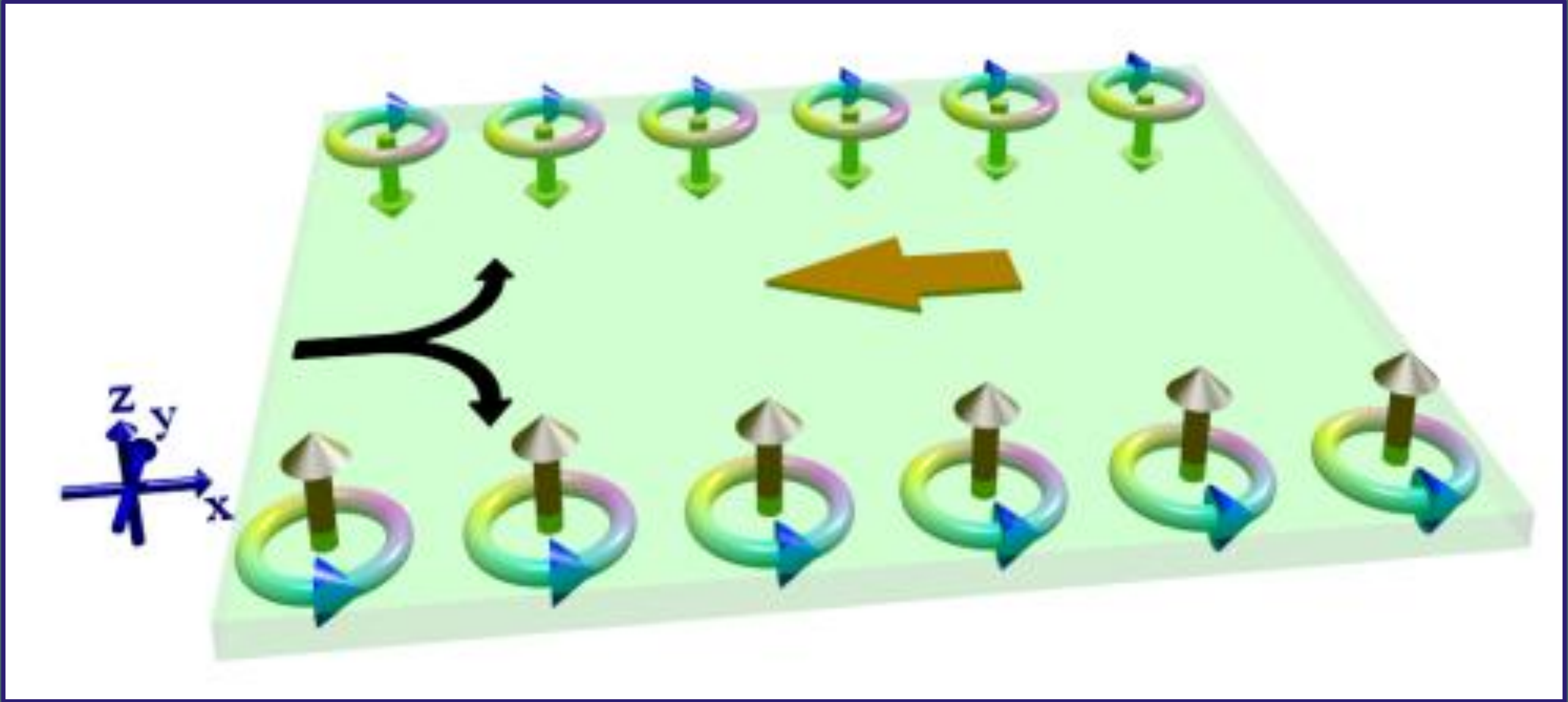
Orbitronics: from transport to topology

Speaker: Tarik P. Cysne (UFF-RJ)

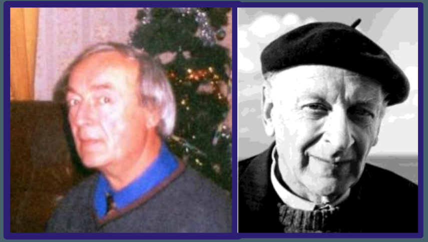
Instituto de Física
Universidade Federal Fluminense



Part I: Introduction

Brief History

Theory: Dyakonov-Perel



(1971)

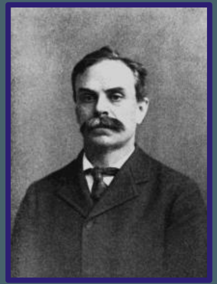
Intense activity in SHE:
- Intrinsic x extrinsic
- Quantum SHE
- Topological Insulators

...

Poor interest in OHE

Direct experimental observation of OHE!

(1879)



Hall effect

(1965)

Mott Scattering

(1999/2000)

Theory/Experiment:
Spin Hall Effect
(Mott mechanism)

(2005/06)

Theory:
Orbital Hall effect
(analog to SHE)

(2016) (2021/22)

Renewed interest in the OHE pushed by theoretical works.

Extrinsic mechanism
(impurity dependent)

Intrinsic mechanism
(Band structure)

Motivation


FUTURE VENTURES
122 YEARS OF MOORE'S LAW
MECHANICAL
RELAY
VACUUM TUBE
TRANSISTOR
INTEGRATED CIRCUIT
1E+13
1E+11
1E+09
1E+07
1E+05
1,000
10
0.1
0.001
1E-05
1E-07
1E-09
ANALYTICAL ENGINE
HOLLERITH TABULATOR
MONROE CALCULATOR
IBM TABULATOR
NATIONAL ELLIS 3000
ZUSE 3
COLOSSUS
ENIAC
WHIRLWIND
UNIVAC 1
IBM 1620
DEC PDP-1
DEC PDP-8
IBM 360
DATA GENERAL NOVA
APPLE II
SUN 1
IBM PC
DEC VAX 11 MODEL 780
APPLE MACINTOSH
COMPAQ DESKPRO 386
PENTIUM PC
IBM ASCI WHITE
POWER MAC G4
IBM BLUE GENE
DELL XPS 630
NVIDIA GTX 280
NVIDIA GTX 680
NVIDIA TITAN X
MYTHIC M.2
TESLA DOJO
GOOGLE TPU4
TESLA FSD
1900
1905
1910
1915
1920
1925
1930
1935
1940
1945
1950
1955
1960
1965
1970
1975
1980
1985
1990
1995
2000
2005
2010
2015
2020
2025

Motivation

Changing the paradigm of information technology

Spintronics: Use the spin of e^- ($\hat{S}$) to store and process information

Fundamentals of spintronics:

1 -spin-injection

2 -spin-manipulation

3 -spin-detection

Preferable by electrical means ($\vec{E}$)

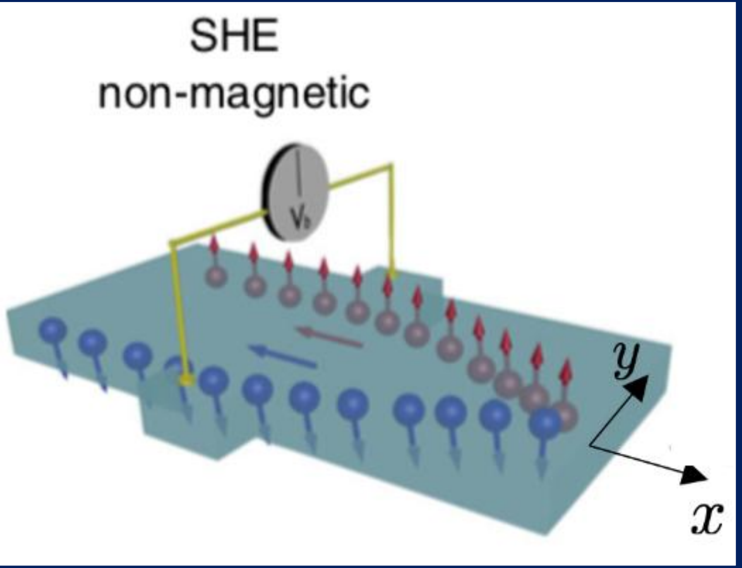
Problem: $\vec{E}$ does not couple directly with $\hat{S}$… ☹ ☹ ☹

The use of materials with strong spin-orbit coupling (SOC). 😐 😐 😐

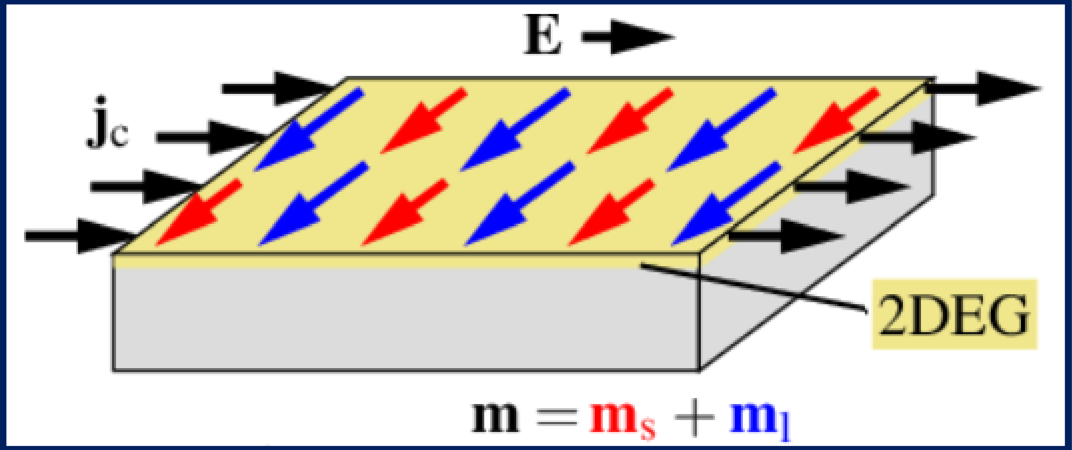
Some Important effects in spintronics

Spin Hall effect

[J. Sinova, et. al. RPM. 87, 1213 (2015)]

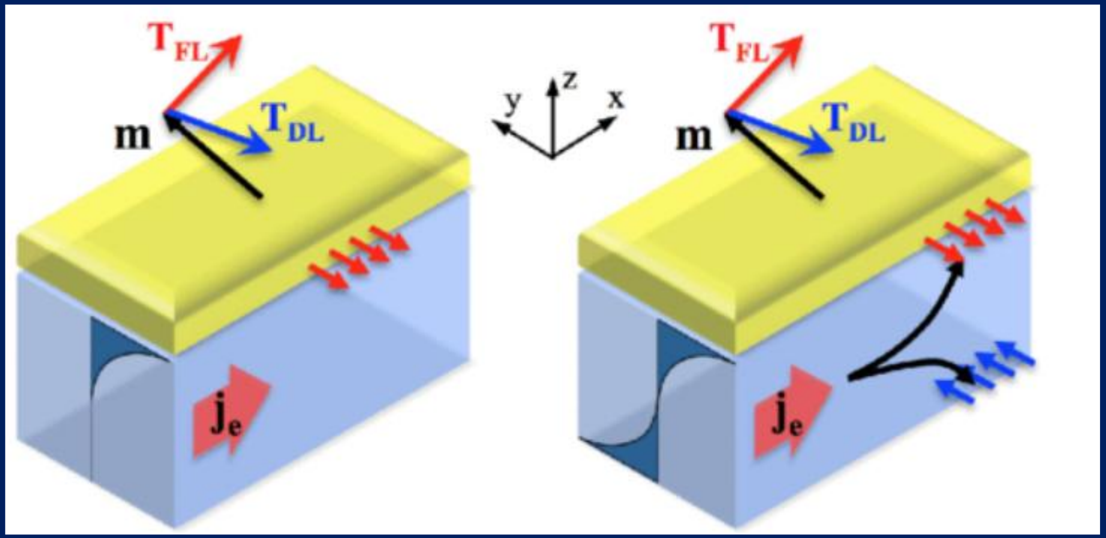


Spin Edelstein effect

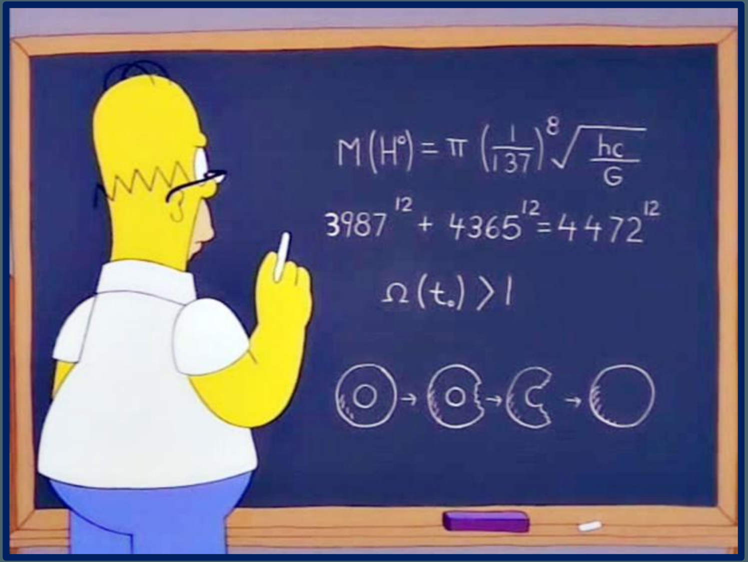


Spin-orbit torque

[A. Manchon, et. al. RPM. 91, 035004 (2019)]

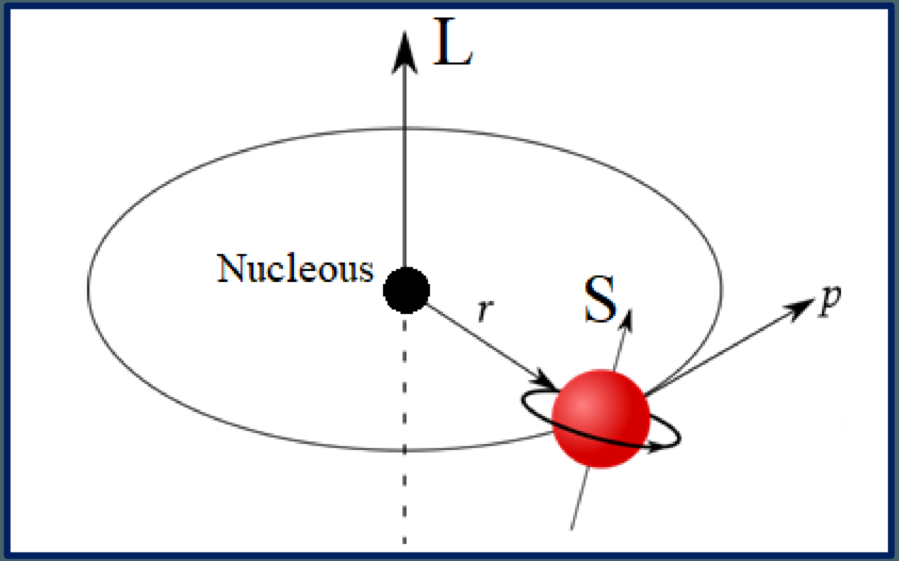


Can we overcome the need for strong spin-orbit coupling?

