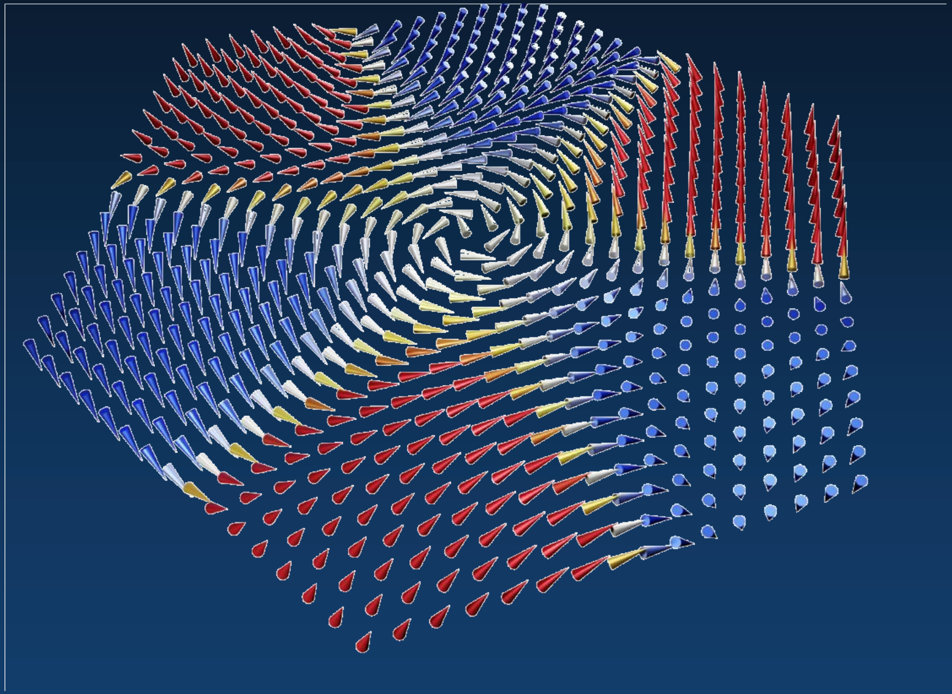


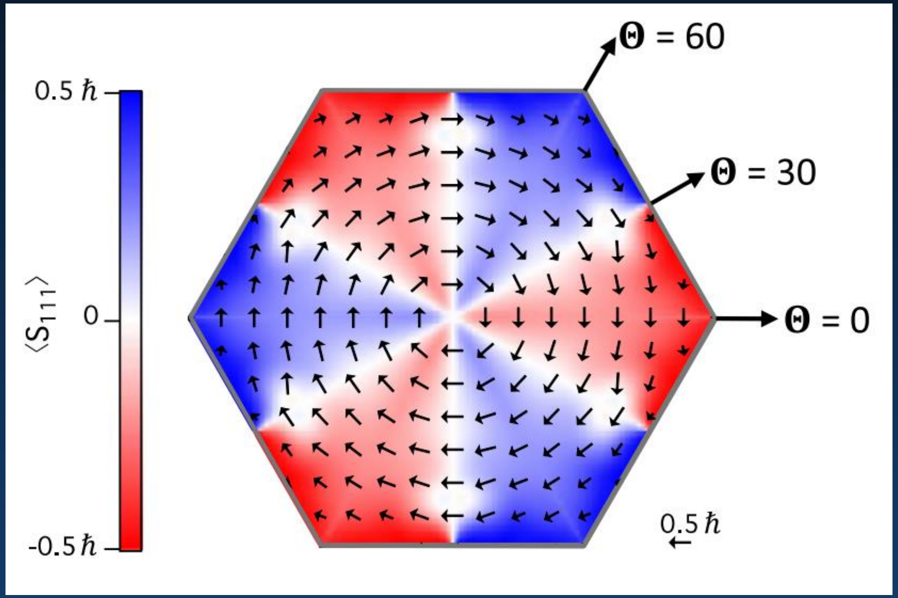
Monteiro et al.
Phys. Rev. B 99, 201102R (2019)

$$\mathcal{H}(\mathbf{k}) = \frac{k^2}{2m}\sigma_0 + (\alpha_{\mathrm{R}} k_x + \mathcal{B}\sin\theta)\sigma_y + (-\alpha_{\mathrm{R}} k_y + \mathcal{B}\cos\theta)\sigma_x + \\ + \frac{\lambda}{2}(k_+^3 + k_-^3)\sigma_z$$

$$k_\pm = k_x \pm i k_y$$

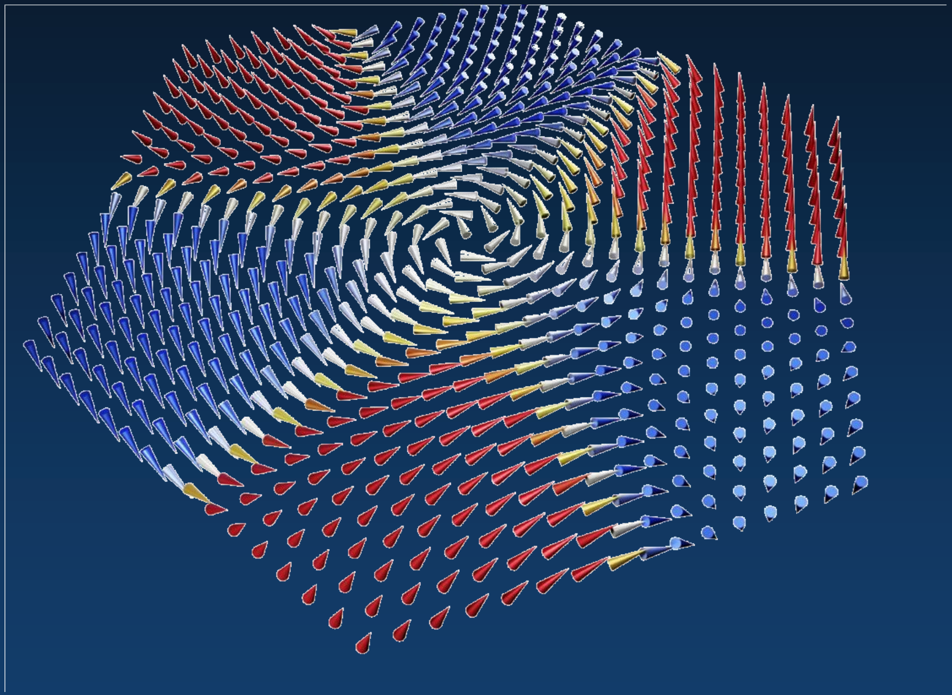
Out-of-plane spin texture

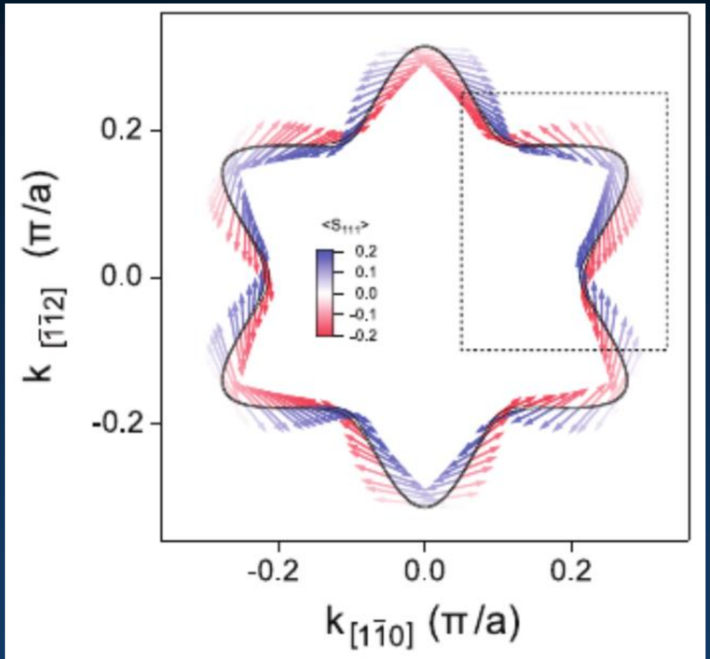




Surface of (111)SrTiO3
He et al. Physical Review Letters 120, 266802 (2018)

