ORBITAL HALL EFFECT IN 2D MATERIALS

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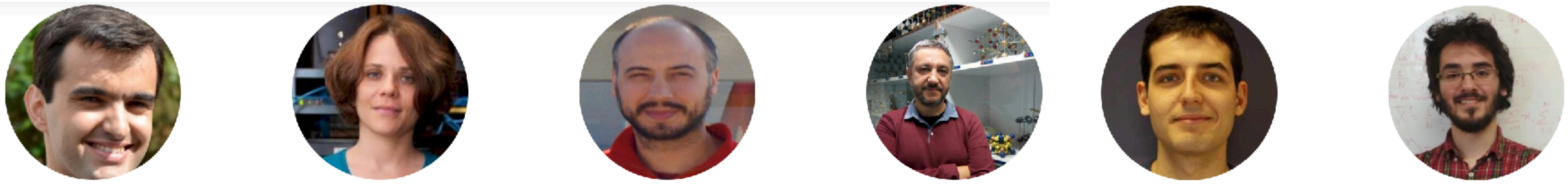
L. M. Canonico, T. G. Rappoport, R. B. Muniz, Phys. Rev. Lett. 122 (2019) 196601.

L. M. Canonico,T. P. Cysne,T. G. Rappoport and R. B. Muniz, Phys. Rev. B 101, 075429 (2020)

L. M. Canonico,T. P. Cysne, A. Molina-Sanchez, R. B. Muniz and T. G. Rappoport
Phys. Rev. B 101, 161409 (2020).

KITE

quantum transport software



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Open Source

Python Scripts

Evaluation of response functions in systems with up to 10^{10} orbitals

https://quantum-kite.com/

KITE: high-performance accurate modelling of electronic structure and response functions of large molecules, disordered crystals and heterostructures

R. Soc. open sci. 7, 191809 (2020)

+

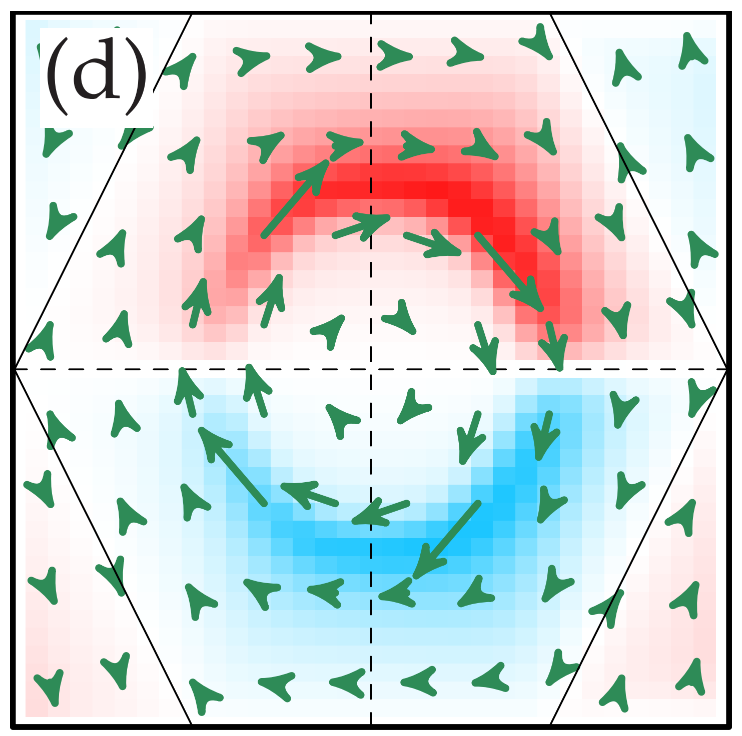
Orbital angular momentum (OAM) can be manipulated like spin

No need of exchange interaction or SOC

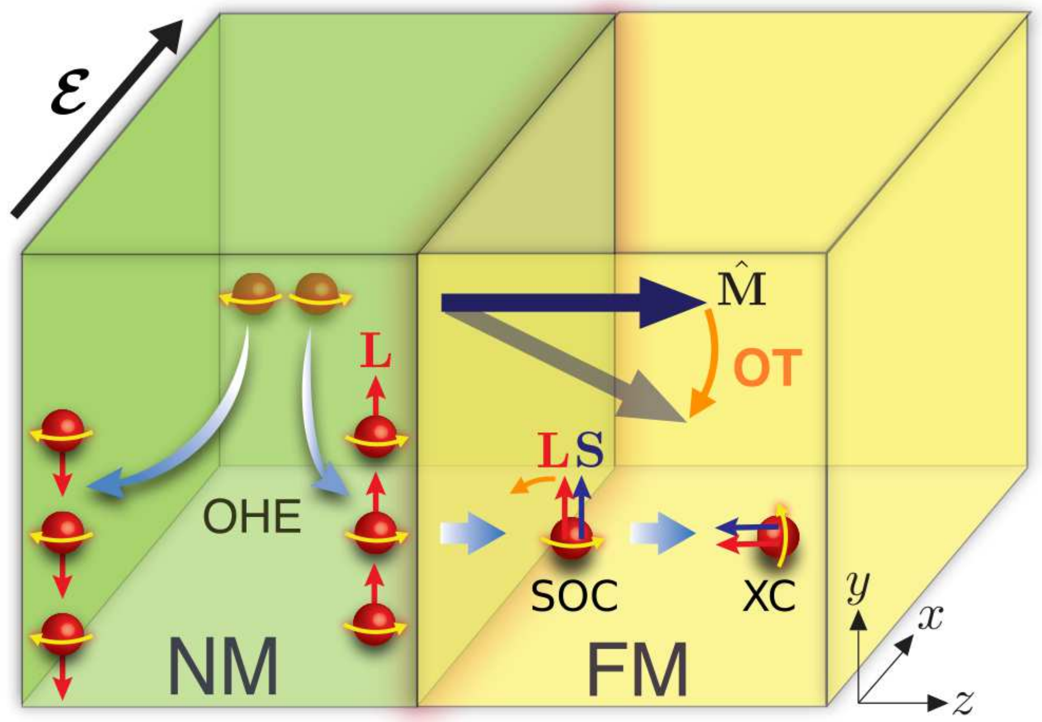
Orbital Hall effect

B. A. Bernevig et al. PRL 2005
H. Kontani et al. PRL 2009
D. Go et al. PRL 2018 ..

Orbital Rashba effect



Jin-Hong Park et al PRB 2012
Sp metals
D. Go et al. Sci.Rep. 2017
Tin Teluride monolayers
Jeongwoo Kim et al, Nature Comm 2019



Orbital Torque

Xi Chen et al. Nature Comm. 2018
D. Go et al. Phys. Rev. Research 2020
Z. C. Zheng et al,PR. Research 2020
Y. Tazaki et al.ArXiv:2004.09165

Orbital Rashba-Edelstein Effect

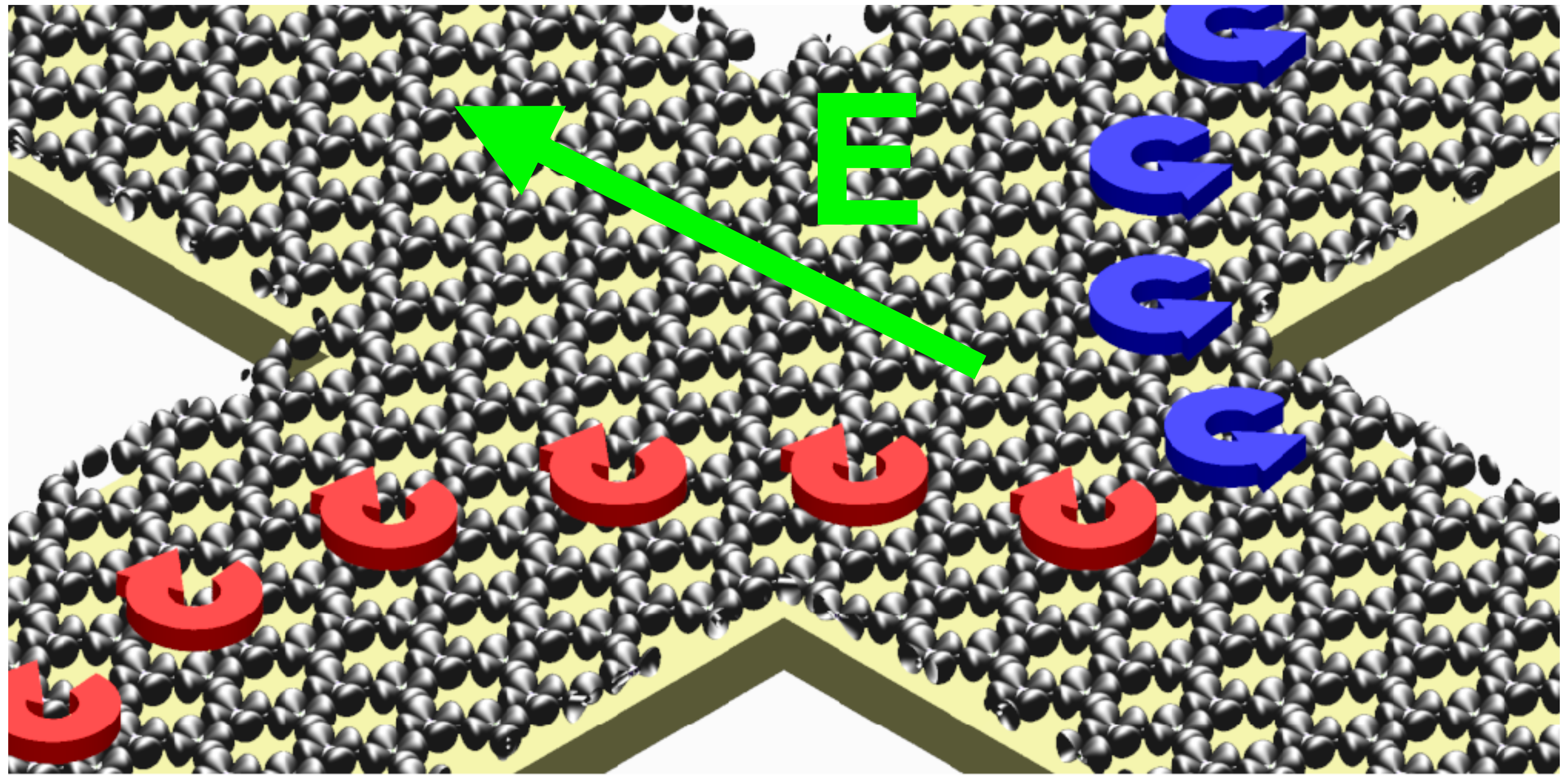
T. Koretsune, PRB 2012
T. Yoda et al Nano Letters 2018
N.Salemi et al. Nature Comm. 2019

Orbital Chern insulators

A. L. Sharpe et al. Science 2019
M. Serlin et al. Science 2019
G. Chen et al. Nature 2020

ORBITAL HALL EFFECT

Orbital angular momentum (OAM) analogous of the spin Hall effect



First proposal (for Silicon): B. A. Bernevig, T. L. Hughes, and S-C. Zhang, PRL (2005)

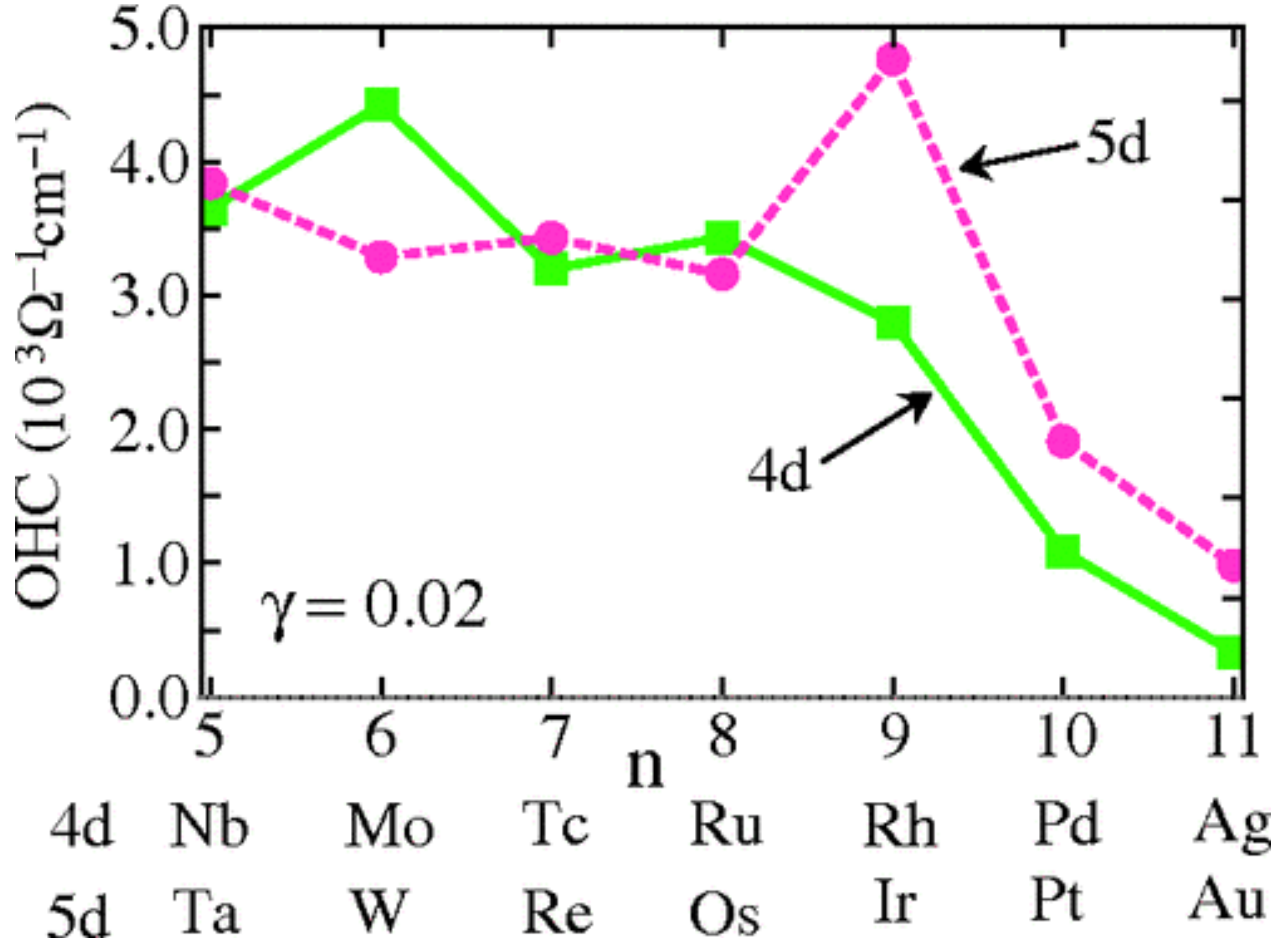
$$\sigma_{\mathrm{OH(SH)}} = \frac{e}{\hbar} \sum_{n \neq m} \int \frac{d^3 k}{(2\pi)^3} \left(f_{m\mathbf{k}} - f_{n\mathbf{k}} \right) \Omega^{X_z}_{nm\mathbf{k}},$$

$$\Omega^{X_z}_{nm\mathbf{k}} = \hbar^2 \mathrm{Im} \left[\frac{\langle u_{n\mathbf{k}} | \, j^{X_z}_y \, | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | \, v_x \, | u_{n\mathbf{k}} \rangle}{\left(E_{n\mathbf{k}} - E_{m\mathbf{k}} + i\eta \right)^2} \right]$$

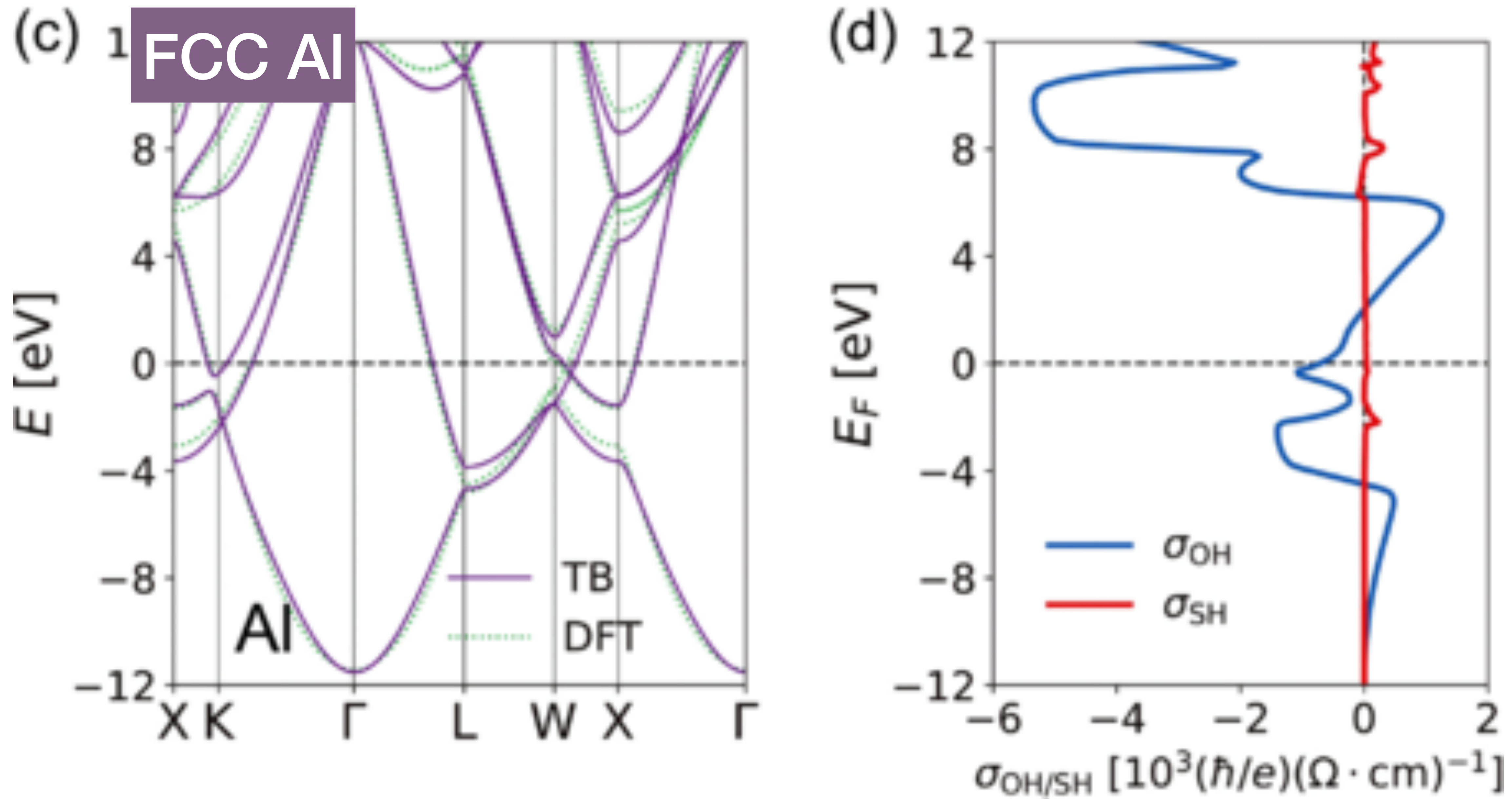
$$j^{X_z}_y = \left(v_y X_z + X_z v_y \right) / 2$$