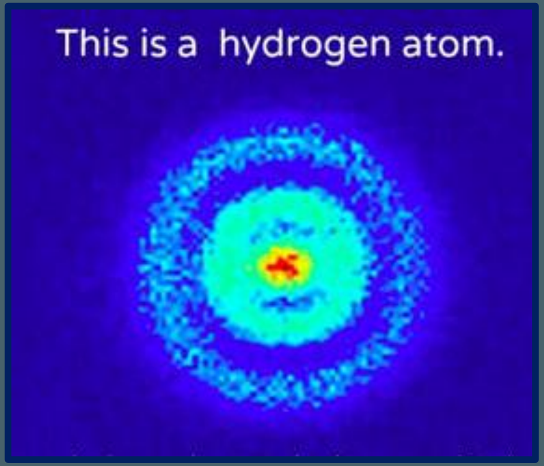


From Beginning

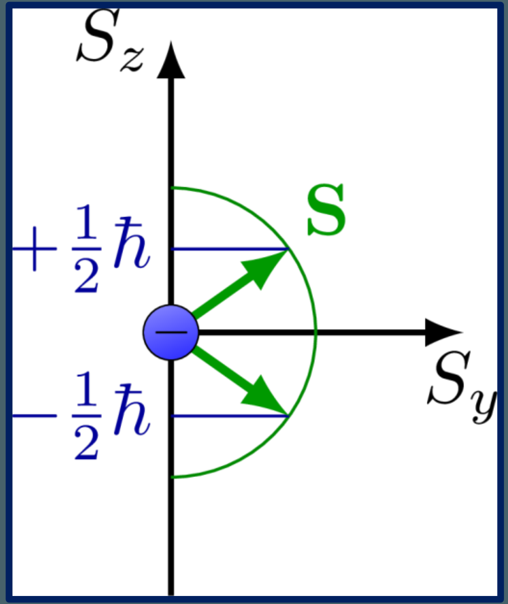
An atom:



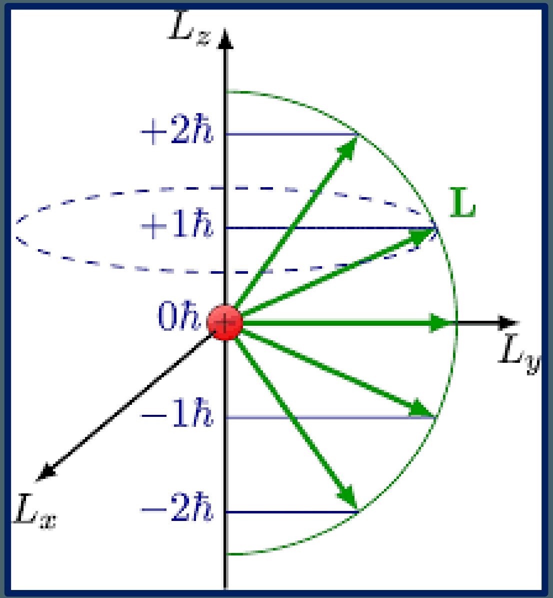
Charge:



e^- -Spin:

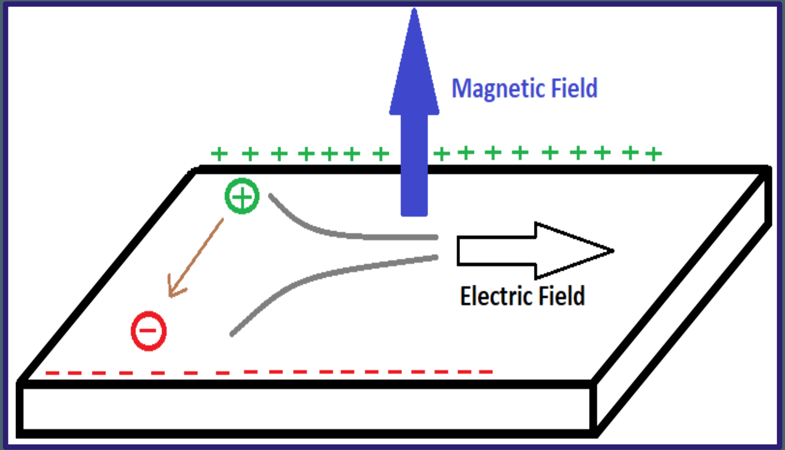


e^- -Orbital angular momentum:



Hall Effects

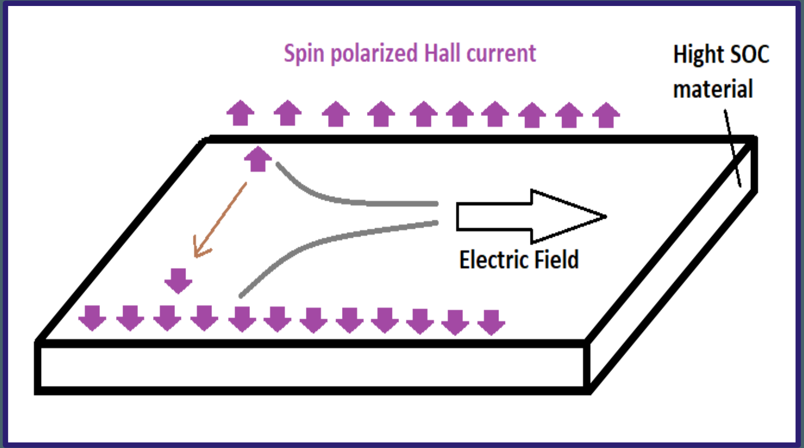
"Charge" Hall Effect



Time Reversal Symmetry Breaking

(E.g. External Magnetic Field)

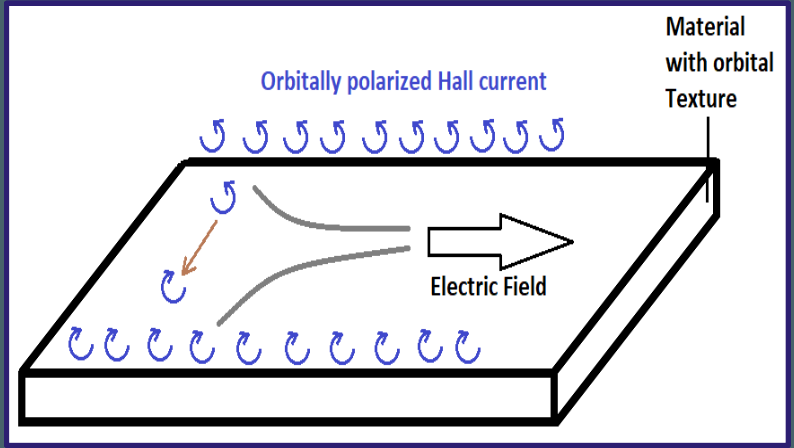
Spin Hall Effect (SHE)



High SOC systems

(E.g. material with a high atomic number Z ☹)

Orbital Hall Effect (OHE)

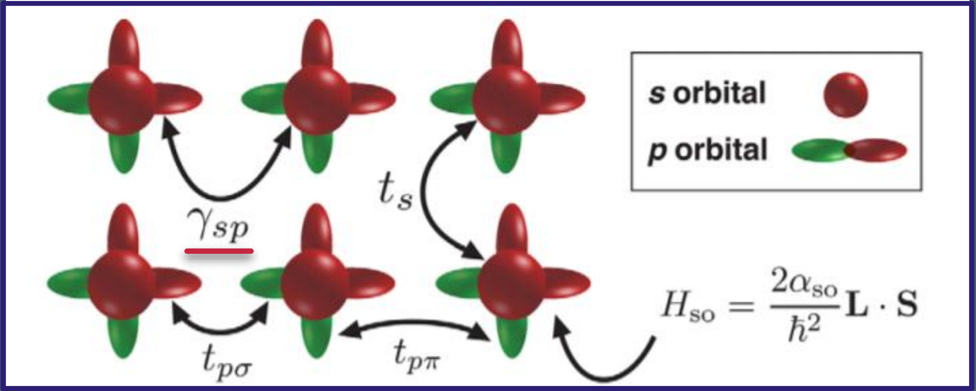


Solids with multi-orbital texture and strong inter-orbital hybridization

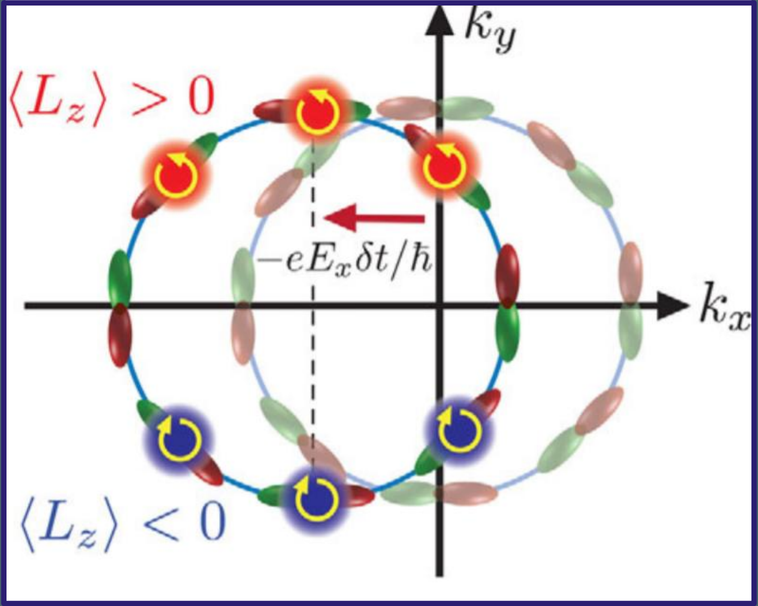
(Occurs even in the absence of SOC ☺)

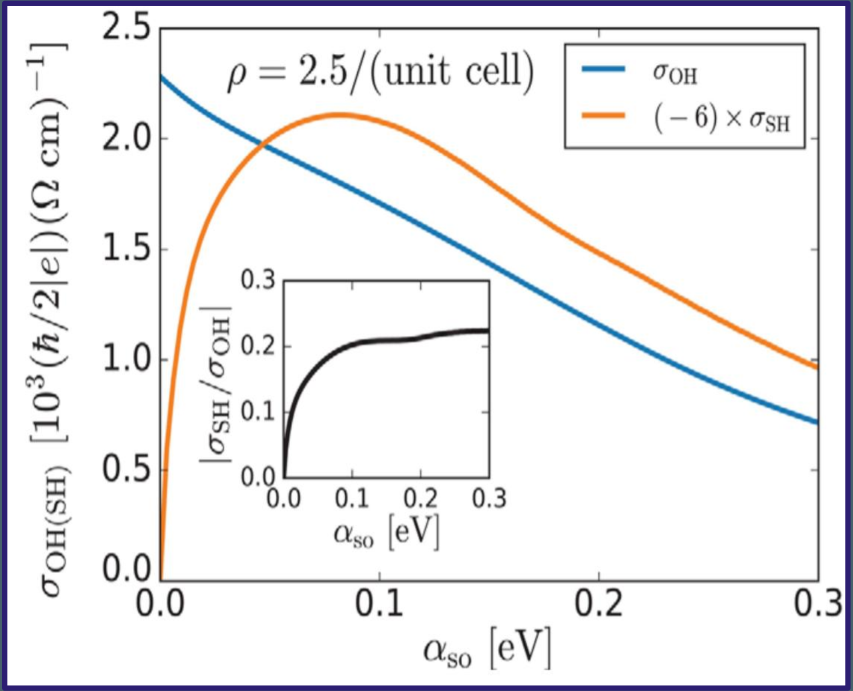
Intrinsic mechanism of OHE ***(3D Metals)***

Multi-orbital solid with sp Hybridization



Intrinsic OHE is a consequence of orbital texture:





(i)- OHE precedes the SHE
(ii)- The OHE is converted in SHE by SOC: $\vec{L}.\vec{S}$
(iii)- The OHE occurs even in absence of SOC! ☺ ☺ ☺

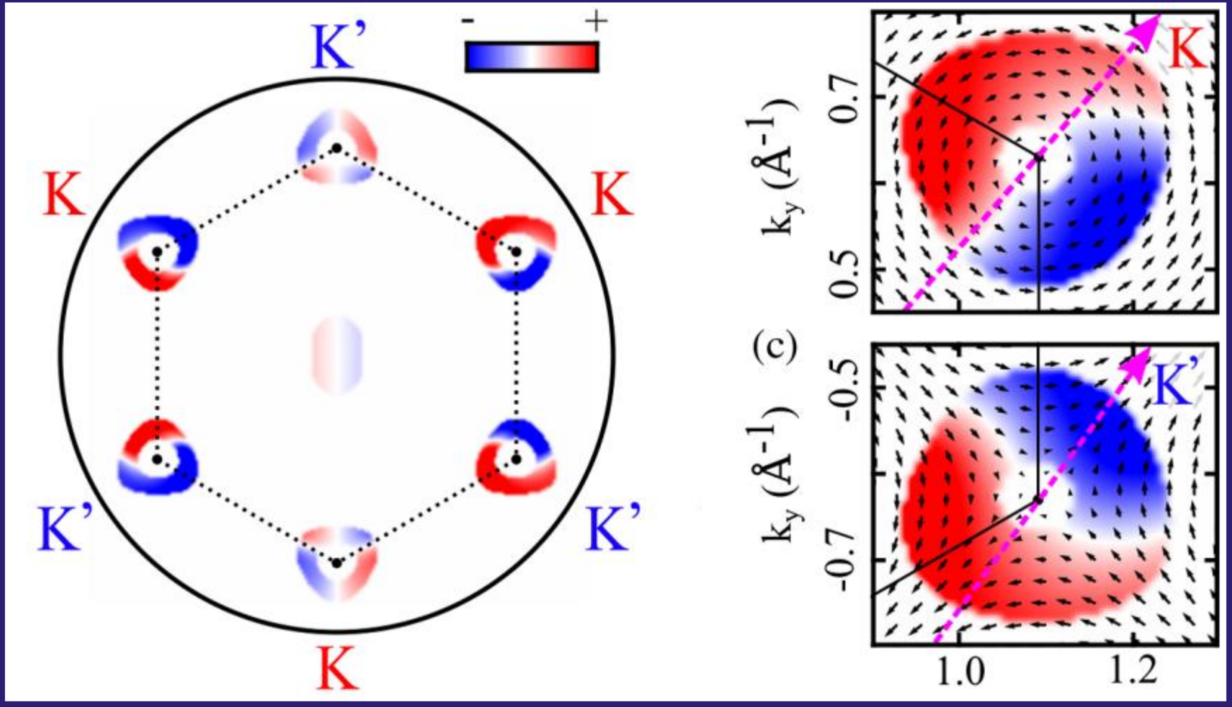
[D. Go, et. al. PRL. 121, 086602 (2018)]

Orbital Textures

OAM texture: $\langle L_{x,y,z} \rangle = \langle u_{nk} | \hat{L}_{x,y,z} | u_{nk} \rangle$

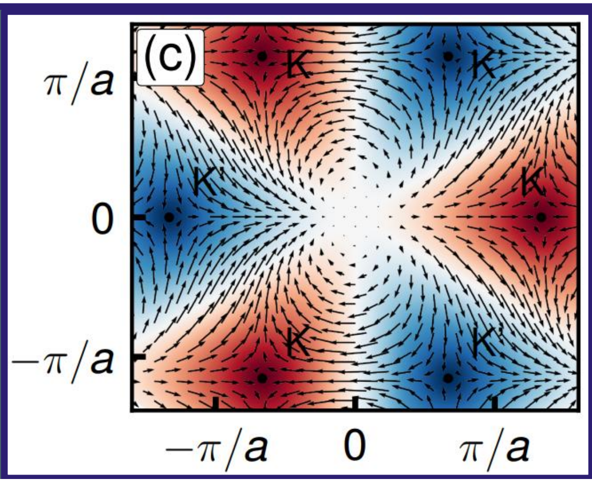
Experiment

Can be measured by TRDPAD (time-reversal dichroism in photoelectron angular distributions):



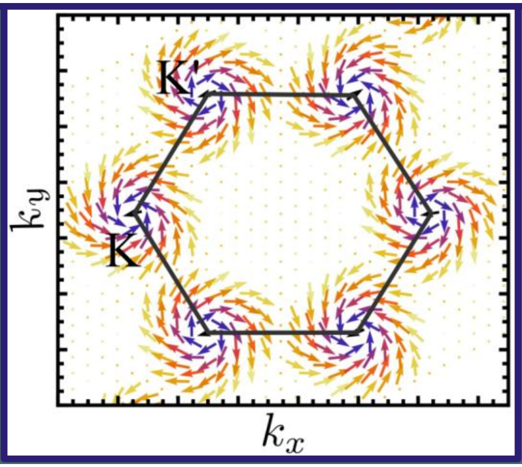
[S. Beaulieu, et.al. PRL 125, 216404 (2020)]

Valence band of 1L-MoS_2 (Theory)



[L. Canonico, et.al. PRB **101**, 161409(R)(2020)]

Borophene monolayer (Theory)



[F. Crasto de Lima, et.al., *Nano Lett.* 19 (9) 6564(2019)]

Important groups are studying orbitronics

nature communications
Article
https://doi.org/10.1038/s41467-024-46405-6

Orbitronics: light-induced orbital currents in Ni studied by terahertz emission experiments

Received: 15 July 2023
Accepted: 26 February 2024
Published online: 06 March 2024

Yong Xu[1,2,3,5], Fan Zhang[3,5], Albert Fert[2,4,5], Henri-Yves Jaffres[4,5], Yongshan Liu[2,3], Renyou Xu[2,3], Yuhao Jiang[2], Houyi Cheng[2,3] & Weisheng Zhao[1,2,3]

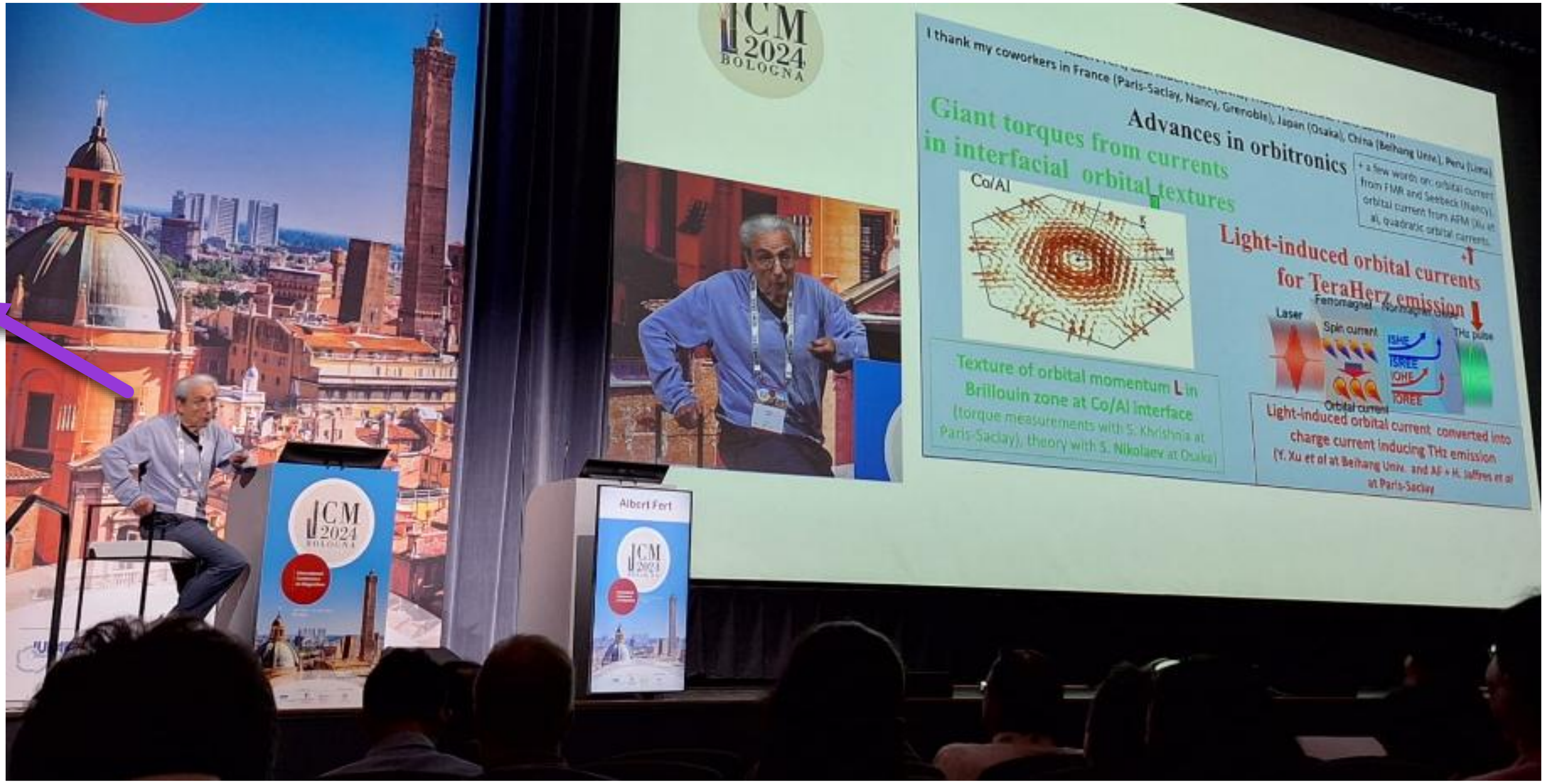
nature

Observation of the orbital Hall effect in a light metal Ti

Young-Gwan Choi, Daegeun Jo, Kyung-Hun Ko, Dongwook Go, Kyung-Han Kim, Hee Gyum Park, Changyoung Kim, Byoung-Chul Min, Gyung-Min Choi & Hyun-Woo Lee