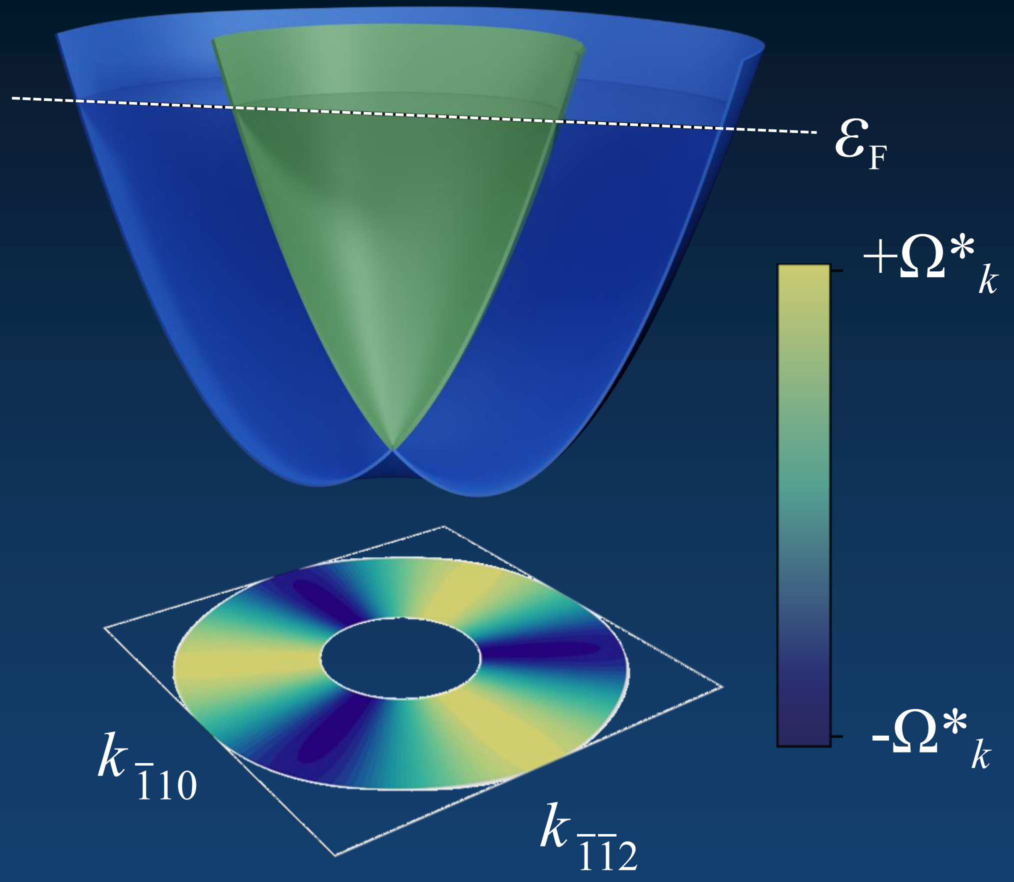
Out-of-plane spin texture



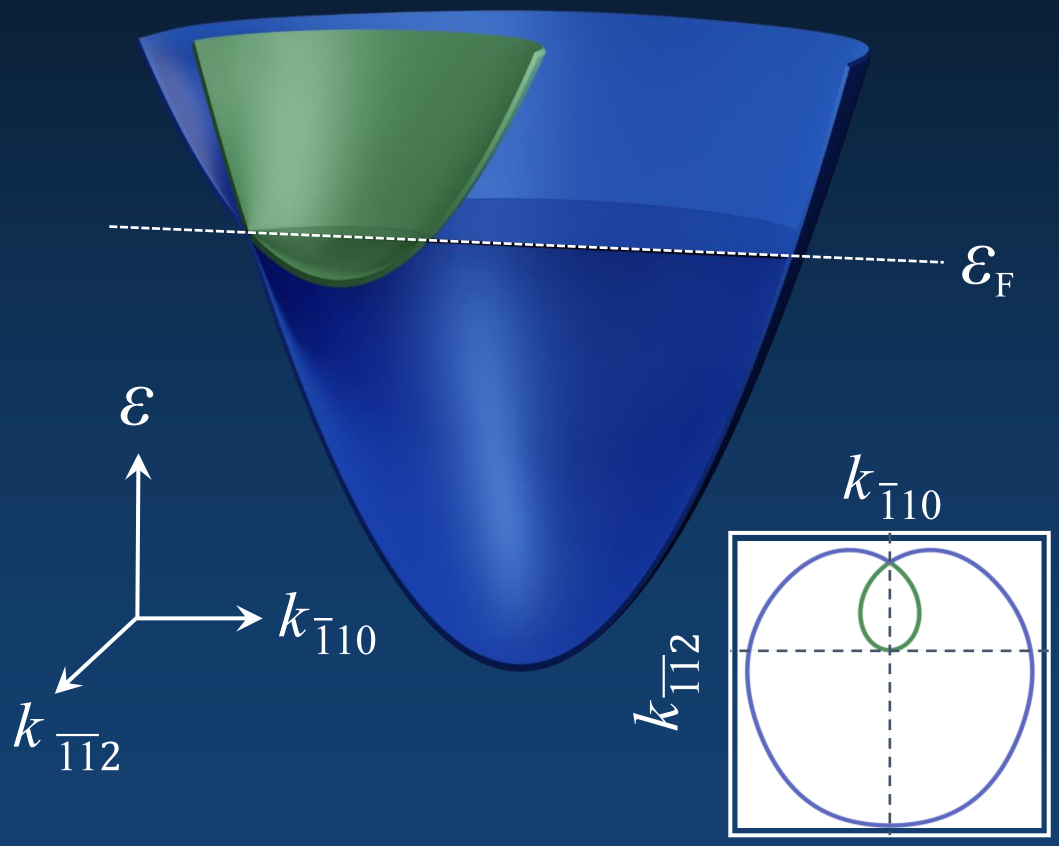


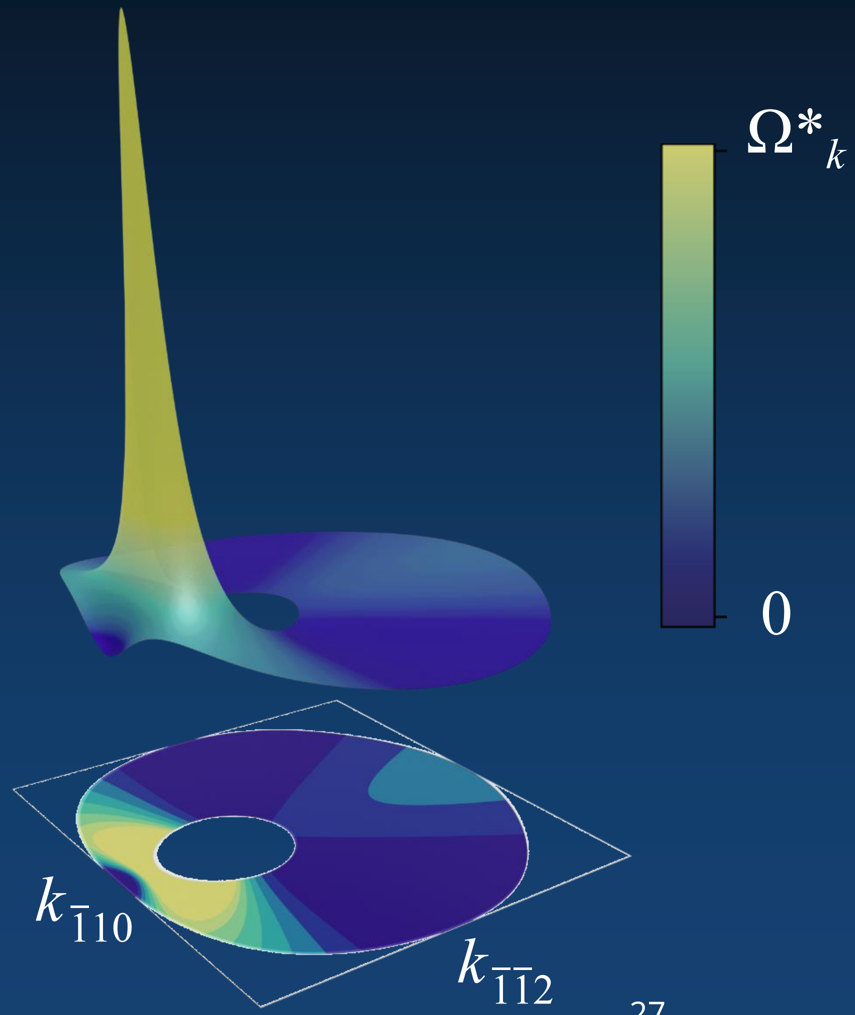
Surface of (111)$KTaO_3$
Bruno et al. Advanced Electronic Materials, 1800860 (2019)

