Room Temperature Quantum Spin Hall Effect

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Outline

Topological matter

- Paradigm: integer quantum Hall effect
- Enhancement, deconstruction, extension

Quantum spin Hall effect

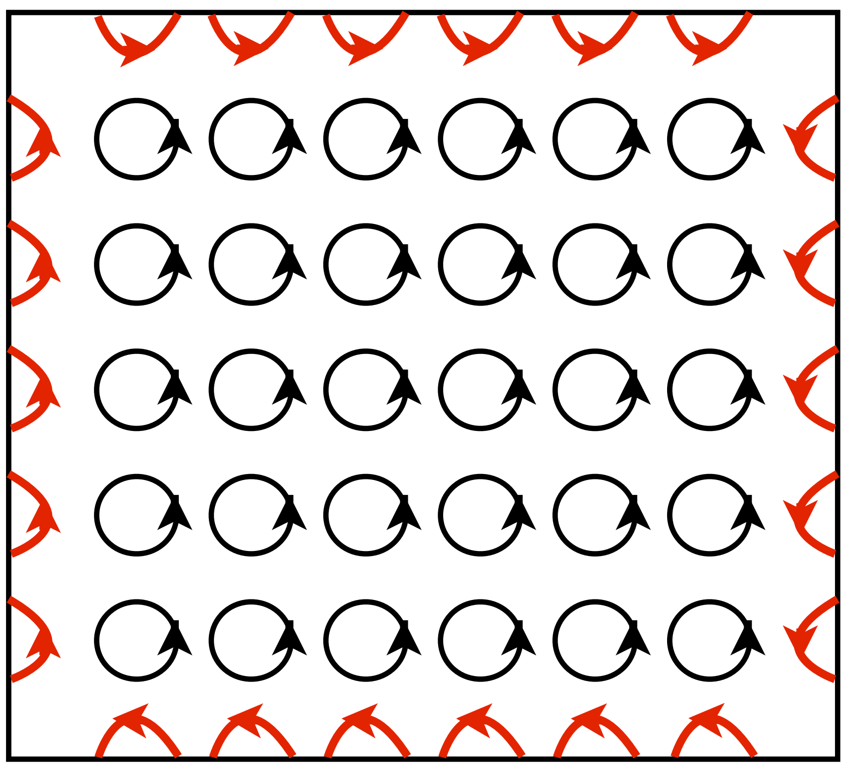
- Bi/SiC heterostructure
- WTe_2 monolayers
- Jacutingaite mineral Pt_2HgSe_3

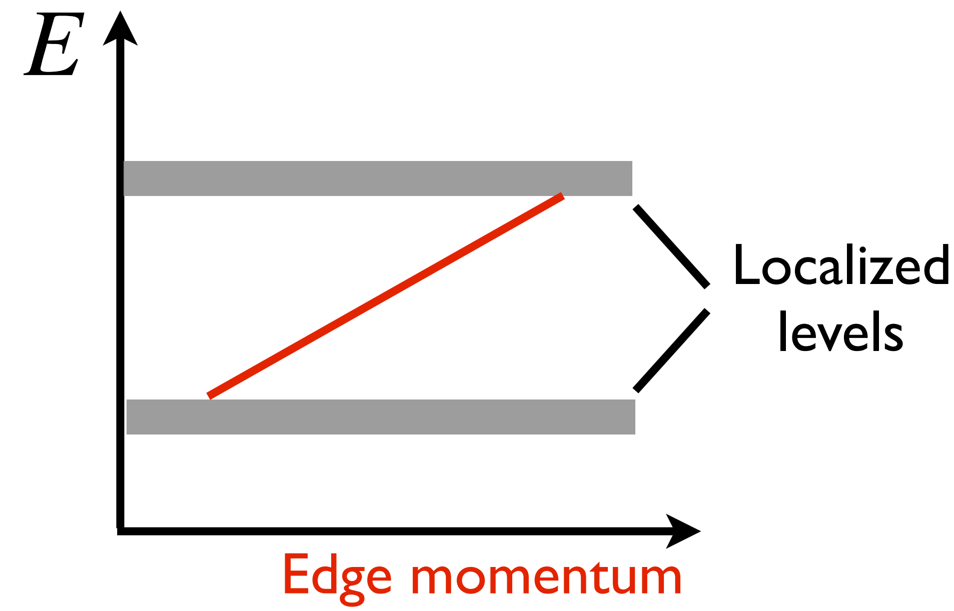
Topological matter

Integer Quantum Hall effect (IQHE)

Von Klitzing 1980; Laughlin 1981; Thouless 1982; Haldane 1988

Chiral mode at the edge of the sample; zero longitudinal resistance

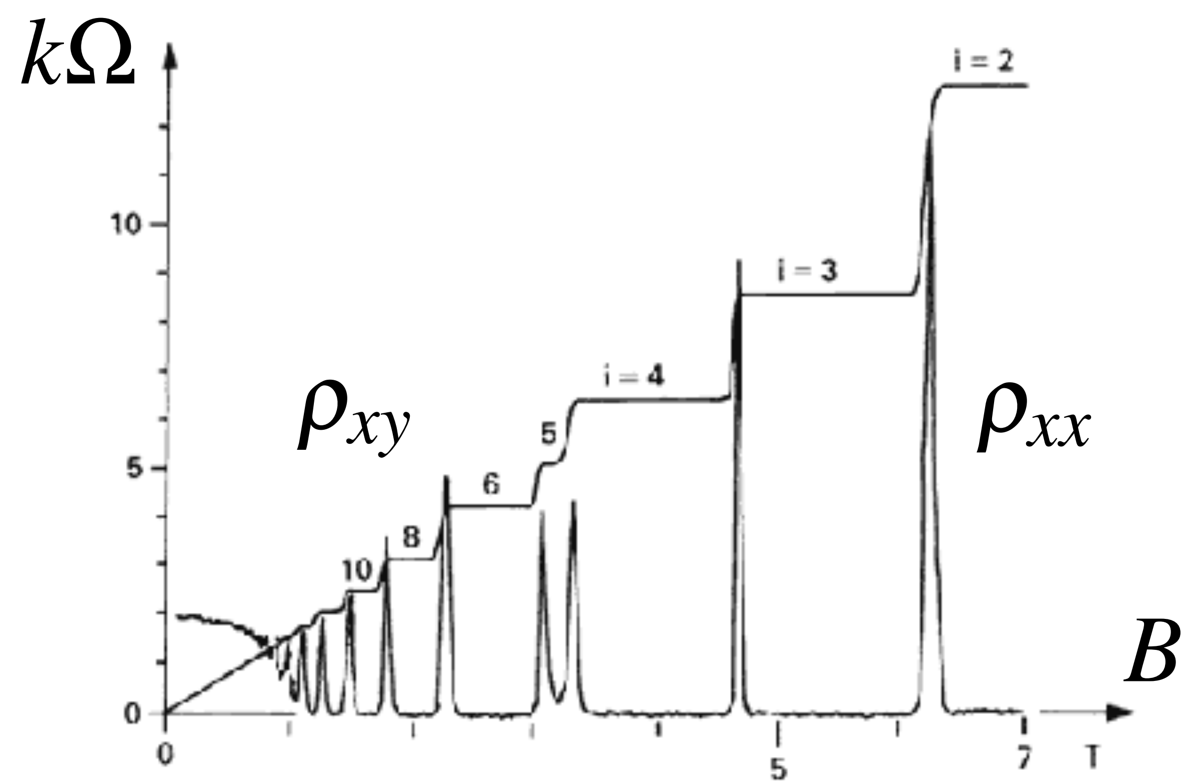




$$\rho_{xy} = \frac{1}{C}\frac{h}{e^2} \qquad \rho_{xx} = 0$$

Chern number $C \in \mathbb{Z}$

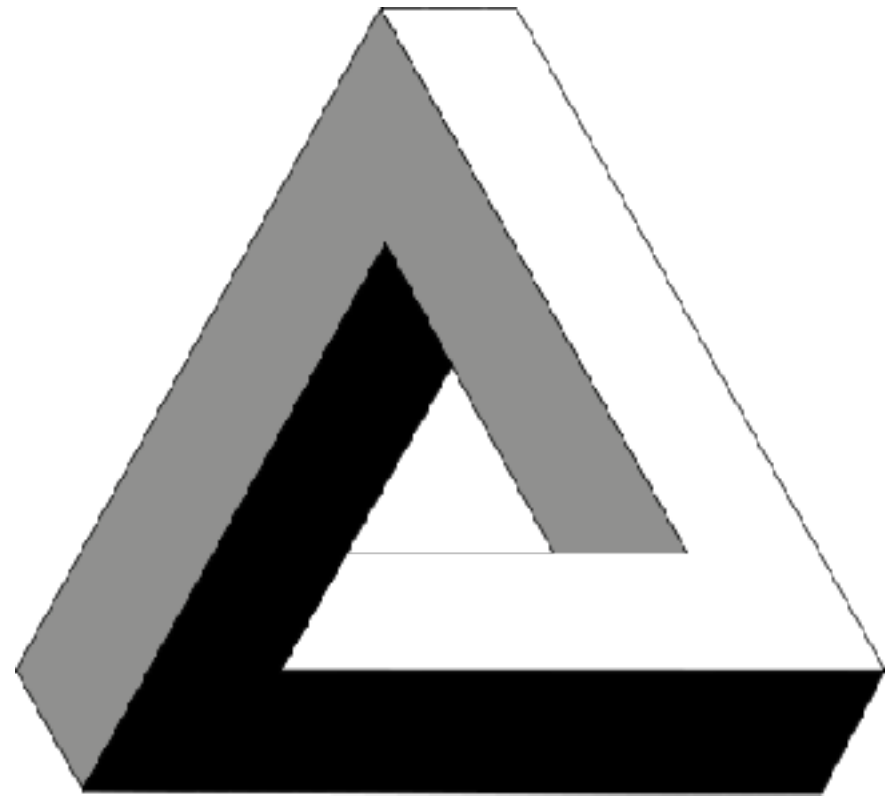
topological invariant



Evolution of topological matter

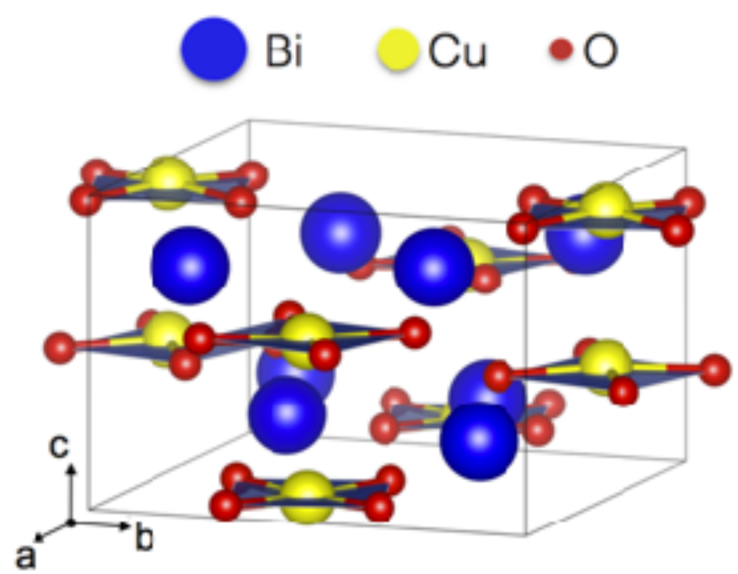
Deconstruction

Symmetry				d							
AZ	Θ	Ξ	Π	1	2	3	4	5	6	7	8
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	−1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AII	−1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	−1	−1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	−1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	−1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