$$X_z = L_z (S_z)$$

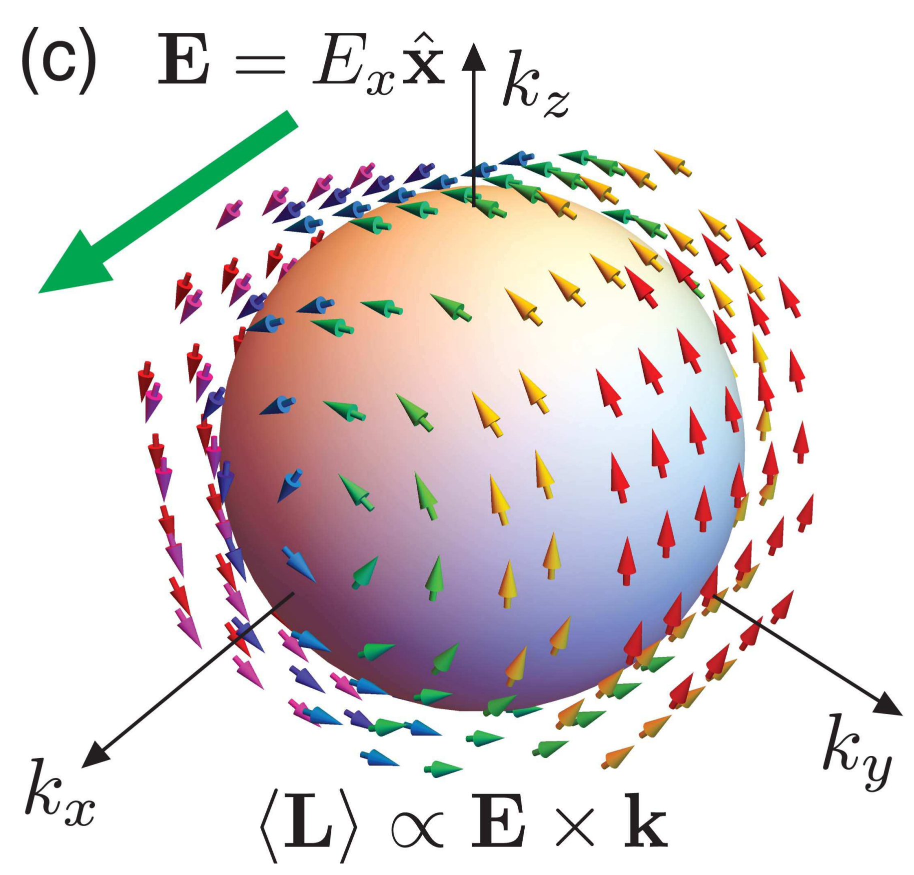
OHE IN METALLIC 3D SYSTEMS



H. Kontani et al. PRL 2009
T. Tanaka et al. PRB 2008



D Go, HW Lee arXiv:1903.01085
D Jo, D Go, HW Lee PRB, 2018



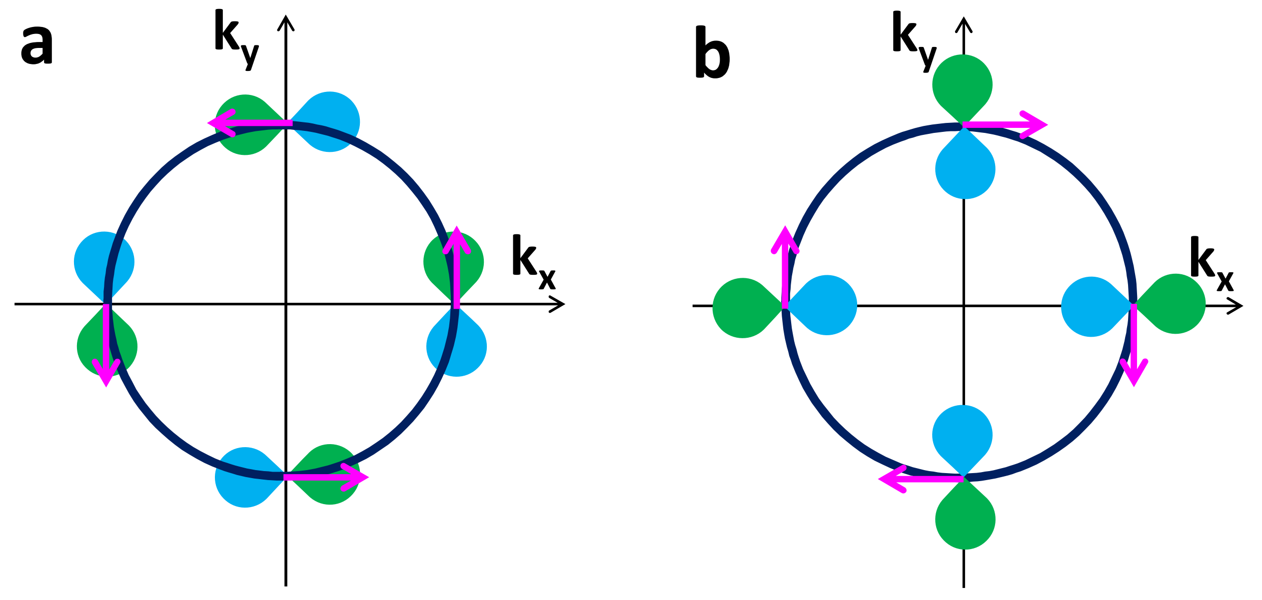
Orbital Texture induce OHE

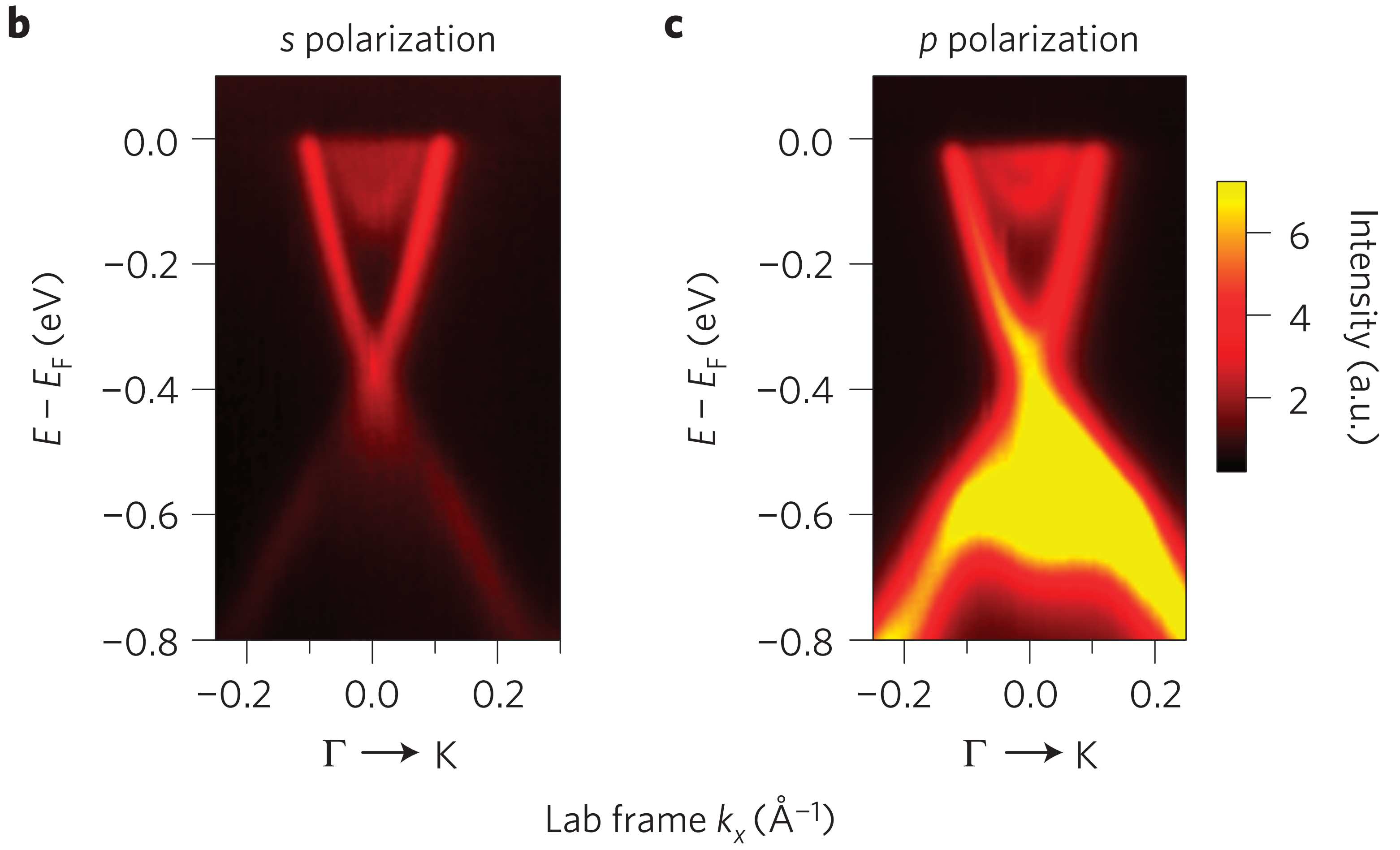
D Jo, D Go, HW Lee PRL, 2018

ORBITAL TEXTURES IN SOLIDS

Topological Insulators

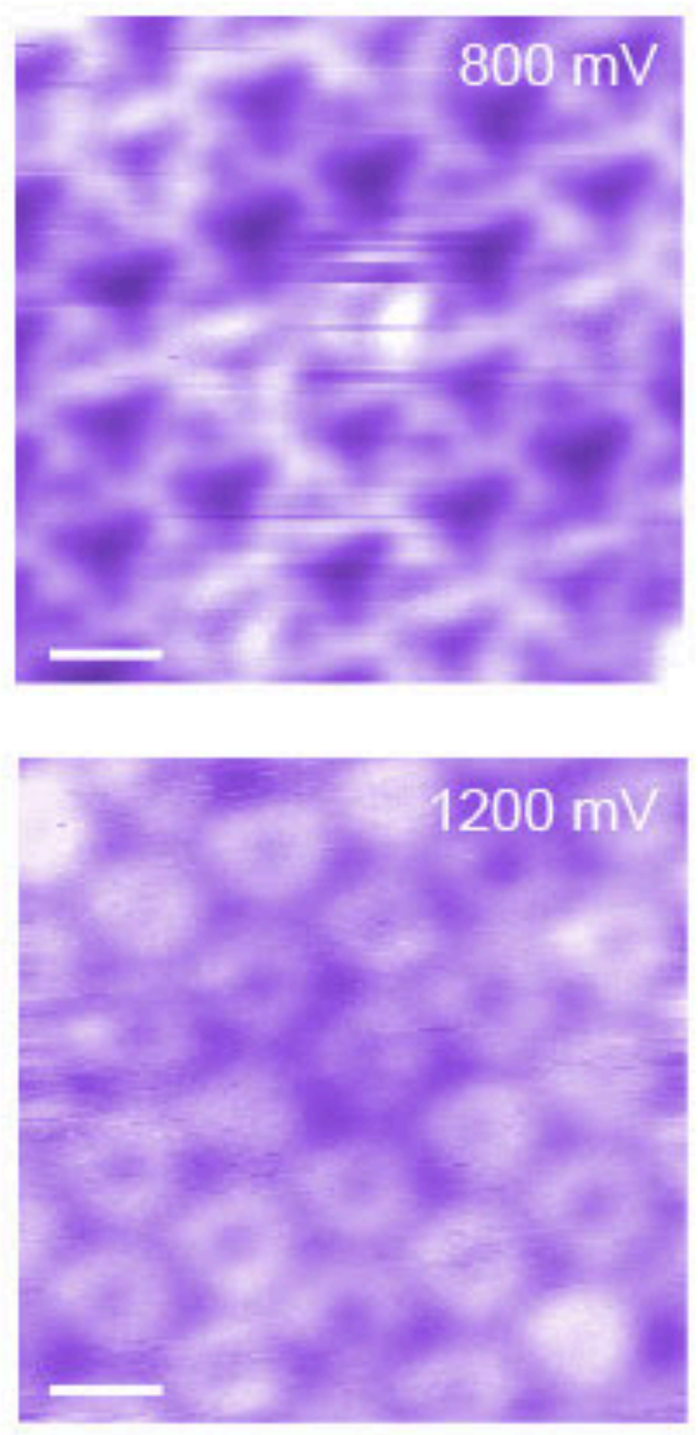
H Zhang, CX Liu, SC Zhang PRL 2013
Yue Cao et al Nat. Phys. 2013