Spin sources of Berry curvature

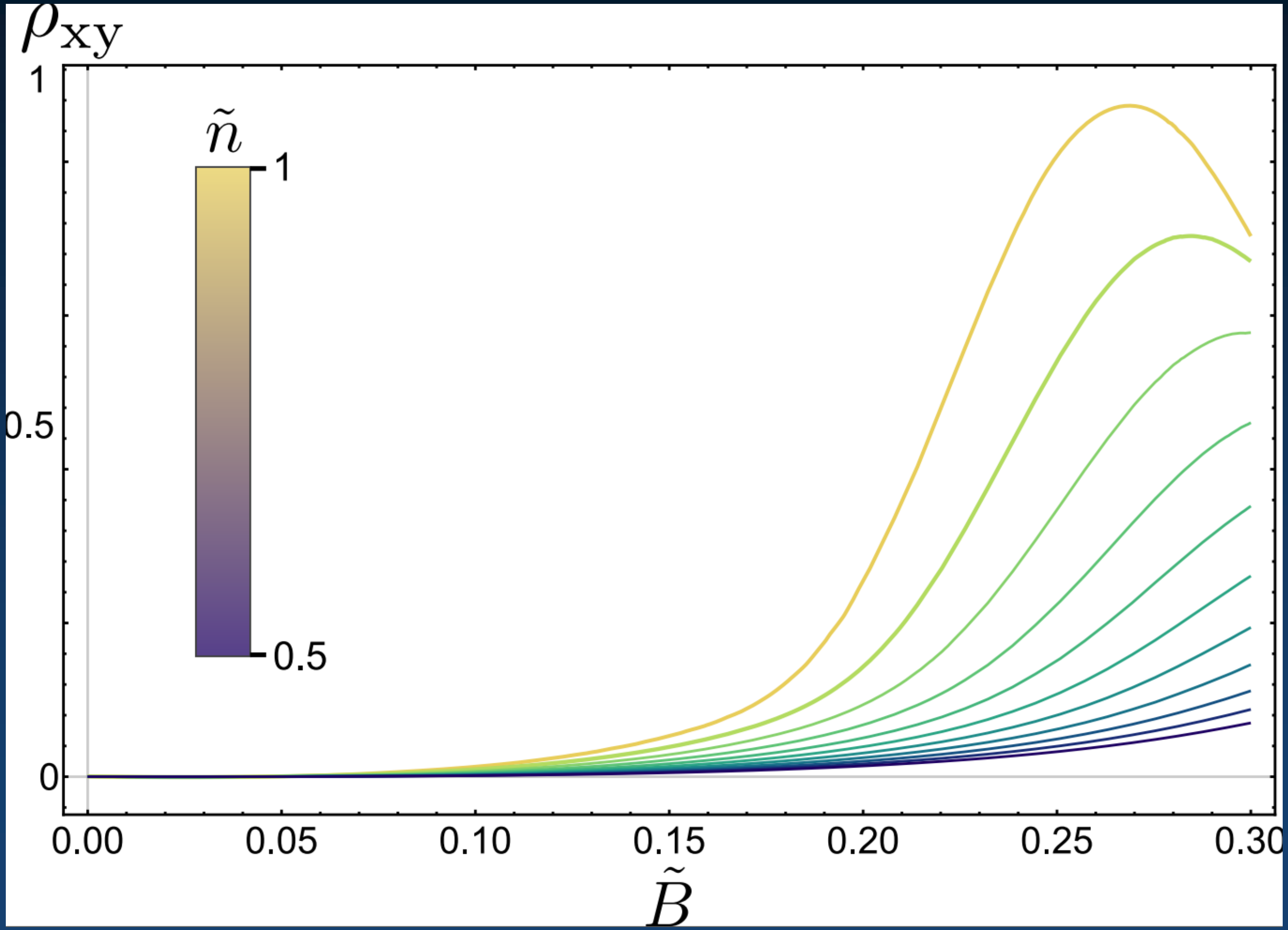


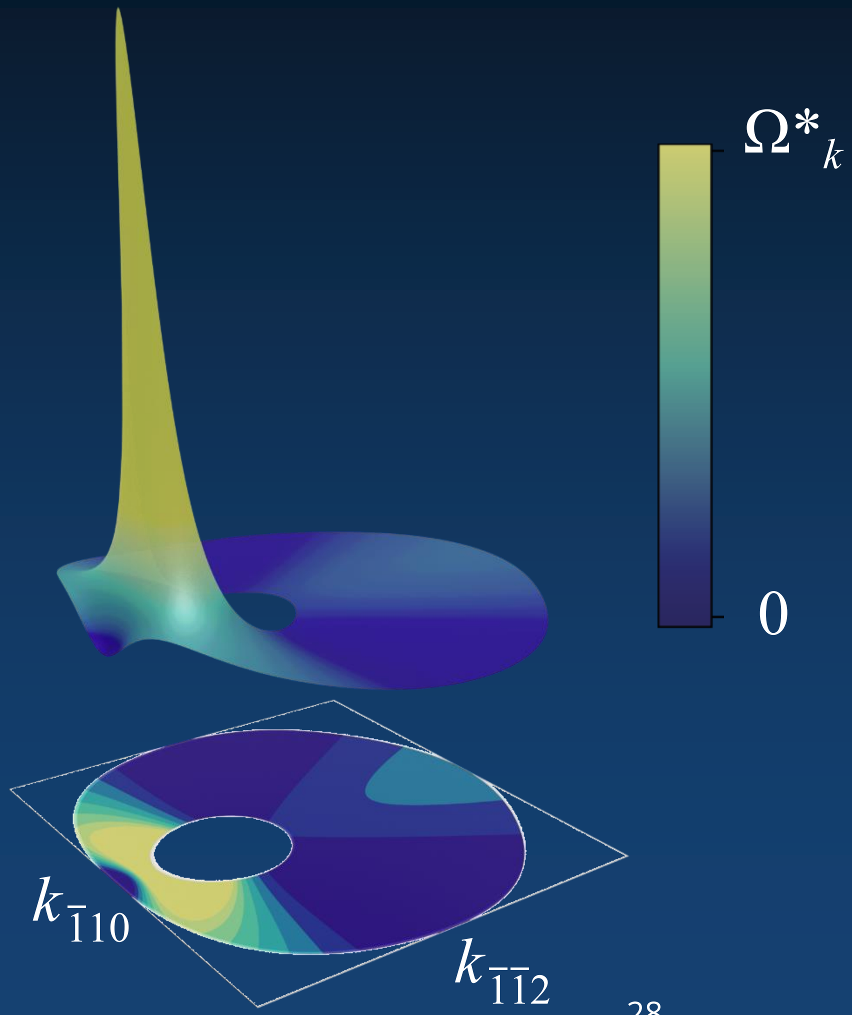
In-plane magnetic field



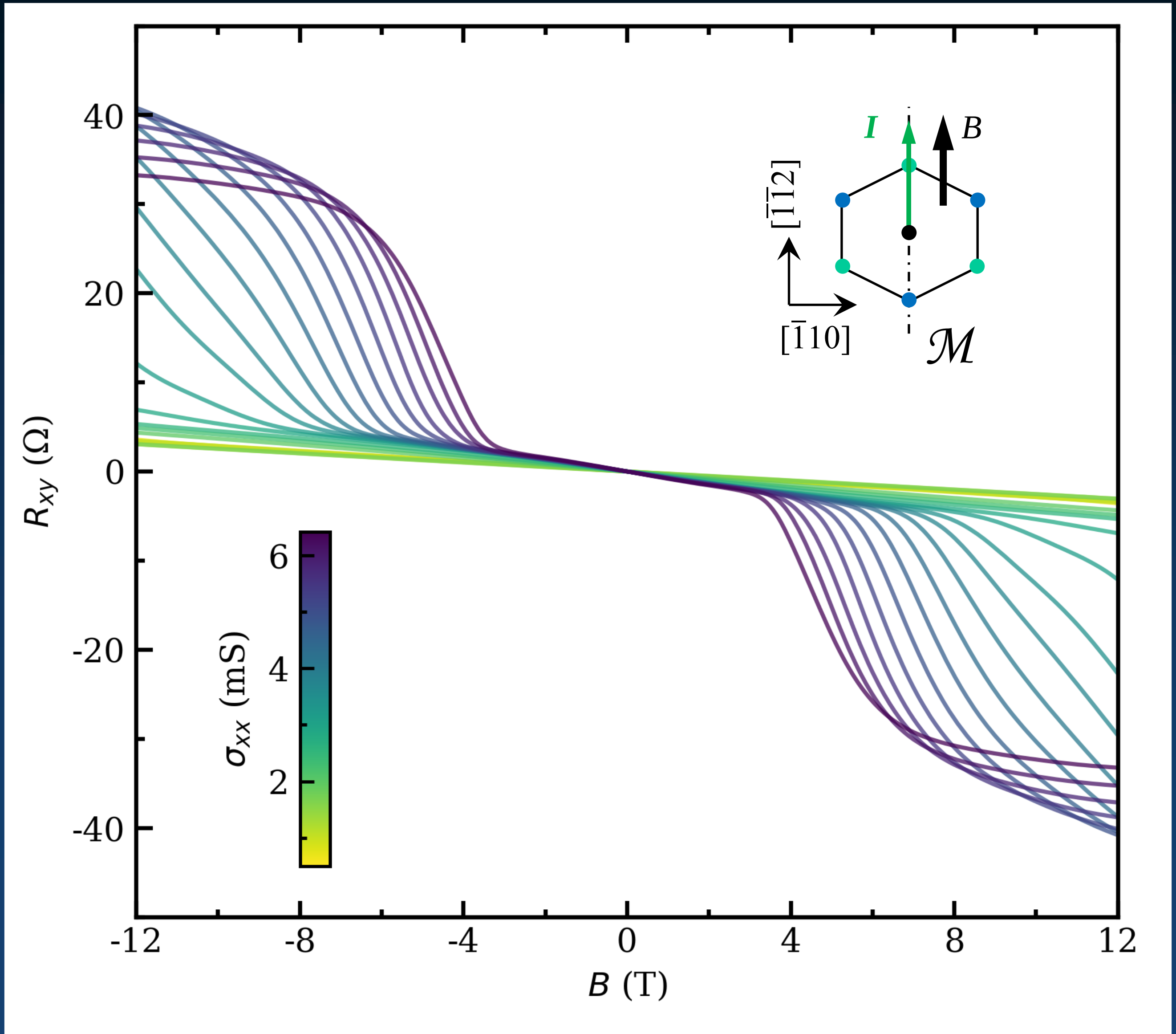


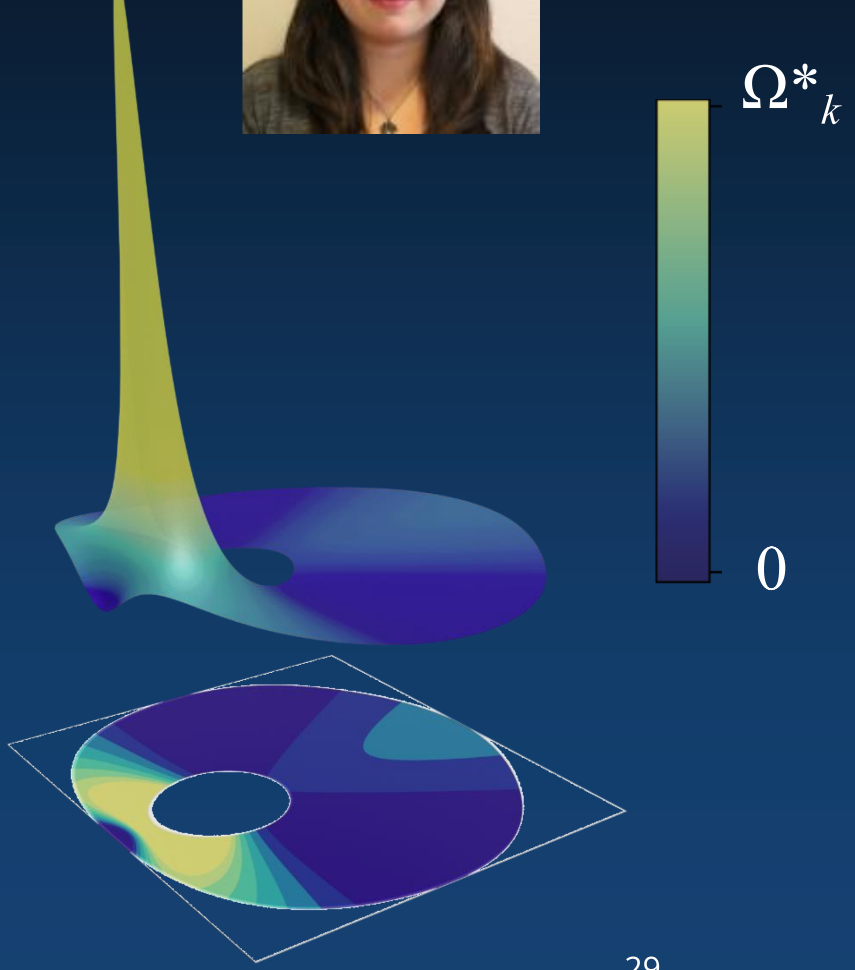
In-plane magnetic field