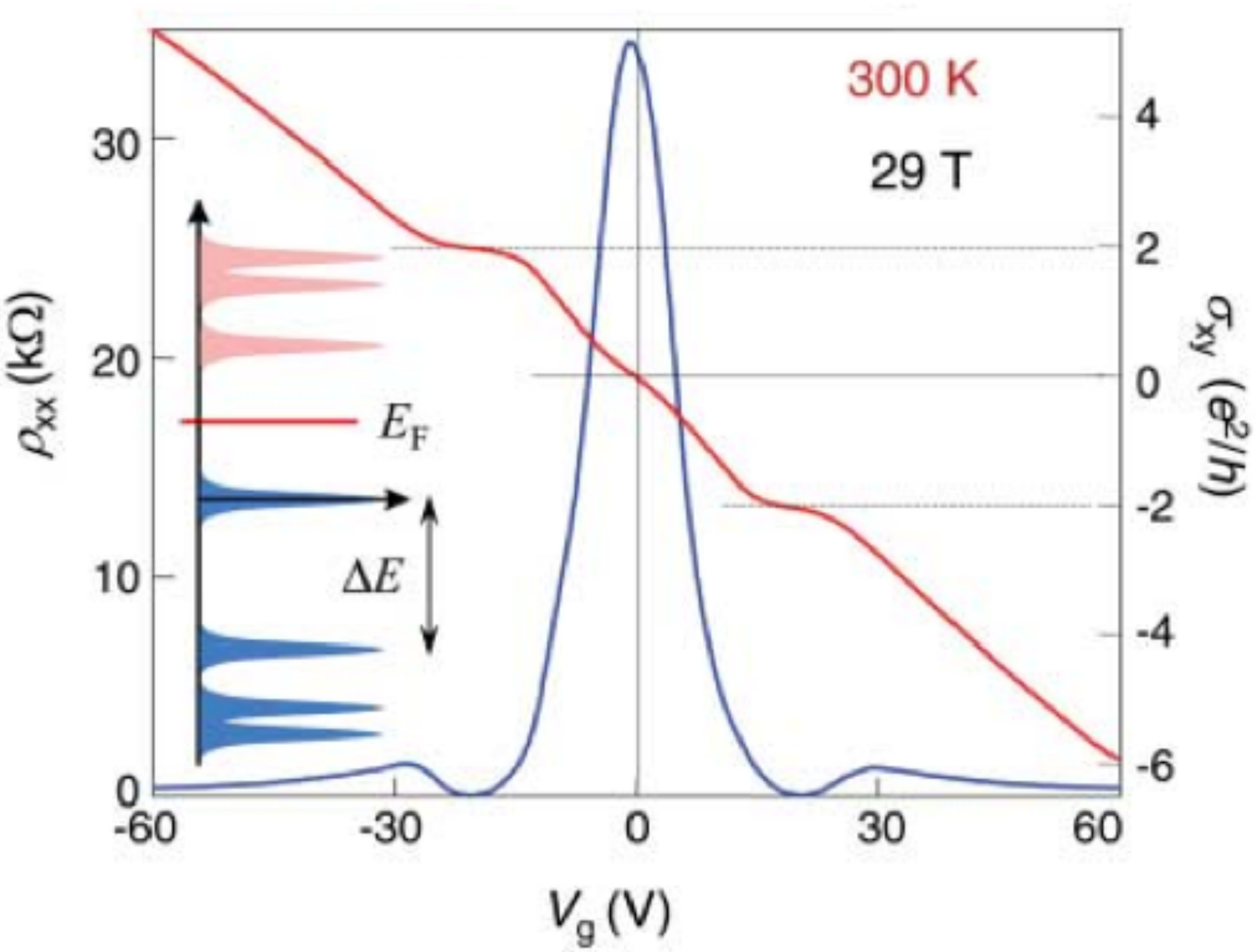


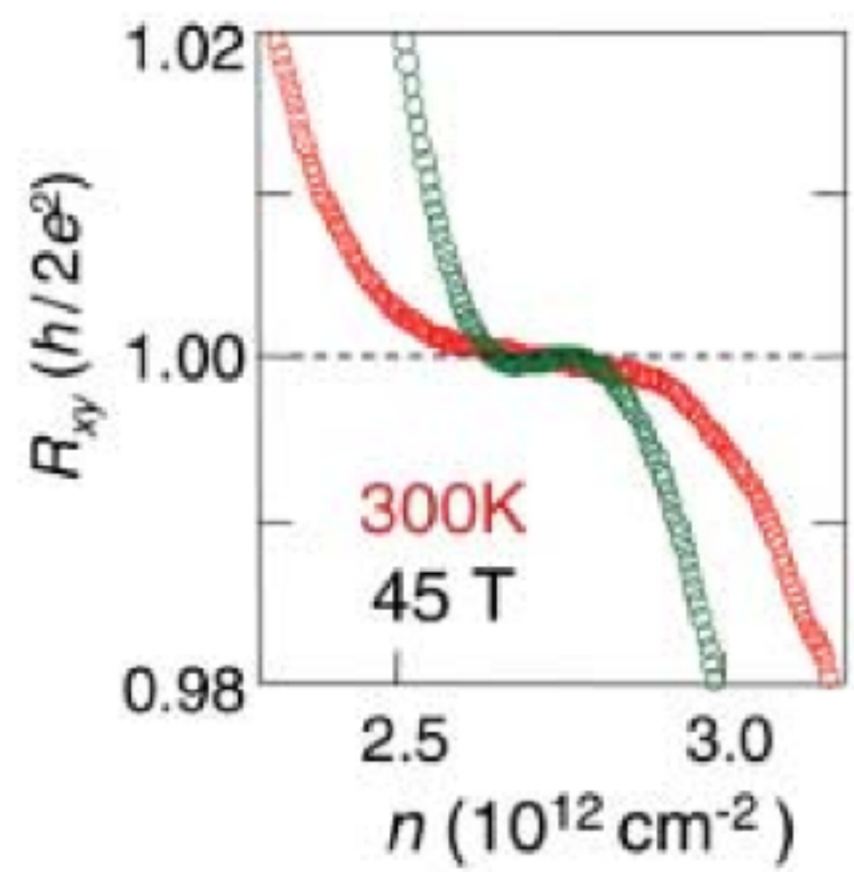
Enhancement

Extension



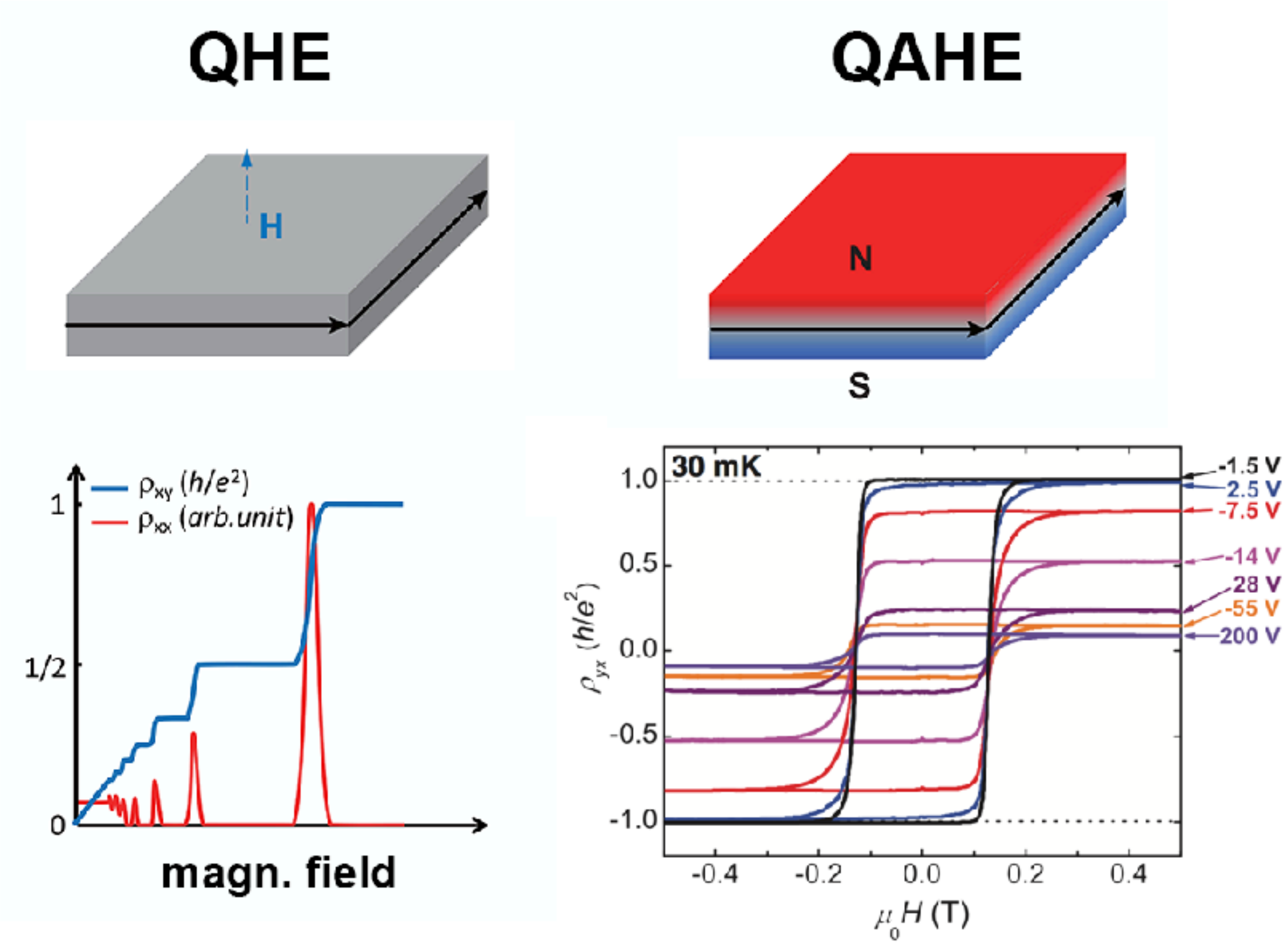
Enhancement: optimize 2DEG conditions





Deconstruction: external field is inessential

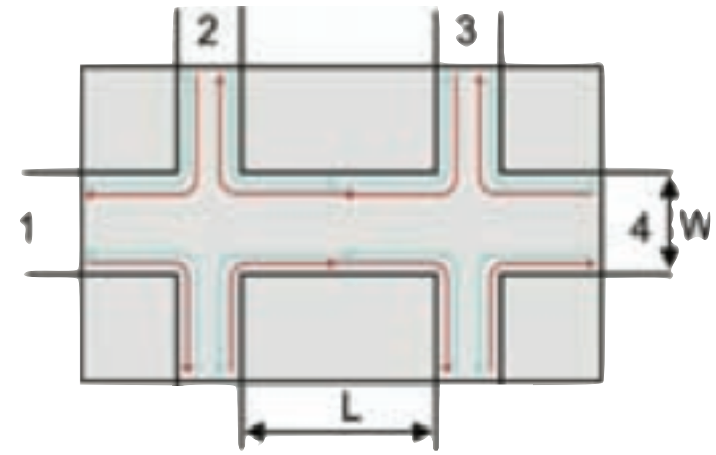
Haldane 1988; Tsinghua group 2013; MIT group 2015