1T Ta-based TMD layers

T. Ritschel et al. Nature Phys. 2015
Yi Chen et al Nature Phys. 2019

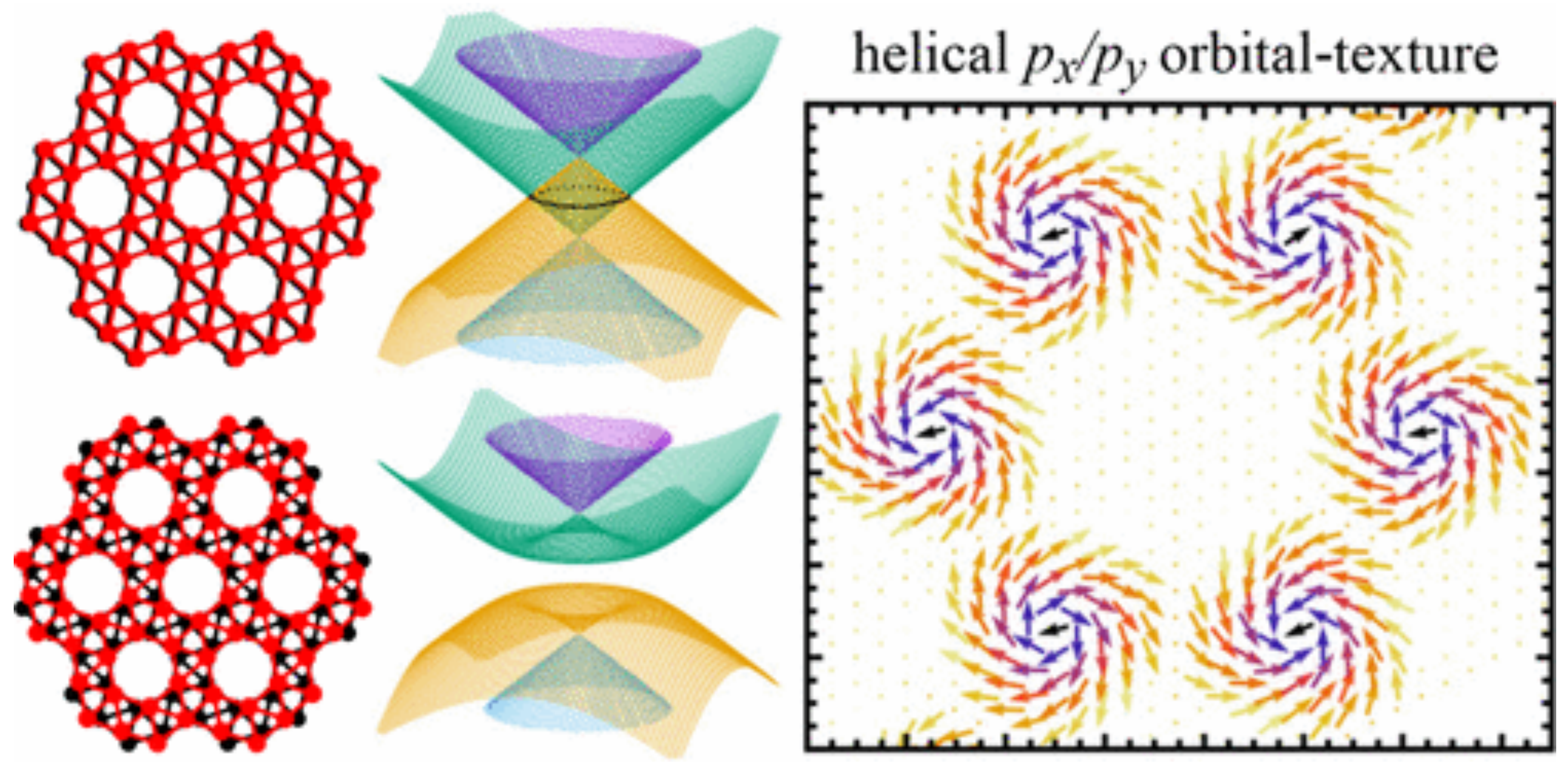


2DEG in Oxides

J.J.Kim et al, Nat. Comm. 2014

Borophene

F. C. de Lima et al., Nanoletters. 2019

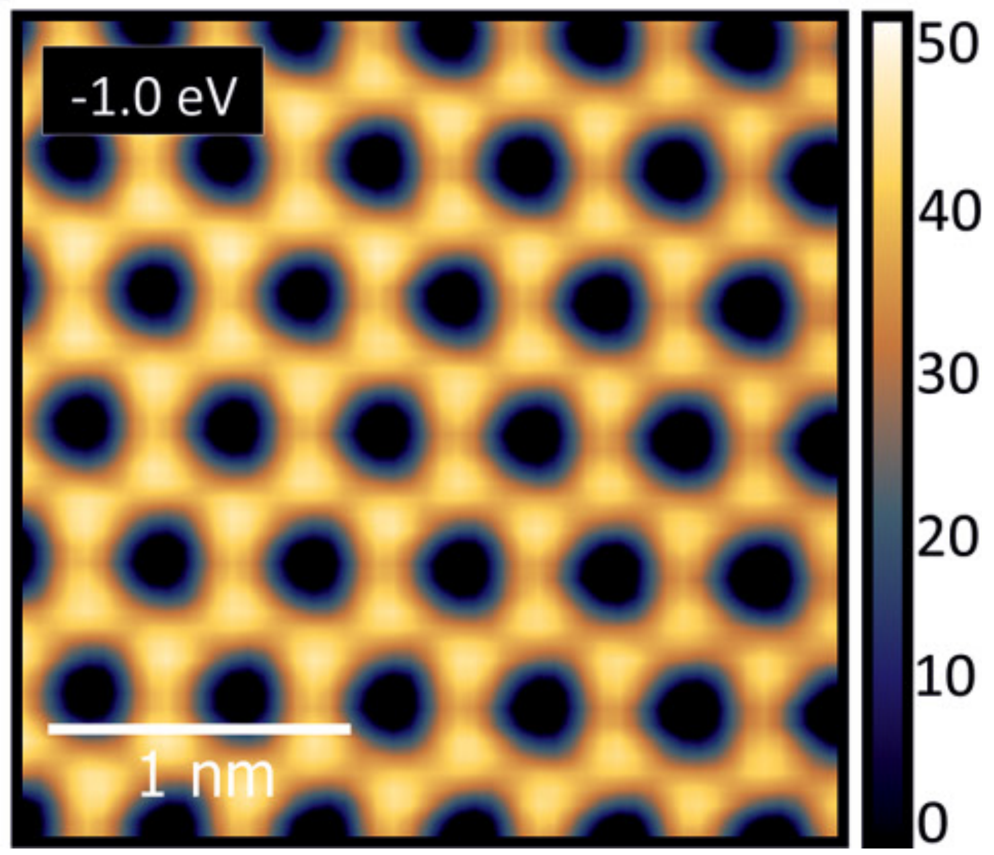


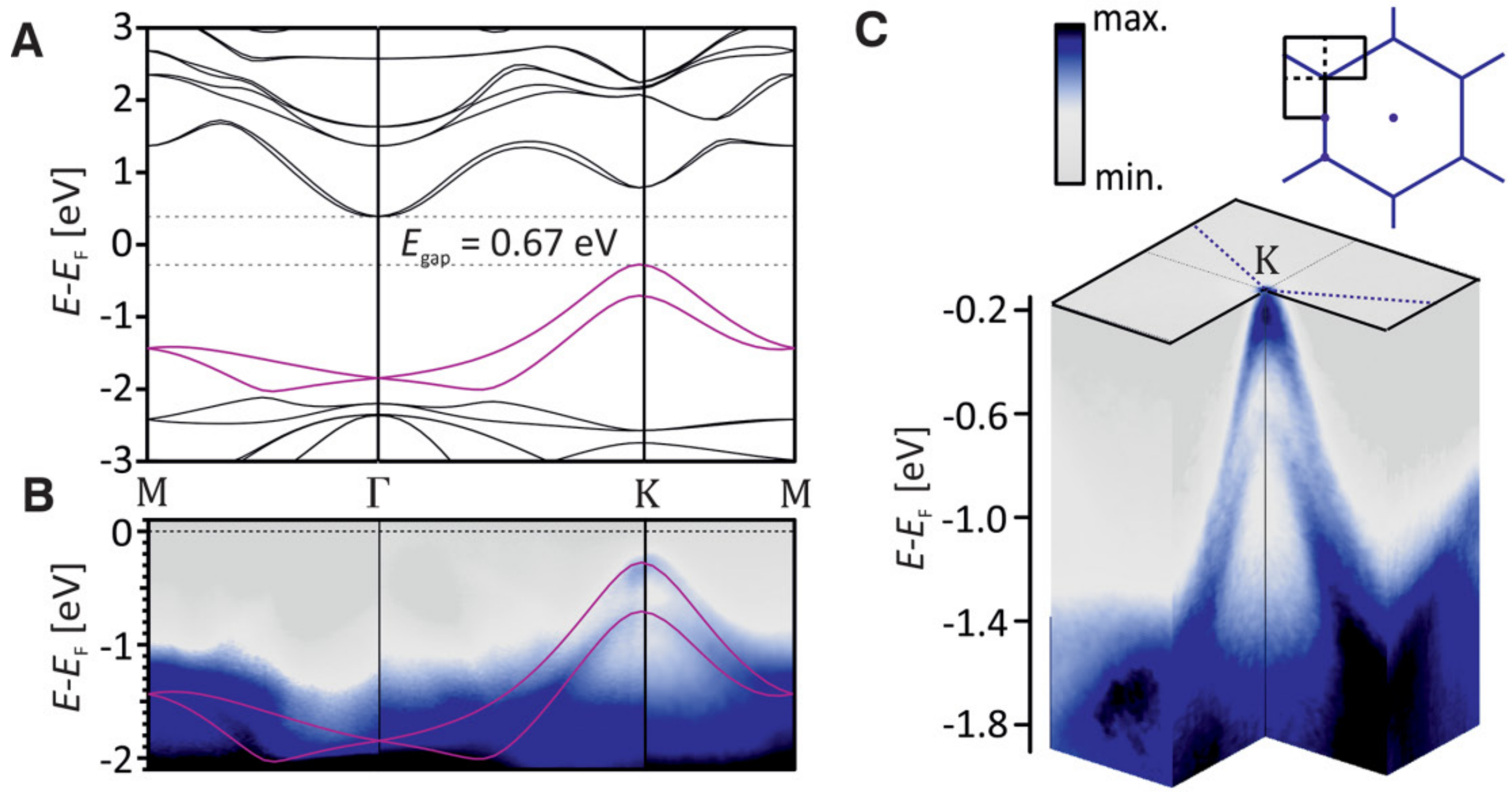
OUR MINIMAL MODEL

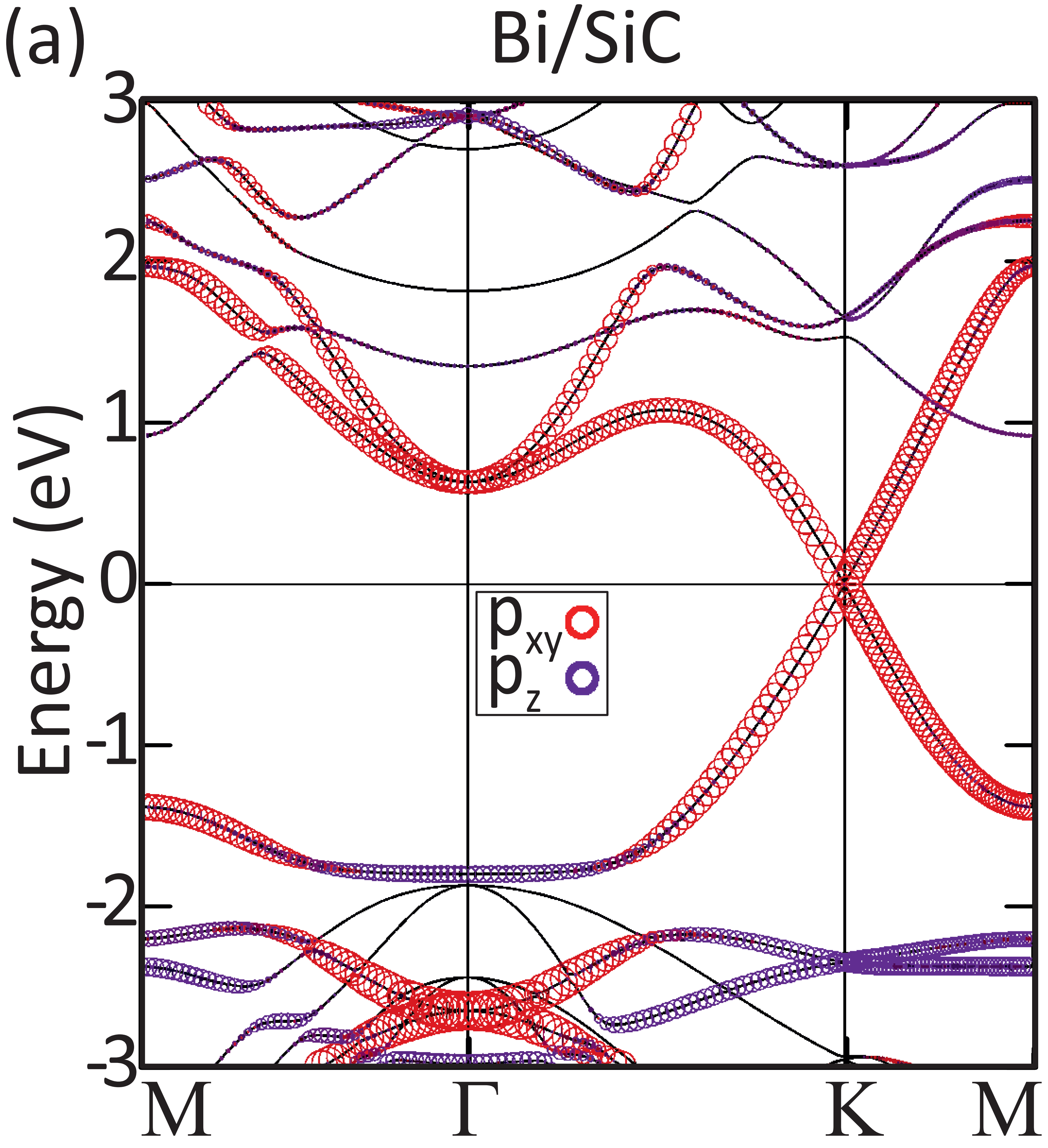
GENERAL ASPECTS

Epitaxy

SiC Substrate







F. Reis, G. Li, L. Dudy, M. Bauernfeind, S. Glass, W. Hanke, R. Thomale, J. Schäfer, R. Claessen, Science 2017

PX-PY HAMILTONIAN + SOC

$$\mathcal{H} = \sum_{\langle ij \rangle} \sum_{\mu\nu s} t_{ij}^{\mu\nu} p_{i\mu s}^{\dagger} p_{j\nu s} + \sum_{i\mu s} \epsilon_i p_{i\mu s}^{\dagger} p_{i\mu s} + \sum_{i\mu s} \mathbf{h}_{\mu s}^{z} p_{i\mu s}^{\dagger} p_{i\mu s},$$

$\lambda_I L_z S_z$

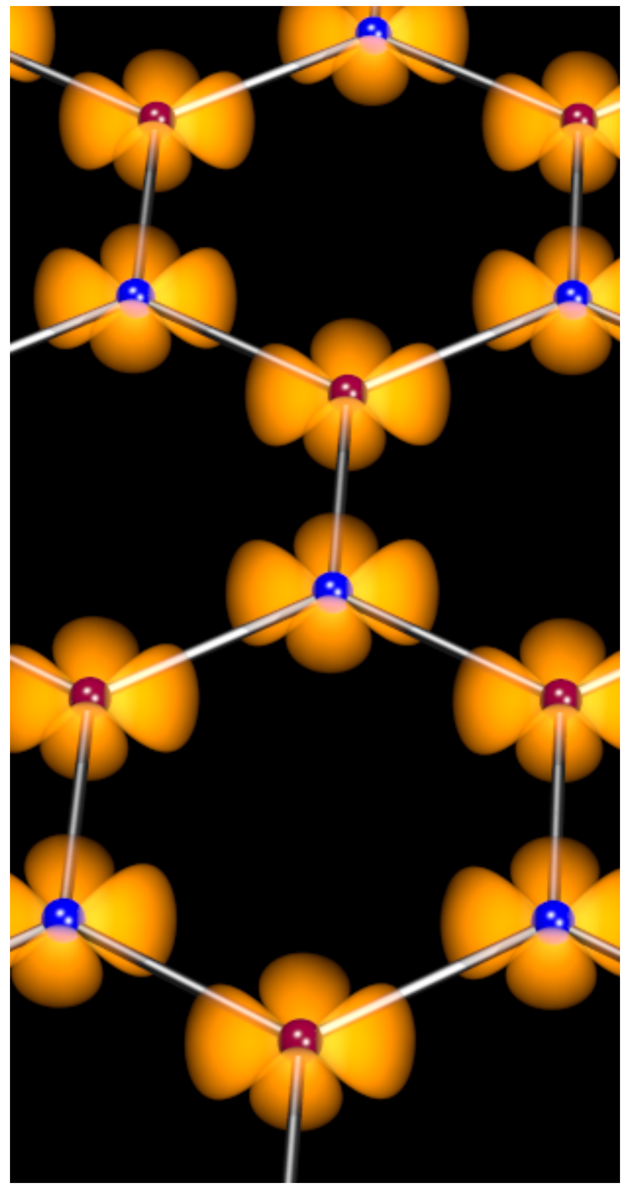
$h_{\rm ex} L_z$

$\epsilon_i = \pm V_{AB}$

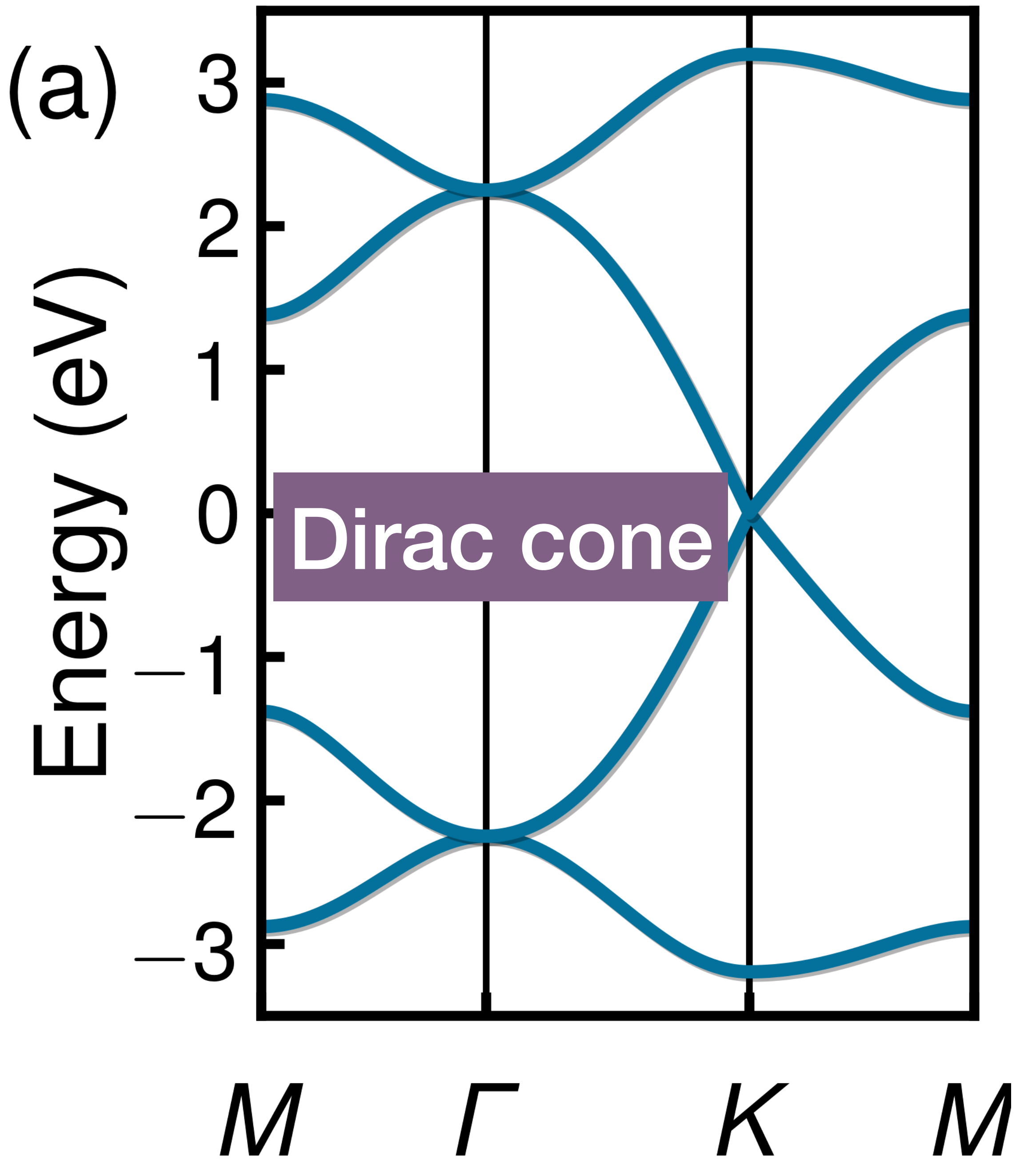
$p_\mu = p_\pm = \frac{1}{\sqrt{2}}(p_x \pm i p_y)$