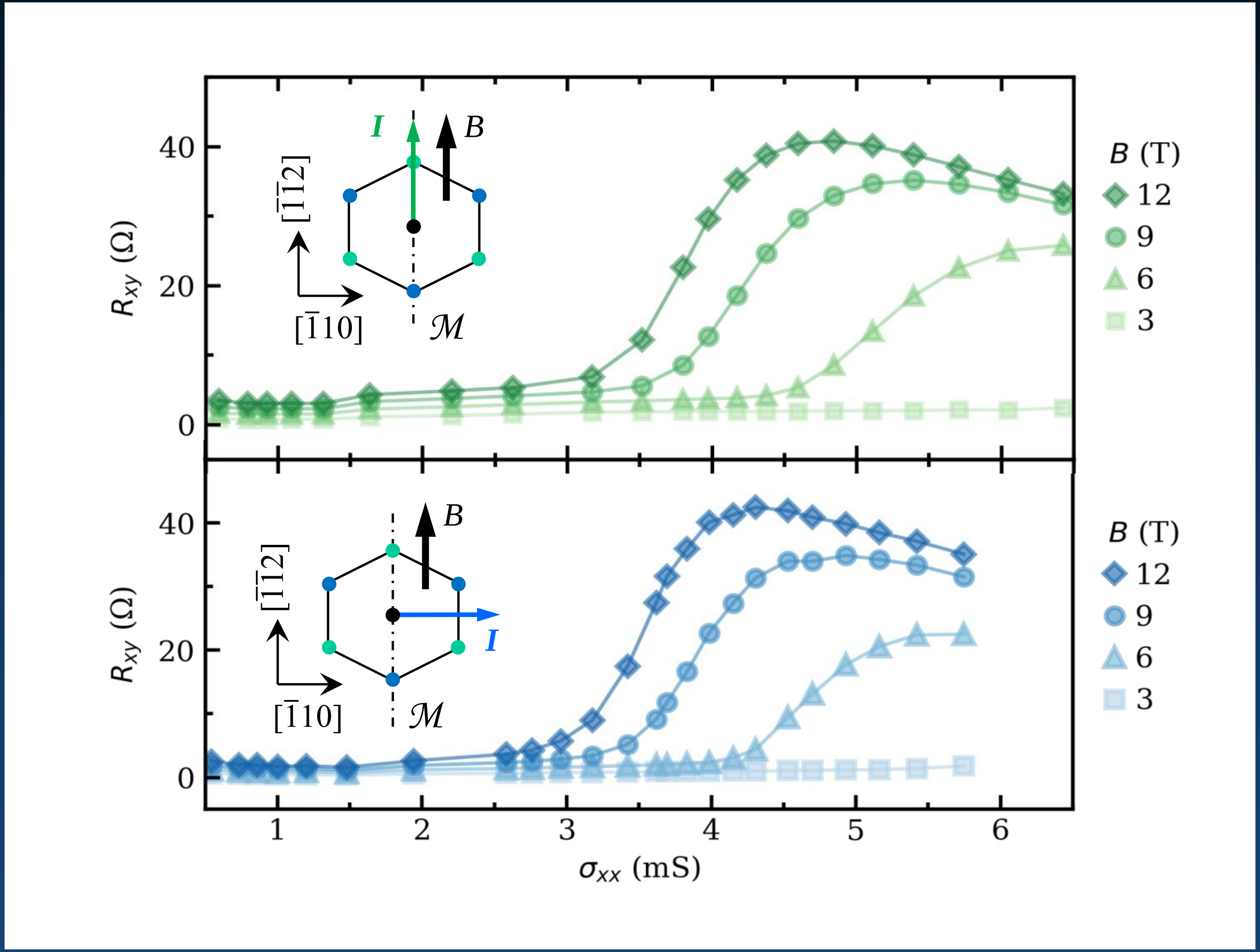


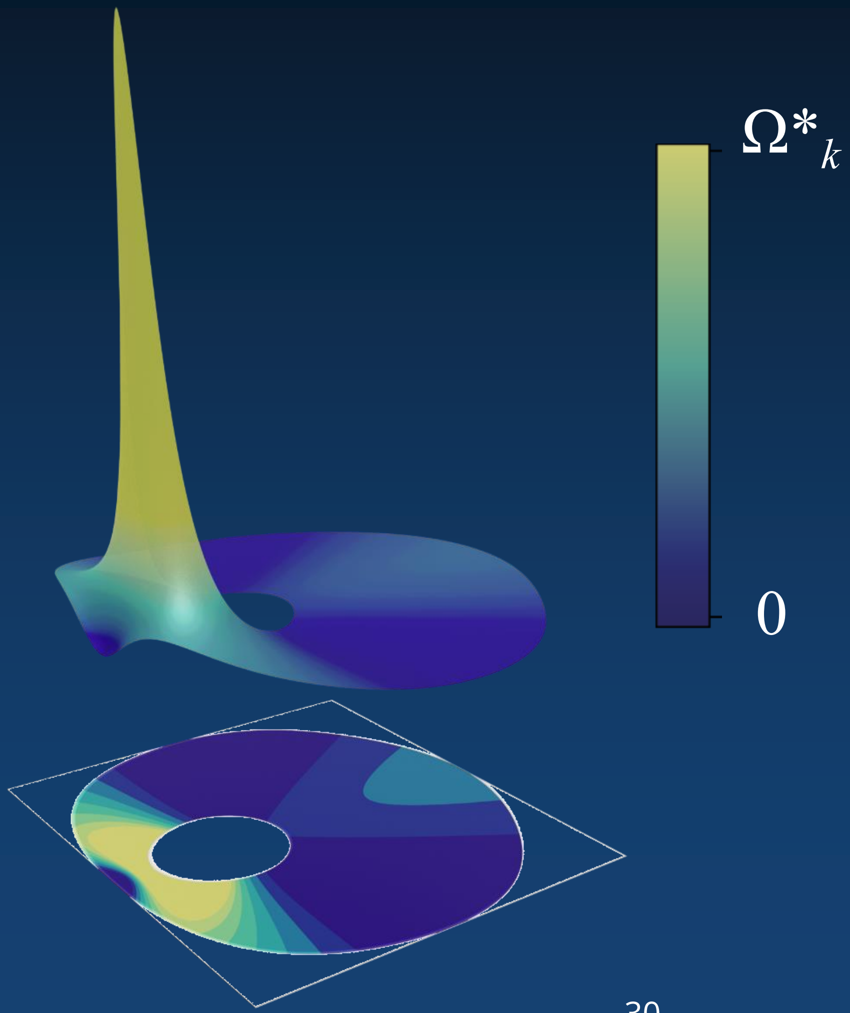
Spin sources of Berry curvature





Spin sources of Berry curvature



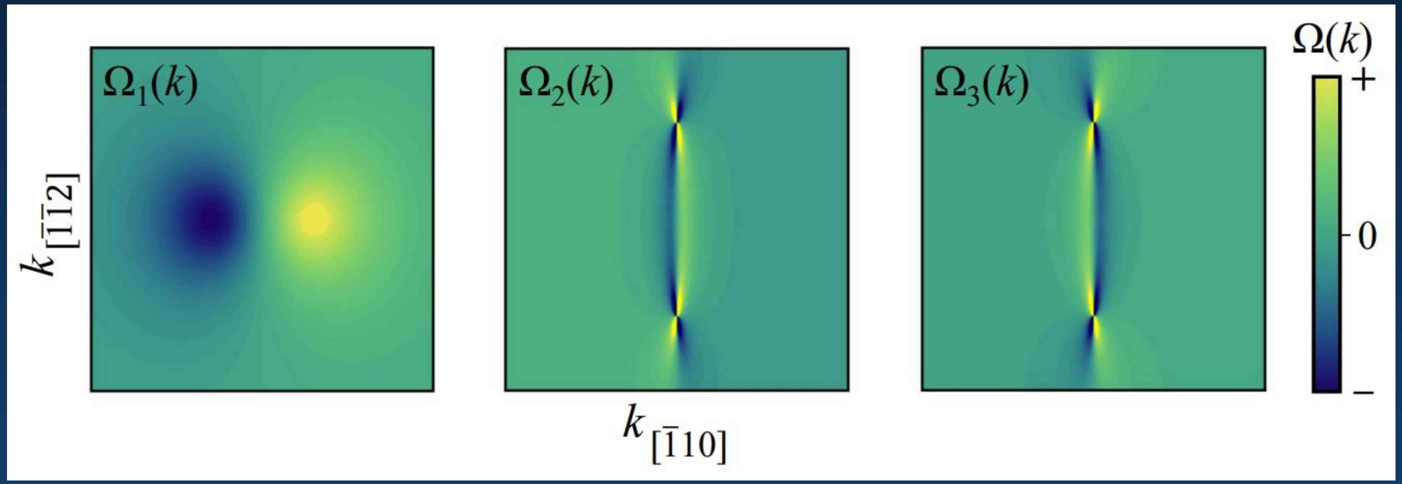


Research question

Are there phenomena manifesting at $B = 0$?

Orbital sources of Berry curvature

t_{2g} orbitals with mixing terms:
Δ trigonal crystal field
Δ_m tetragonal distortion (T < 105 K),
α_{OR} interfacial breaking of inversion symmetry with polar axis (T < 30 K)