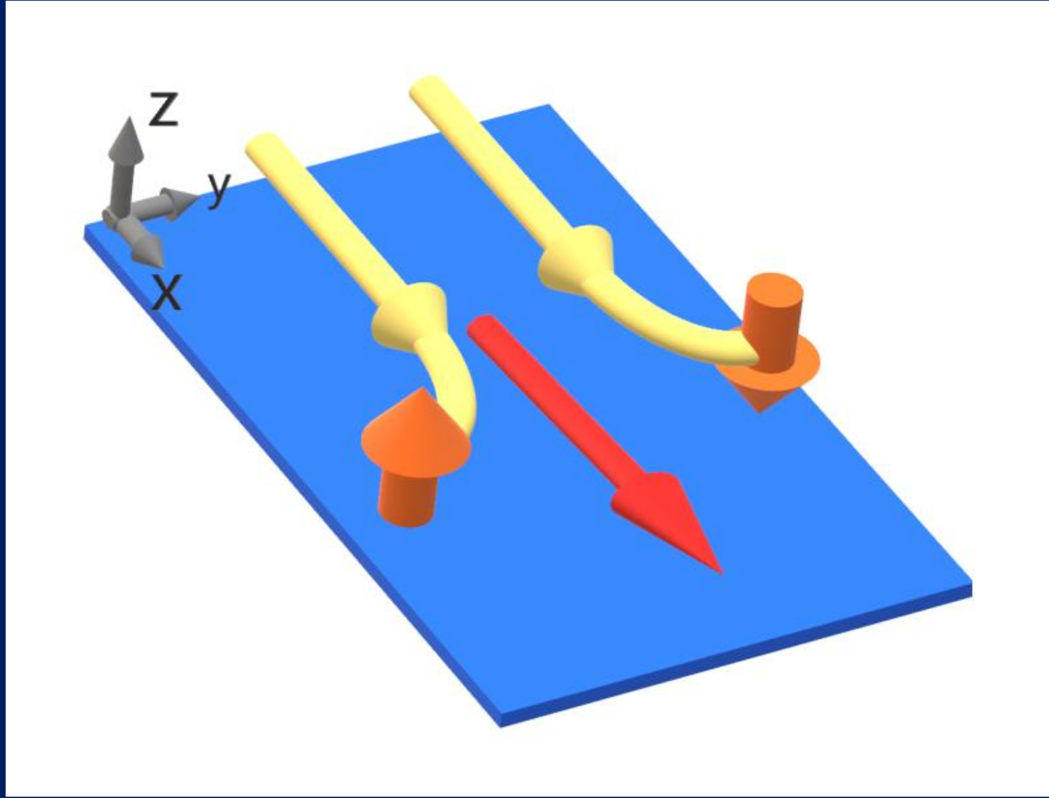
Nature **619**, 52–56 (2023) | Cite this article

Albert Fert !



Now… let’s talk about some of our work works : Orbitronics in 2D materials

Part II:
Orbital Hall effect



Orbital Hall Conductivity

$$\frac{\Omega^{X_z}_{n,\vec{k}}}{2\hbar} = \sum_{m\neq n} \mathrm{Im}\left[\frac{\langle u_{n,\vec{k}}|\hat{v}_x(\vec{k})|u_{m,\vec{k}}\rangle\langle u_{m,\vec{k}}|\hat{J}^{X_z}_y(\vec{k})|u_{n,\vec{k}}\rangle}{(E_{n,\vec{k}} - E_{m,\vec{k}})^2}\right]$$

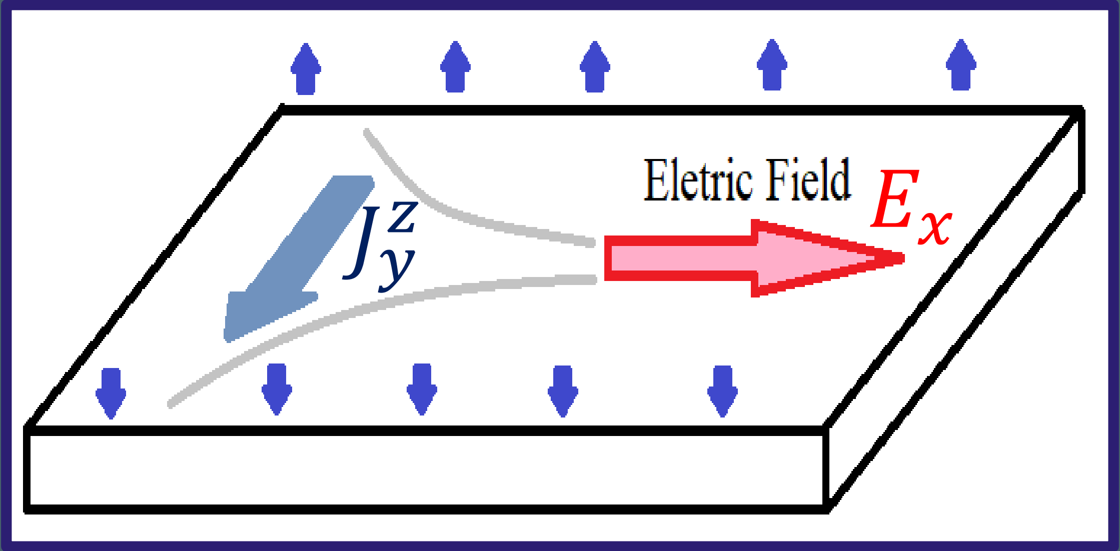
$$\sigma^{X_z}_{\mathrm{OH}} = e\sum_n \int \frac{d^2k}{(2\pi)^2} f_{n,\vec{k}}\Omega^{X_z}_{n,\vec{k}}$$

[T. P. Cysne, et. al., PRB 105, 195421 (2022)]

Orbital current operator:

$$\hat{J}^{L_z}_y(\vec{k}) = \frac{1}{2}[L_z\hat{v}_y(\vec{k}) + \hat{v}_y(\vec{k})L_z]$$

Intra-atomic approximation
(Localized electronic orbits)



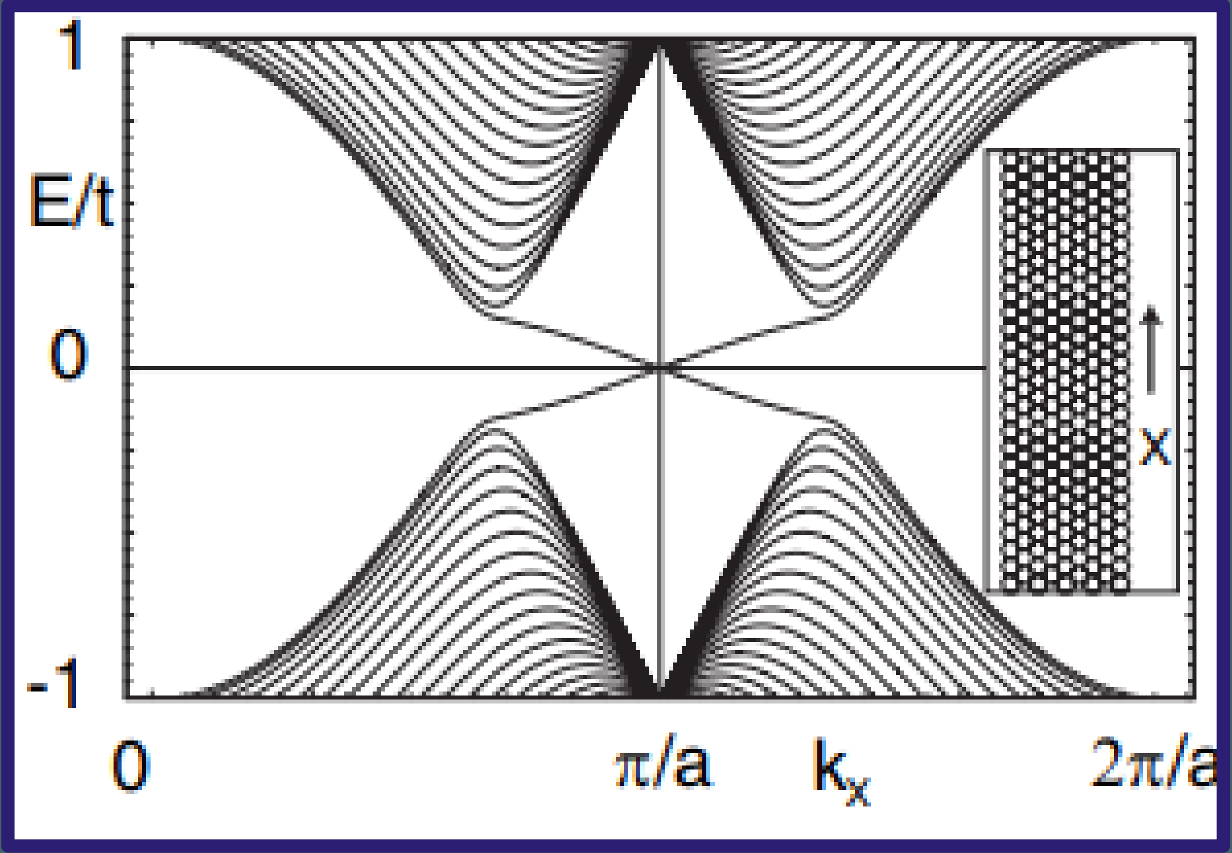
$$\langle J^{L_z}_y\rangle = \sigma^{L_z}_{OH}\mathcal{E}_x$$

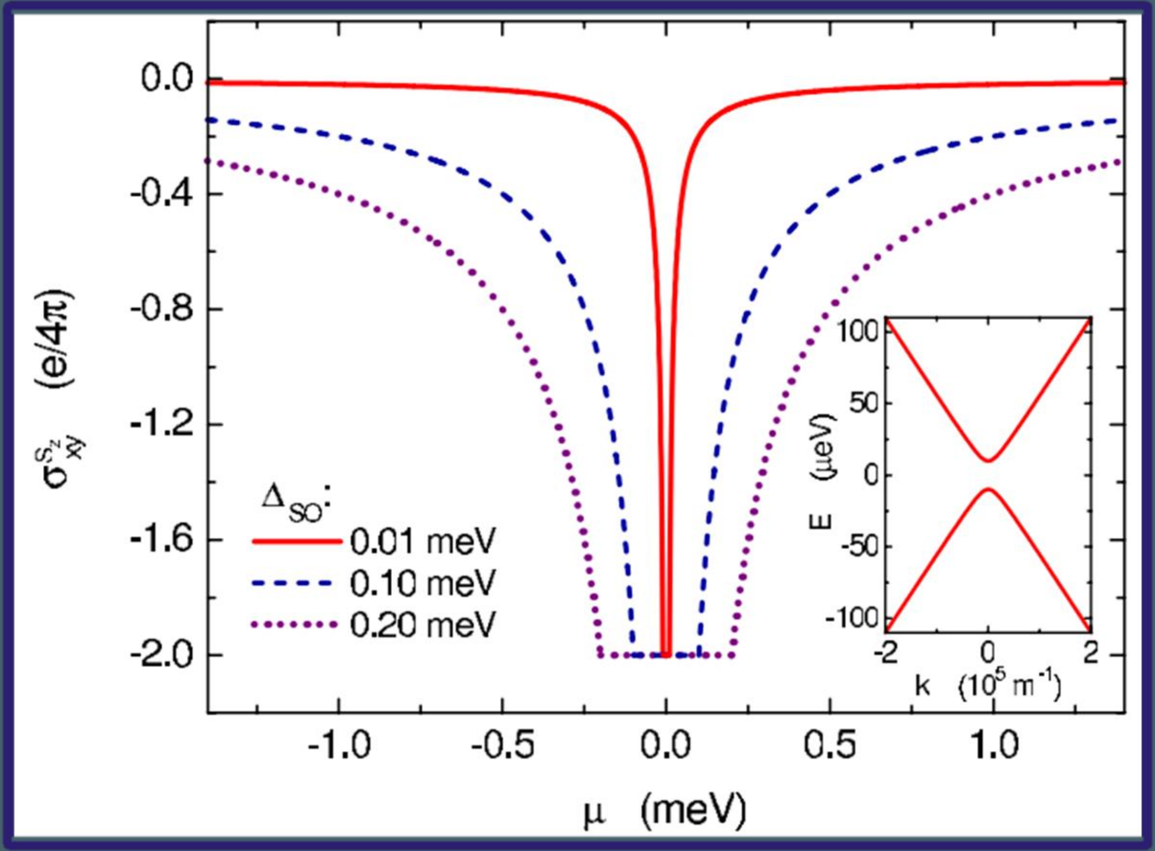
Talking about spin again (Quantum Spin Hall insulators Paradigm)

$$\langle J_y^{S_z} \rangle = \sigma_{SH}^{S_z} \mathcal{E}_x$$

$$\sigma_{SH}^{S_z} = \frac{e}{2\pi} C_S$$

Spin Chern number

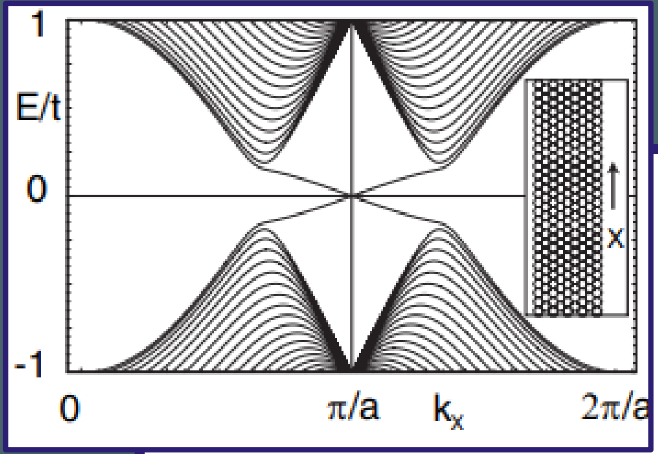




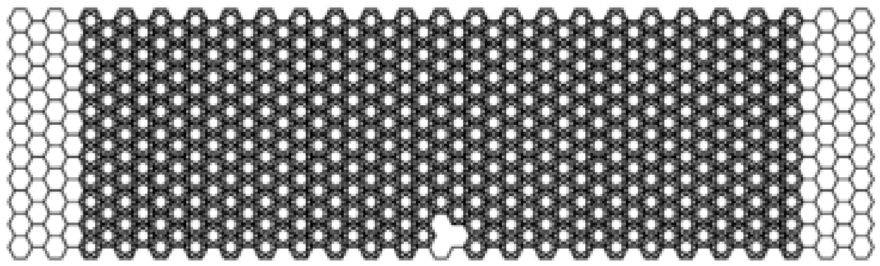
Talking about spin again (Quantum Spin Hall insulators Paradigm)