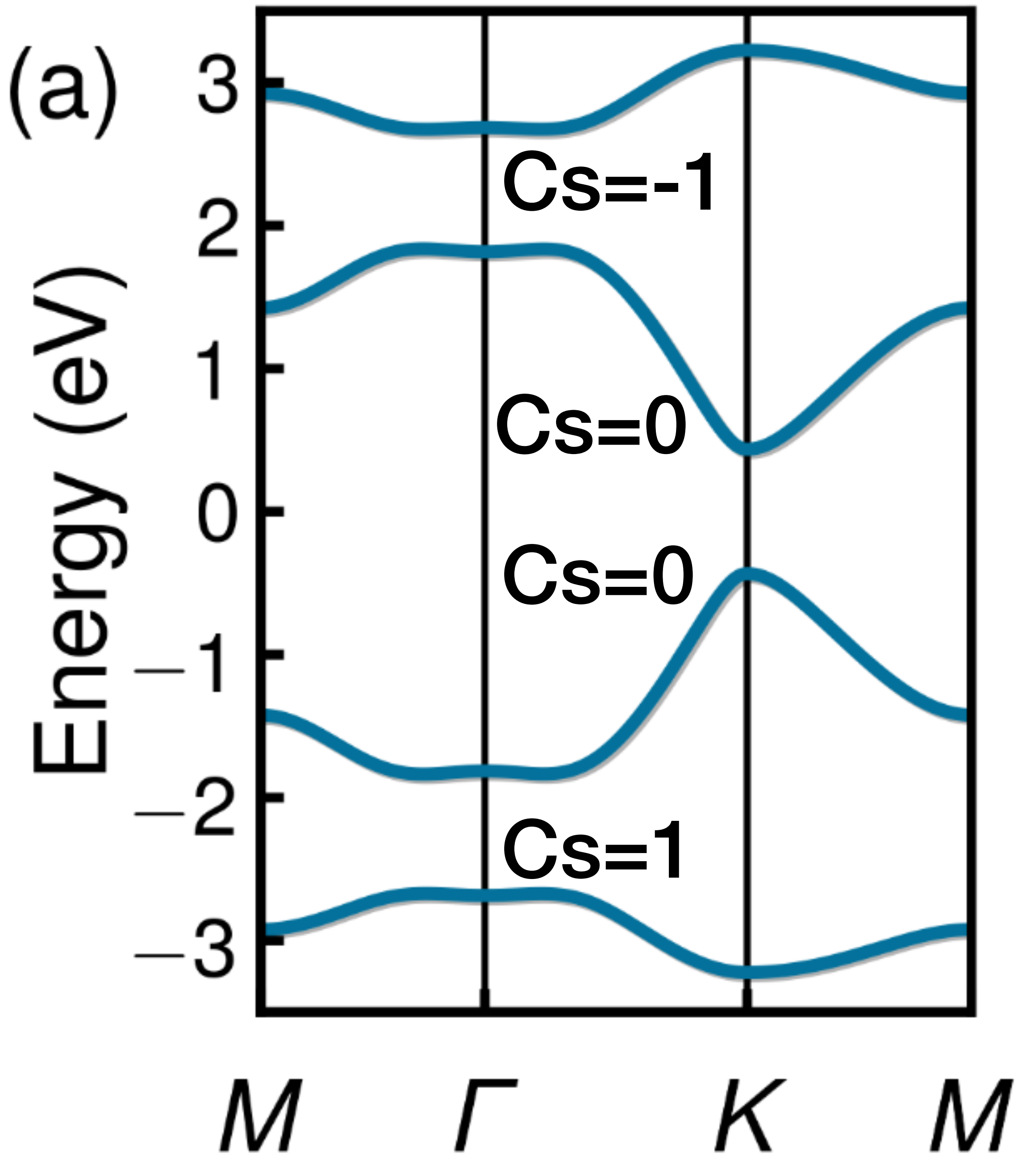
On-site

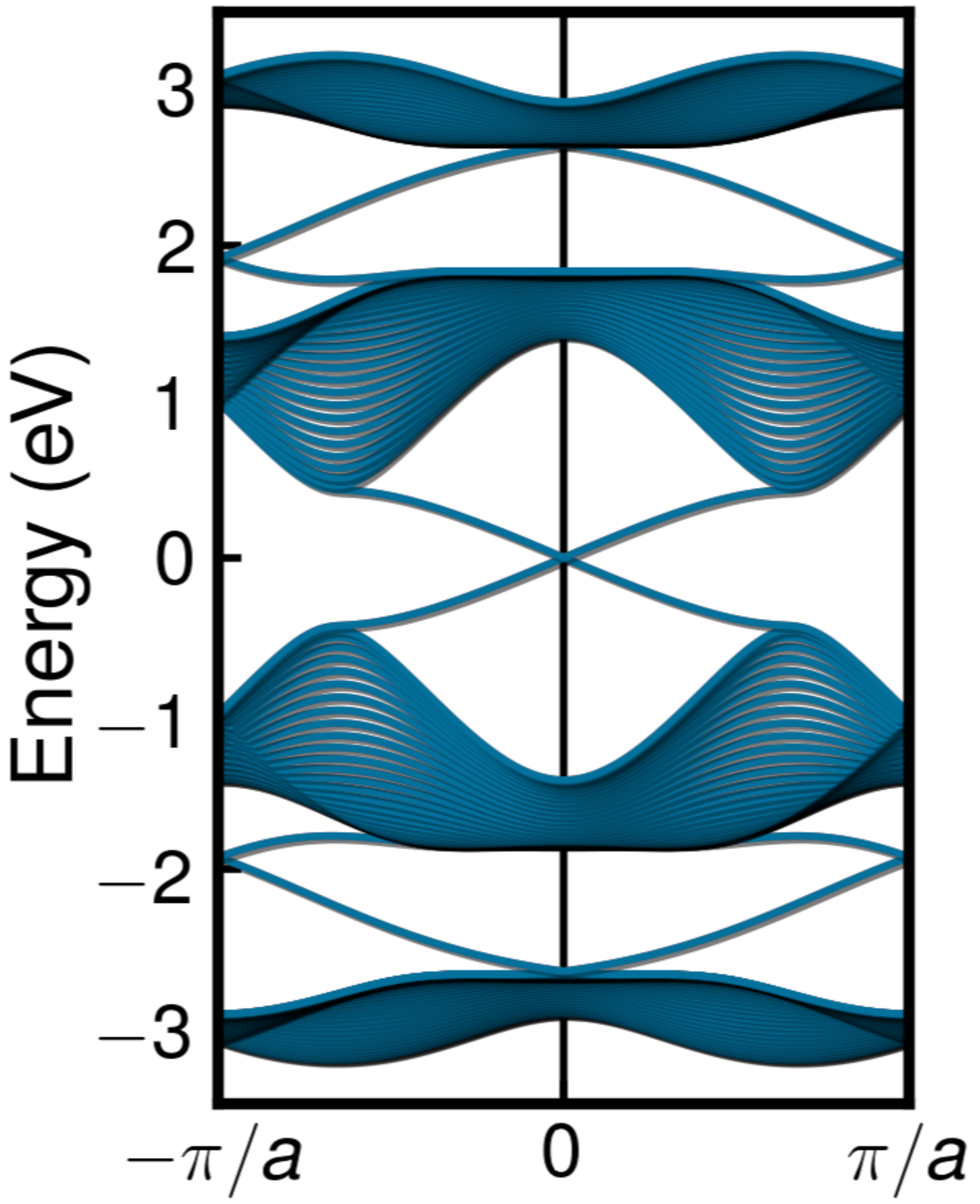
S_z is a good quantum number



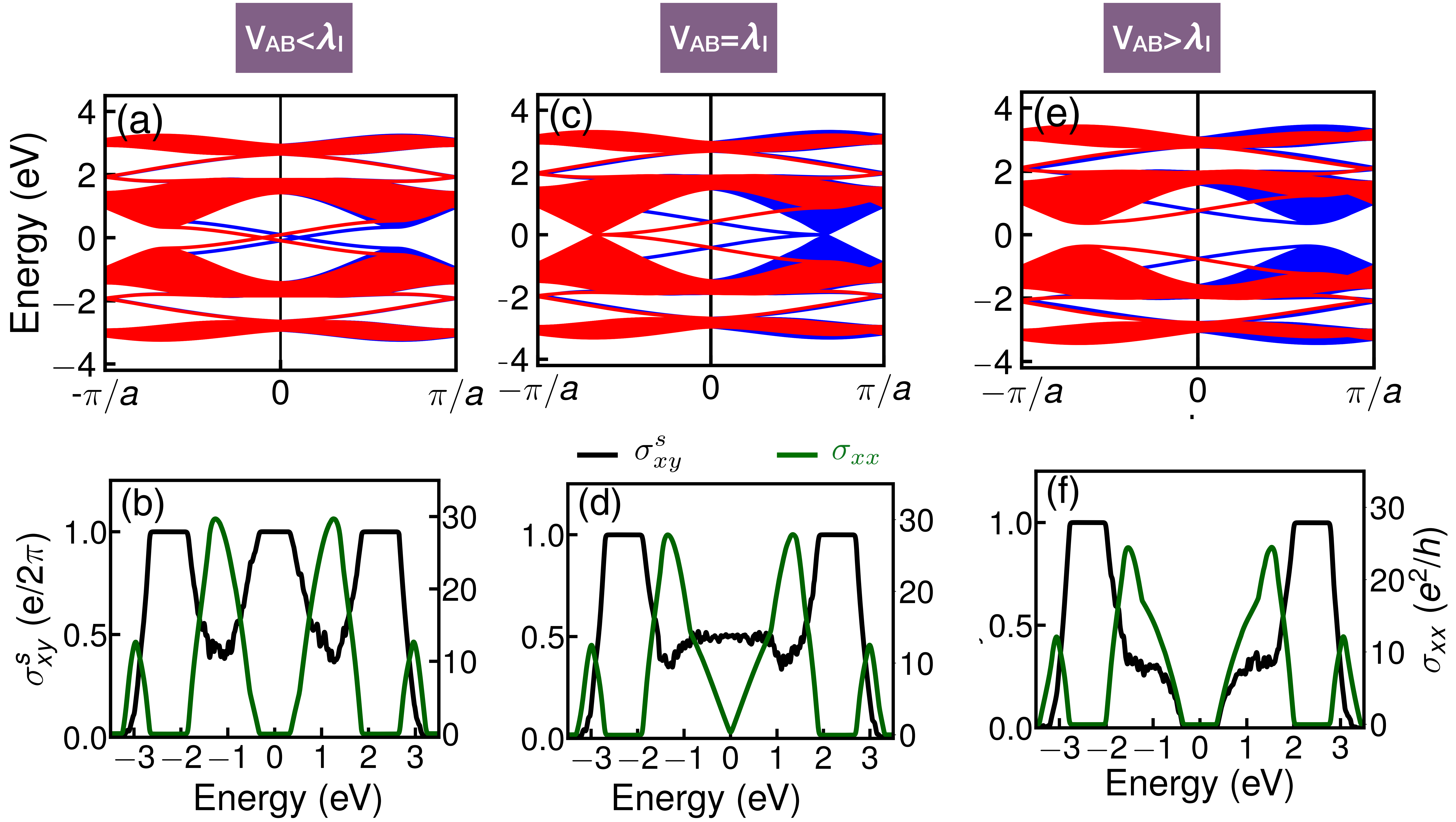
C. Wu, PRL (2008)





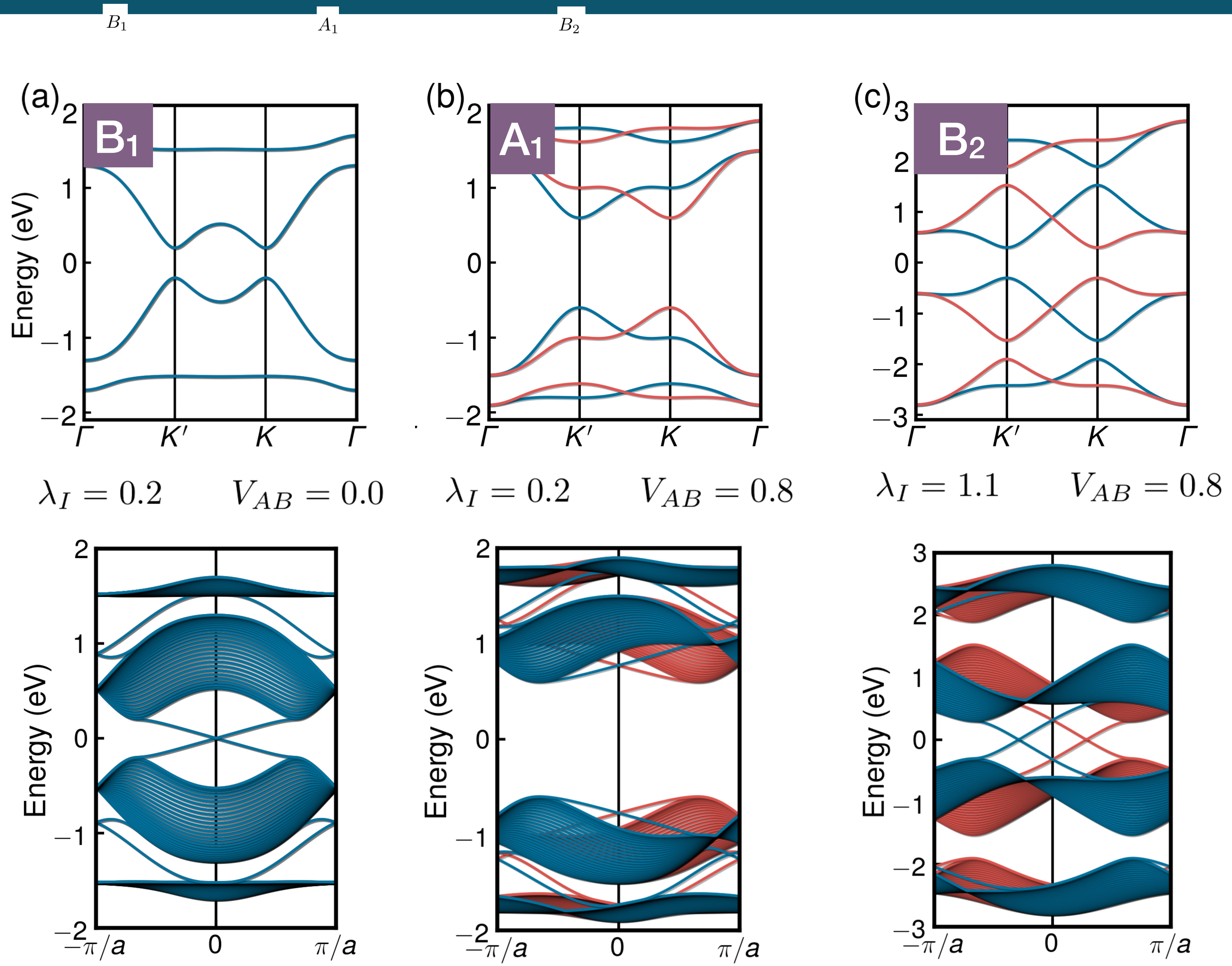


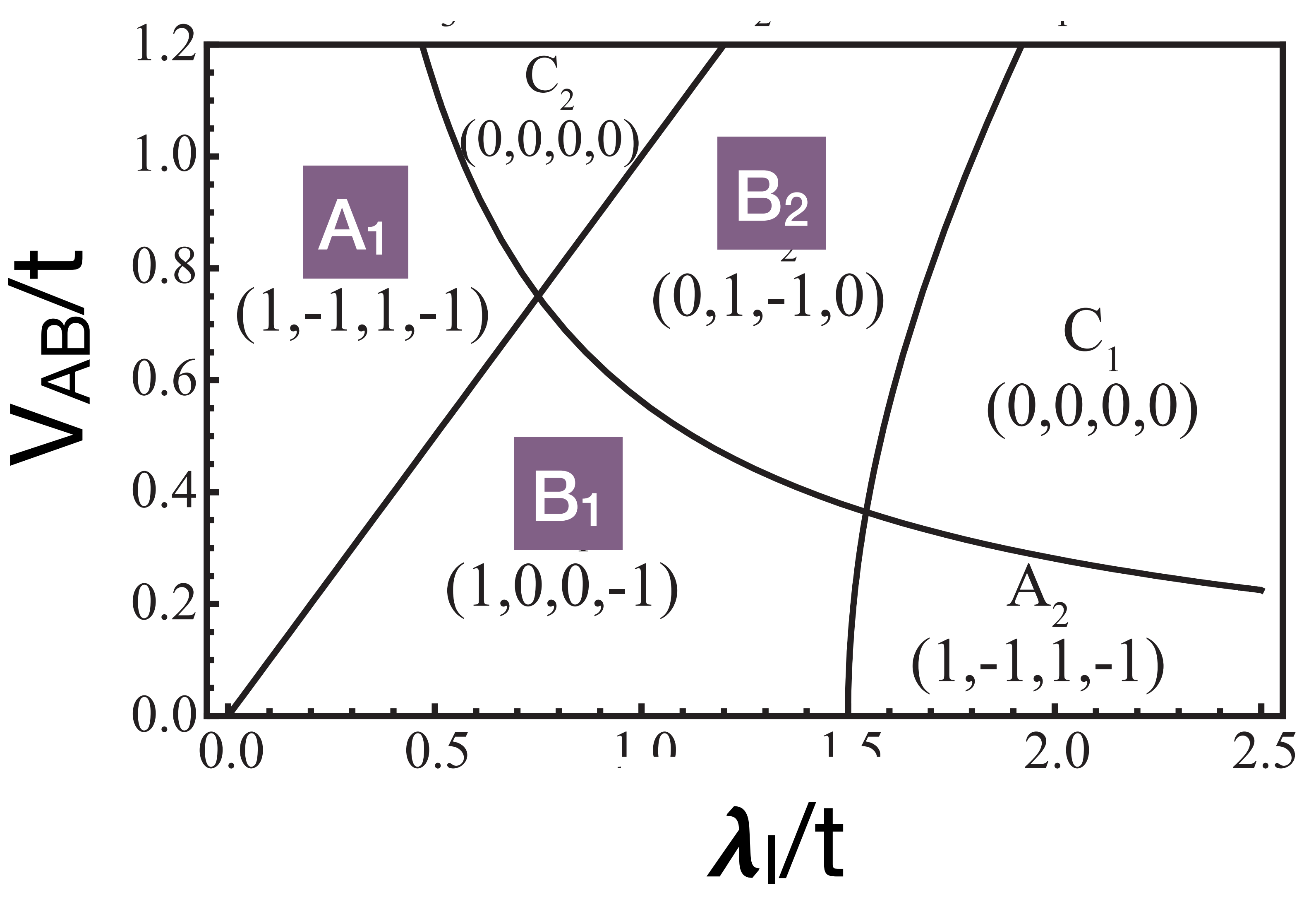
SUBLATTICE SYMMETRY BREAKING



Luis M. Canonico, Tatiana G. Rappoport, R. B. Muniz, Phys. Rev. Lett. 122 (2019) 196601.

P_X–P_Y: TOPOLOGICAL PHASE DIAGRAM





ORBITAL ANGULAR MOMENTUM

P_X–P_Y– ORBITAL TEXTURES

Because of the restricted Hilbert space, we define the spinors:

$$l_z = |p_+\rangle\langle p_+| - |p_-\rangle\langle p_-|,$$

$$l_x = |p_+\rangle\langle p_-| + |p_-\rangle\langle p_+|,$$

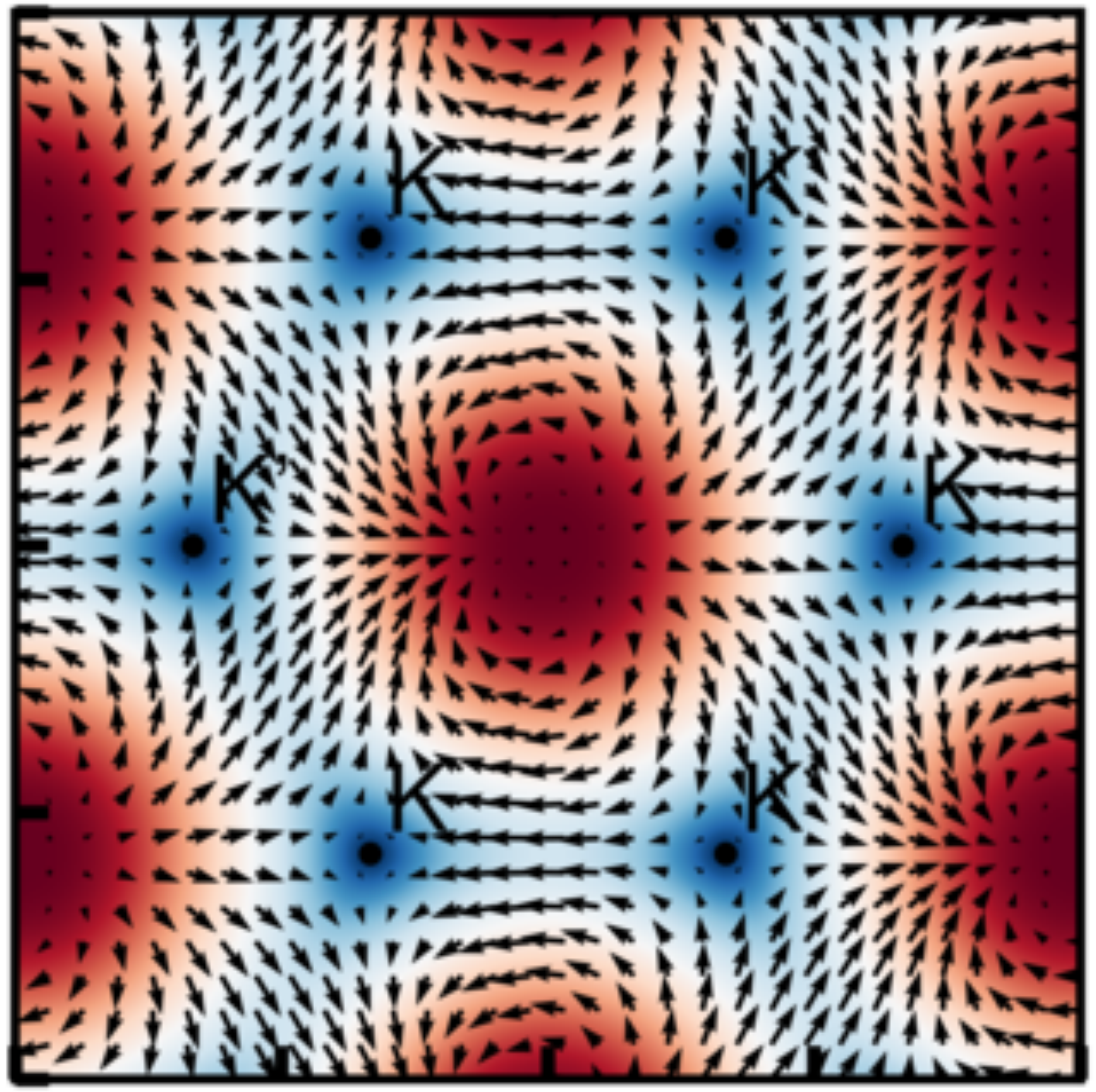
$$l_y = i\Big(|p_-\rangle\langle p_+| - |p_+\rangle\langle p_-|\Big).$$

$$\vec{l}_n(\vec{k}) = \langle l_x\rangle_n(\vec{k})\hat{x} + \langle l_y\rangle_n(\vec{k})\hat{y} + \langle l_z\rangle_n(\vec{k})\hat{z},$$

$$\langle l_i\rangle_n(\vec{k}) = \sum_{\sigma=A,B} \langle \psi_n(\vec{k})|l_i(\sigma)|\psi_n(\vec{k})\rangle,$$