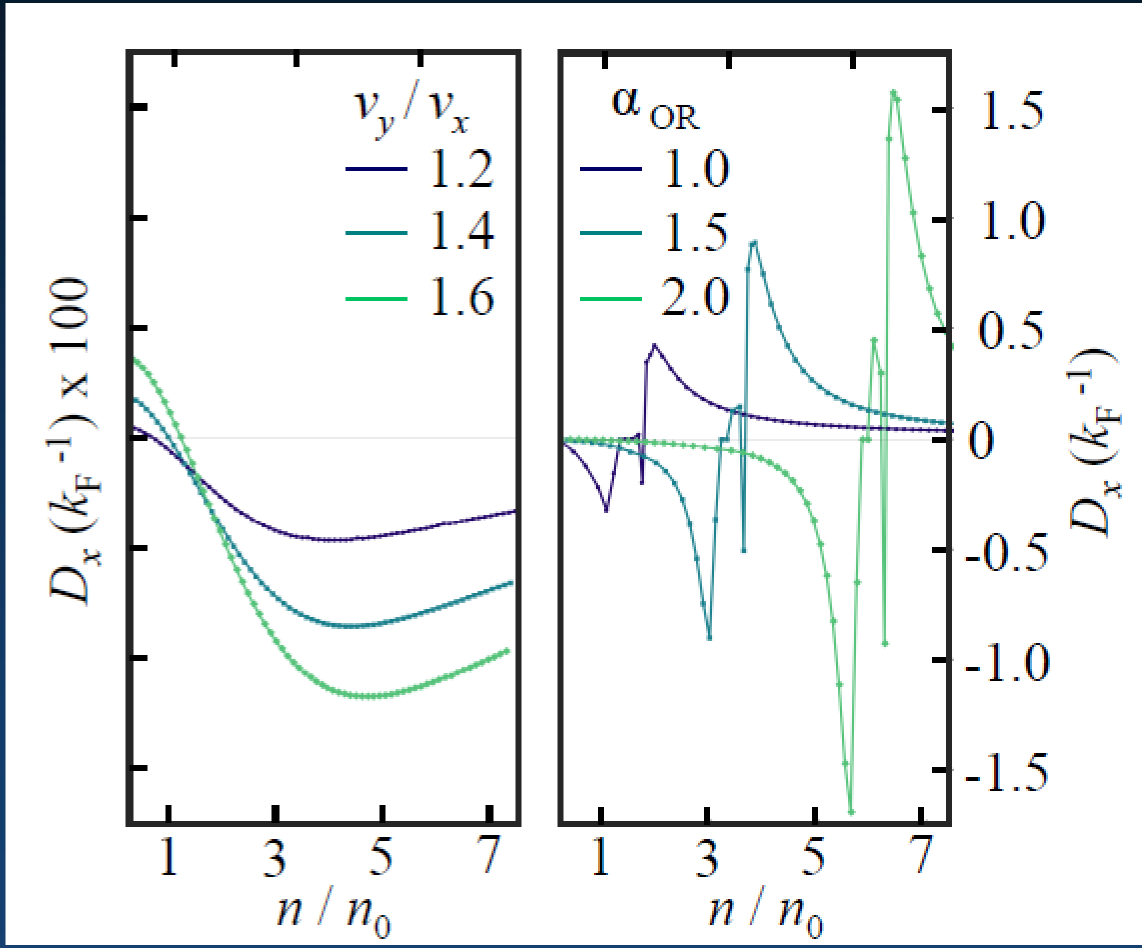


Hot spots

Singular pinch points

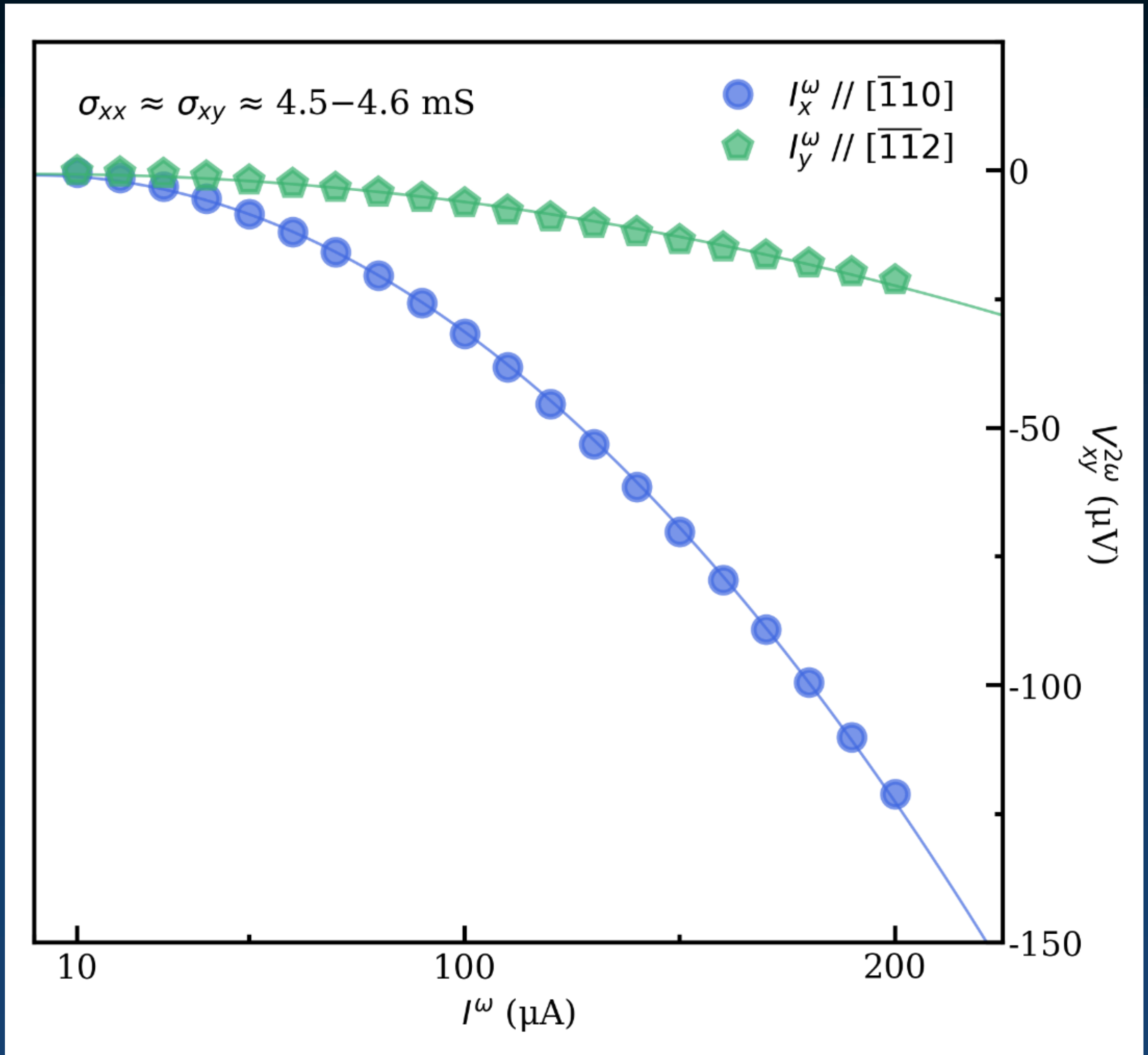
$$\mathscr{H}_{\mathrm{OR}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\Lambda_0 + \Delta\left(\Lambda_3 + \frac{1}{\sqrt{3}}\Lambda_8\right) + \Delta_m\left(\frac{1}{2}\Lambda_3 - \frac{\sqrt{3}}{2}\Lambda_8\right) - \alpha_{\mathrm{OR}}\left[k_x\Lambda_5 + k_y\Lambda_2\right] - \alpha_m k_x \Lambda_7$$

Orbital sources of Berry curvature

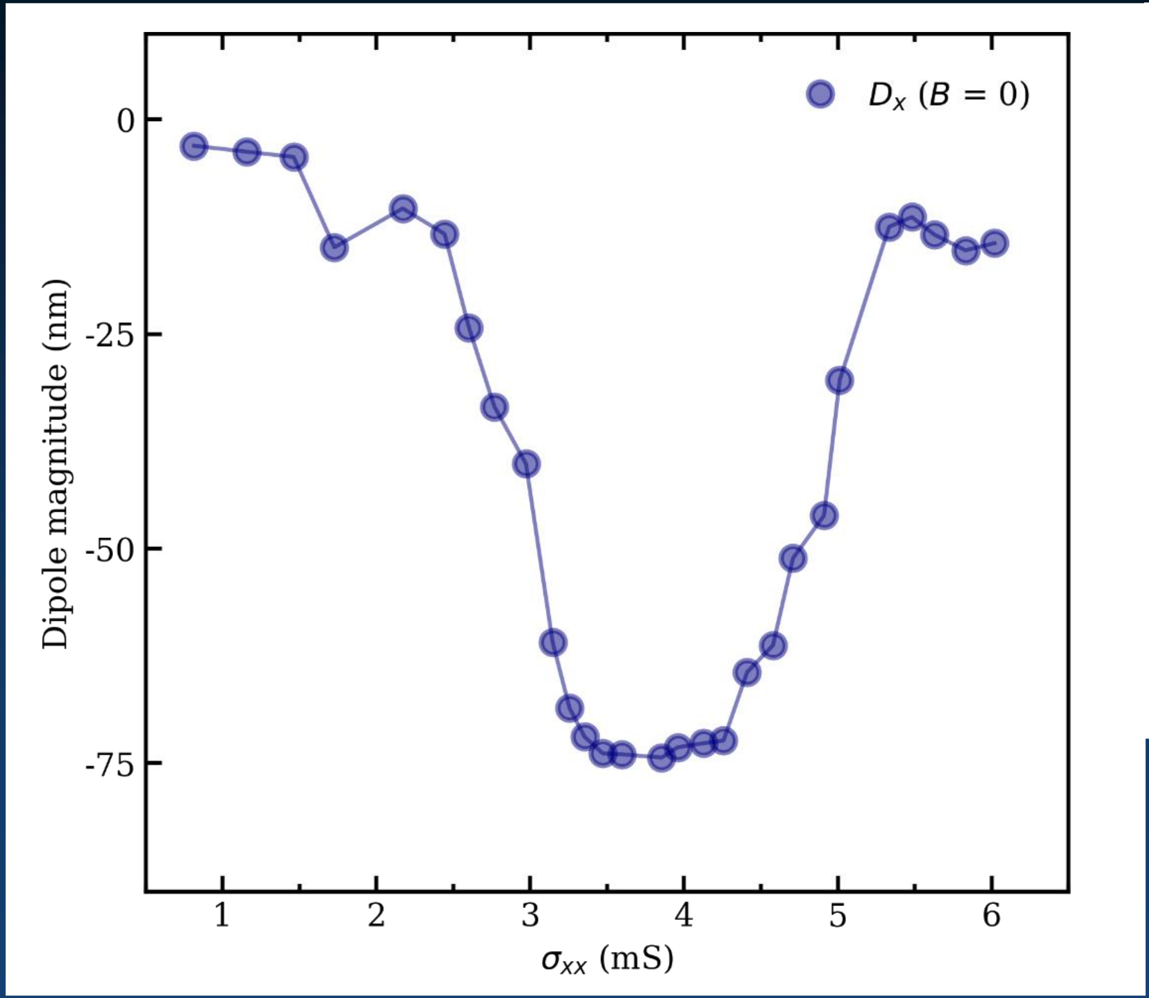


Prediction:
BCD in the 10s nm range!