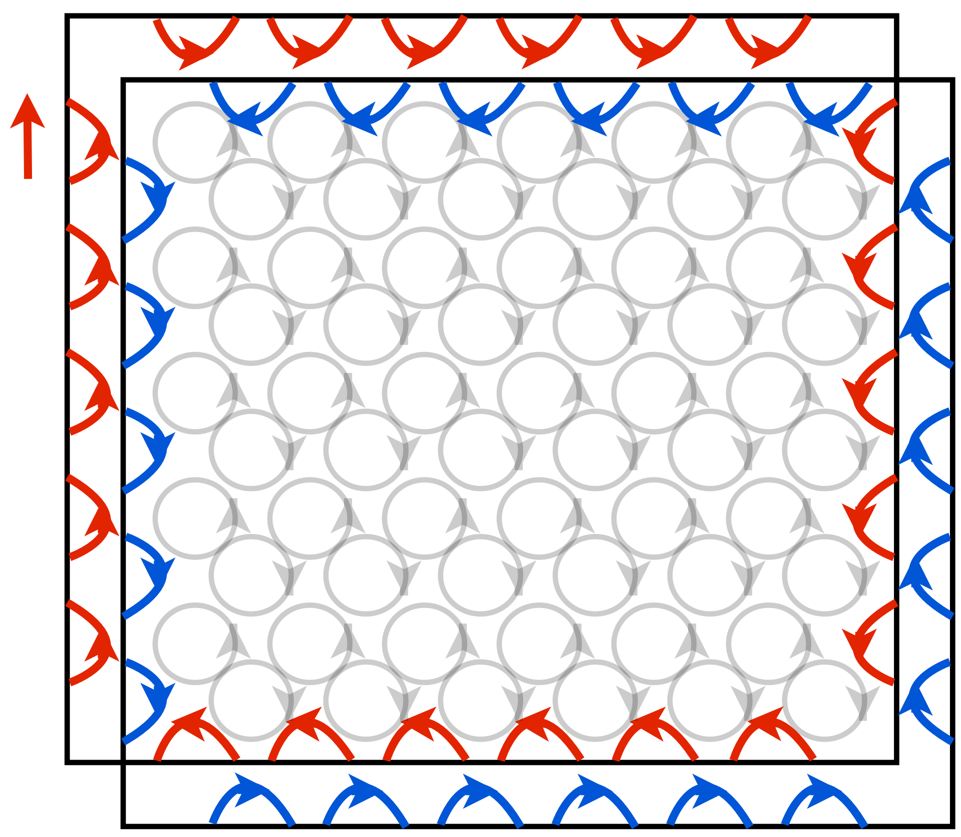


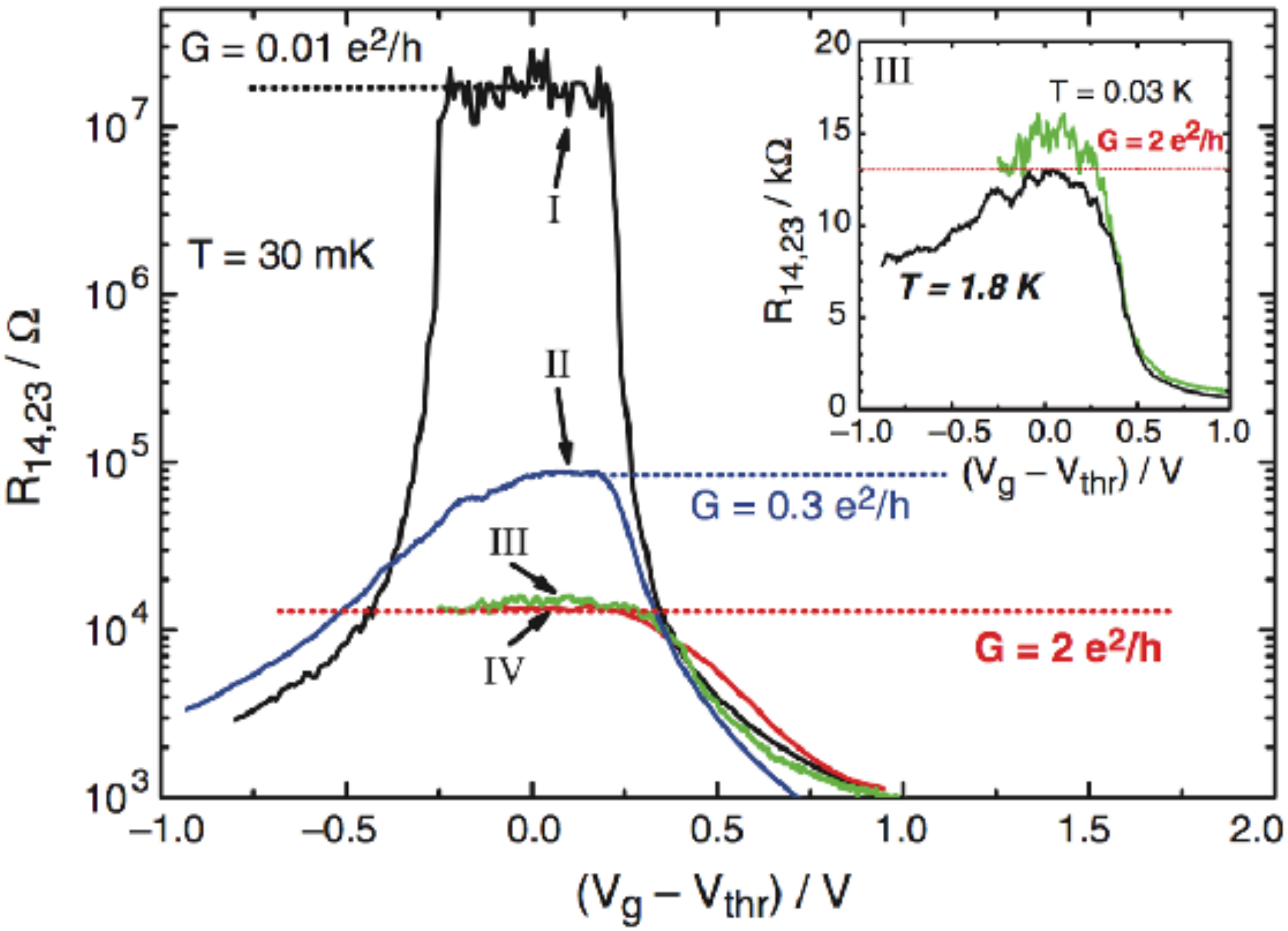
Extension: quantum spin Hall effect (QSHE) in HgTe