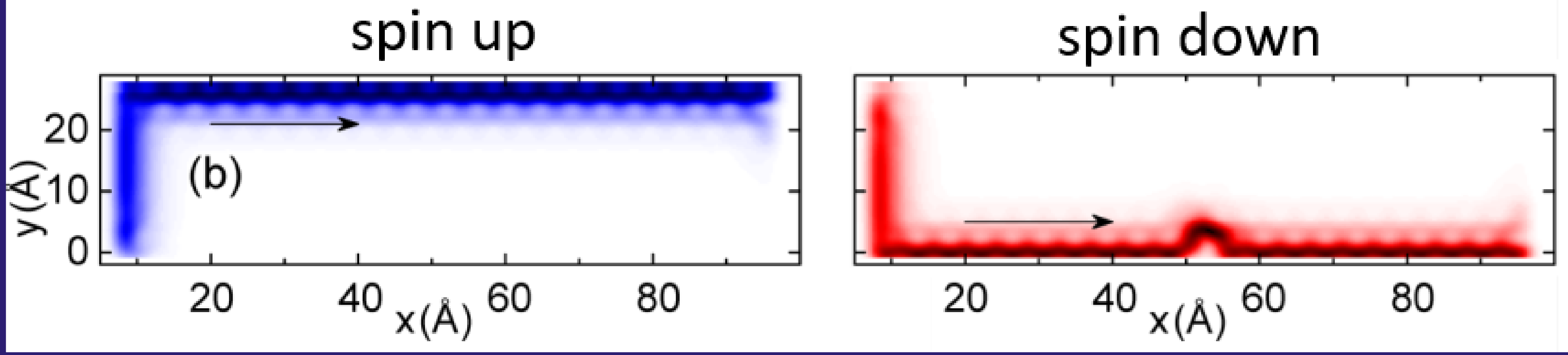
$$\langle J_y^{S_z} \rangle = \sigma_{SH}^{S_z} \mathcal{E}_x$$

$$\sigma_{SH}^{S_z} = \frac{e}{2\pi} C_S$$



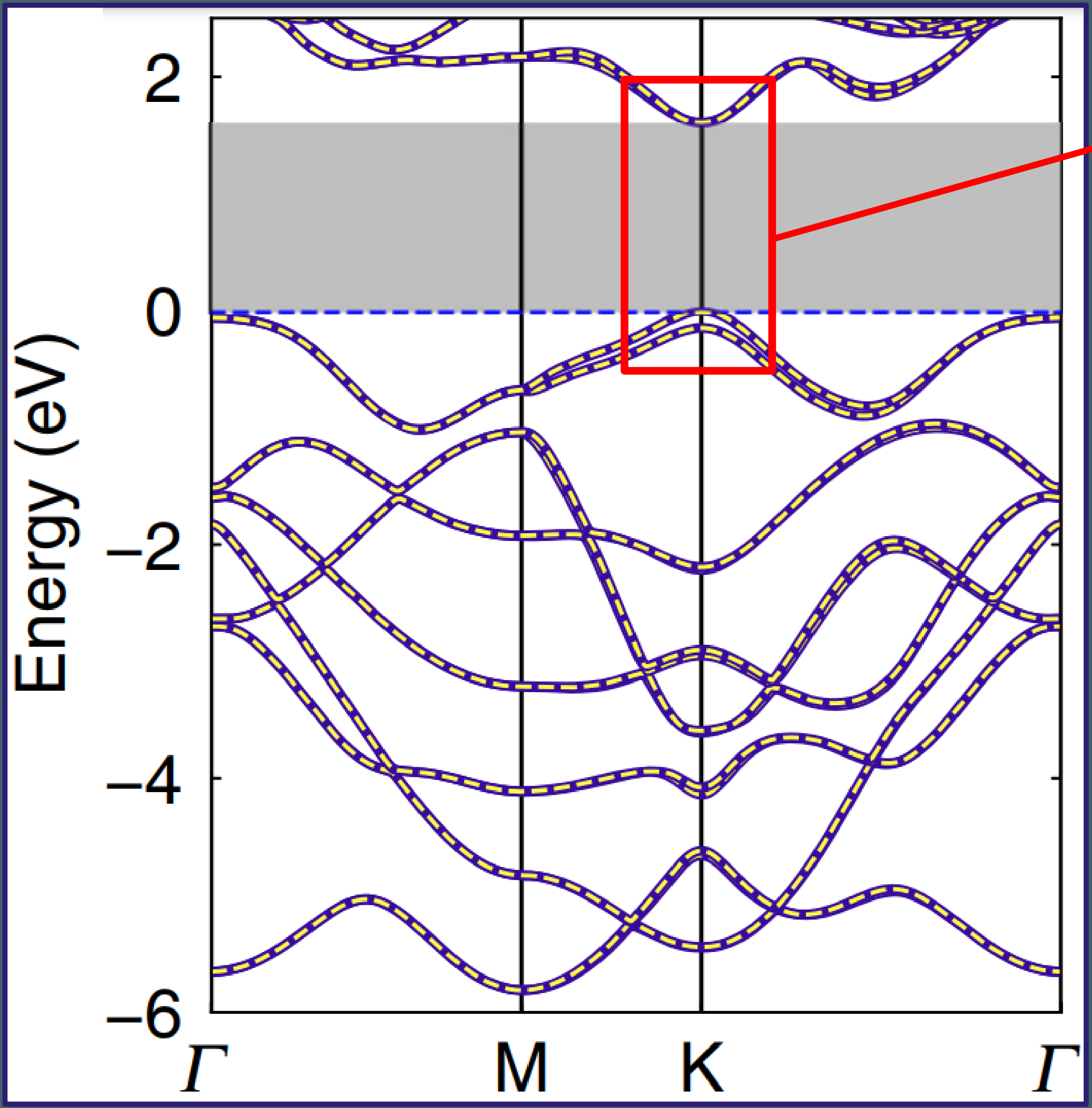
[L.F. Lima and C. Lewenkopf PRB 106, 245408 (2022)]





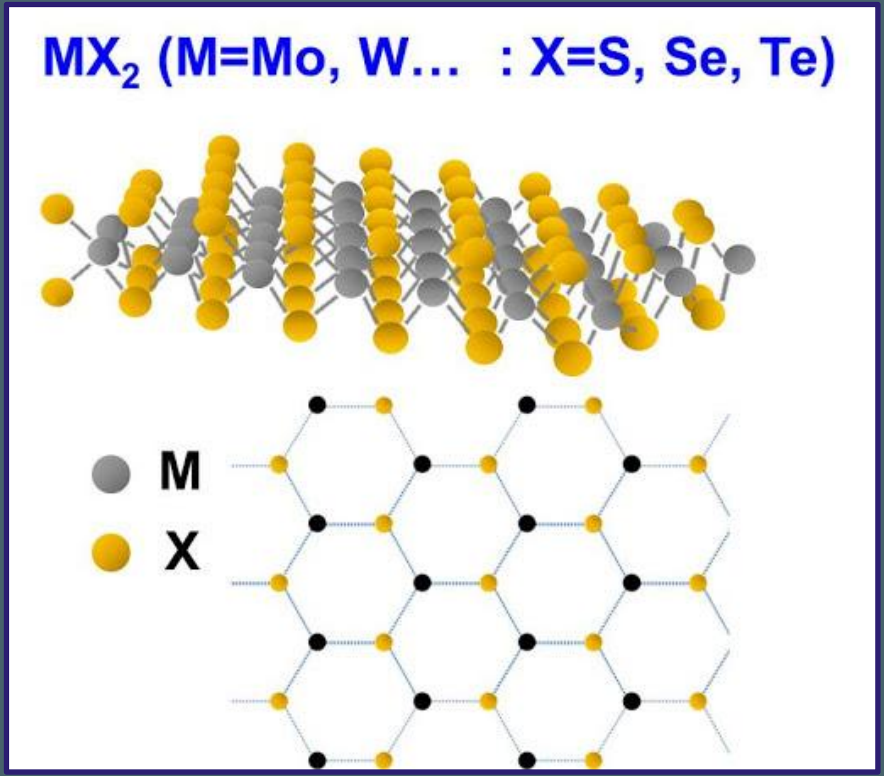
Multi-Orbital Two-dimentional materials

Monolayer of 2H-MoS_2

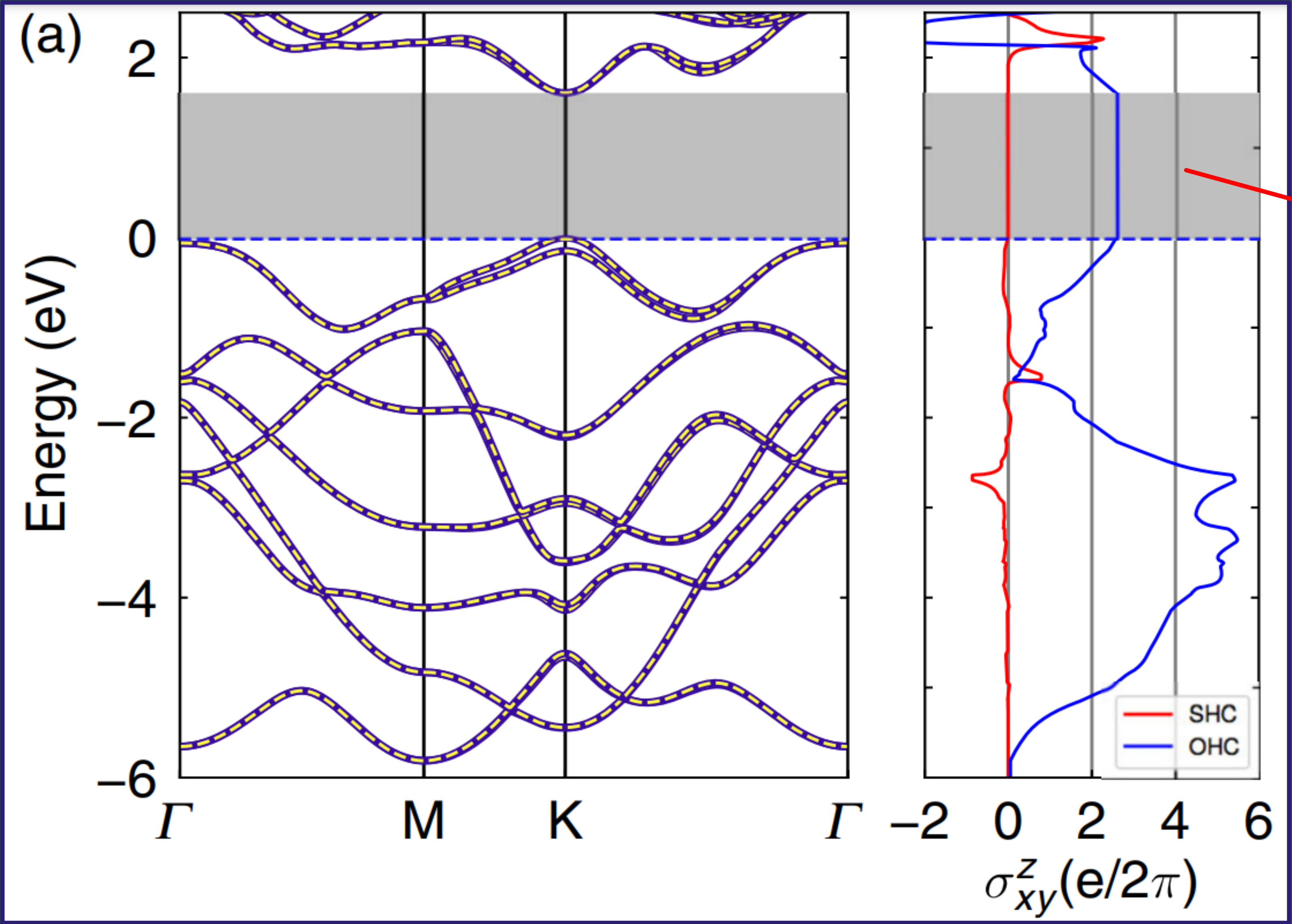


Conduction band: $\{d_{z^2}\}$

Valence band: $\{d_{x^2-y^2} \pm i d_{xy}\}$



OHE in Two-Dimensional Materials



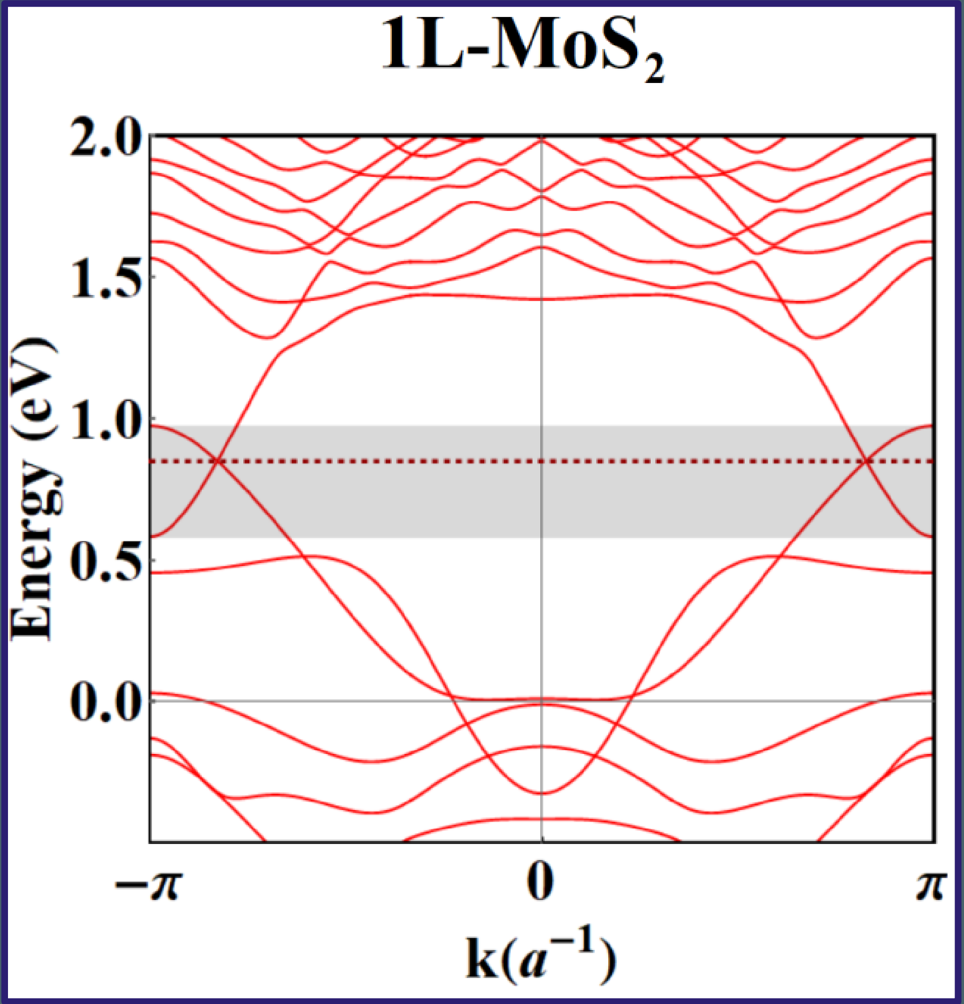
OH insulator

$\sigma_{OH} \neq 0$
For
$E_F \in$ Band-gap

[see. L. M. Canonico et. al., PRB **101**, 075429 (2020) and PRB **101**, 161409(R) (2020)]:

Orbital Chern number

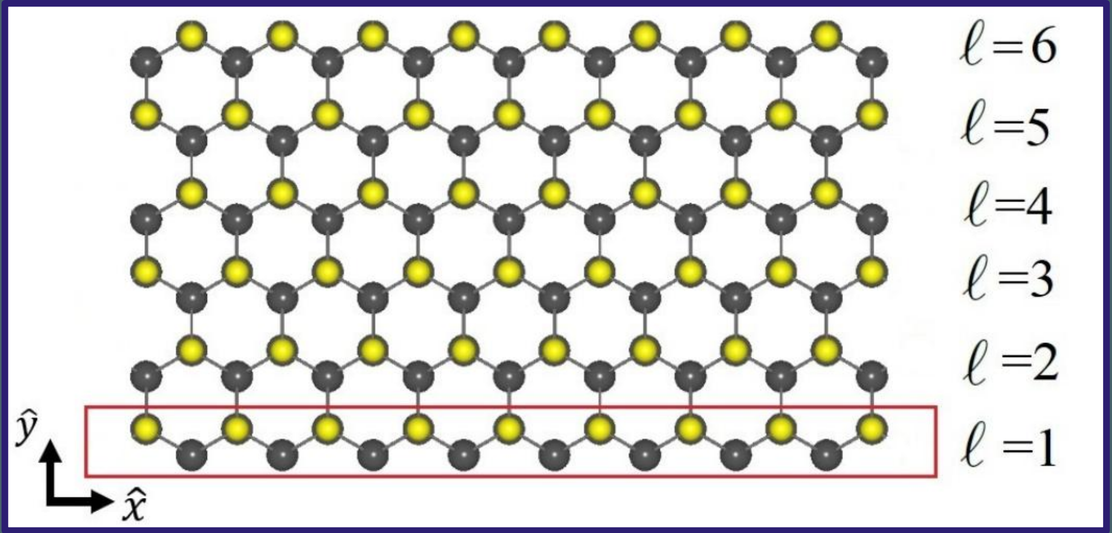
Zigzag Nanoribbons of 2H-TMDs has Lz-polarized edge-states. The **orbital Hall insulating phase** can be indexed by **Orbital Chern Number** [T. P. Cysne, et. al., PRL 126, 056601 (2021) and PRB 105, 195421 (2022)]:



Orbital Chern number:

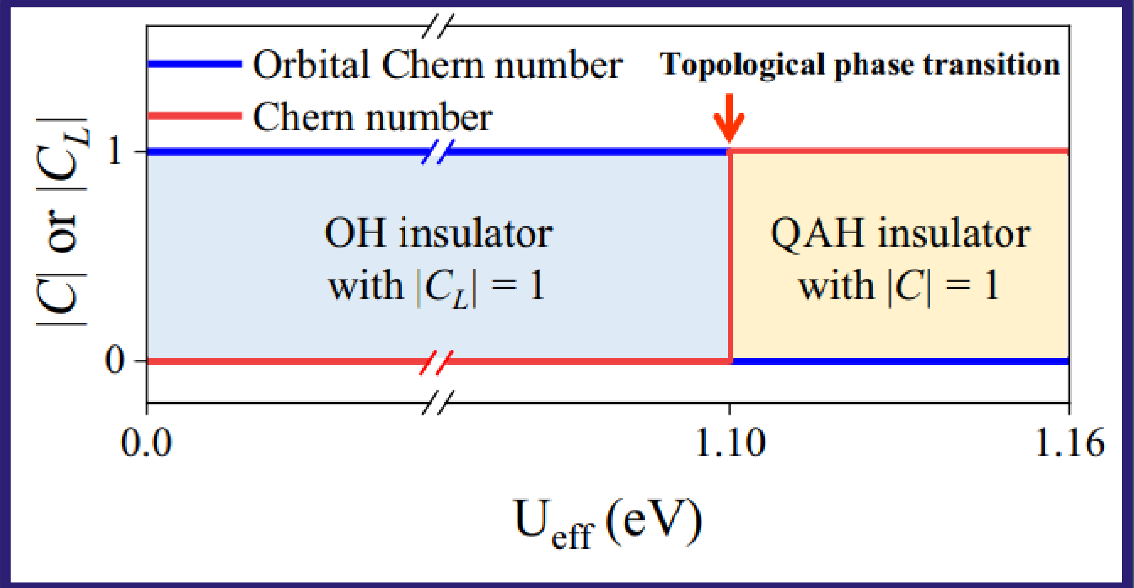
$$C_L = +1$$

Zigzag Nanoribbons:

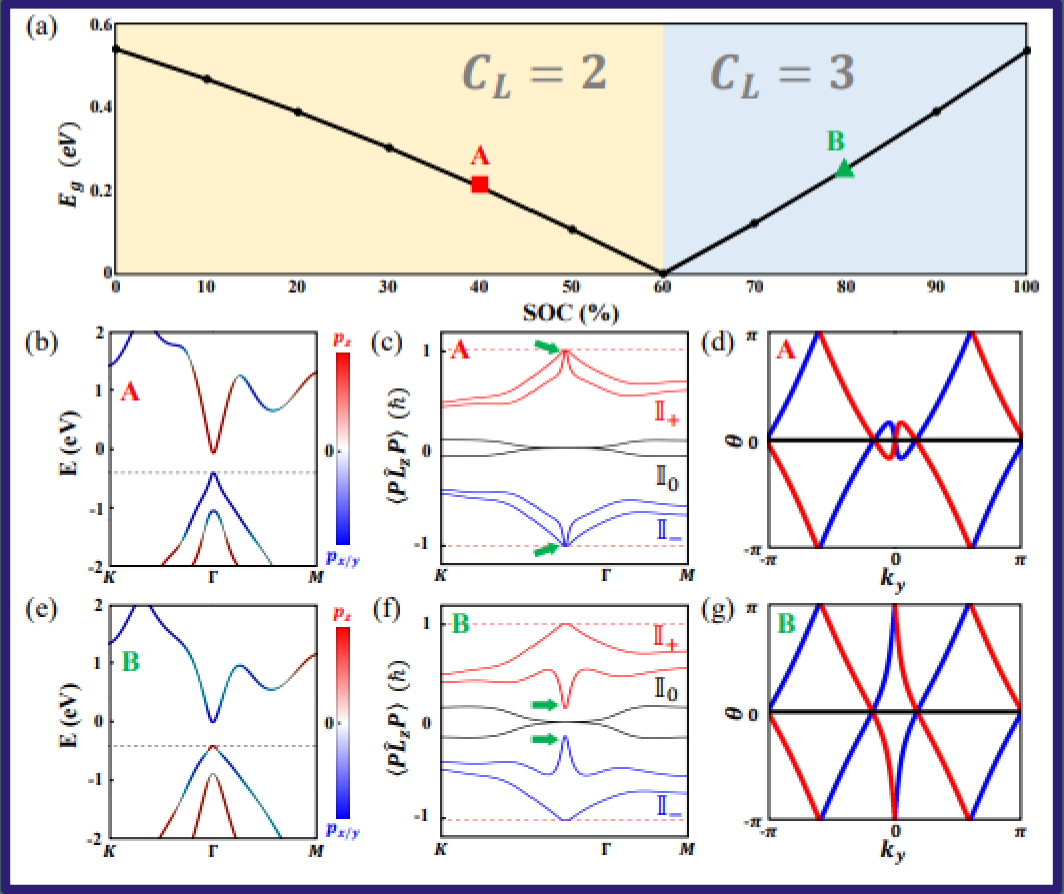


Orbital Chern number

Orbital Chern numbers can undergo topological phase transitions:



[Shilei Ji, et. al. , Phys. Rev. B 108, 224422 (2023)]

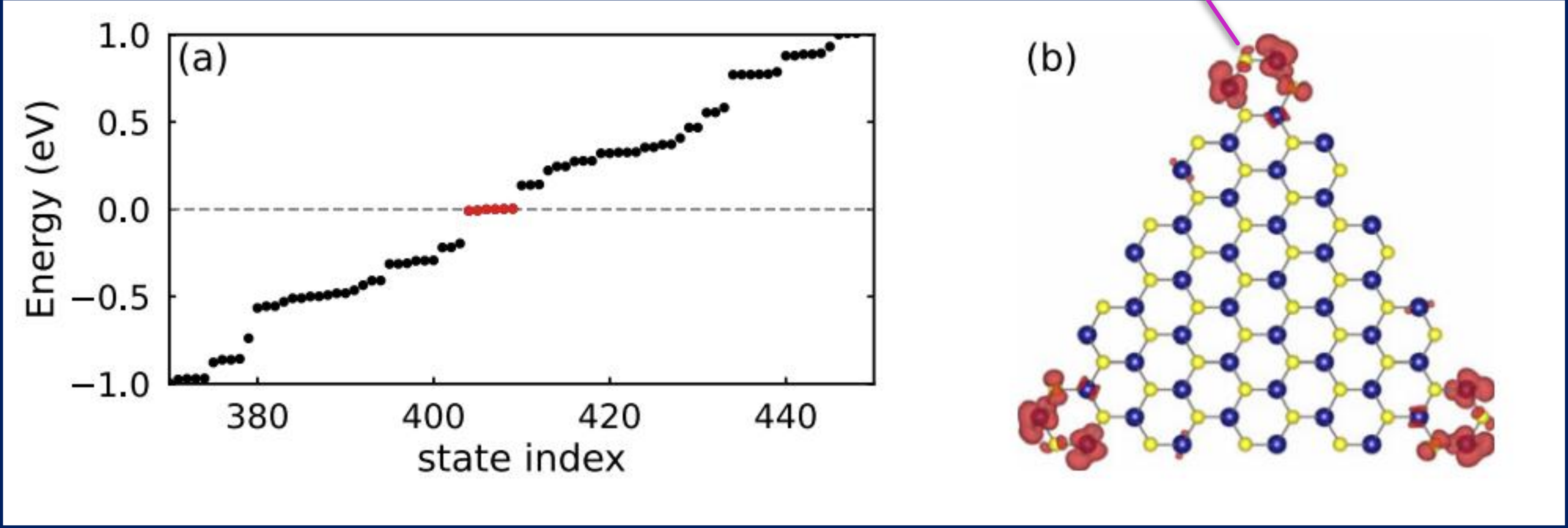


[Y.-T. Yao , et. al. , arXiv:2503.08138 (2025)]

Orbital Hall insulators and high Order topological insulators

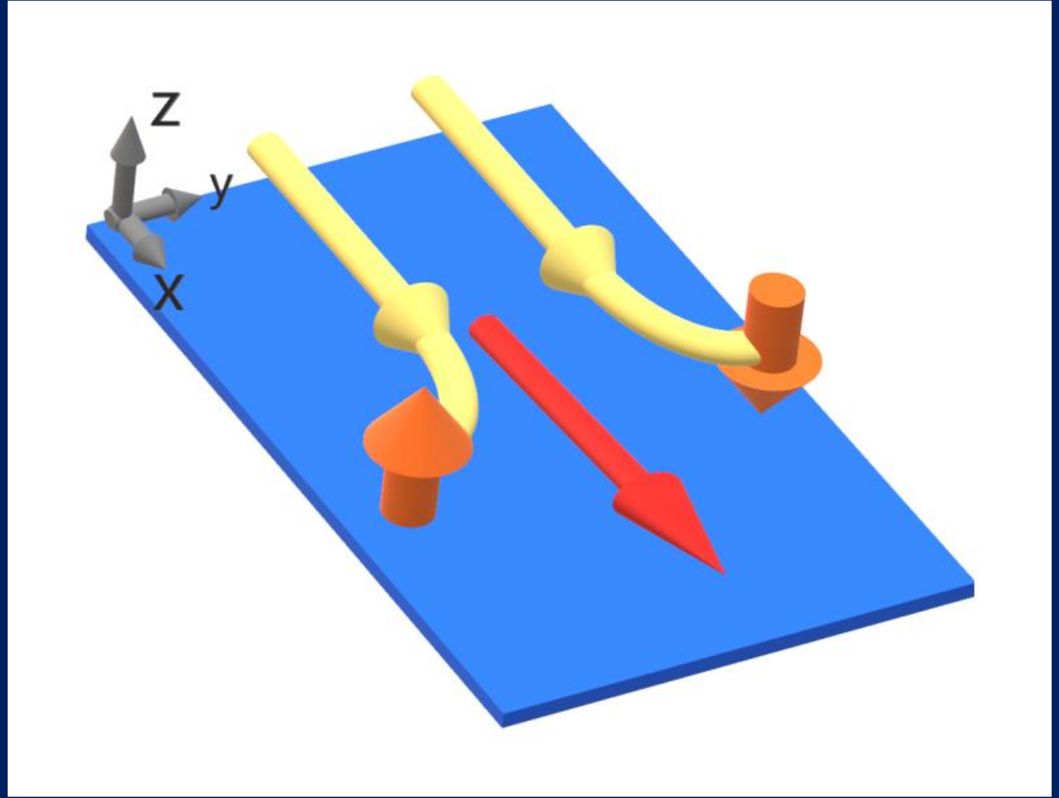
M. Costa, et. al., Phys. Rev. Lett. **130**, 116204 (2023)

$$Q_c^{(3)} = \frac{e}{3}[K_2^{(3)}] \bmod e$$



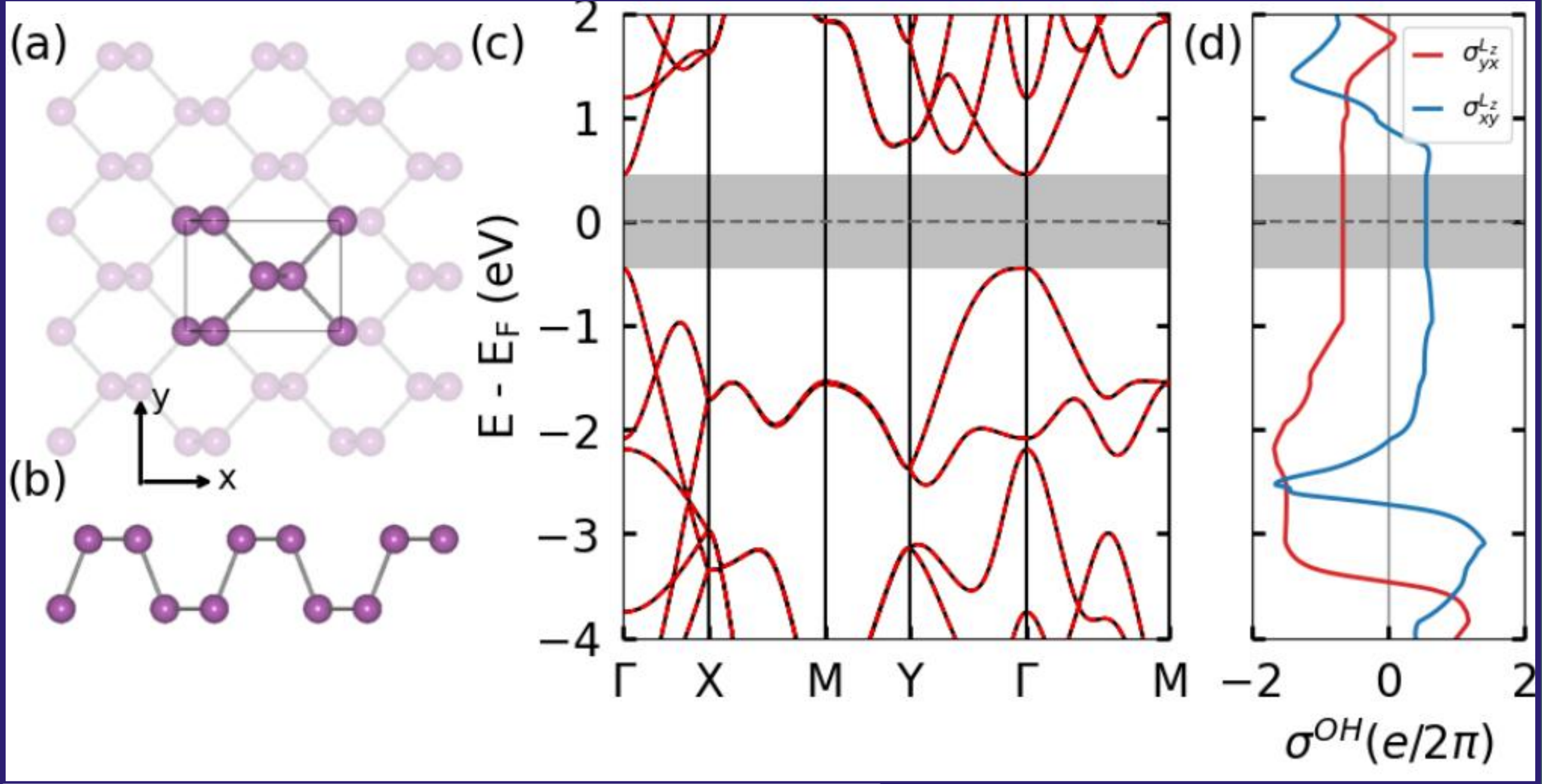
-2H-TMDs are higher-order topological insulators with protected corner states
-This HOTI phase appears to be related to the orbital Hall insulator phase

Part III:
OHE in other 2D materials



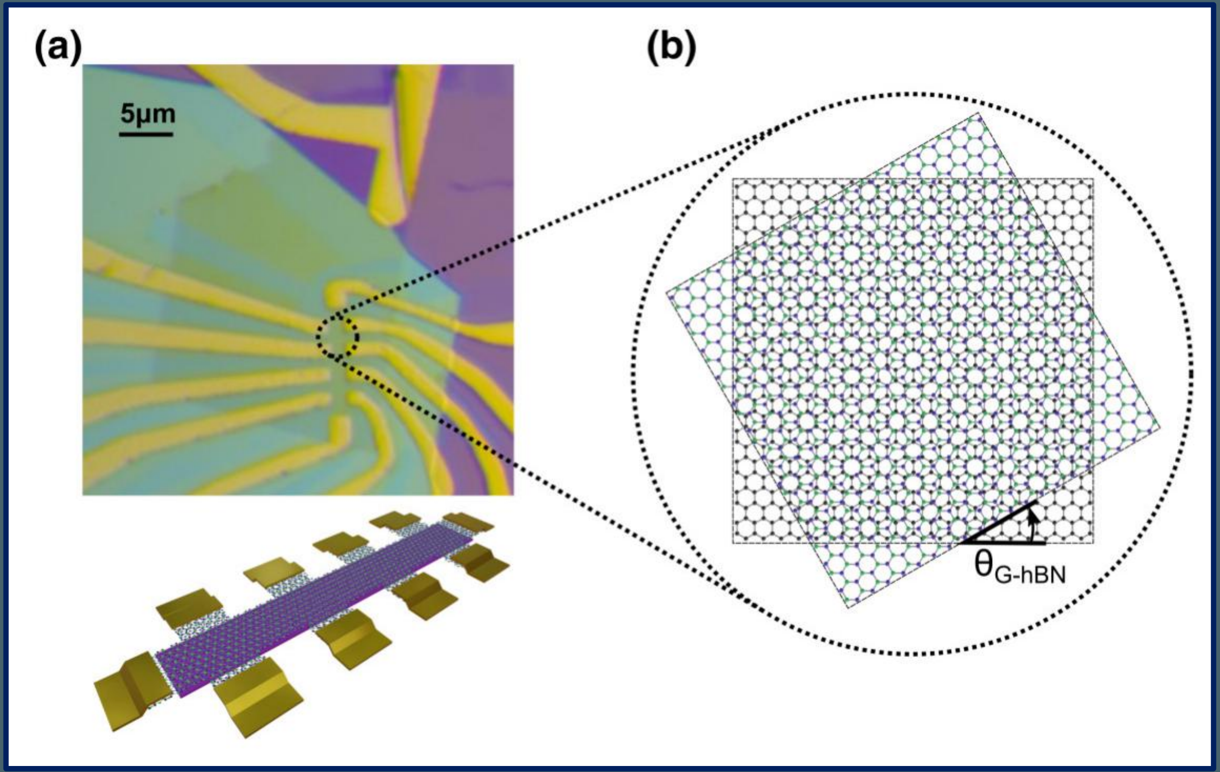
We found other two-dimensional orbital Hall insulators …