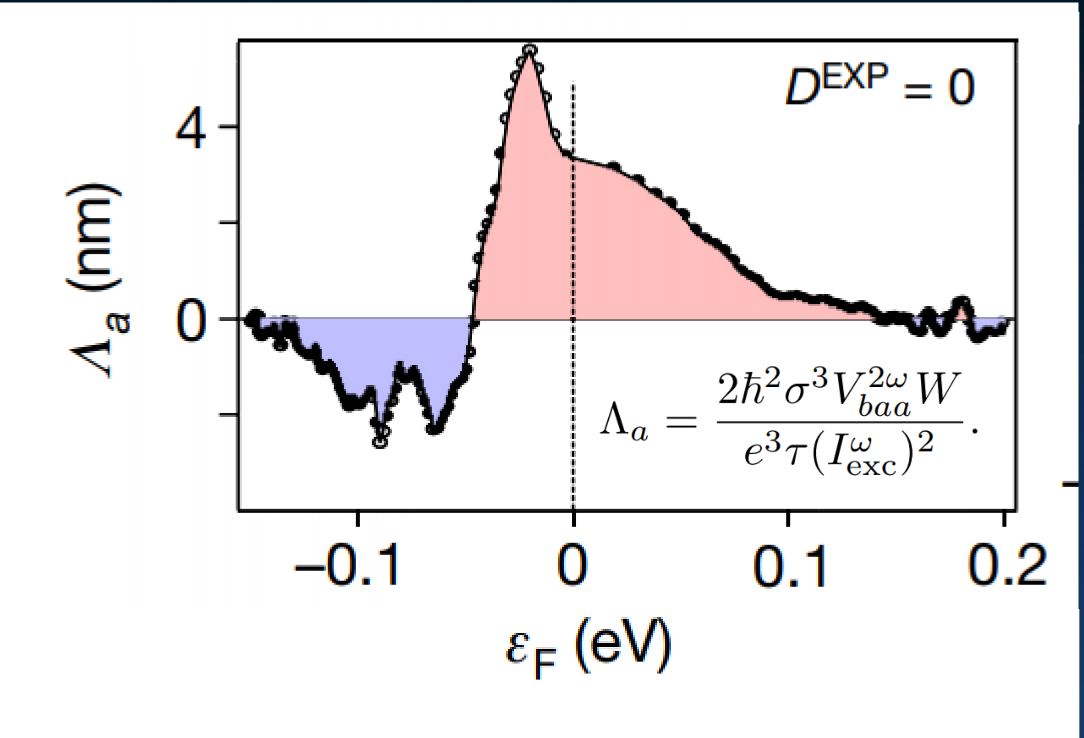
Non linear Hall effect at B=0



Dipole magnitude



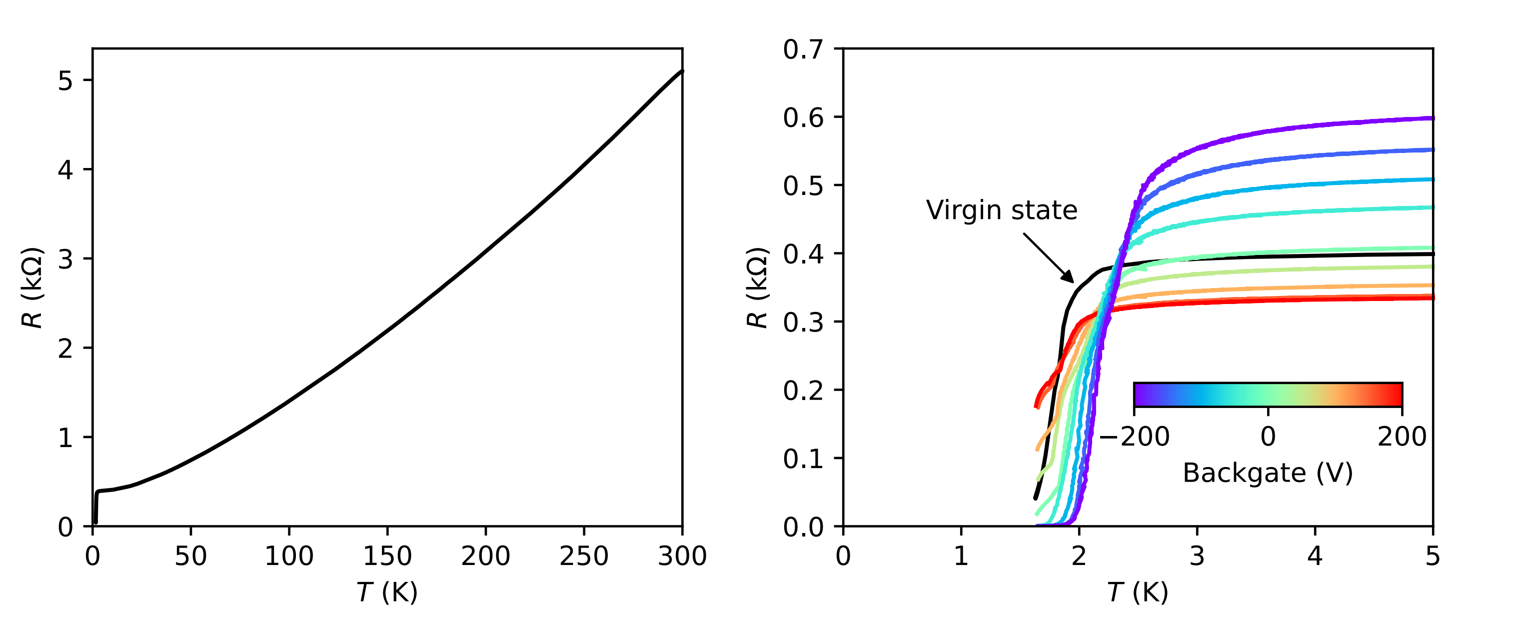
(111)$LaAlO_3$/$SrTiO_3$



WTe_2
Ma et al. Nature 565, 337 (2019)
Sodemann, I. & Fu, L.. Phys. Rev. Lett. 115, 216806 (2015)

Conclusions and future directions

- Curved momentum-space leads to an emergent magnetic field, anomalous velocity and Hall effect
- Ultrathin $SrRuO_3$ hosts topological bands
- Real-space charge reconstruction modifies the momentum-space Berry curvature in $SrRuO_3$, driving a reorganization of the topological charges in the band structure
- (111)$LaAlO_3$/$SrTiO_3$ is the first example of a material system hosting coexisting spin and orbital sources of Berry curvature



(111)$KTaO_3$

Collaborators and funding

Thierry van Thiel, Yildiz Saglam, Edouard Lesne,
Ulderico Filippozzi, Patrick Blah, Graham Kimbell

Carmine Autieri,
Wojciech Brzezicki, **Mario Cuoco**
CNR Spin

Nicolas Gauquelin, J. Verbeeck
University of Antwerp

Marc Gabay
Uni Paris Sud

Raffaele Battilomo, **Carmine Ortix**
Uni Utrecht
Uni Salerno

erc
European Research Council
Established by the European Commission

GORDON AND BETTY MOORE FOUNDATION

UNIVERSITÉ DE GENÈVE