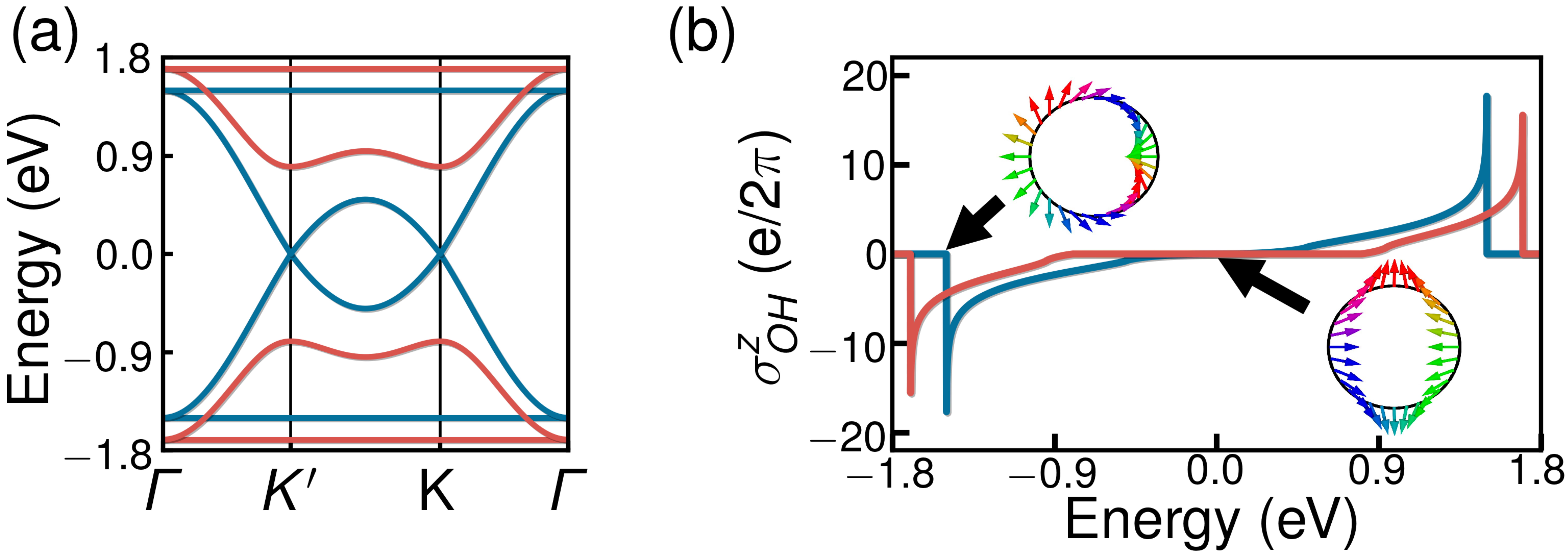
$$H_D = -\frac{\sqrt{3}\hbar v_F}{2a}\left(\ell_x\sigma_x + \tau\ell_y\sigma_y\right).$$

$$p_\mu = p_\pm = \frac{1}{\sqrt{2}}(p_x \pm i p_y)$$



OHE WITHOUT SOC

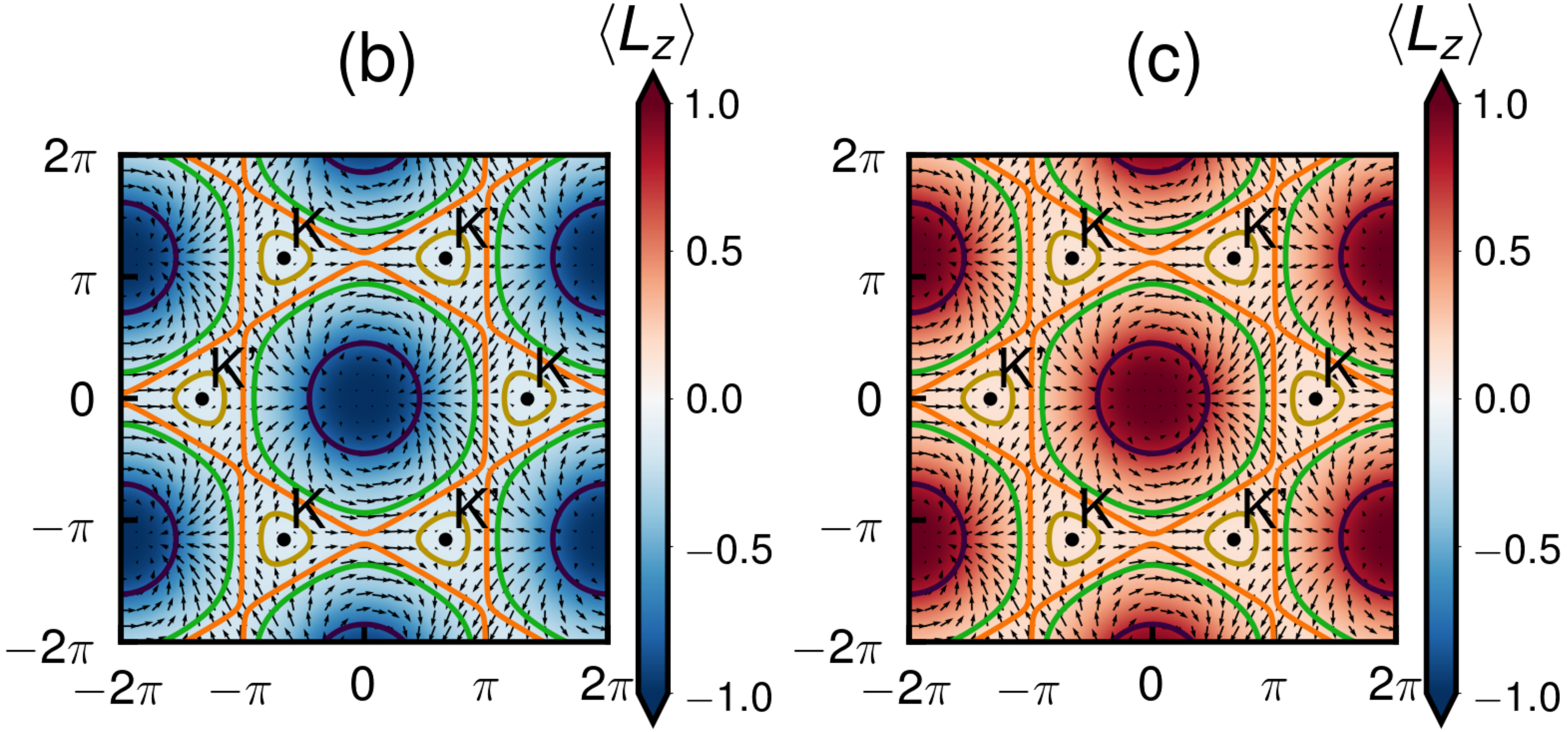
$\lambda_I = 0$



$V_{AB} = 0.0$ $V_{AB} = 0.8$

J. Sinova et al. PRL 2004

ORBITAL TEXTURES FOR INVERTED SPIN DIRECTIONS



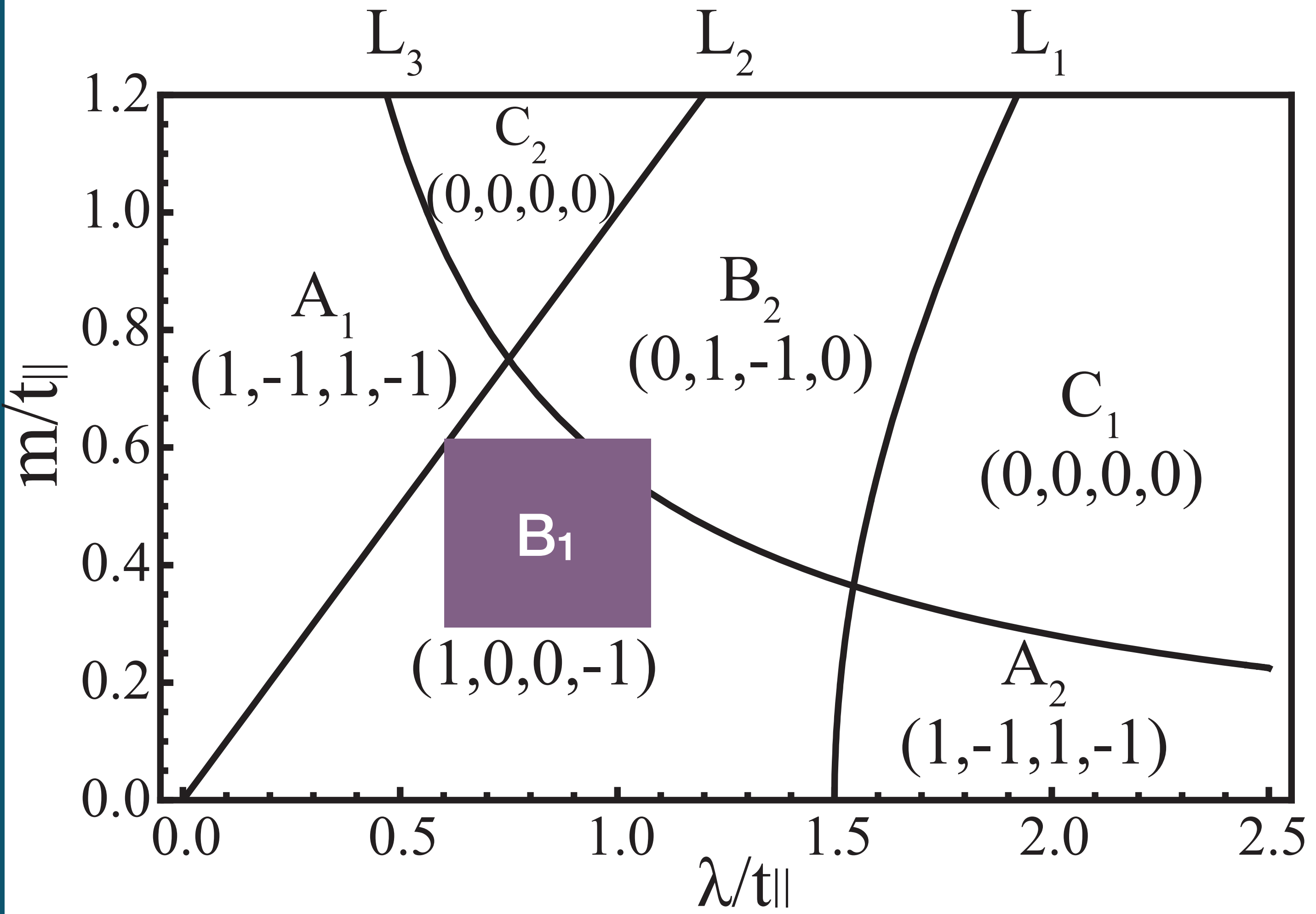
Dresselhaus “SOC"

Degenerate bands: $\Rightarrow \langle \ell_t^z \rangle = 0$

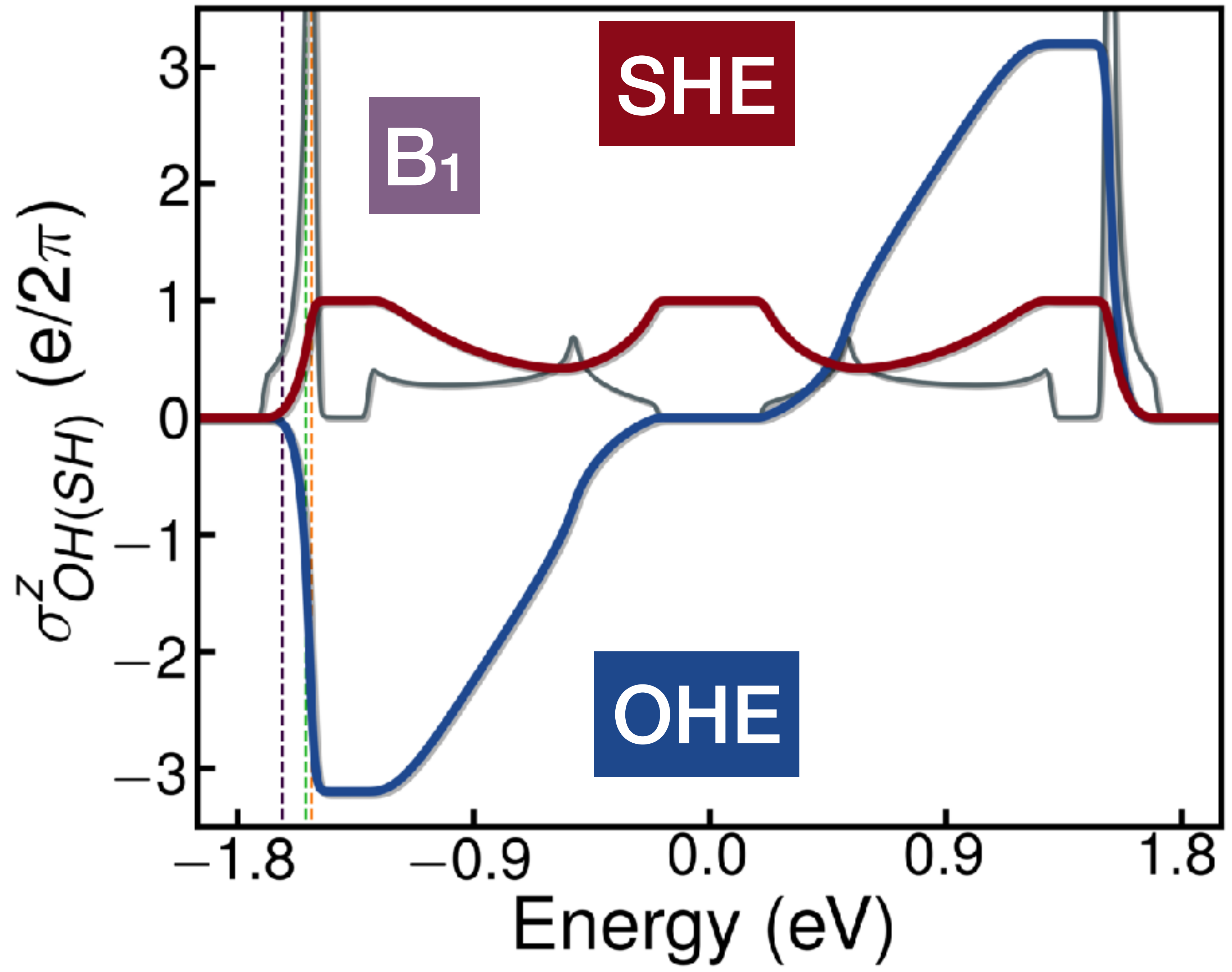
In-plane orbital texture survives

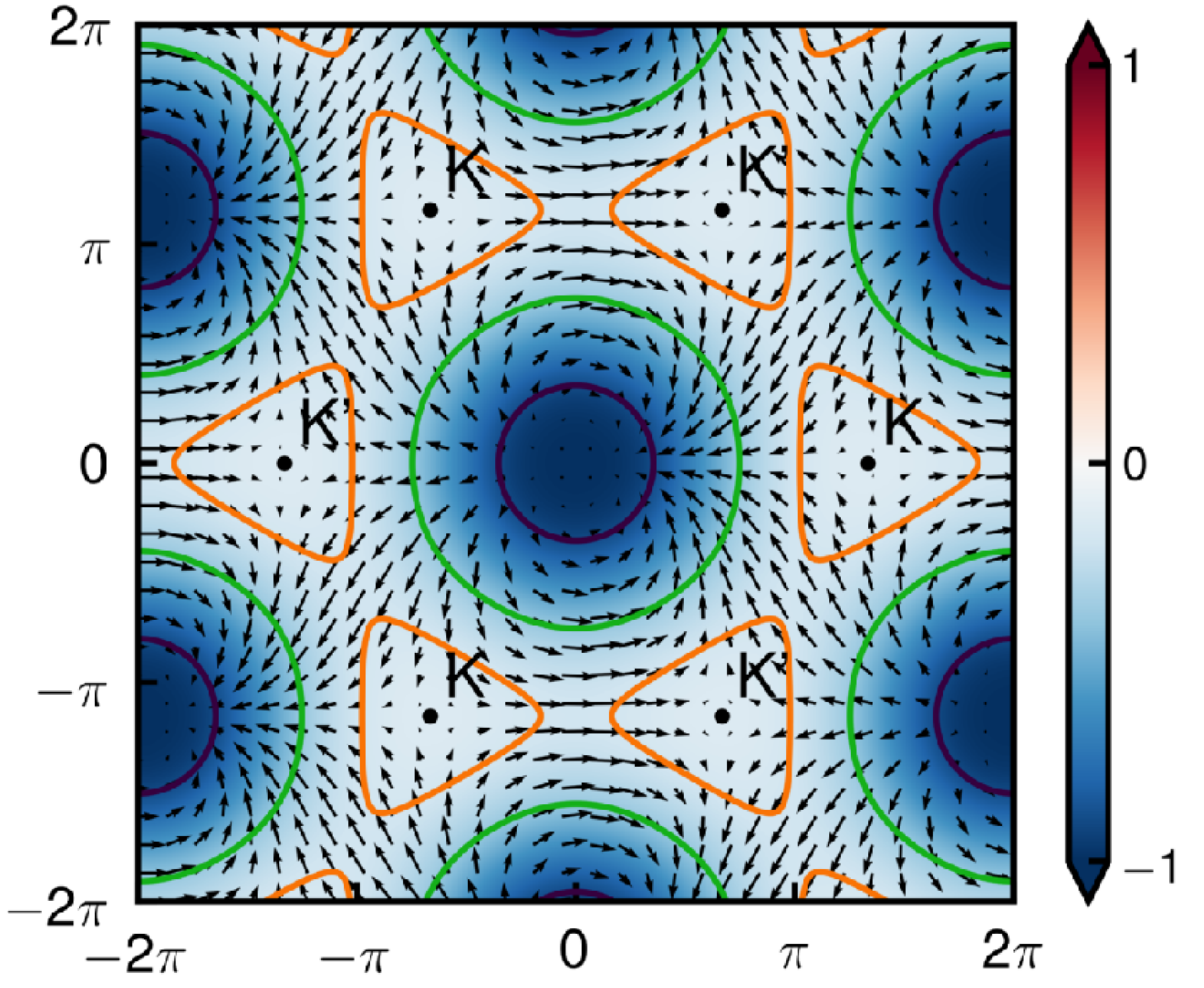
$$H_D = -\frac{\sqrt{3}\hbar v_F}{2a}\left(\ell_x \sigma_x + \tau \ell_y \sigma_y\right).$$