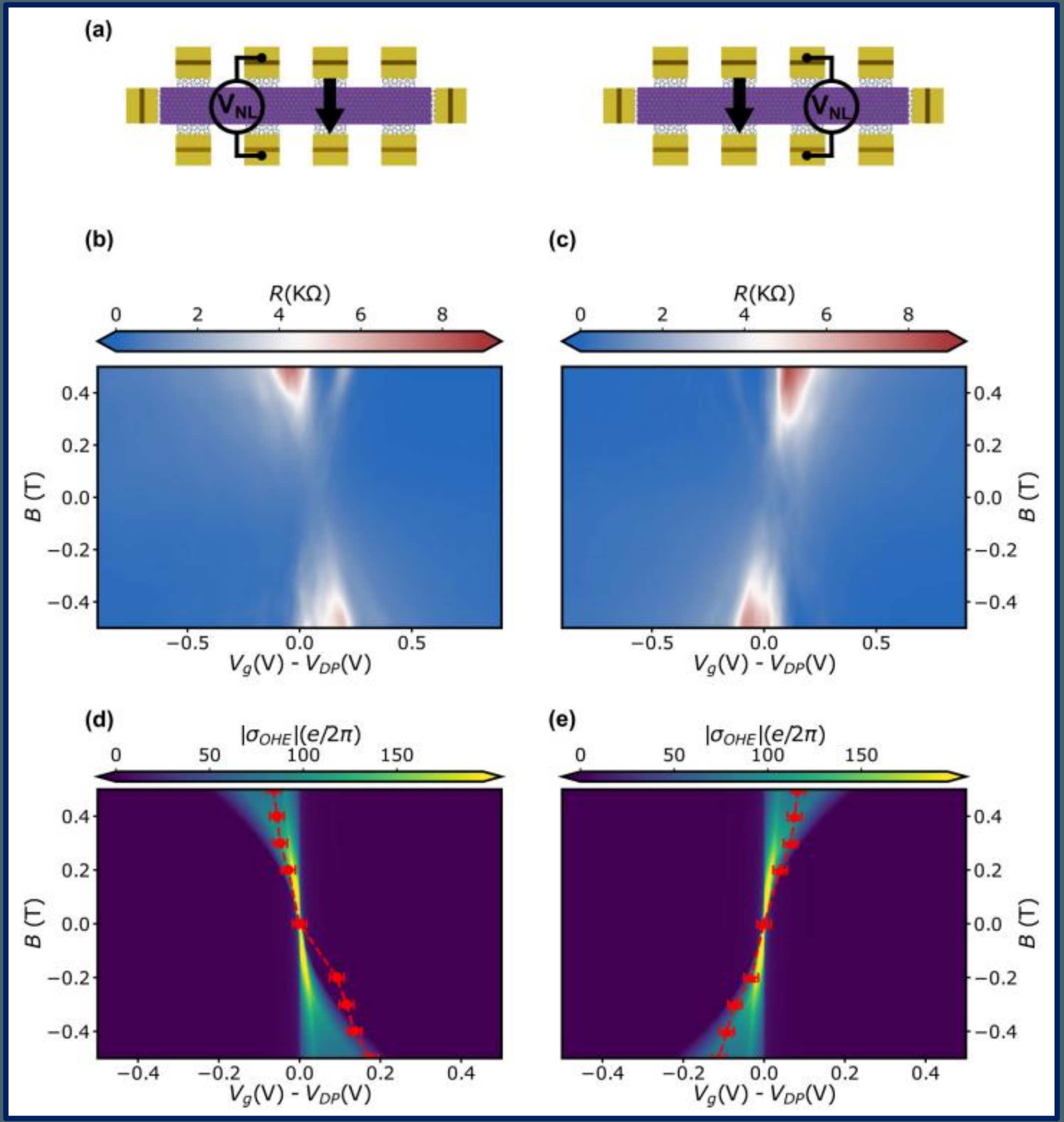
Phosphorene monolayer: anisotropic orbital Hall insulating plateau



[T. P. Cysne, et. al., PRB **108**, 165415 (2023)]

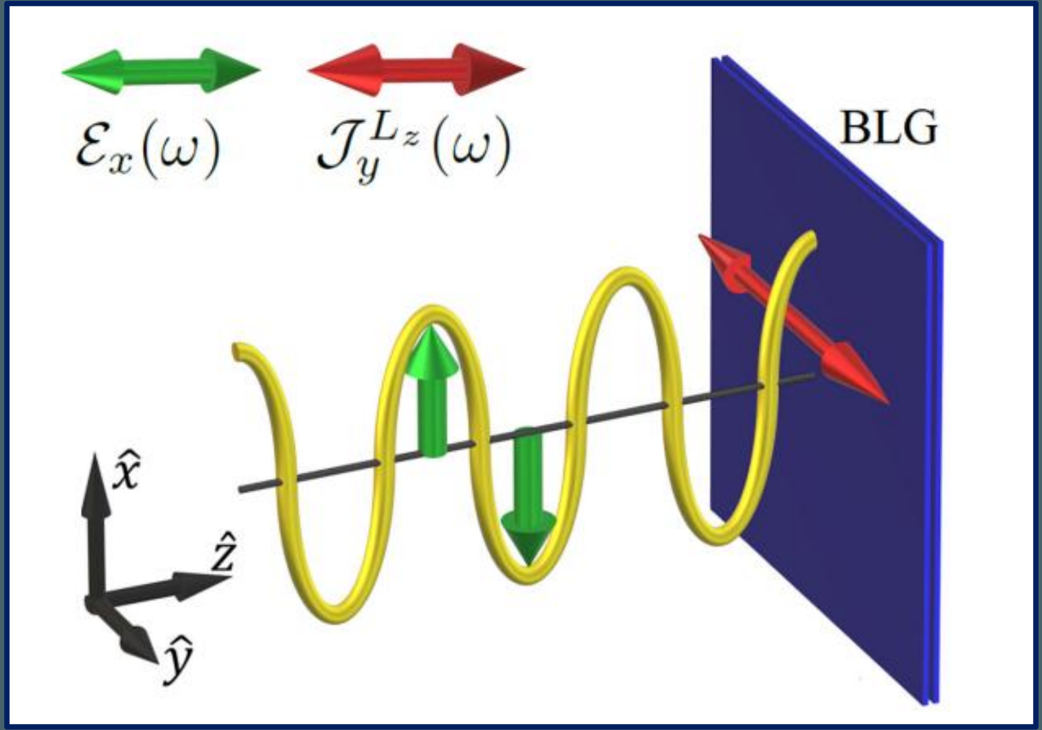
Experimental signature of OHE



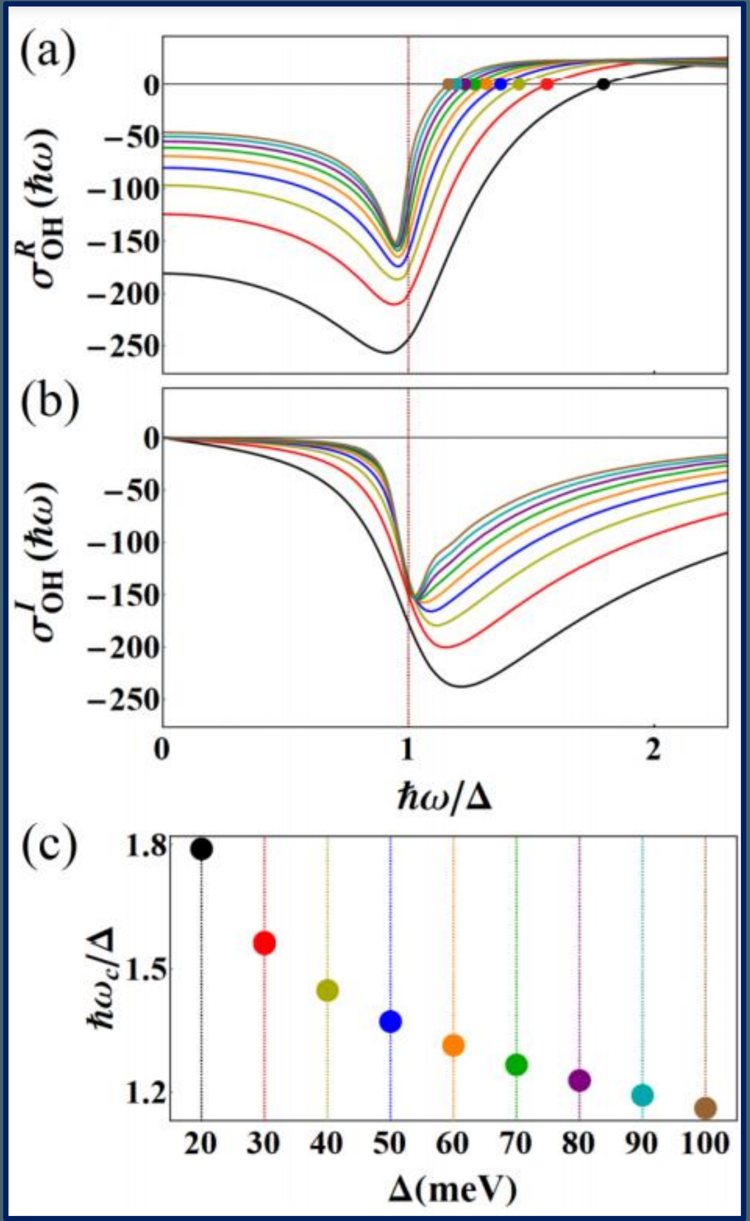


[J. Salvador-Sánchez, et. al., Phys. Rev. Research **6**, 0232 (2024)]

Interaction of materials with light



[T. P. Cysne, W. J. M. Kort-Kamp, and T. G. Rappoport, Phys. Rev. Research **6**, 023271 (2024)]



Final: Perspective for the future

1- Treatment of Disorder: How Disorder can impact the orbital response in materials?

2- Real space calculations: Numerical methods to compute the orbital accumulations in real space.

3- Going beyond intra-atomic approximation: Rigorous treatment of orbital angular momentum operator on the modern theory of orbital magnetization. For what condition intra-atomic approximation is good or bad?

Review on 2D-materials orbitronics

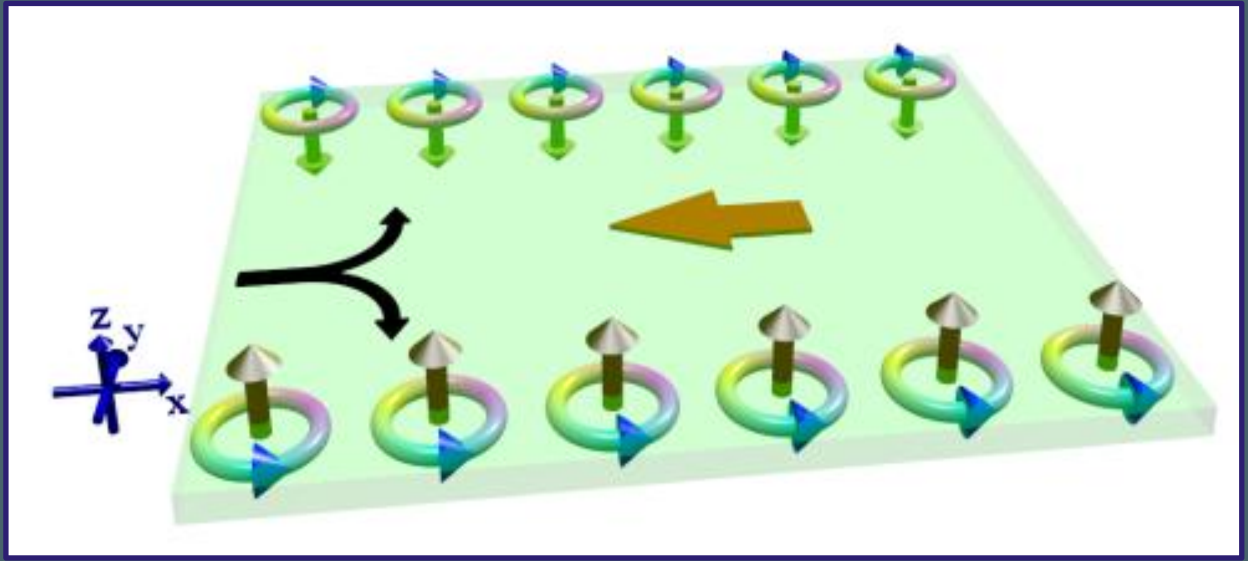
npj | spintronics

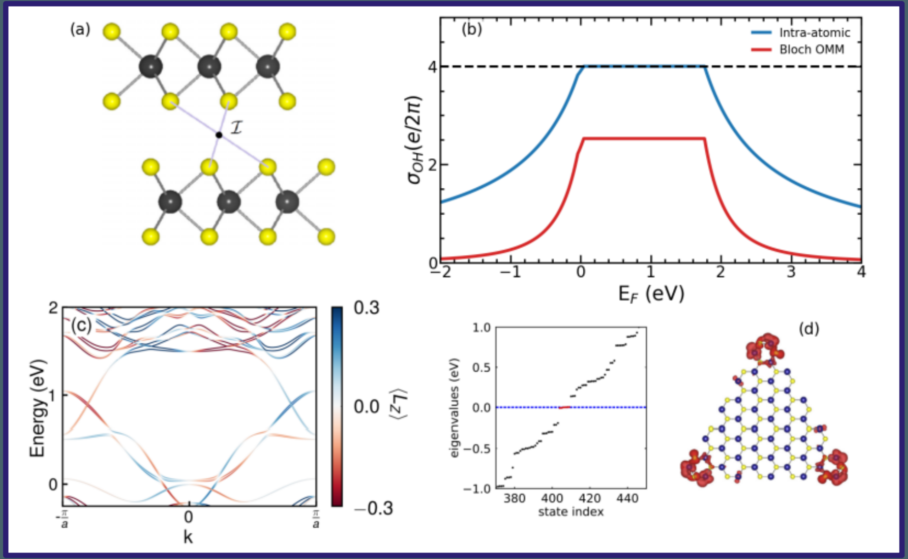
Review

https://doi.org/10.1038/s44306-025-00103-1

Orbitronics in two-dimensional materials

Tarik P. Cysne[1] ✉, Luis M. Canonico[2], Marcio Costa[1], R. B. Muniz[1] & Tatiana G. Rappoport[3,4,5] ✉





People involved

Prof. R. B. Muniz
(UFF/BR)

Profa. T. G. Rappoport
(UFRJ/BR)

Prof. M. Costa
(UFF/BR)

Dr. L. M. Canonico
(ICN-2/spain)

Dr. T. P. Cysne
(UFF/BR)

Collaborators:

- Filipe Guimarães (Peter Grunberg Institute/Germany)
- M. Buongiorno Nardelli (University of North Texas/USA)

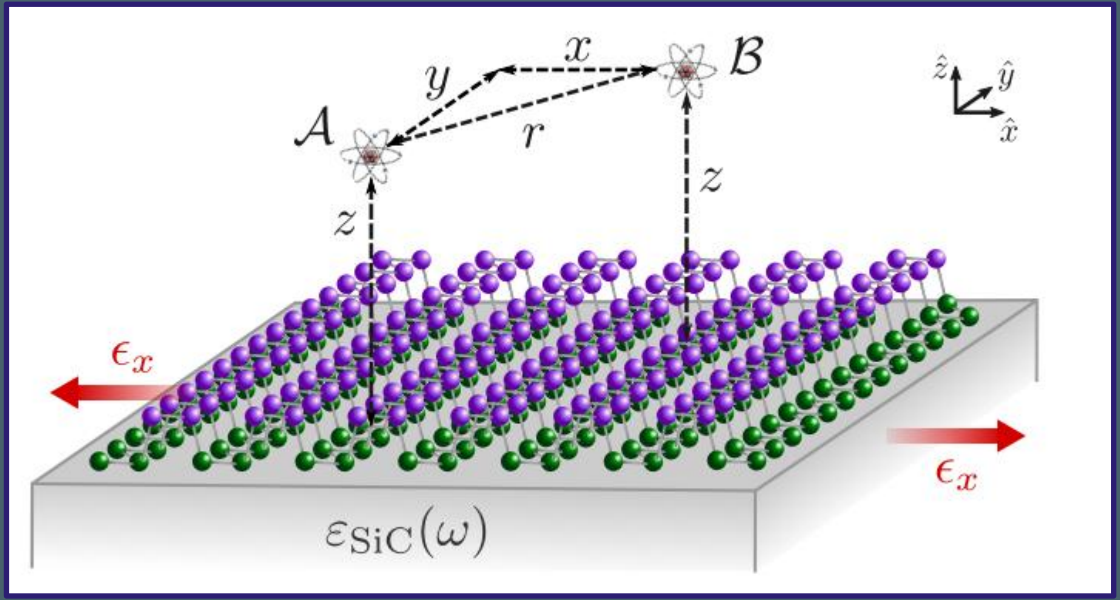
Part IV:
Other research topics

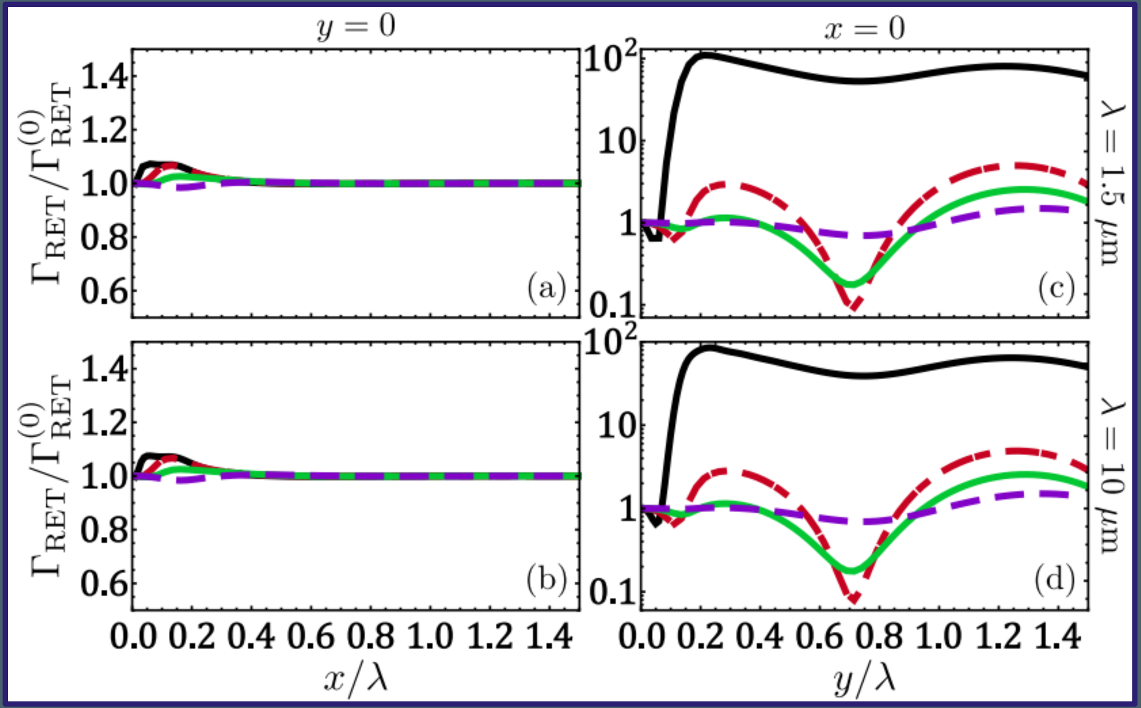
Nanofotônica em materiais 2D

PHYSICAL REVIEW B **111**, 205422 (2025)