König et al. (Molenkamp/Zhang group), Science 2007

Time-reversed counterpropagating edge modes of unpolarized electrons



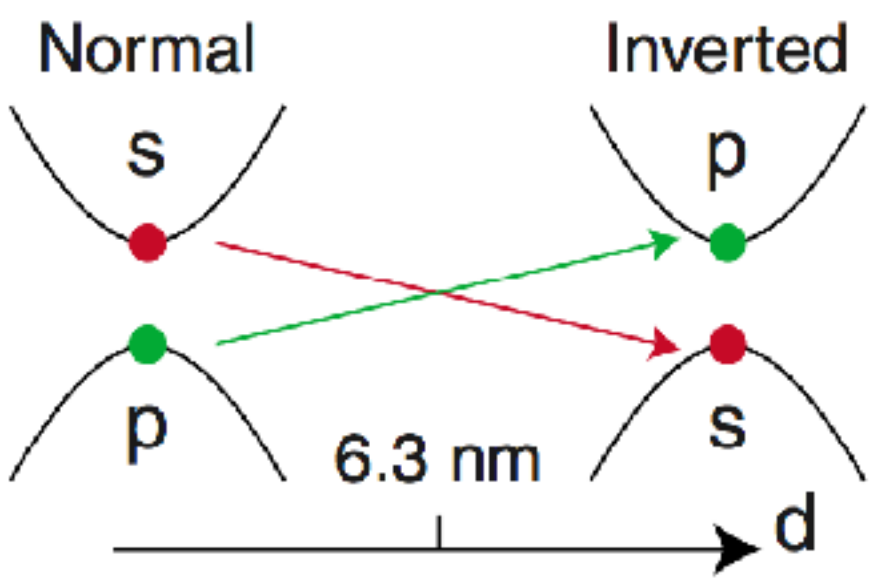


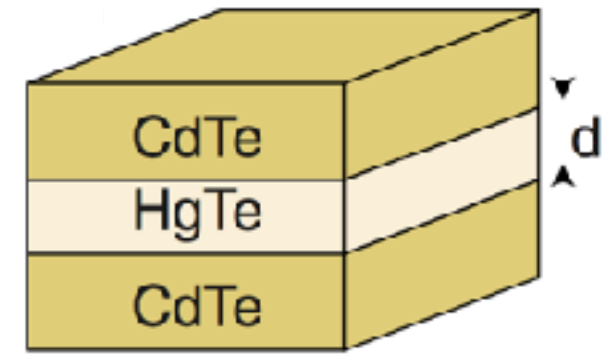


Mechanisms of QSHE

Band inversion

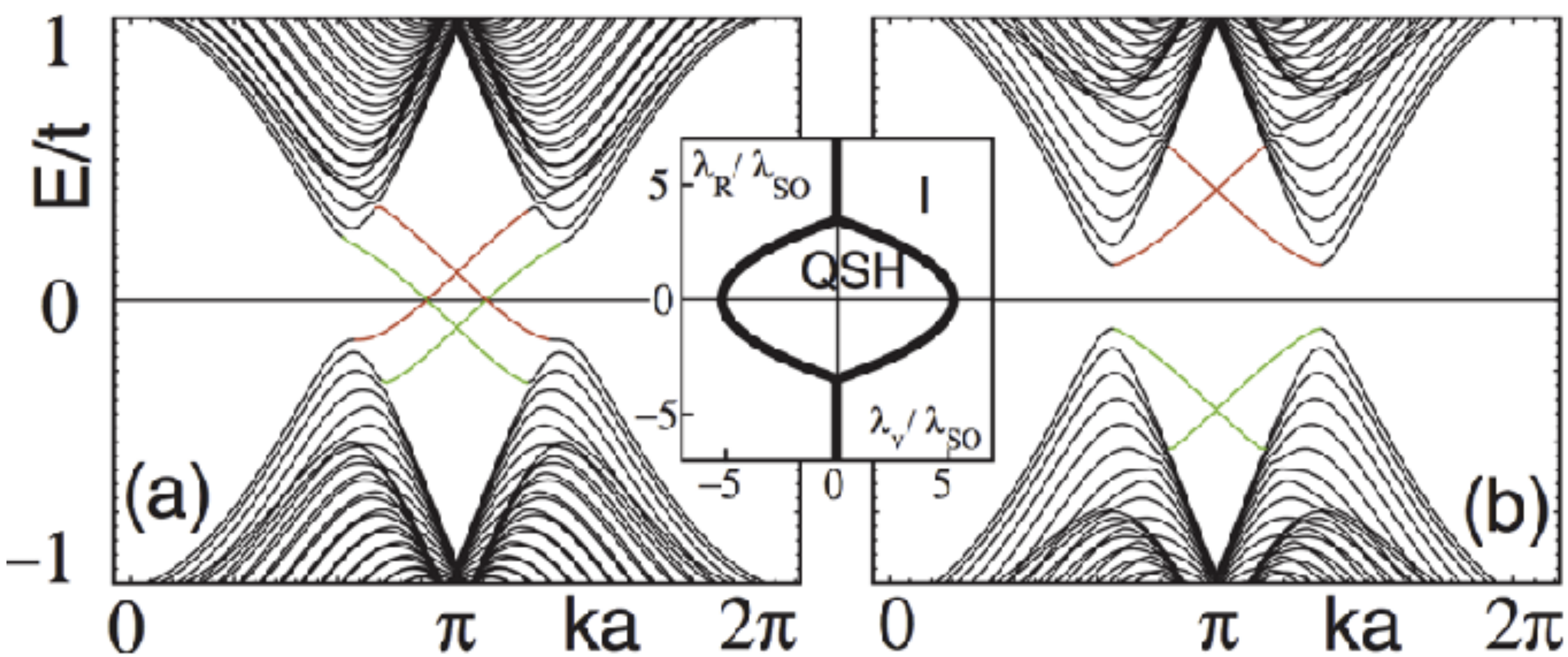
Bernevig, Hughes, Zhang, Science 2006





Dirac electron mass due to SOC

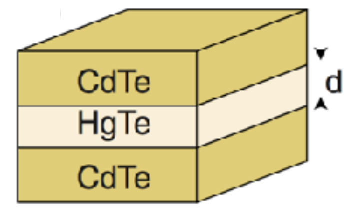
Kane & Mele PRL 2005



$$\Delta = \frac{t_s}{9t_{sp\sigma}^2}\lambda_{\mathrm{SOC}}$$

$$= 0.03\lambda_{\mathrm{SOC}}$$

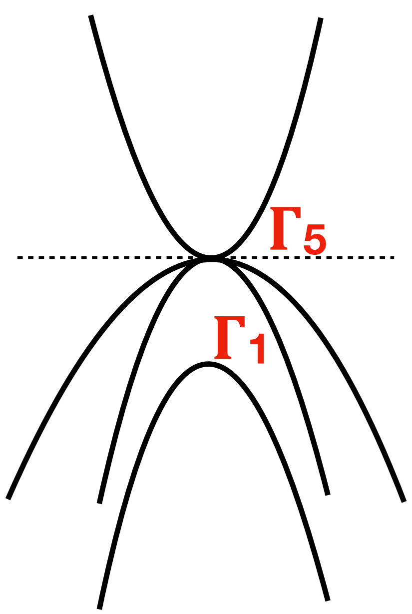
Symmetry analysis of HgTe/CdTe



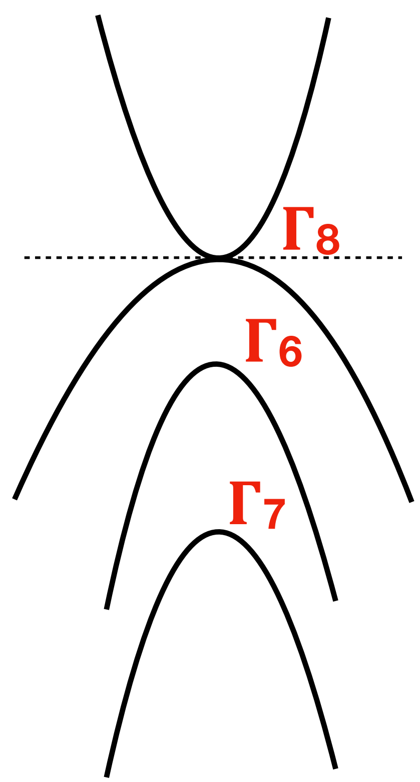
Zinc blende Symmetry: T_d

Dihedral Symmetry: D_{2d}

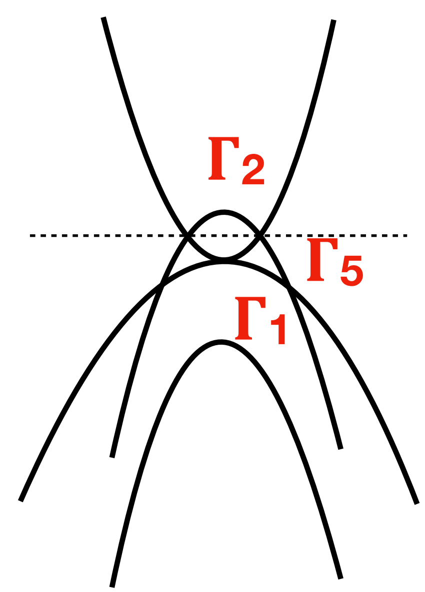
w/o SOC



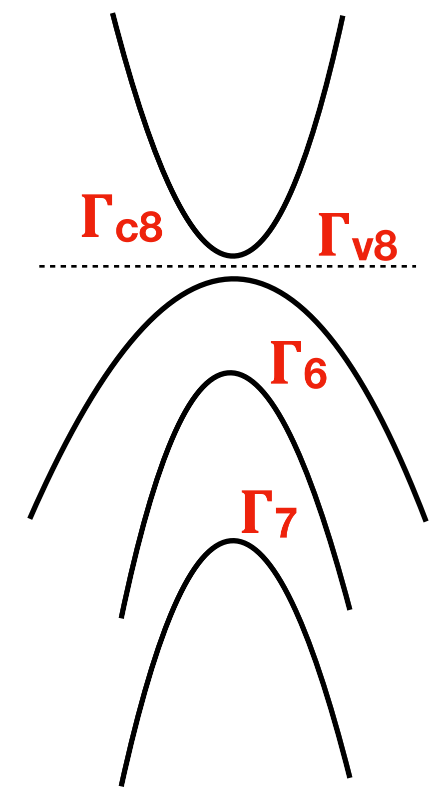
w SOC



w/o SOC



w SOC



Mapping to the double space group:

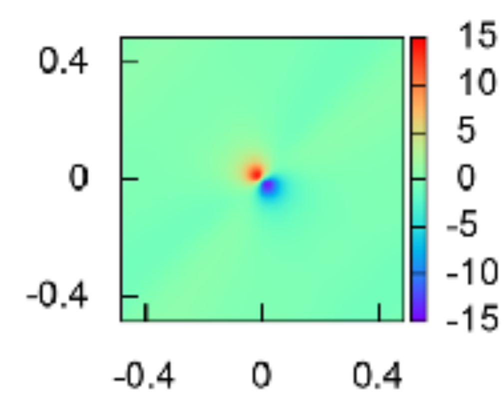
$\Gamma_1(1) \longrightarrow \Gamma_6(2)$

$\Gamma_5(3) \longrightarrow \Gamma_7(2)+\Gamma_8(4)$

$\Gamma_1(1) \longrightarrow \Gamma_6(2)$

$\Gamma_2(1) \longrightarrow \Gamma_7(2)$

$\Gamma_5(2) \longrightarrow \Gamma_{v8}(2)+\Gamma_{c8}(2)$



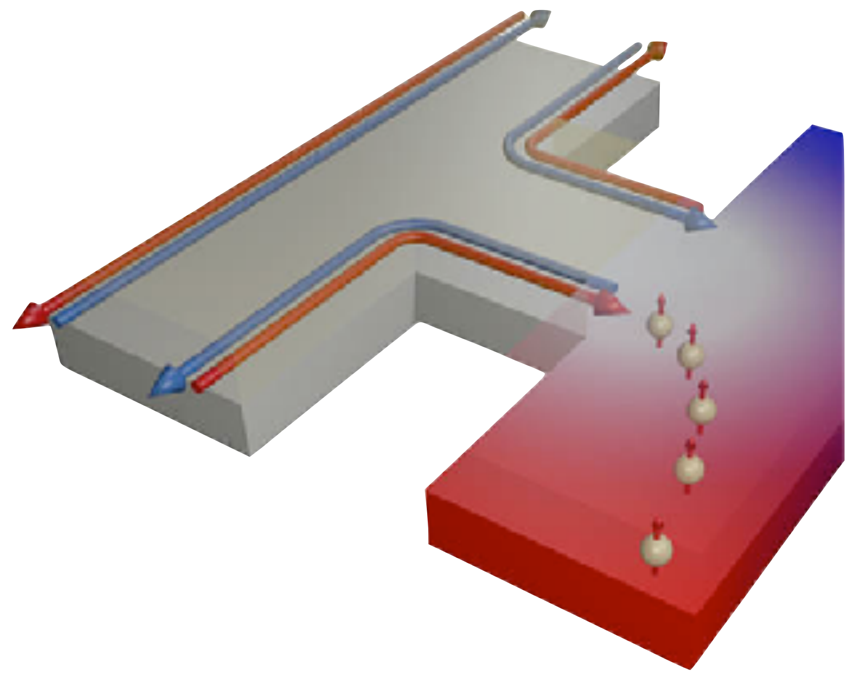
Theoretical Paradigm for
High Temperature Quantum Spin Hall Effect