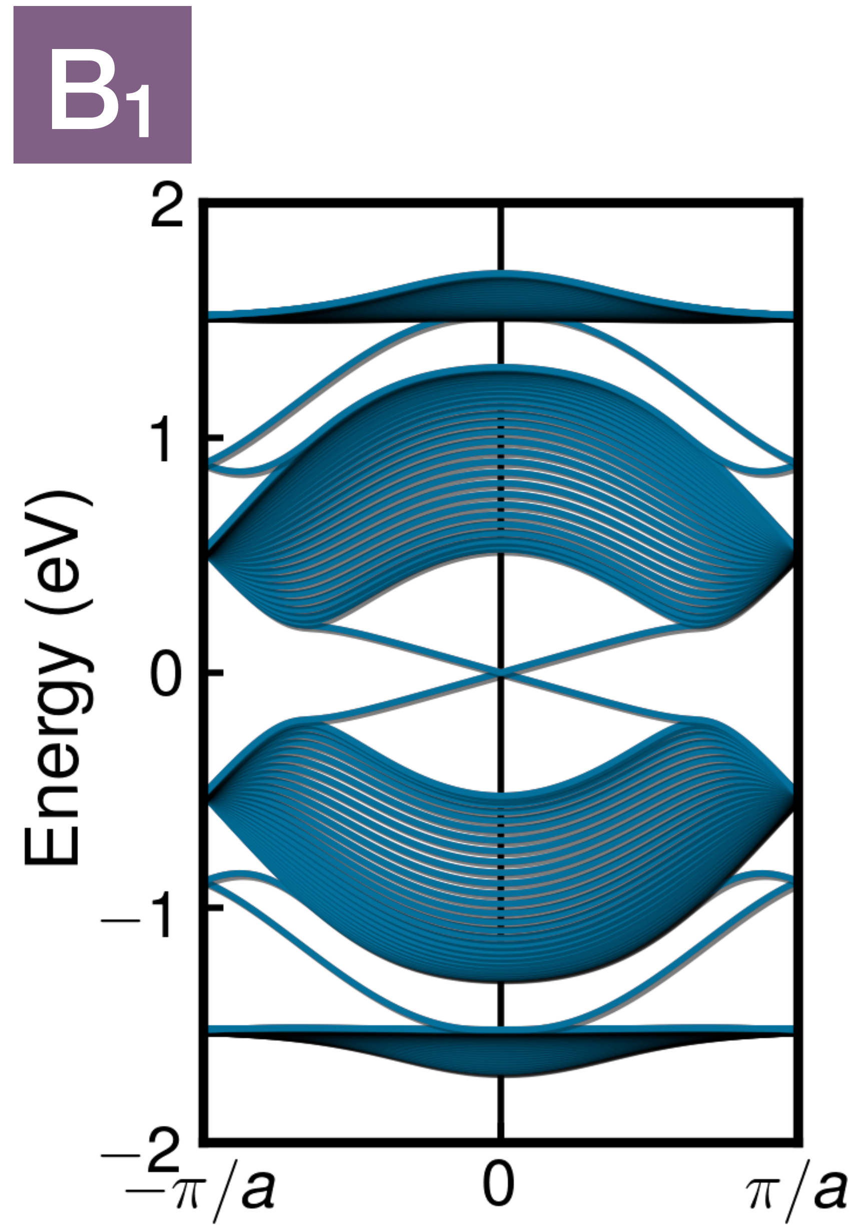
OHE – PHASE B1



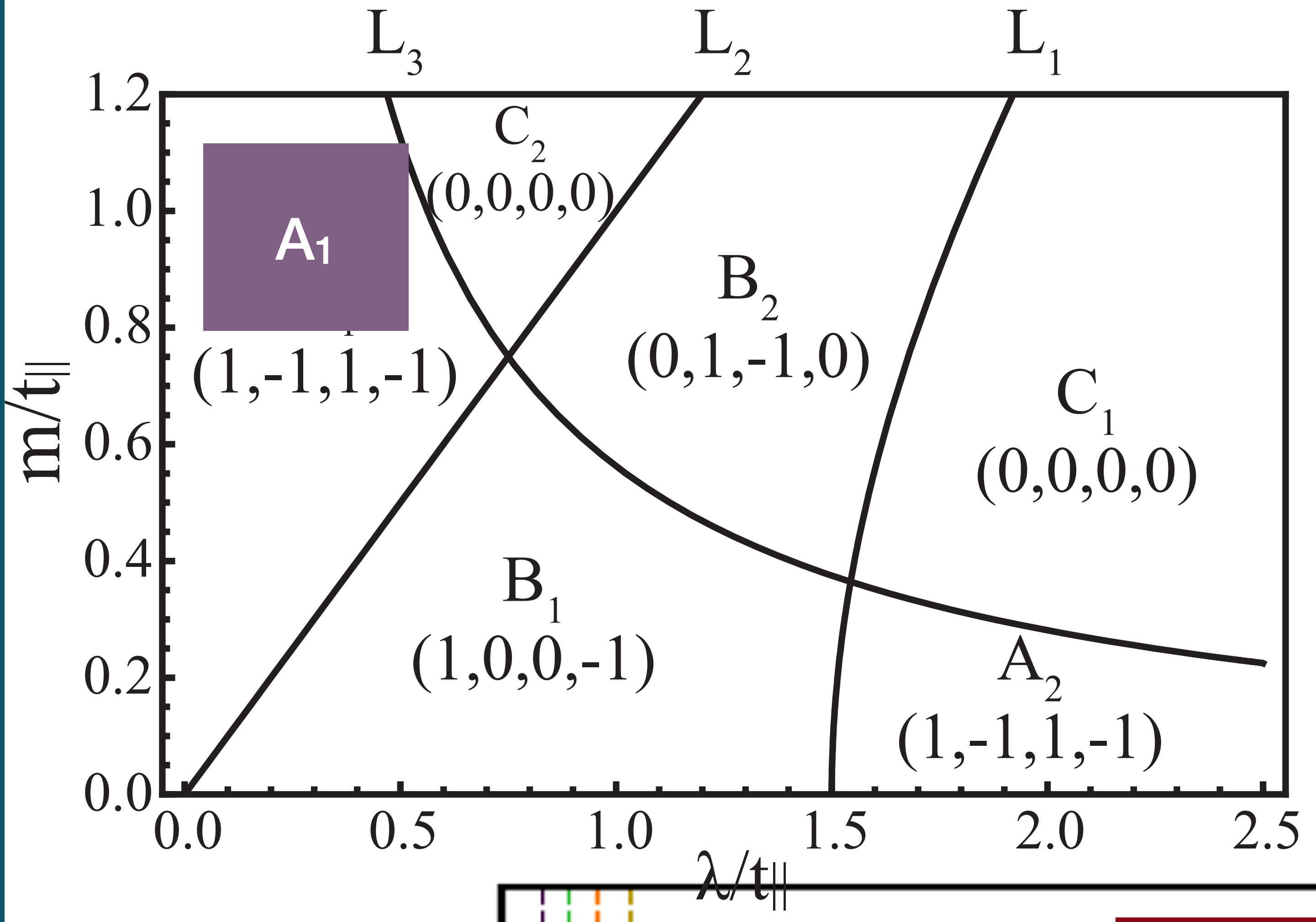
B1 with $\lambda_I = 0.2V_{pp\sigma}$ and $V_{AB} = 0.$