Anisotropic resonance energy transfer with strained phosphorene

J. Oliveira-Cony,[1,*] C. Farina,[1] P. P. Abrantes,[1,2] and Tarik P. Cysne[2,†]
[1]*Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Rio de Janeiro 21941-617, Brazil*
[2]*Instituto de Física, Universidade Federal Fluminense, Niterói, Rio de Janeiro 24220-900, Brazil*



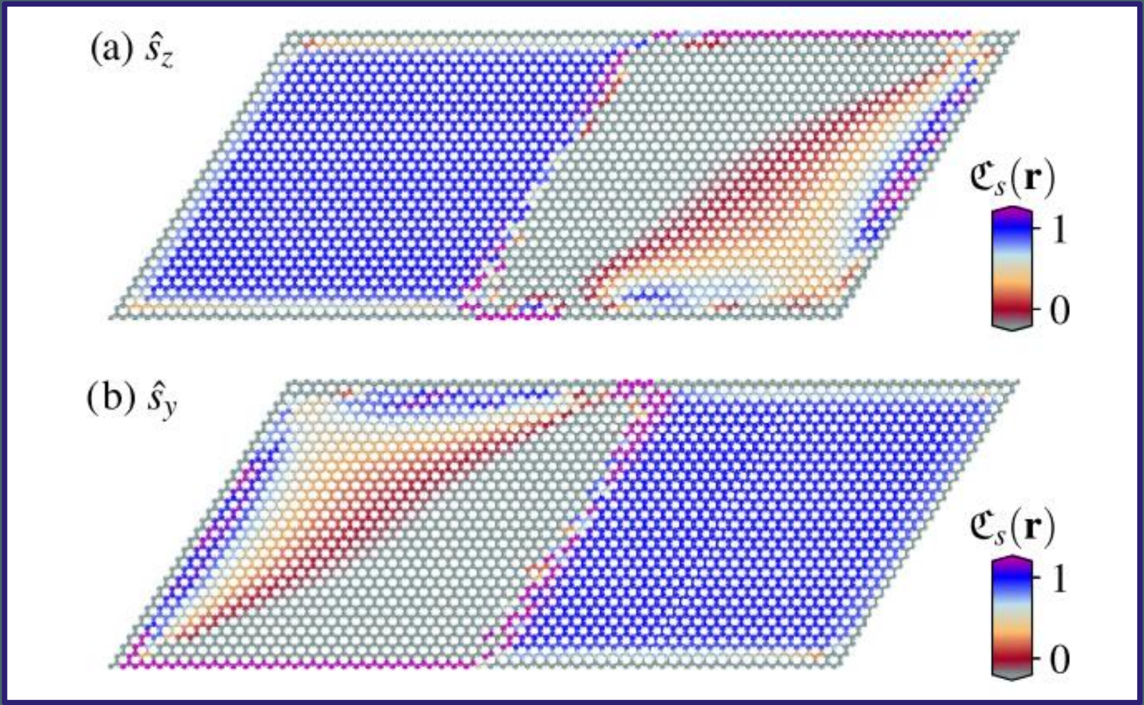


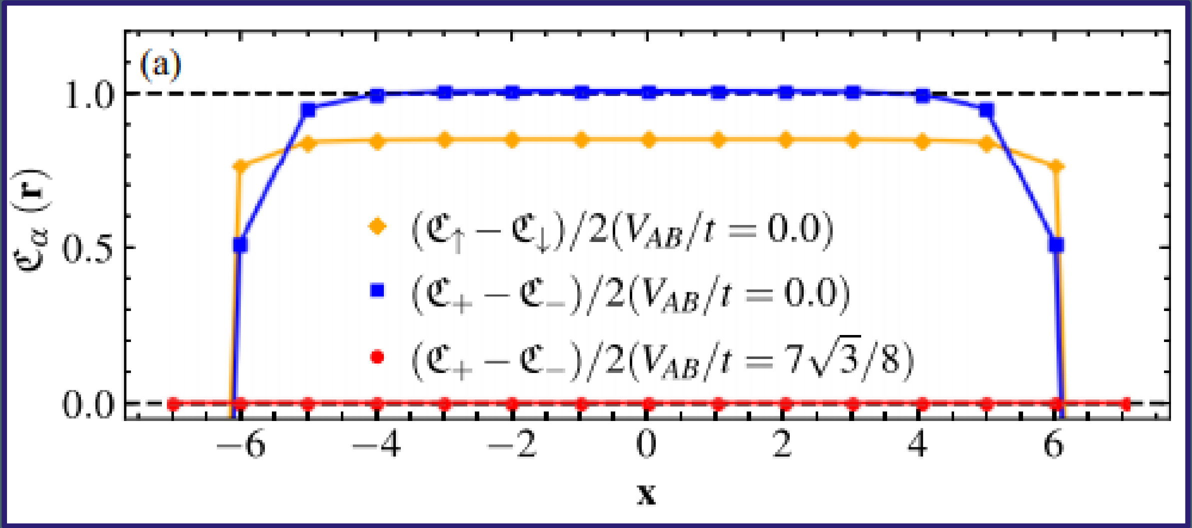
Local markers for topological phases

PHYSICAL REVIEW B **111**, 035411 (2025)

Topological characterization of modified Kane-Mele-Rashba models via local spin Chern marker

Sebastião dos Anjos Sousa-Júnior,[1,*] Marcus V. de S. Ferraz,[2] José P. de Lima,[2] and Tarik P. Cysne[3,†]
[1]Department of Physics, University of Houston, Houston, Texas 77004, USA
[2]Departamento de Física, Universidade Federal do Piauí, 64049-550 Teresina, Piauí, Brazil
[3]Instituto de Física, Universidade Federal Fluminense, 24210-346 Niterói RJ, Brazil



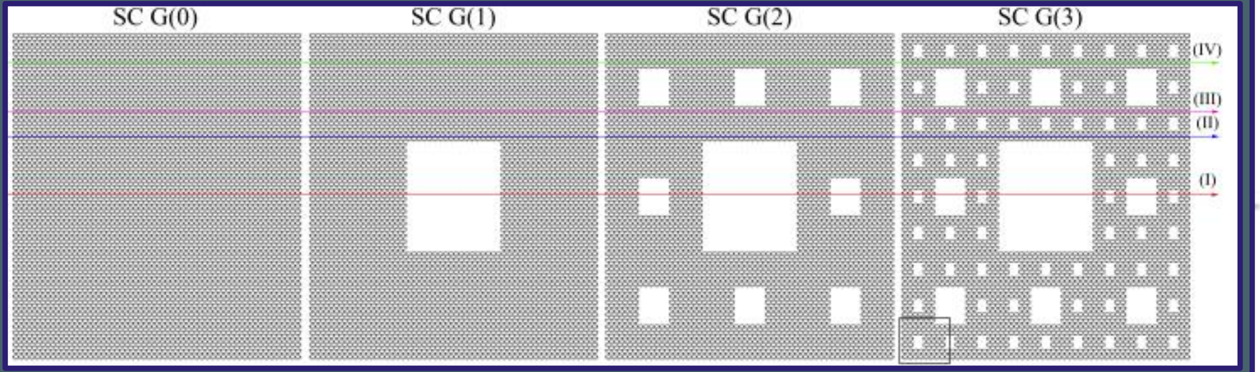


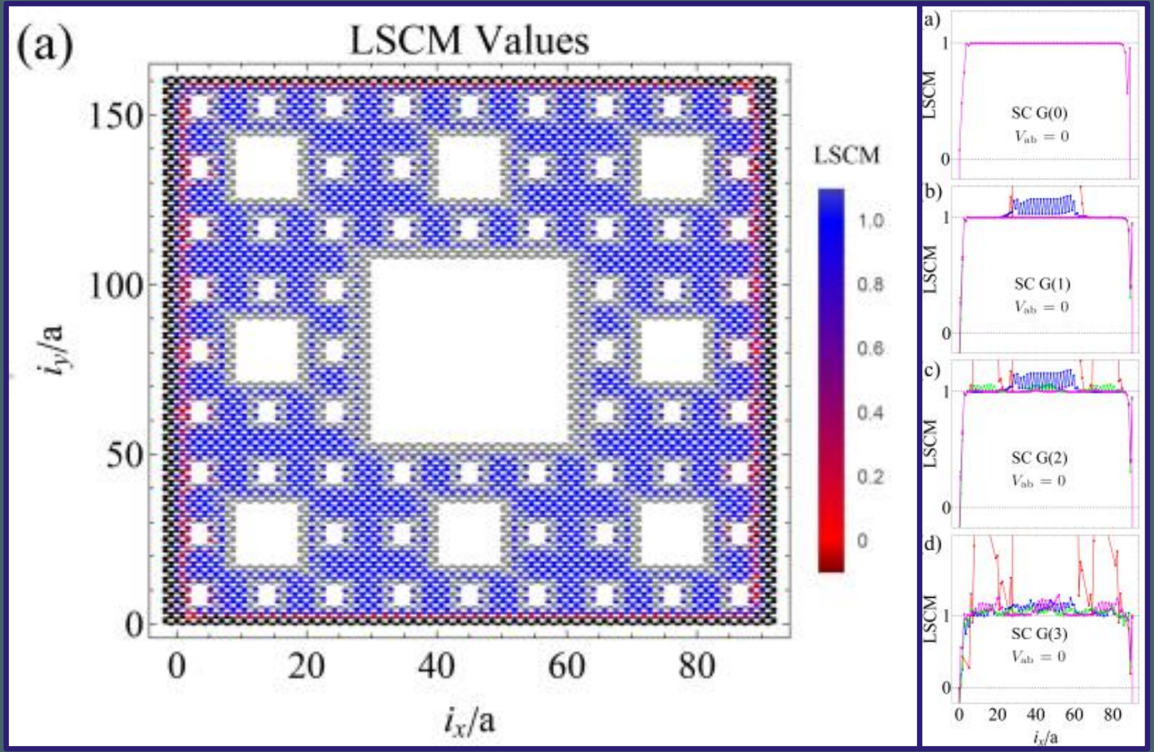
Local markers for topological phases

PHYSICAL REVIEW B **111**, 245418 (2025)

Topological phases in fractals: Local spin Chern marker in the Kane-Mele-Rashba model on the Sierpinski carpet

L. L. Lage,[1,*] A. B. Félix,[1] S. dos A. Sousa-Júnior,[2] A. Latgé,[1] and Tarik P. Cysne[1,†]
[1]*Instituto de Física, Universidade Federal Fluminense, Niterói, Avenida Litorânea sn 24210-340, Rio de Janeiro, Brazil*
[2]*Department of Physics, University of Houston, Houston, Texas 77204, USA*





Instituto de Física da UFF – Niterói/RJ

Instituto de Física

Universidade Federal Fluminense

Thanks for your attention!

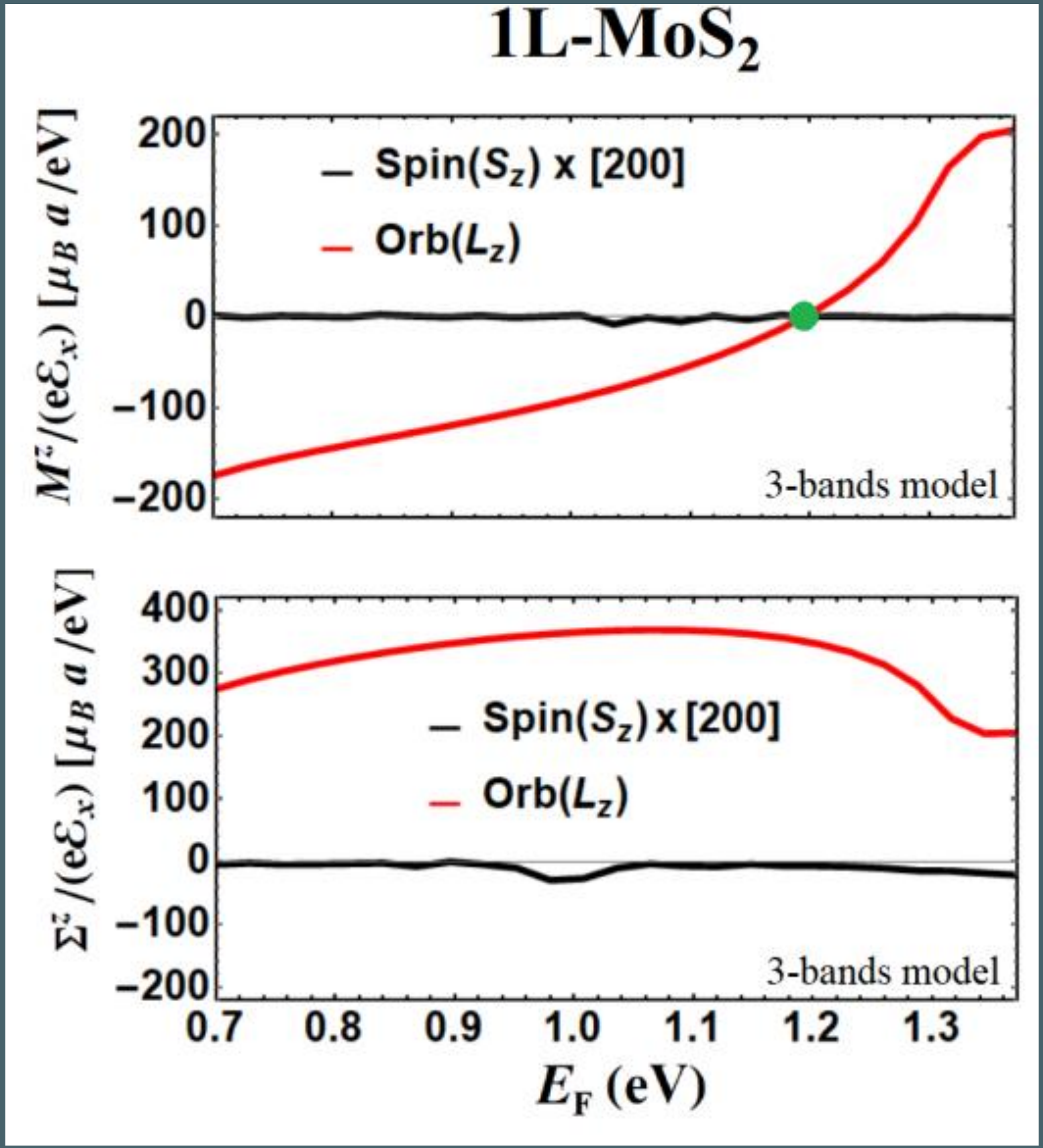
acknowledgements

CNPq

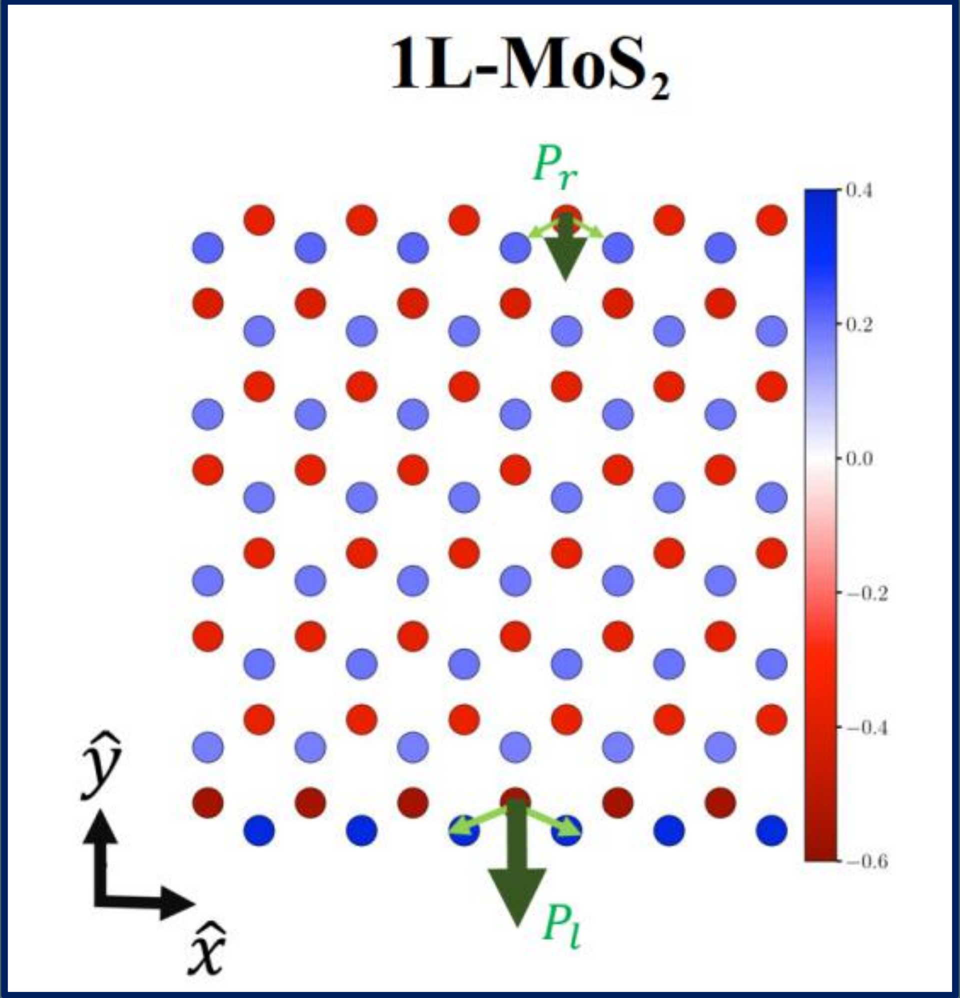
FAPERJ
Fundação Carlos Chagas Filho de Amparo
à Pesquisa do Estado do Rio de Janeiro