RT Quantum spin Hall effect

Insulating gap

Maximize odd-parity matrix elements

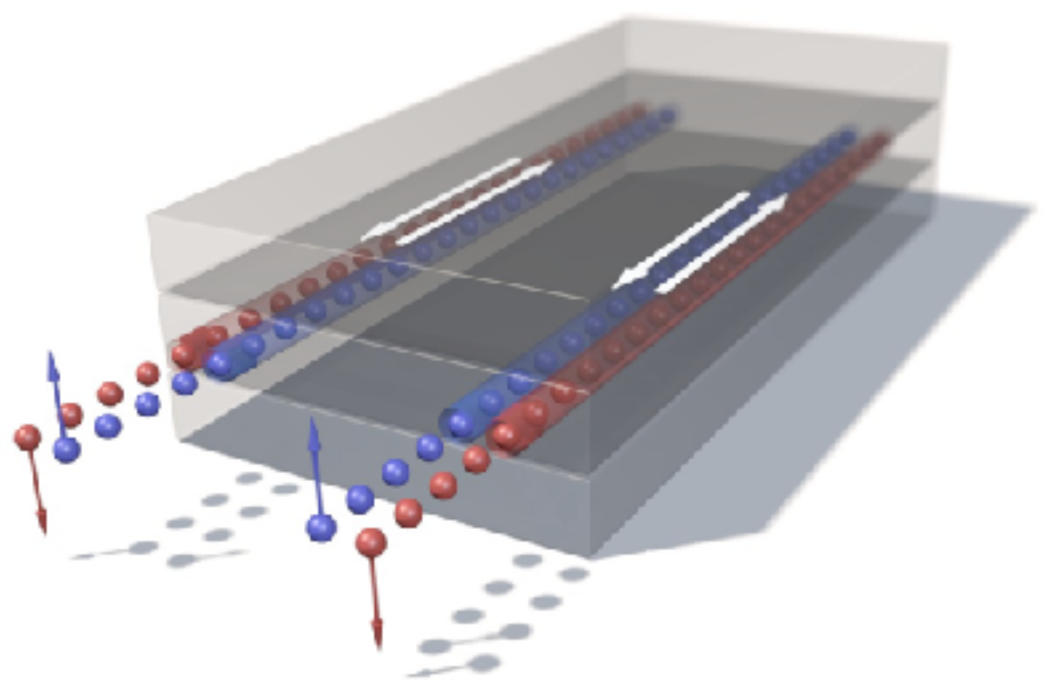
$$\Delta = \frac{t_s}{9t_{sp\sigma}^2}\lambda_{\mathrm{SOC}}$$



Edge states

Minimize localization length

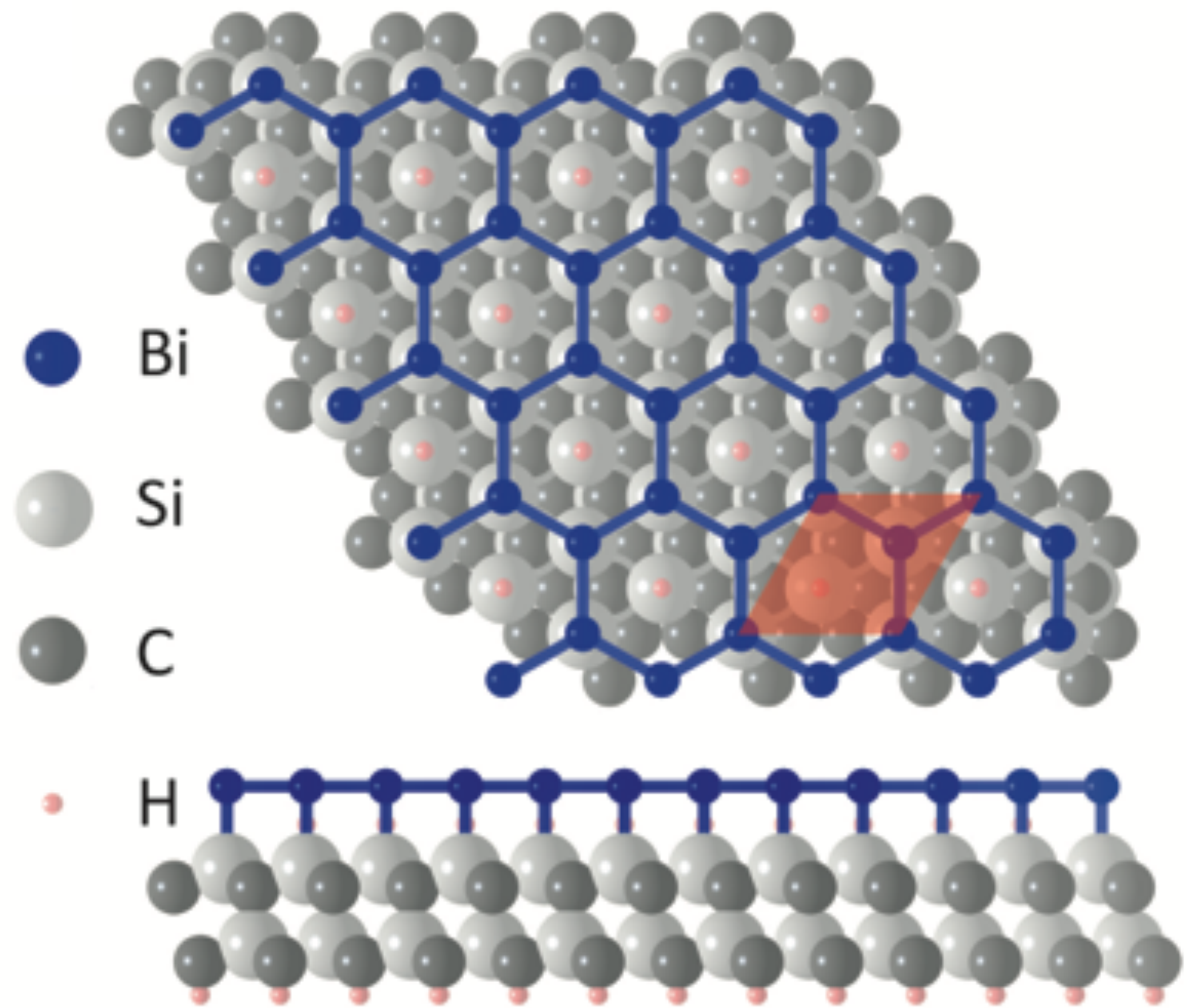
$$\xi = \hbar v_{\mathrm{D}}/\Delta_{\mathrm{d}}$$