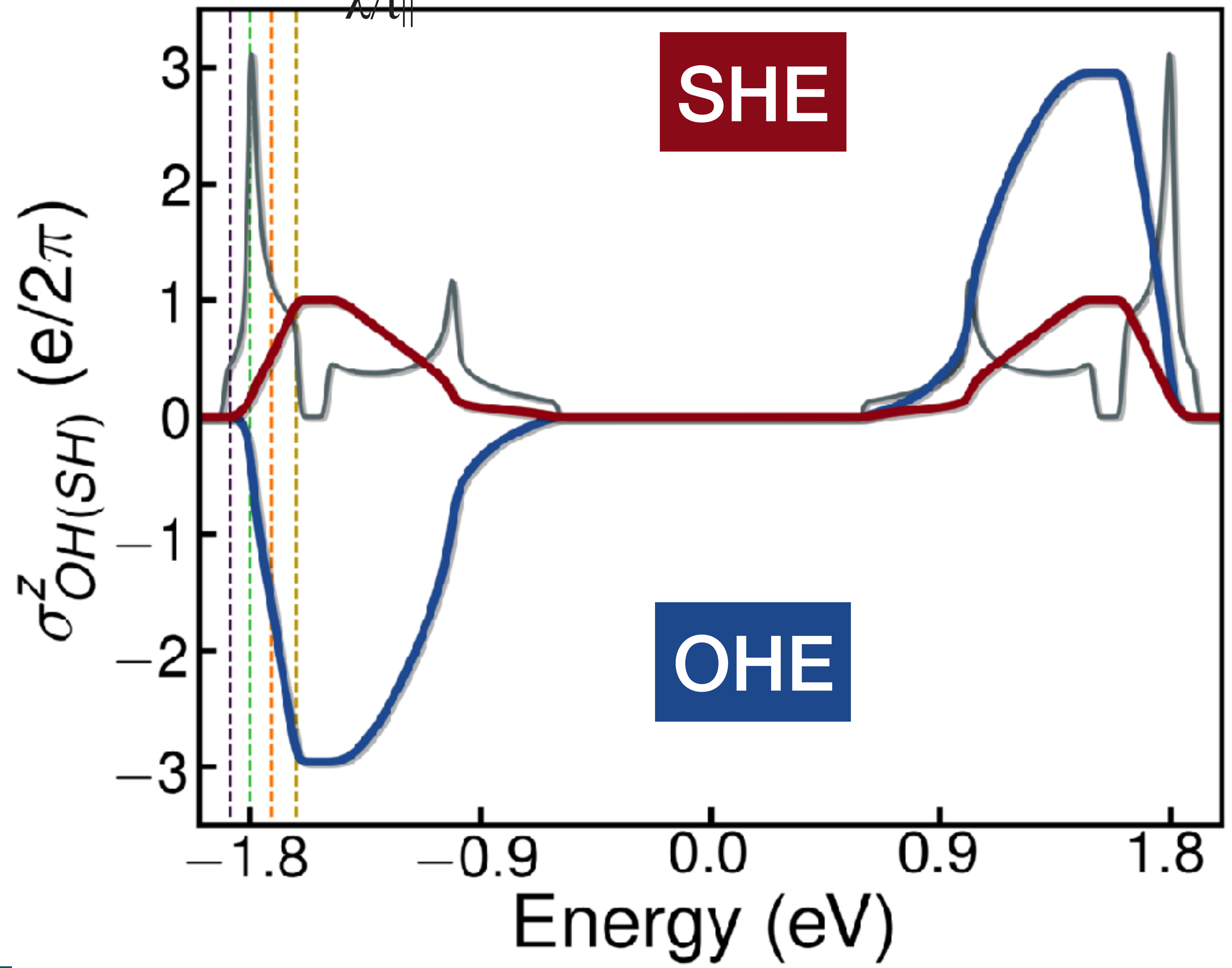


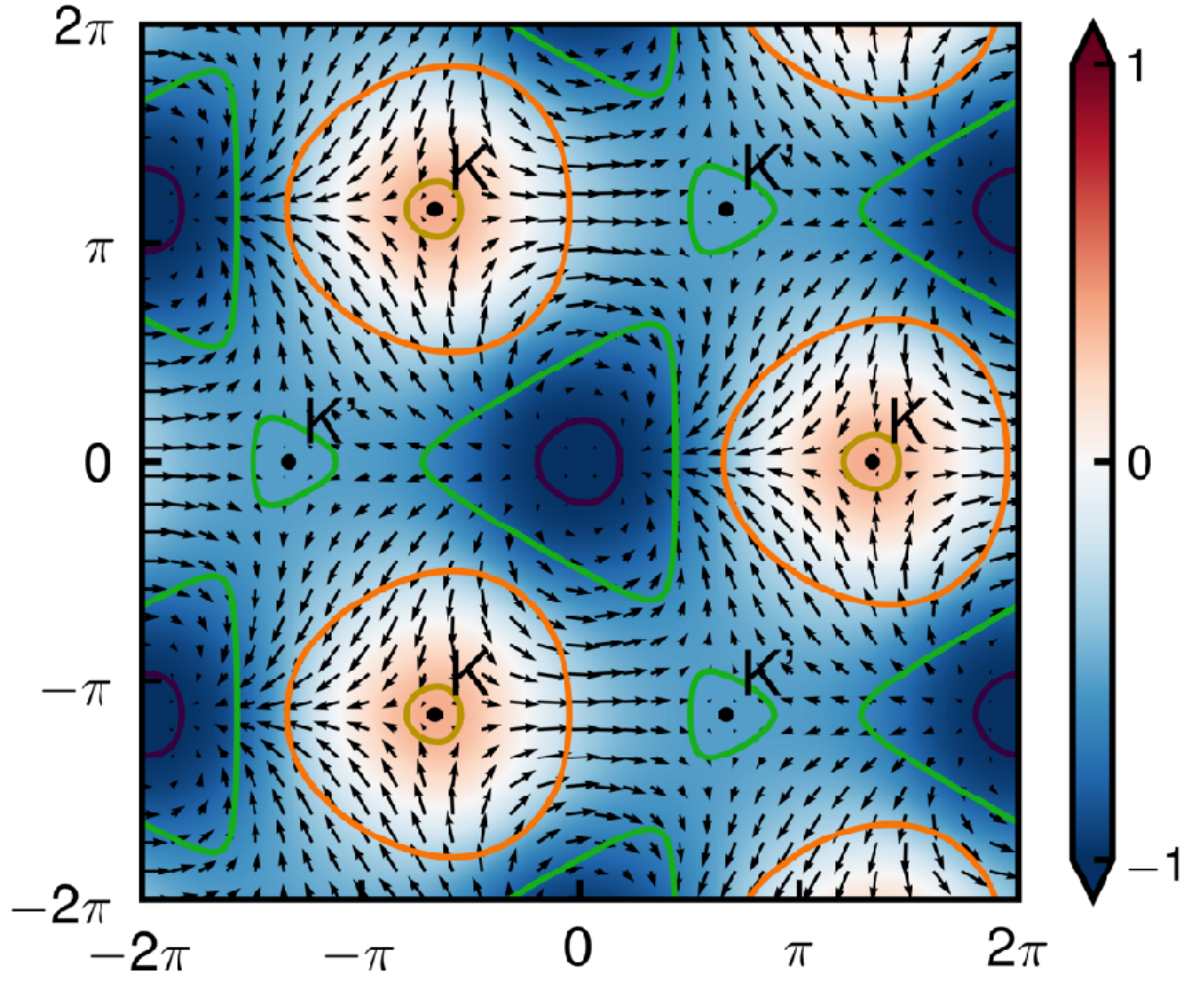


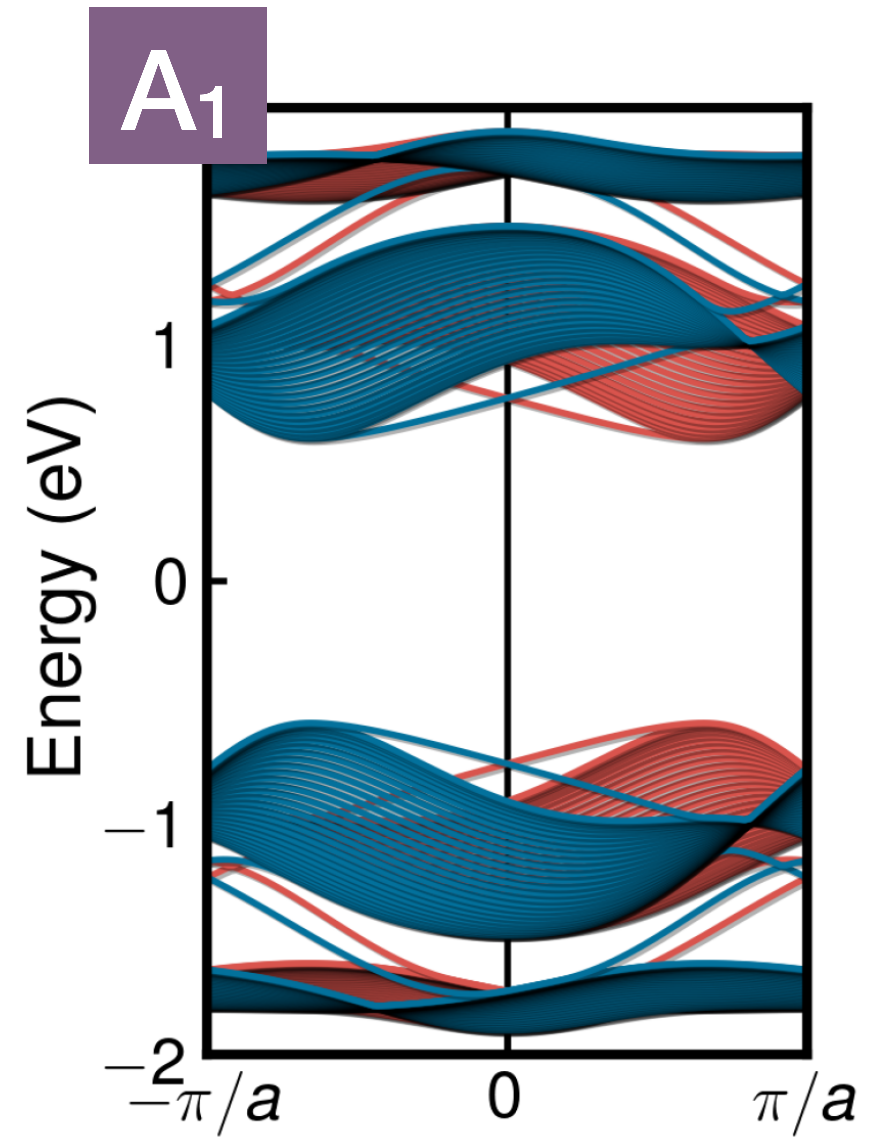
OHE – PHASE A1

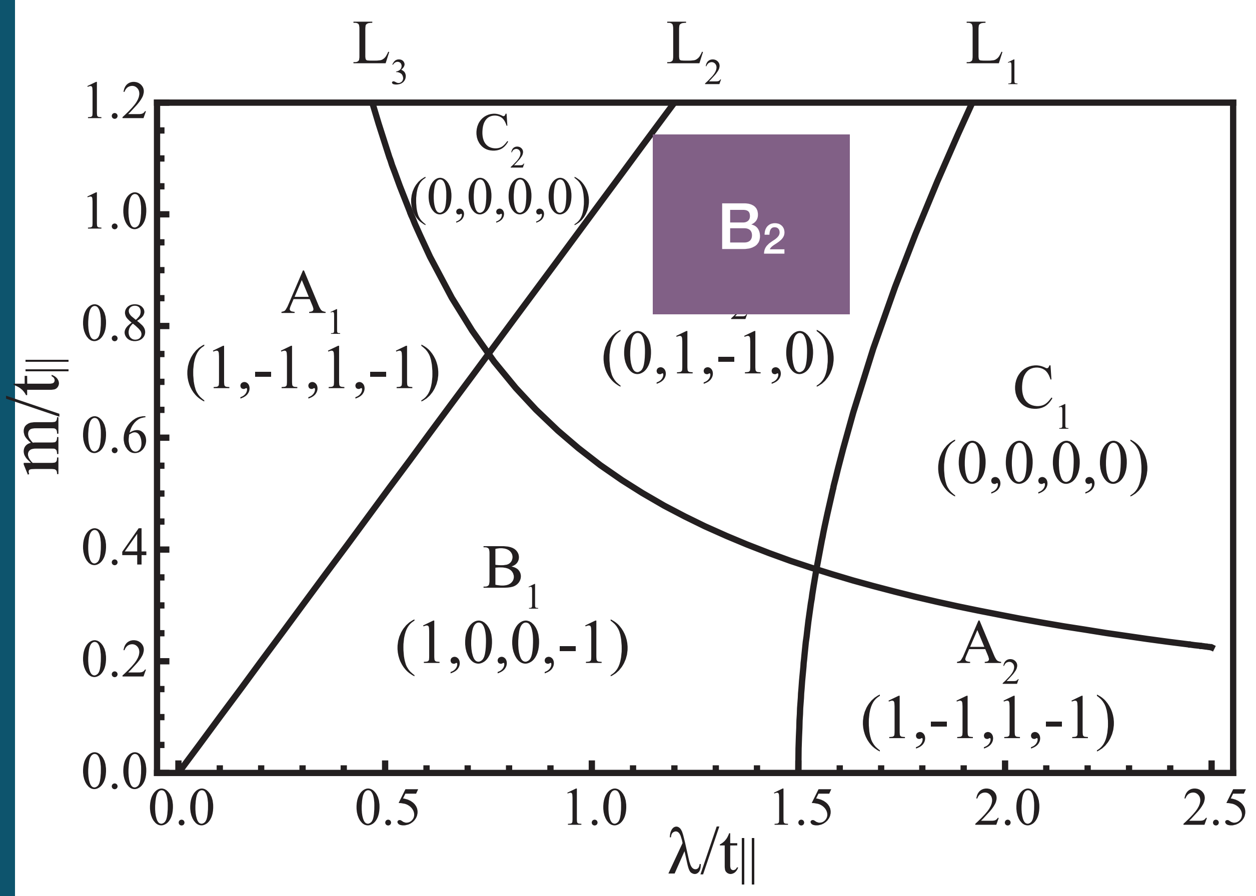


A1 with $\lambda_I = 0.2V_{pp\sigma}$ and $V_{AB} = 0.8V_{pp\sigma}$

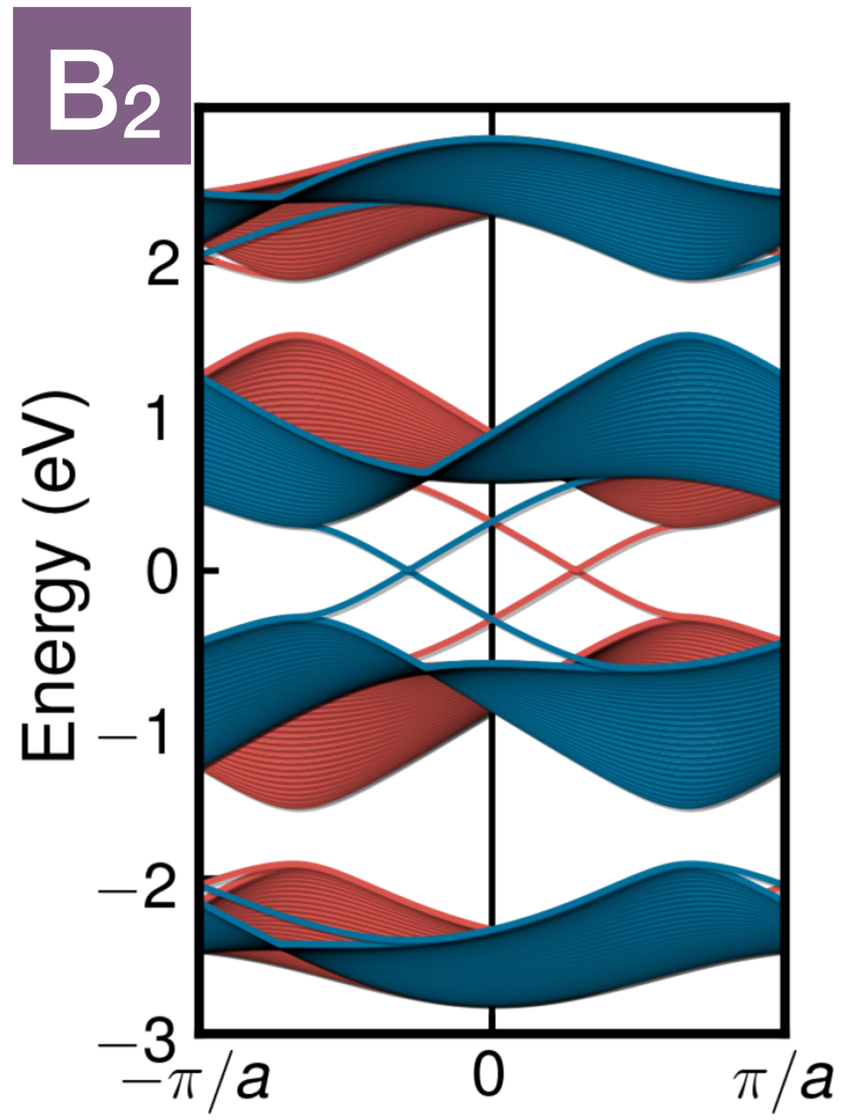


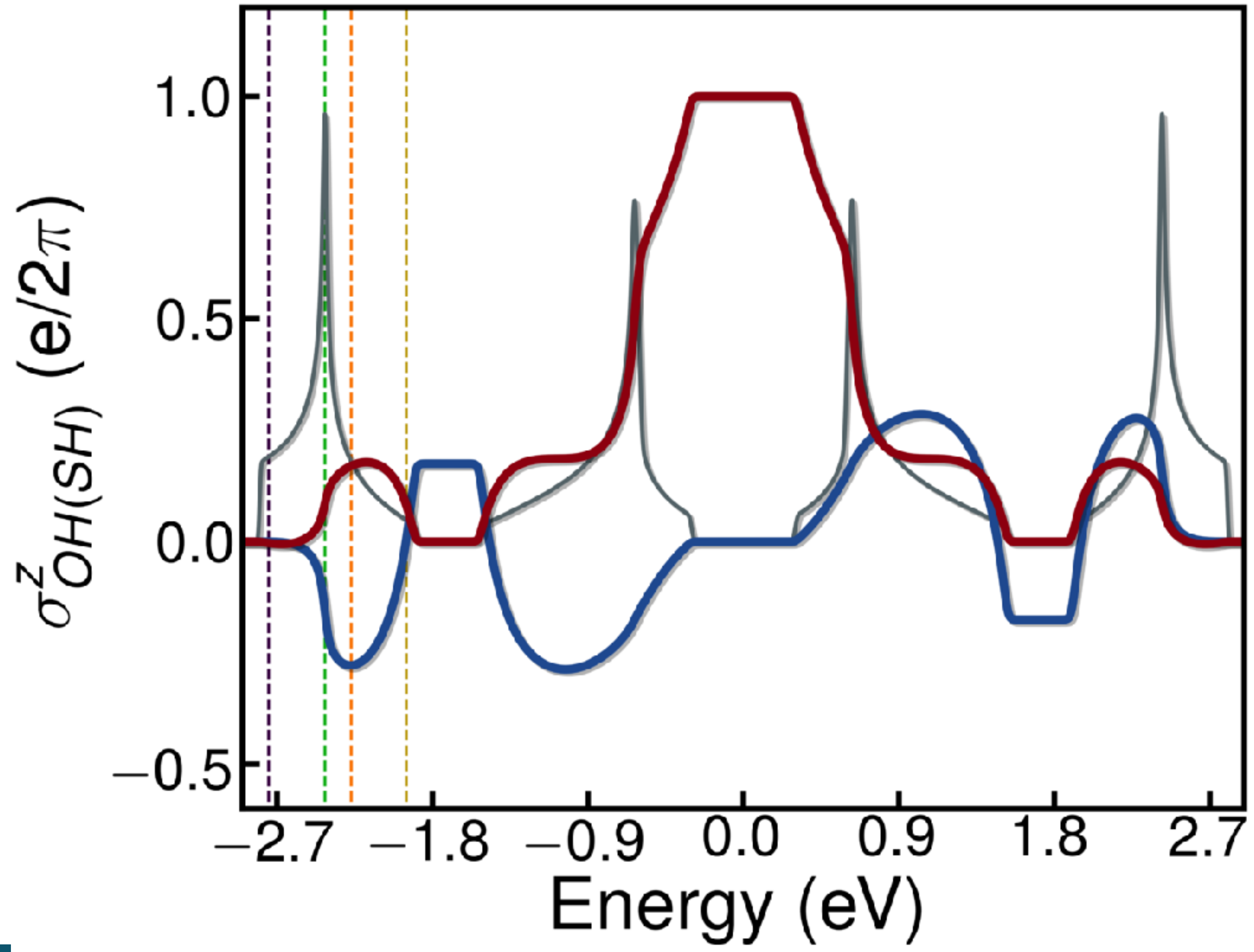


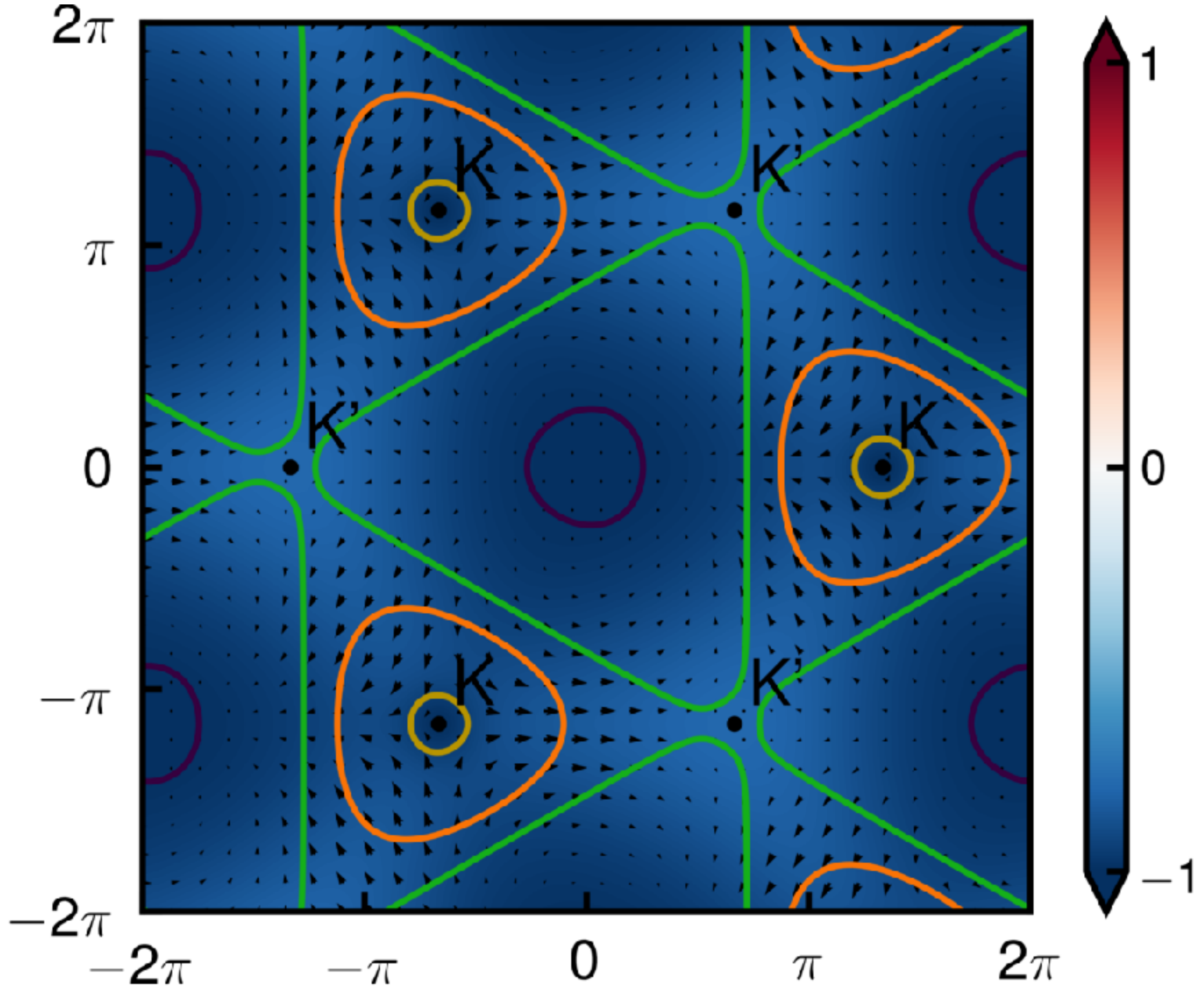




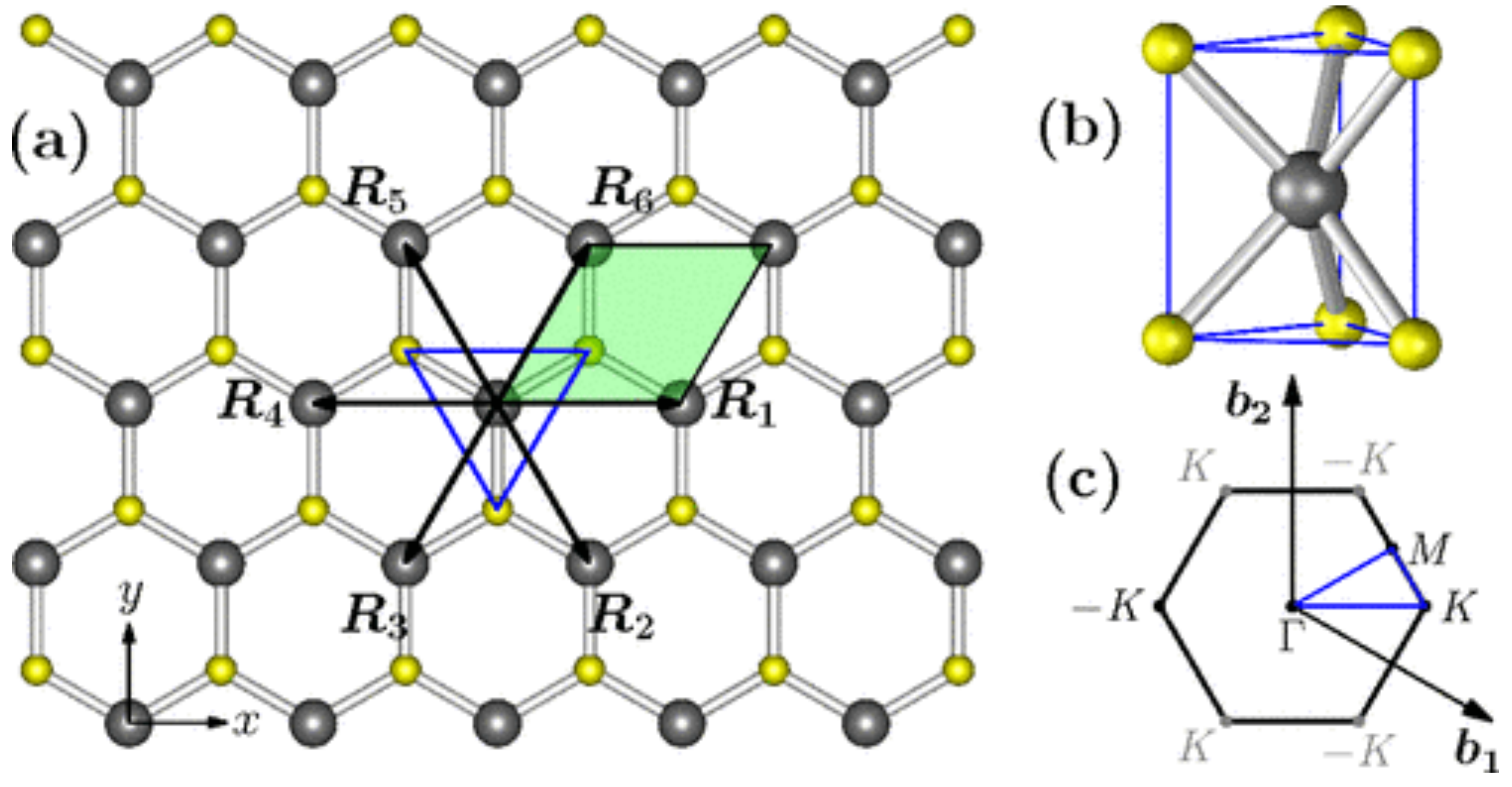
B2 with $\lambda_I = 1.1V_{pp\sigma}$ and $V_{AB} = 0.8V_{pp\sigma}$