CAPES

Contribution from spin sector to magnetoelectric effect in ZZ-NR



Electric polarization x OME in ZZ-NR



Heisenberg's Equation of motion

$$\hat{V}(t) = -\mathrm{e}\,\mathbf{E}(t)\cdot\hat{\mathbf{r}}$$

$$\frac{\mathrm{d}\hat{\mathbf{L}}^{\mathrm{ind}}}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\left[\hat{\mathbf{L}}^{\mathrm{ind}}, \hat{V}(t)\right] = \hat{\mathbf{r}}\times \mathrm{e}\,\mathbf{E}(t)$$

$$\vec{M}_{orb} = \vec{P}_e \times \vec{E}$$

Topology

Low energy theory near valleys

$$\tilde{H}(\vec{q}_\tau) = \begin{bmatrix} \Delta & \gamma_+ & 0 & 0 \\ \gamma_- & -\tau s_z\lambda & 0 & t_\perp \\ 0 & 0 & \Delta & \gamma_- \\ 0 & t_\perp & \gamma_+ & \tau s_z \lambda \end{bmatrix} \begin{array}{l} |d^1_{z^2}\rangle \\ (|d^1_{x^2-y^2}\rangle - i\tau|d^1_{xy}\rangle)/\sqrt{2} \\ |d^2_{z^2}\rangle \\ (|d^2_{x^2-y^2}\rangle + i\tau|d^2_{xy}\rangle)/\sqrt{2} \end{array}$$

Δ ---- **Energy Gap**

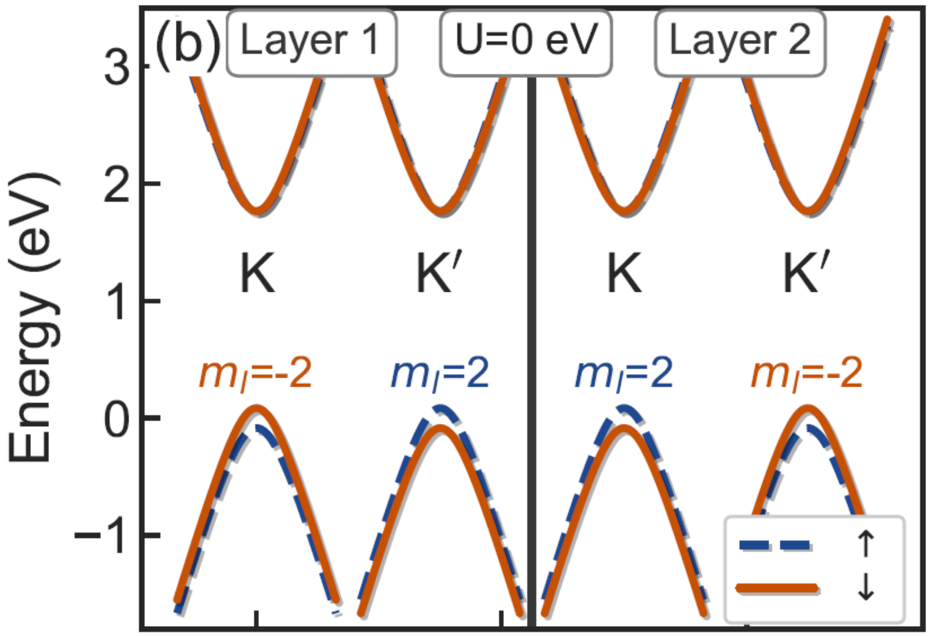
λ ---- **SOC (not considered in this talk)**

$t_\perp$ ---- **Interlayer hopping**

$$\gamma_\pm = at(\tau q_x \pm i q_y)$$

Orbital Angular momentum operator:

$$L_z = \mathrm{diag}(0, -2\hbar\tau, 0, 2\hbar\tau)$$



Topology

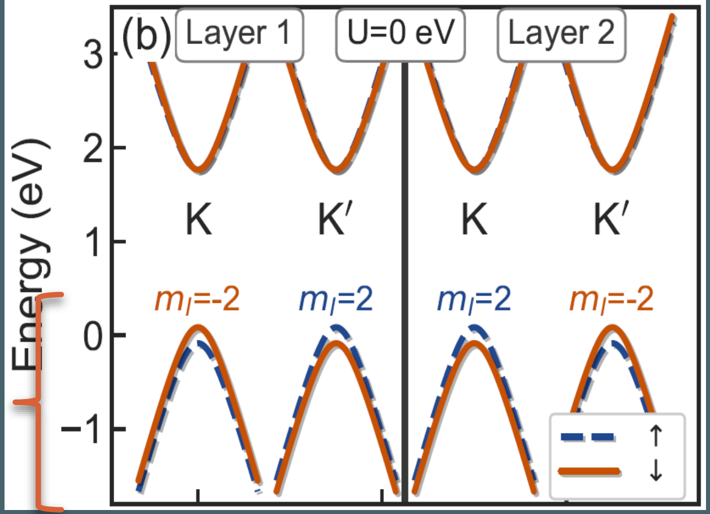
$$\mathbb{L}^{\mathrm{v}}(\vec{k}) = P(\vec{k}) L_z P(\vec{k})$$

Eigenstates of
this matrix

$$\left|\Phi^{\pm}_{n,\tau}(\vec{q})\right\rangle$$

$$P(\vec{k})$$

Valence Band
Projector



$$\mathcal{C}^{\pm}_L = \frac{1}{2\pi}\int d^2q \sum_{n,\tau} F^{\pm}_{n,\tau}(q)$$

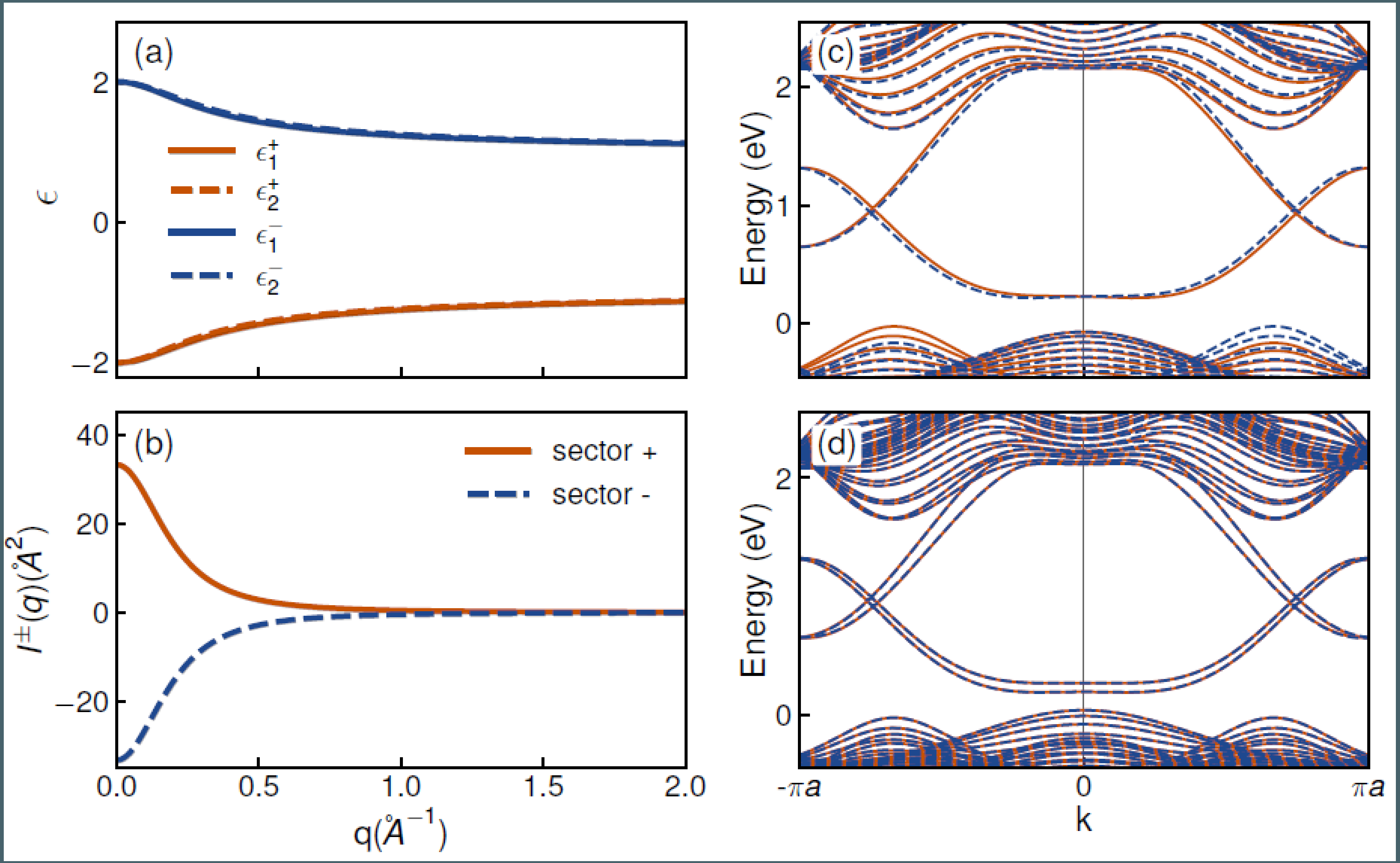
$$F^{\pm}_{n,\tau}(q) = -2\mathrm{Im}[\langle \partial_{q_x}\Phi^{\pm}_{n,\tau}(\vec{q})|\partial_{q_y}\Phi^{\pm}_{n,\tau}(\vec{q})\rangle]$$

Orbital Chern number!

$$\mathcal{C}_L = (\mathcal{C}^{+}_L - \mathcal{C}^{-}_L)/2$$

Topology

$C_L = 2$ for 2L-TMD. $C_L = 1$ for 1L-TMD.



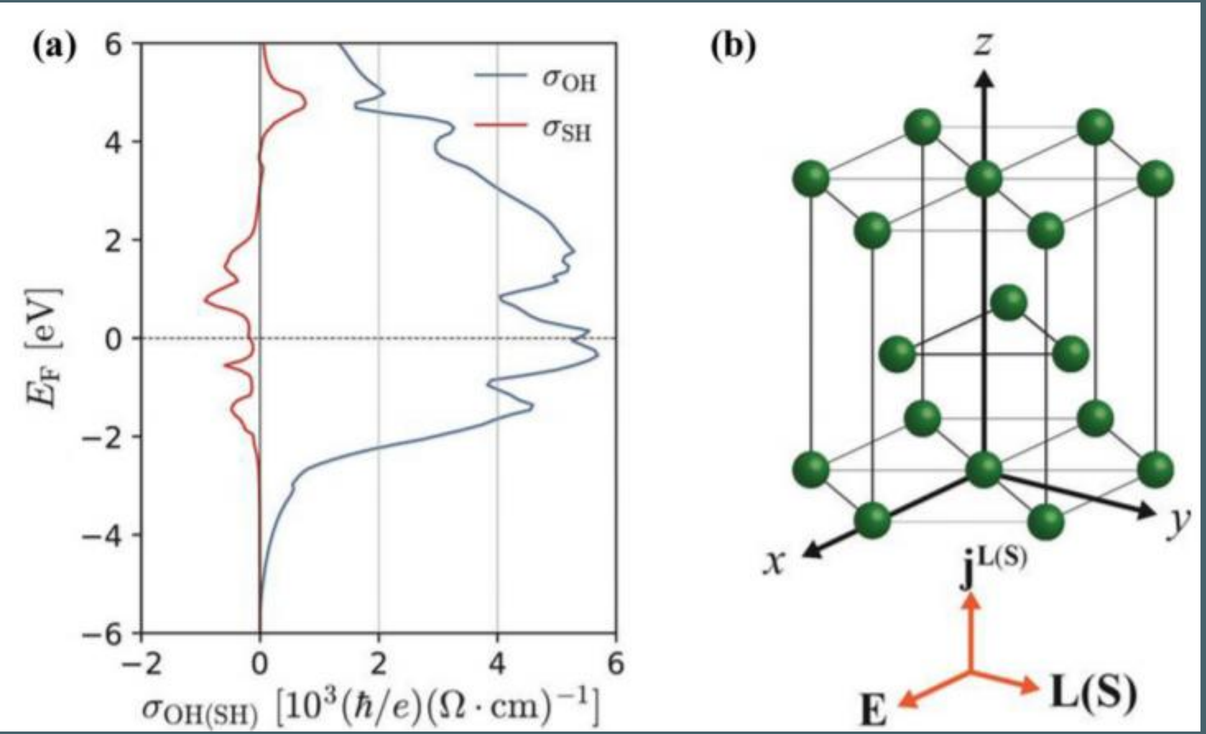
Experiments

PHYSICAL REVIEW RESEARCH **2**, 013127 (2020)

Magnetization switching driven by current-induced torque from weakly spin-orbit coupled Zr

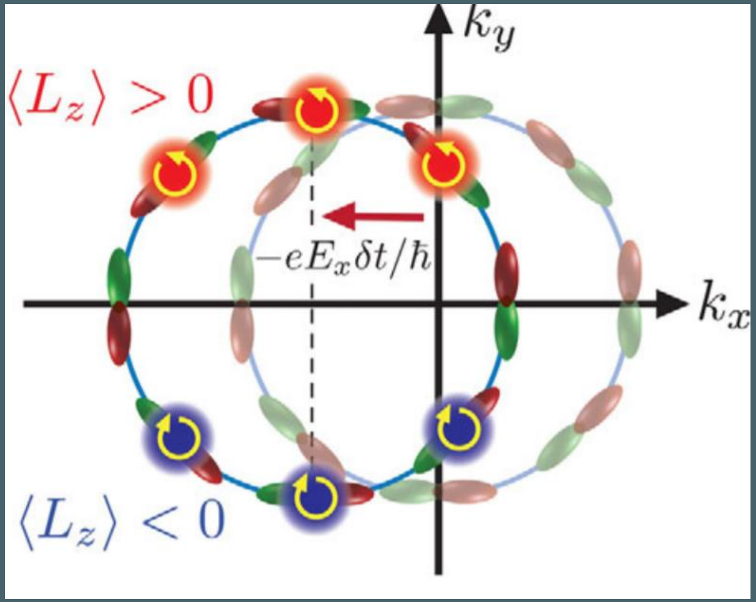
Z. C. Zheng,[1,*] Q. X. Guo,[1,2,*] D. Jo,[3] D. Go,[3,†] L. H. Wang,[4] H. C. Chen,[5] W. Yin,[5] X. M. Wang,[6]
G. H. Yu,[1] W. He,[2] H.-W. Lee,[3] J. Teng,[1,‡] and T. Zhu[2,5,7,§]

Low SOC on Zr. The phenomena should be related to OHE.



Intrinsic mechanism of OHE (3D Metals)

-Intrinsic Mechanism: OHE is a consequence of orbital texture [Figs From "Phys. Rev. Lett. **121**, 086602 (2018)"]:



- Even for solids with quenched OAM, the electric field shifts band structure which causes recombination of its orbital texture and produces a transverse flux of OAM.

- Mechanism analogous to spin texture in SHE, but it is robust against dilute disorder (vertex corrections) in centrosymmetric systems.

- OHE precedes the SHE.

- The OHE is converted in SHE by SOC: $\vec{L}.\vec{S}$

- The OHE occurs even in absence of SOC.