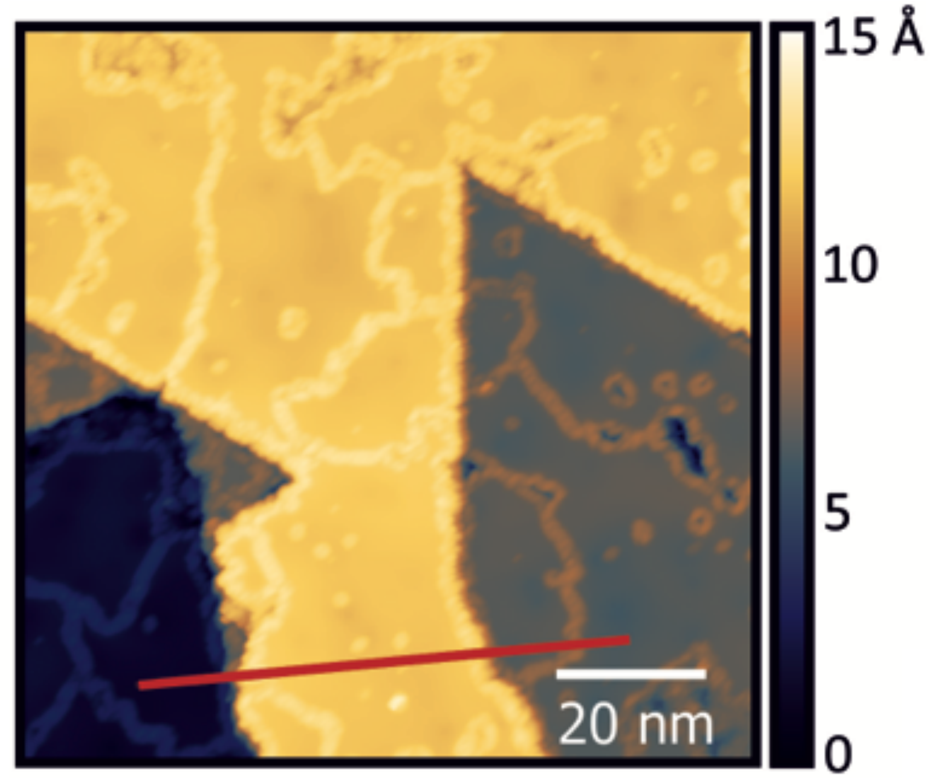


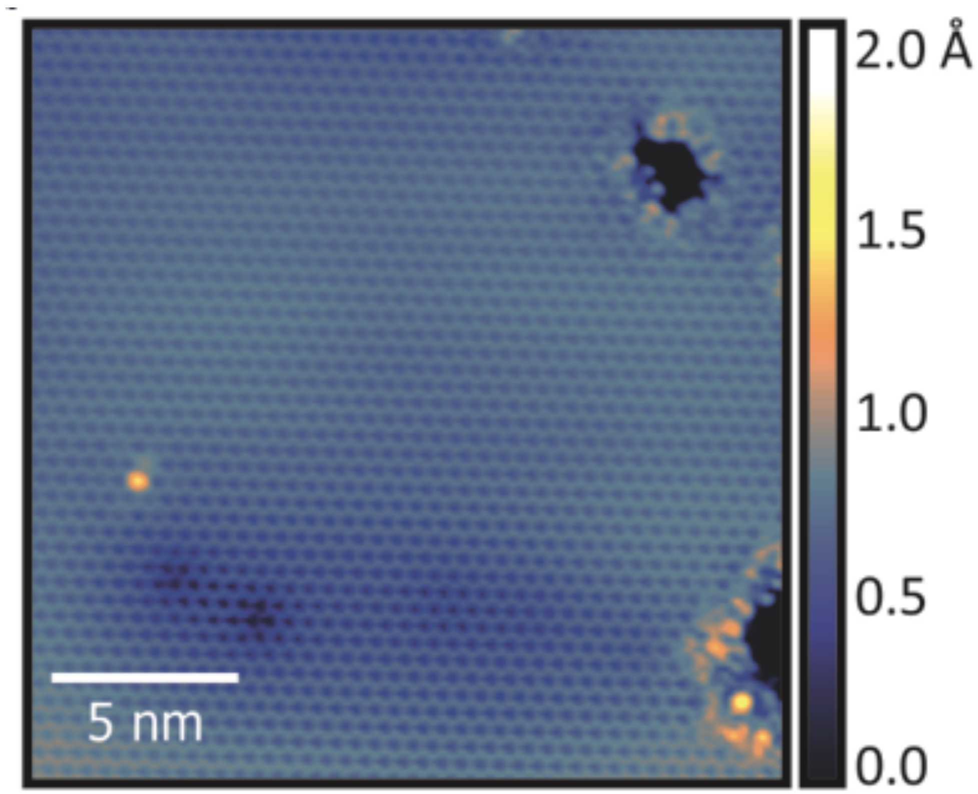
Bi/SiC heterostructure

Structural setup

Reis, *et int.*, Thomale & Claessen,
Science 2017







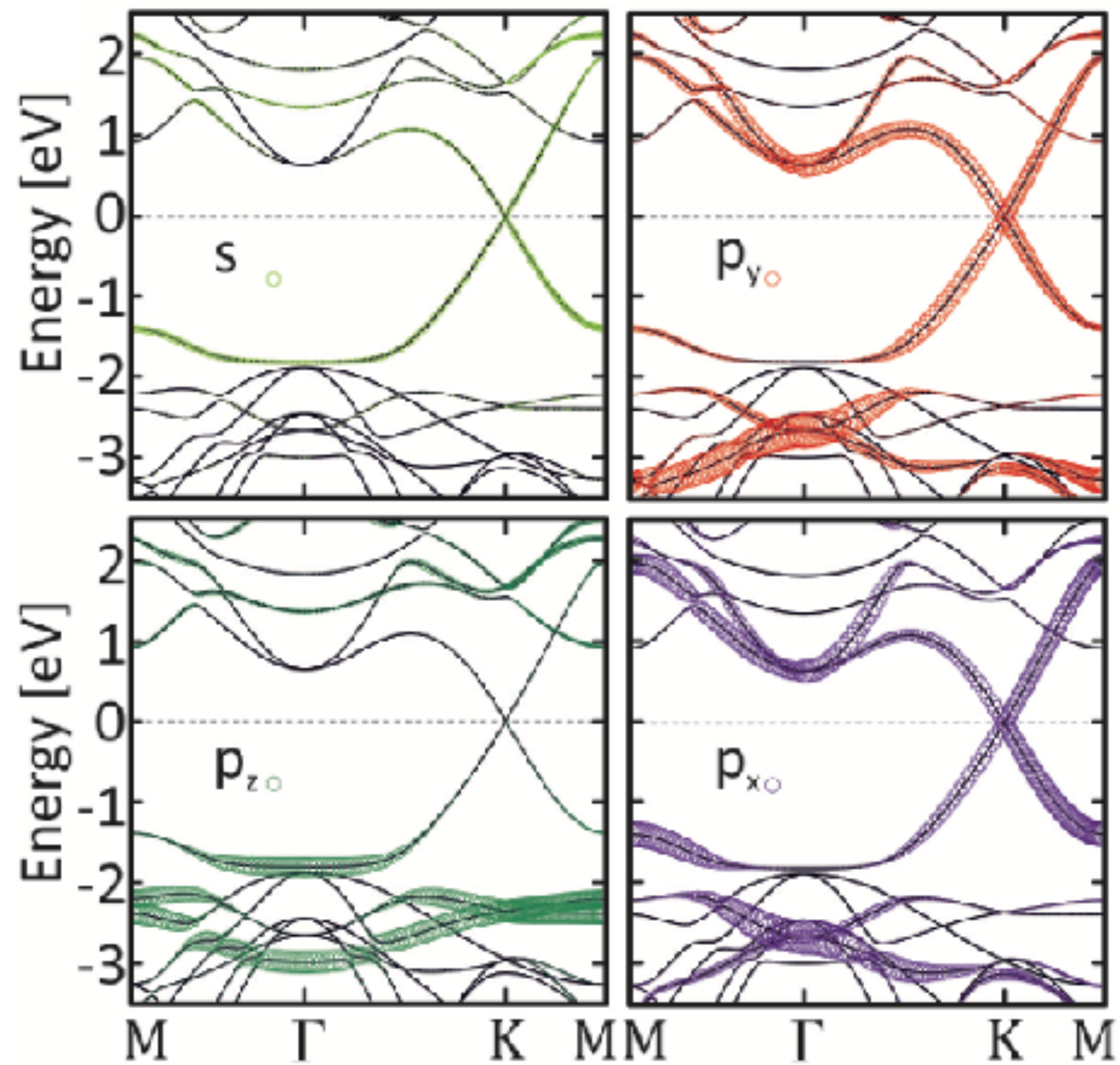
Band structure analysis w/o spin-orbit coupling

Orbital filtering at low energies:

px and py orbital content dominates

substrate removes pz from Fermi level

propagation of local $L^z S^z$ atomic SOC



Effective σ band model:

$$|p^A_{x\uparrow}\rangle, |p^A_{y\uparrow}\rangle, |p^B_{x\uparrow}\rangle, |p^B_{y\uparrow}\rangle; \qquad |p^A_{x\downarrow}\rangle, |p^A_{y\downarrow}\rangle, |p^B_{x\downarrow}\rangle, |p^B_{y\downarrow}\rangle \ .$$

Effective model for the Bi monolayer

$$|p^A_{x\uparrow}\rangle, |p^A_{y\uparrow}\rangle, |p^B_{x\uparrow}\rangle, |p^B_{y\uparrow}\rangle; \qquad |p^A_{x\downarrow}\rangle, |p^A_{y\downarrow}\rangle, |p^B_{x\downarrow}\rangle, |p^B_{y\downarrow}\rangle \,.$$

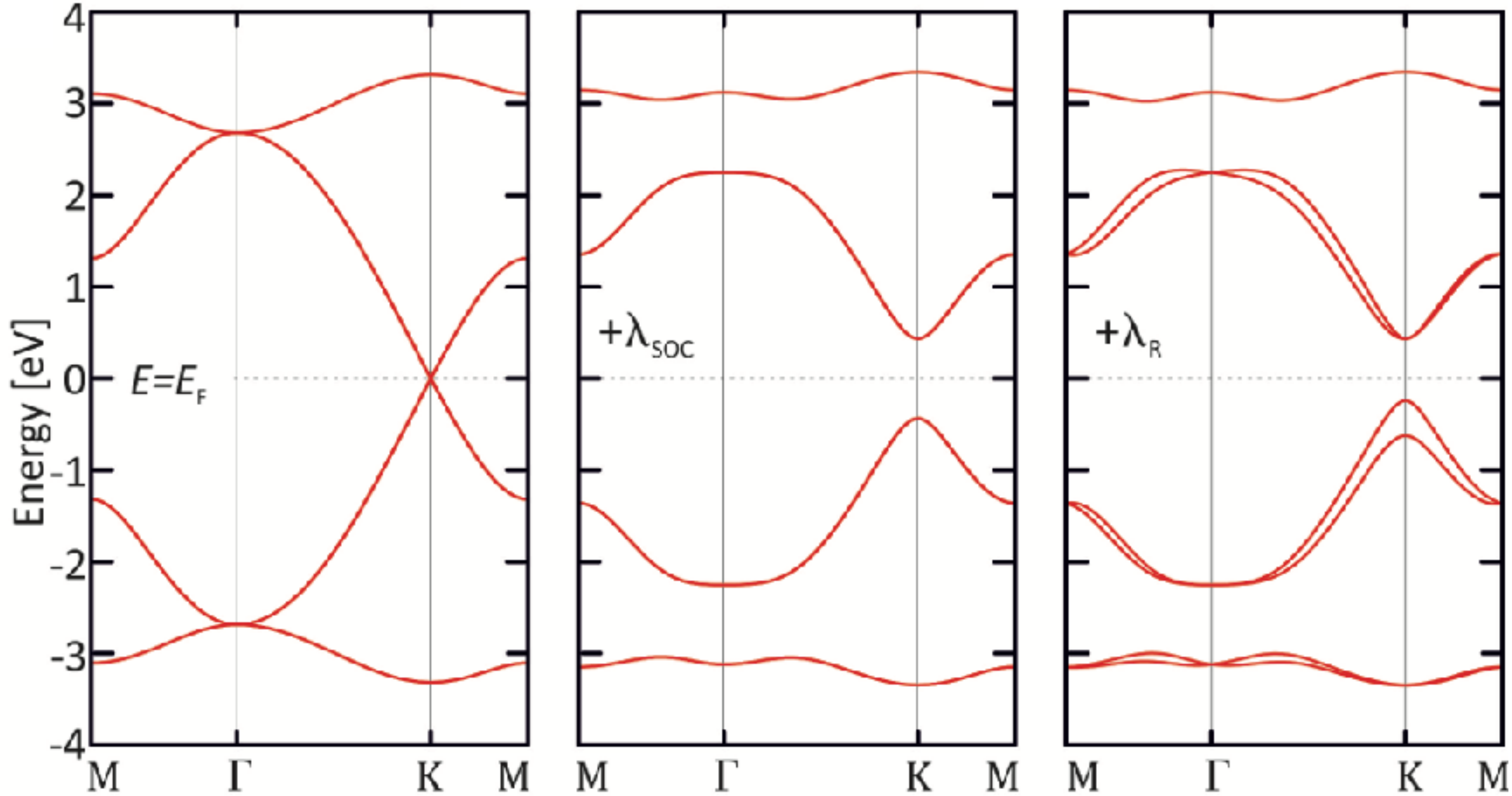
$$H^{\sigma\sigma}_{\text{eff}} = \begin{pmatrix} H^{\sigma\sigma}_{\uparrow\uparrow} & H^{\sigma\sigma}_{\uparrow\downarrow} \\ H^{\sigma\sigma}_{\downarrow\uparrow} & H^{\sigma\sigma}_{\downarrow\downarrow} \end{pmatrix}$$

$$H^{\sigma\sigma}_{\uparrow\uparrow/\downarrow\downarrow} = H^{\sigma\sigma}_{0,\uparrow\uparrow/\downarrow\downarrow} \pm \lambda_{\text{SOC}} \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$