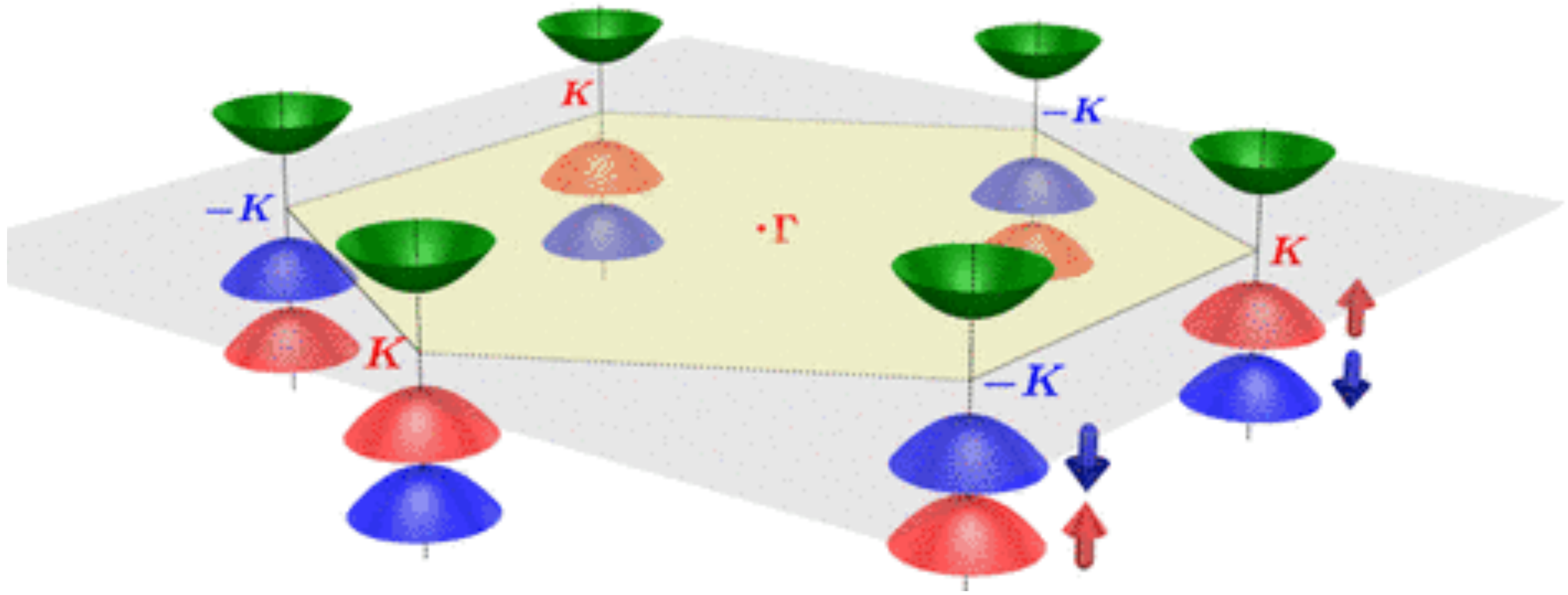




OHE IN TMDS



Spin-valley locking



3 bands model based on TM ***d*** orbitals

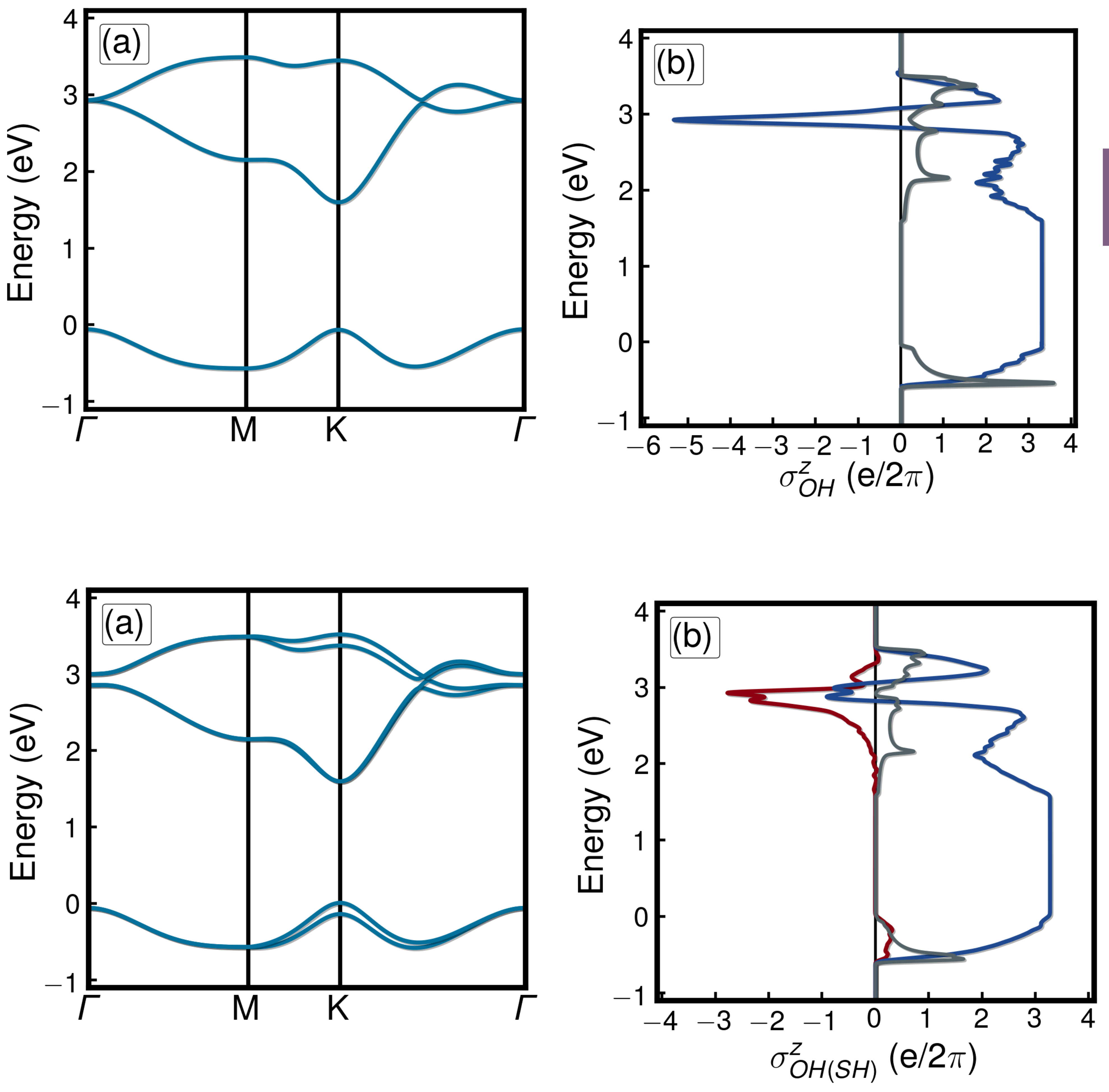
$$d_{z^2},\ d_{xy}\ \text{and}\ d_{x^2+y^2},\qquad \mathbf{L}^z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 2i \\ 0 & -2i & 0 \end{bmatrix}$$

G. B. Liu et al, PRB 2012
Di Xiao, PRL 2012

ORBITAL TEXTURES

MoS_2

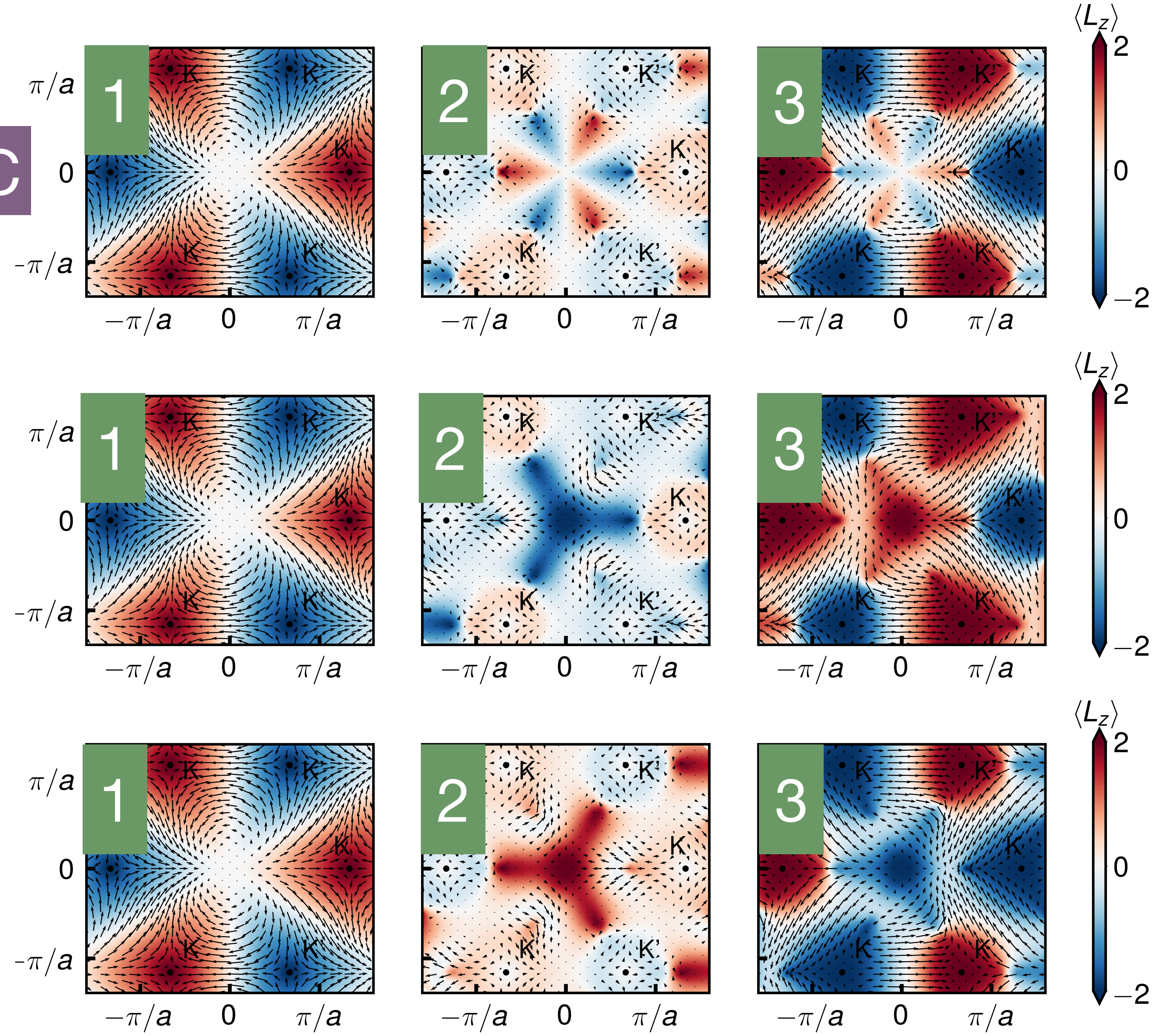
Orbital-Valley locking in the valence band!



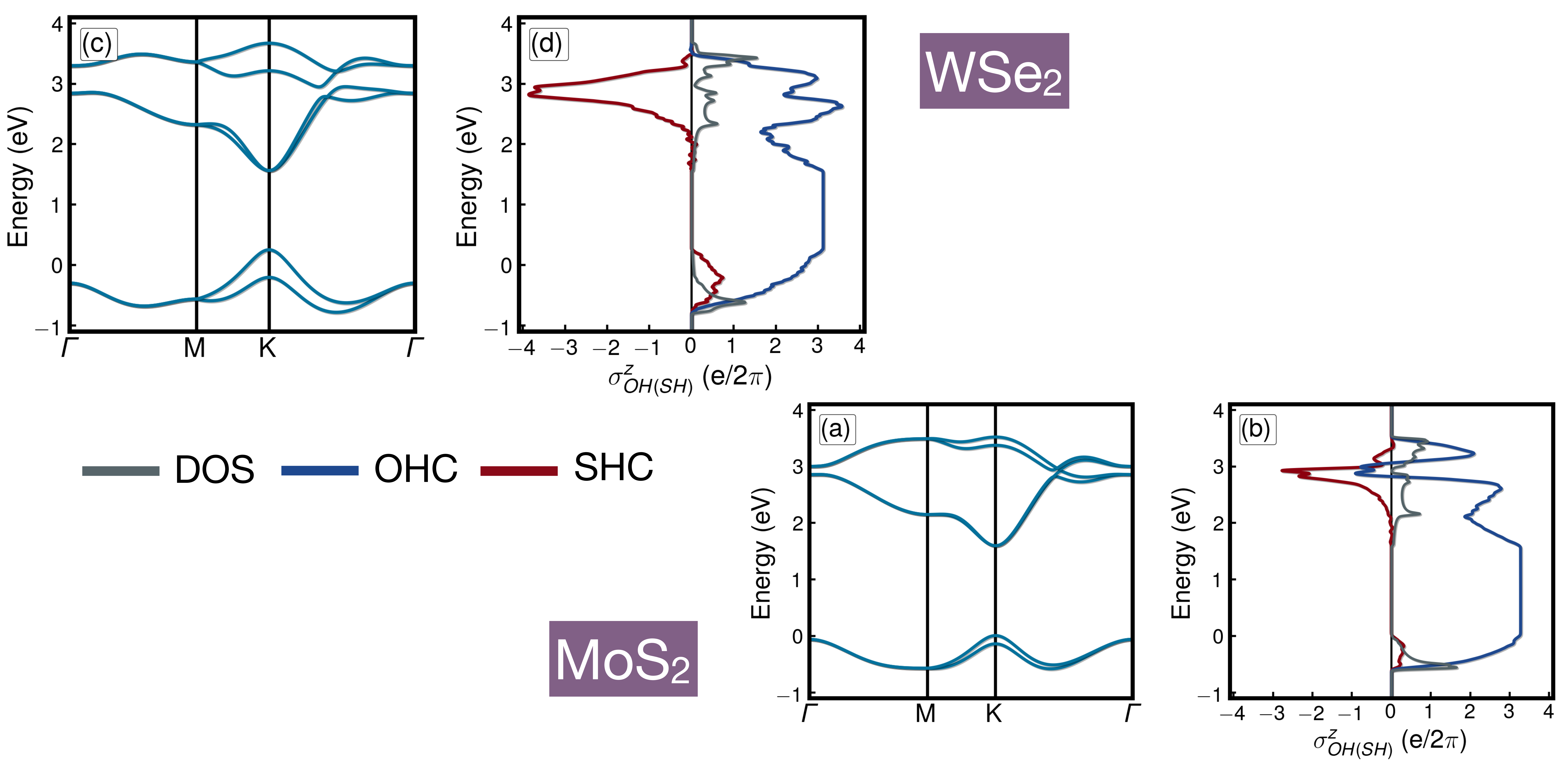
Zero SOC

SOC

SOC



OHE IN TRANSITION METAL DICHALCOGENIDES(1H)



OHE – FIRST PRINCIPLES HAMILTONIAN

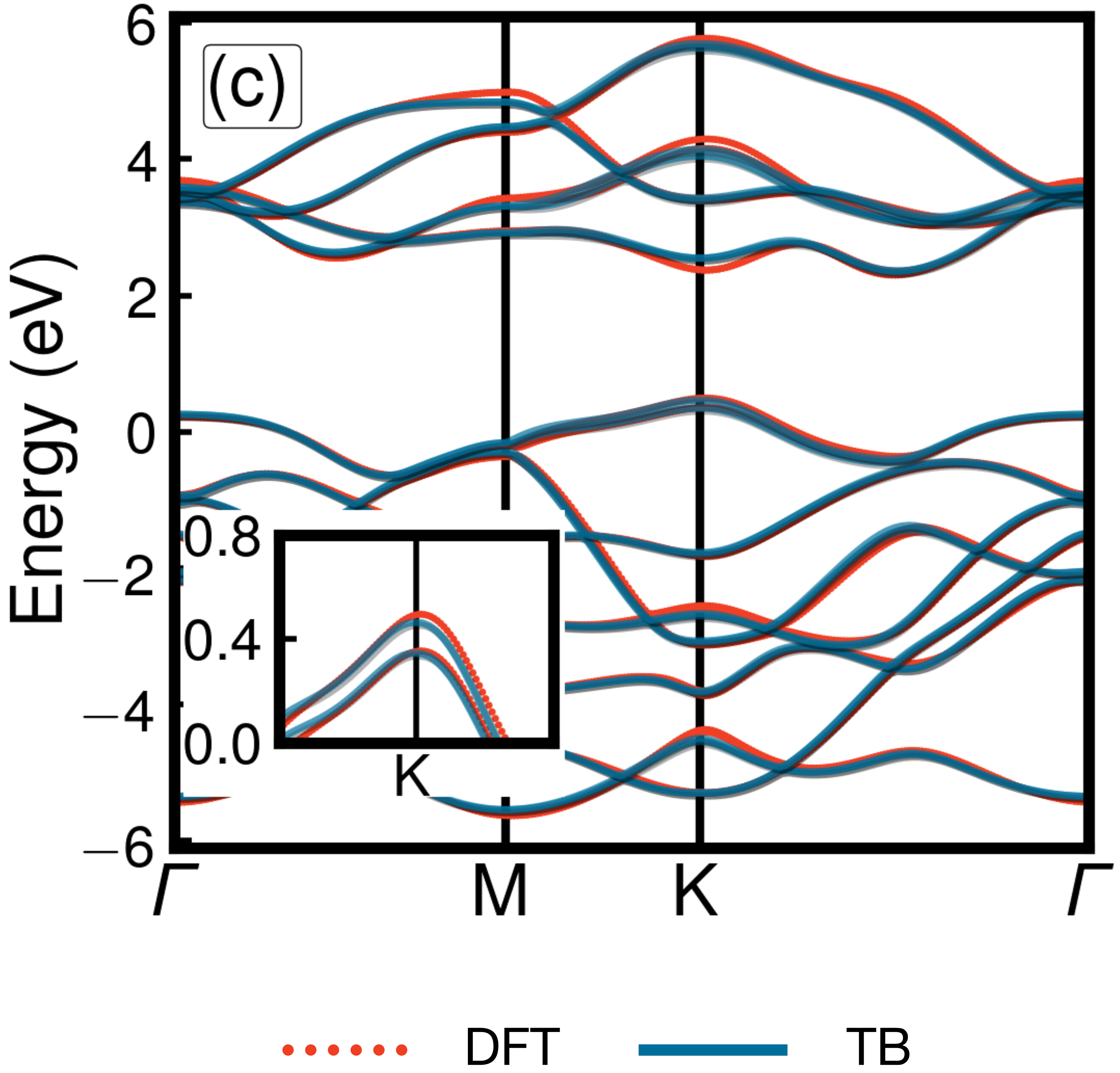
Chalcogen atoms

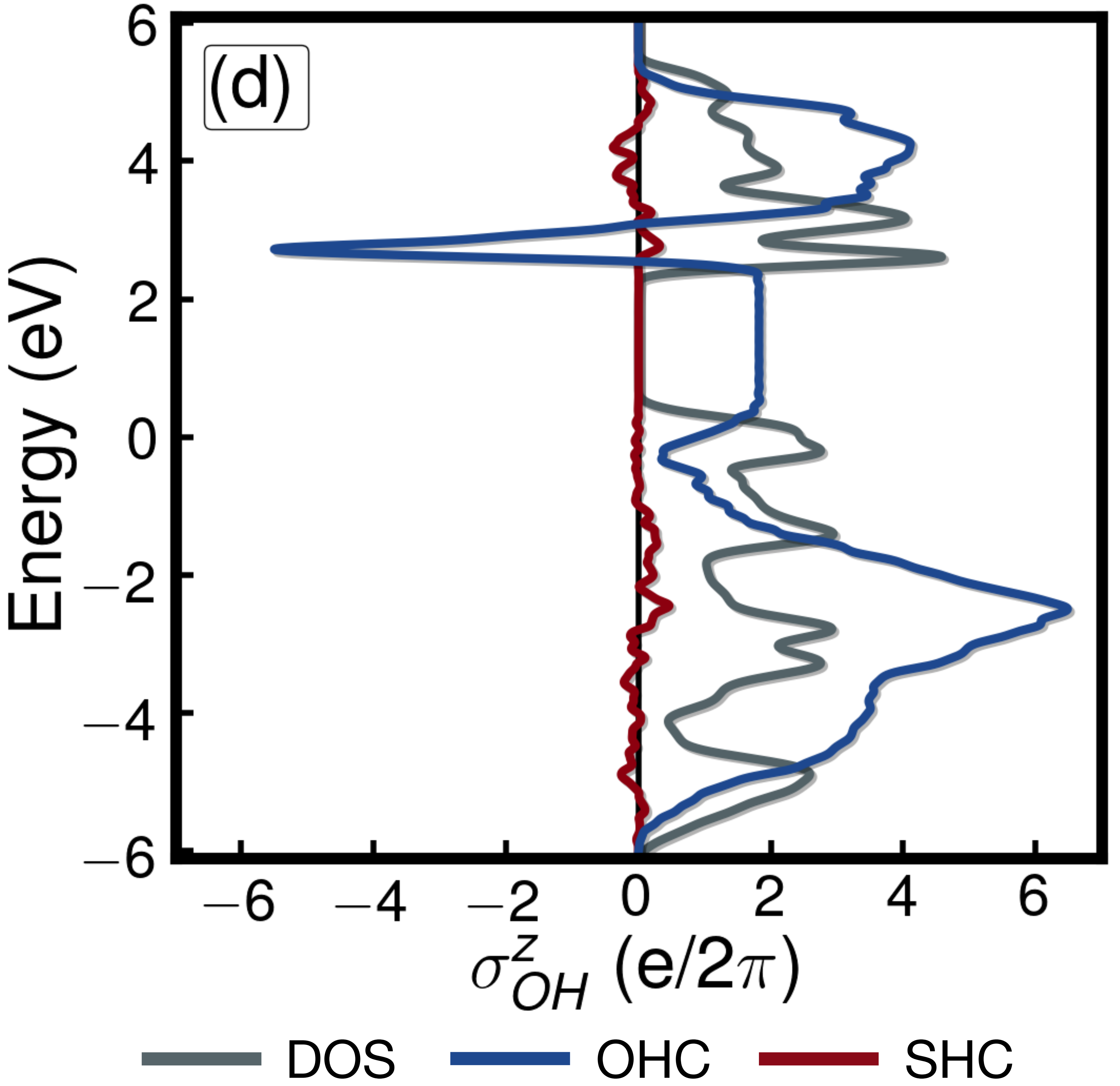
$s,\ p_x,\ p_y$ and p_z

TM atoms

$d_{xy},\ d_{xz}, d_{yz},\ d_{x^2-y^2}$ and d_{z^2}

MoS_2





$$L = 768 \times 768$$

$$M = 768$$

$$R = 10$$

Wannier90

$$t_{cutoff} = 0.0125 \times |t_{max}|$$

CONCLUSIONS/ PERSPECTIVES

- Metallic multi-orbital 2D materials can host large OHE in the **absence** of SOC
- Trivial multi-orbital 2D insulators can host OHE
  - Non-quantized orbital Hall plateaus
- TMDs present sizeable orbital Hall plateaus
- OHE can be used for example, for orbital torque transfer
- OHE widens the pool of materials that can be used for spin-orbitronics.


THANK YOU FOR
YOUR ATTENTION