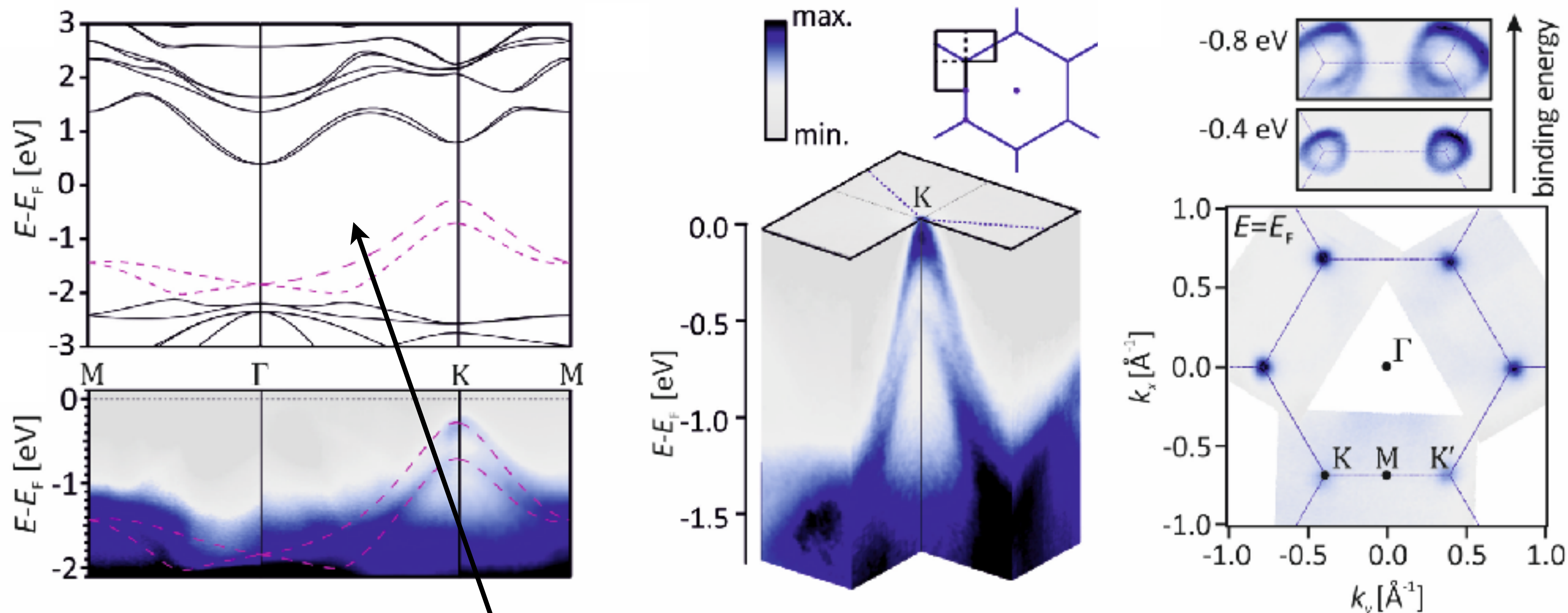
$$H^{\sigma\sigma}_{\uparrow\downarrow} = (H^{\sigma\sigma}_{\downarrow\uparrow})^{\dagger} = \lambda_{\text{R}} \begin{pmatrix} 0 & 0 & m_1 & m_2 \\ 0 & 0 & m_2 & m_3 \\ m_4 & m_5 & 0 & 0 \\ m_5 & m_6 & 0 & 0 \end{pmatrix}$$

Effective model with full SOC

$$H_{\text{eff}}^{\sigma\sigma} = H_0^{\sigma\sigma} + \lambda_{\text{SOC}} H_{\text{SOC}}^{\sigma\sigma} + \lambda_{\text{R}} H_{\text{R}}^{\sigma\sigma}$$



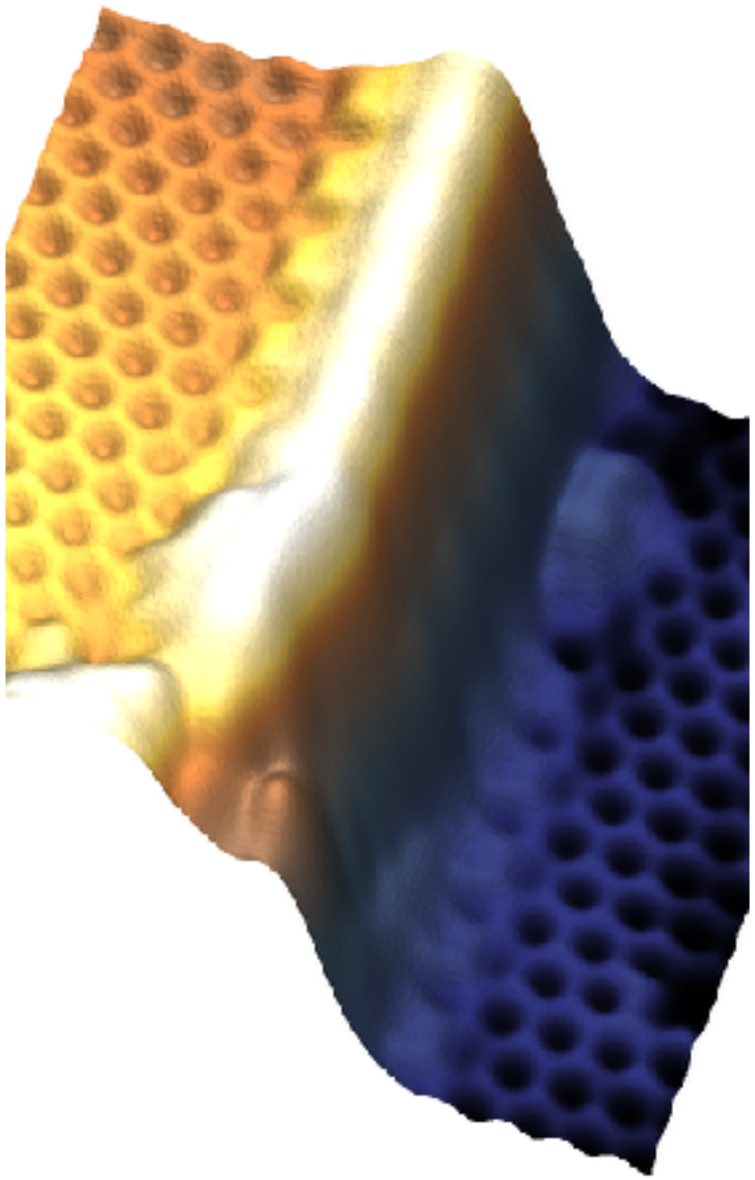
Theory vs. ARPES



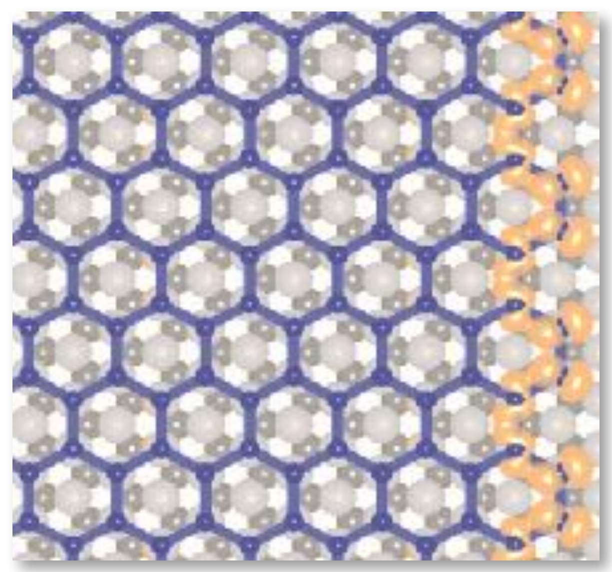
band gap: 0.67 eV!

Theory vs. STM

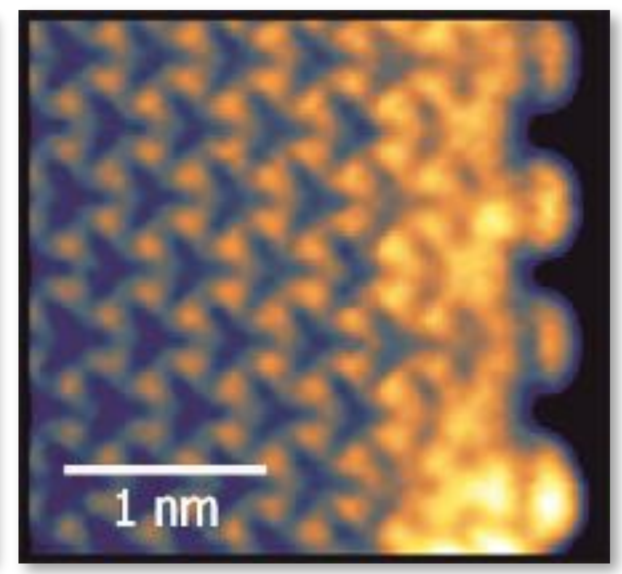
Stühler et al., Nature Physics (2019)



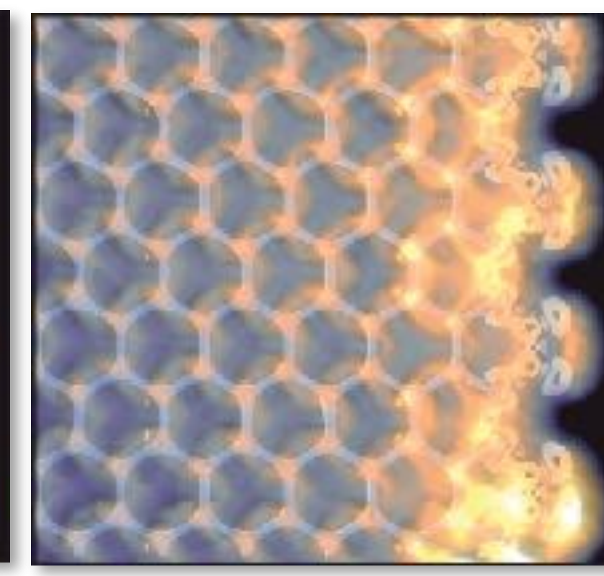
DFT ribbon calculation



STM



Overlay DFT/STM



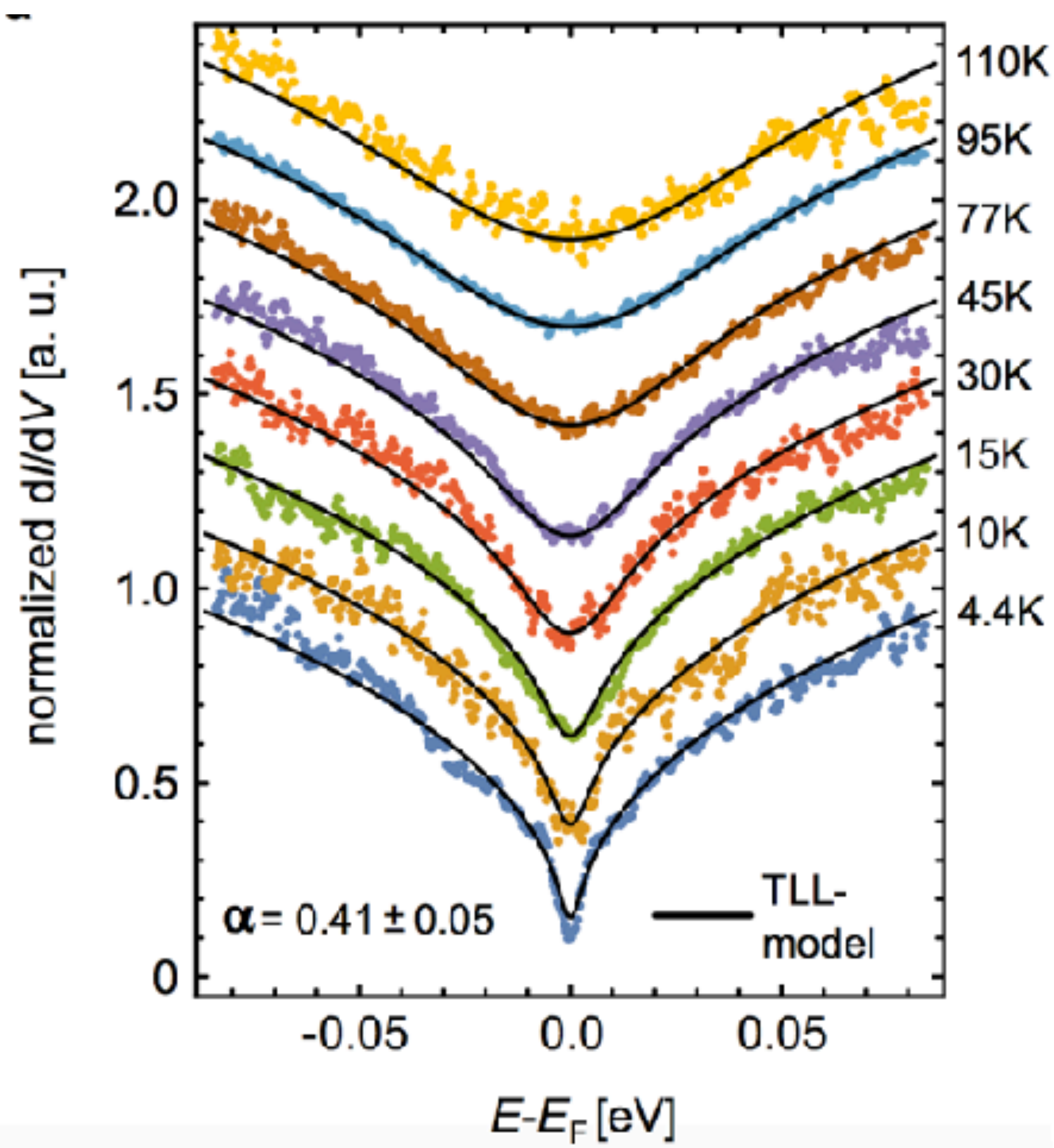
$$\xi = 4.1 \mathring{A}$$

Periodicity and symmetry of the STM charge density matches the ribbon calculation

Open problem: quantitative modeling of twin boundaries

QSH Edge channel interaction

Stühler et al., Nature Physics (2019)



670 meV bulk gap ensures a truly 1D confined edge channel

Quenched Coulomb interactions imply a correlated helical Luttinger liquid

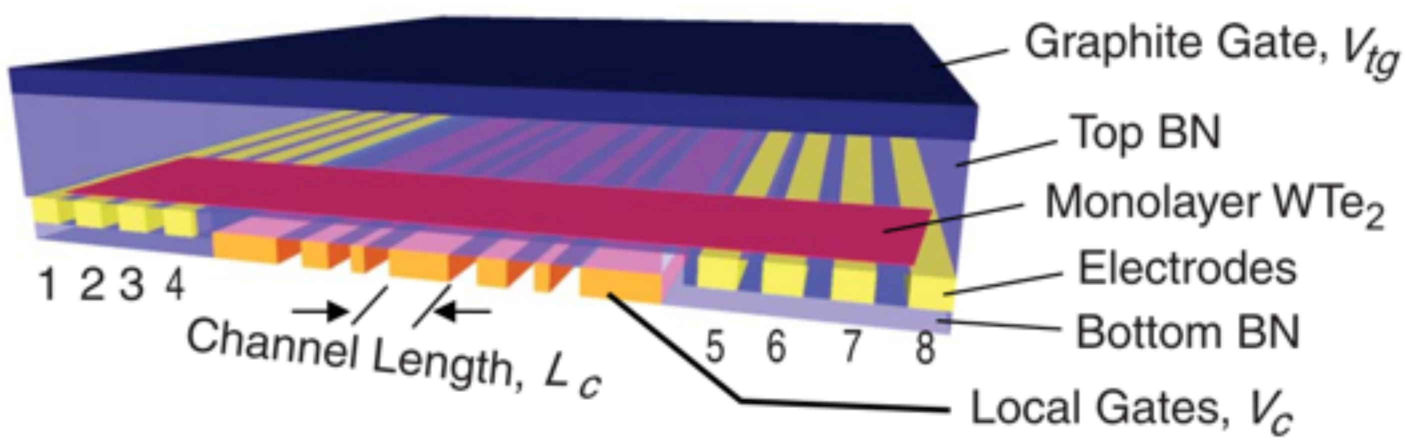
$$\rho \sim |E - E_{\mathrm{F}}|^{\alpha}$$

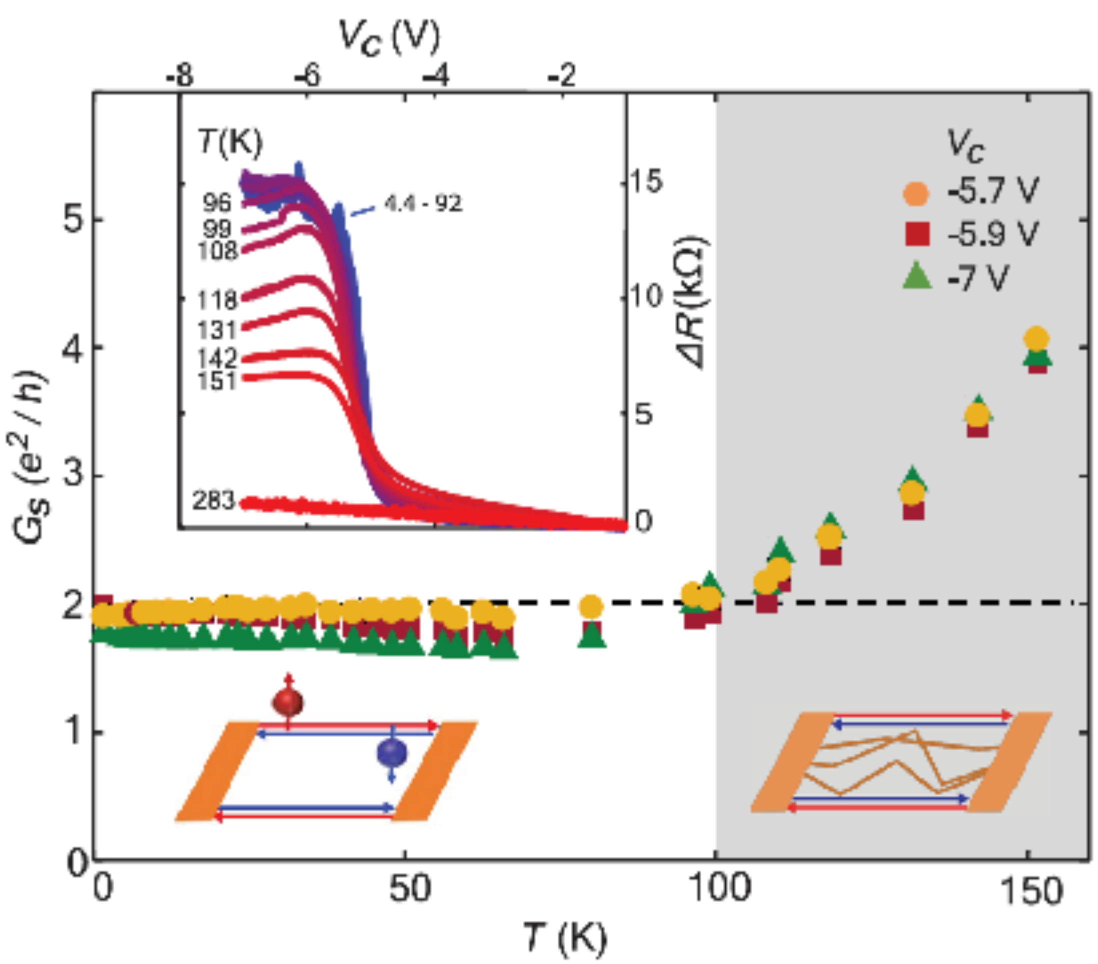
Electron-phonon coupling becomes relevant at RT

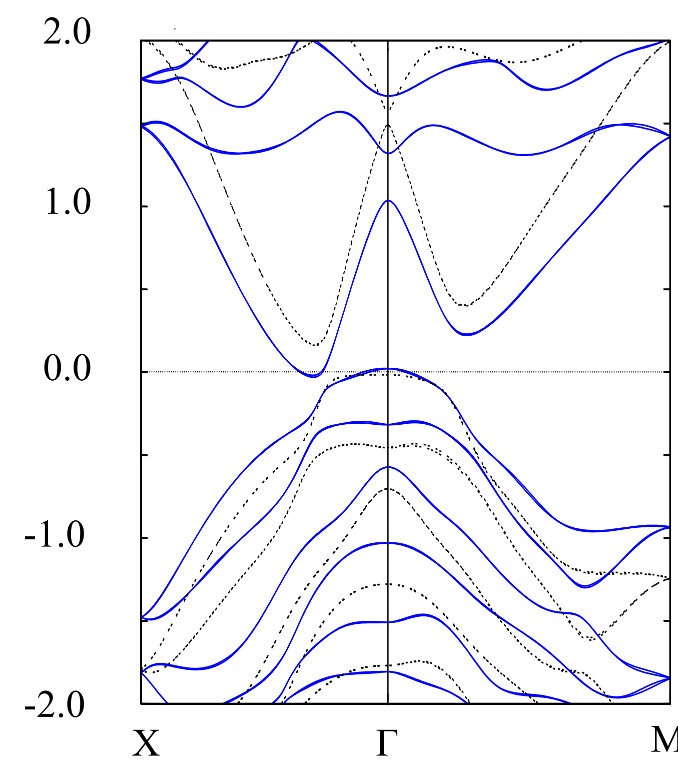
WTe_2 monolayers

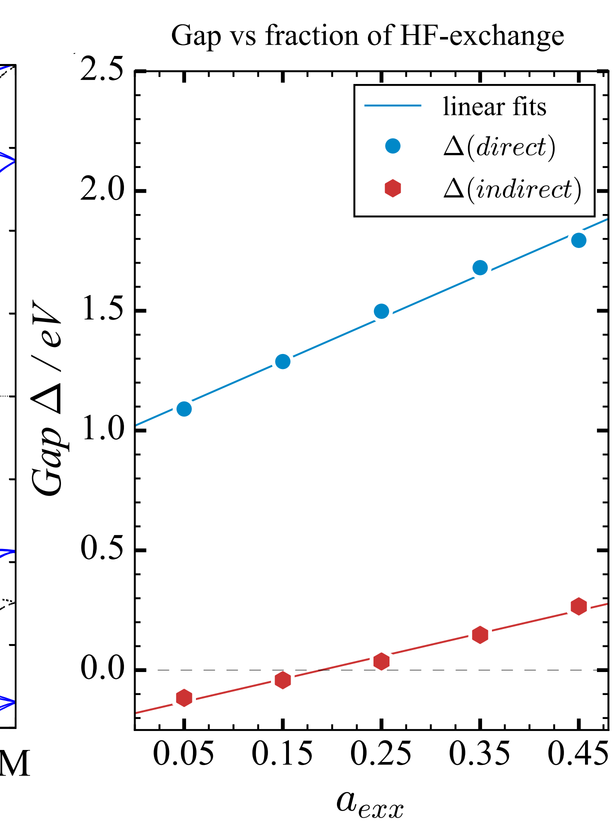
Close-to-metal QSHE at 100K?

S.Wu et al., Science 2018



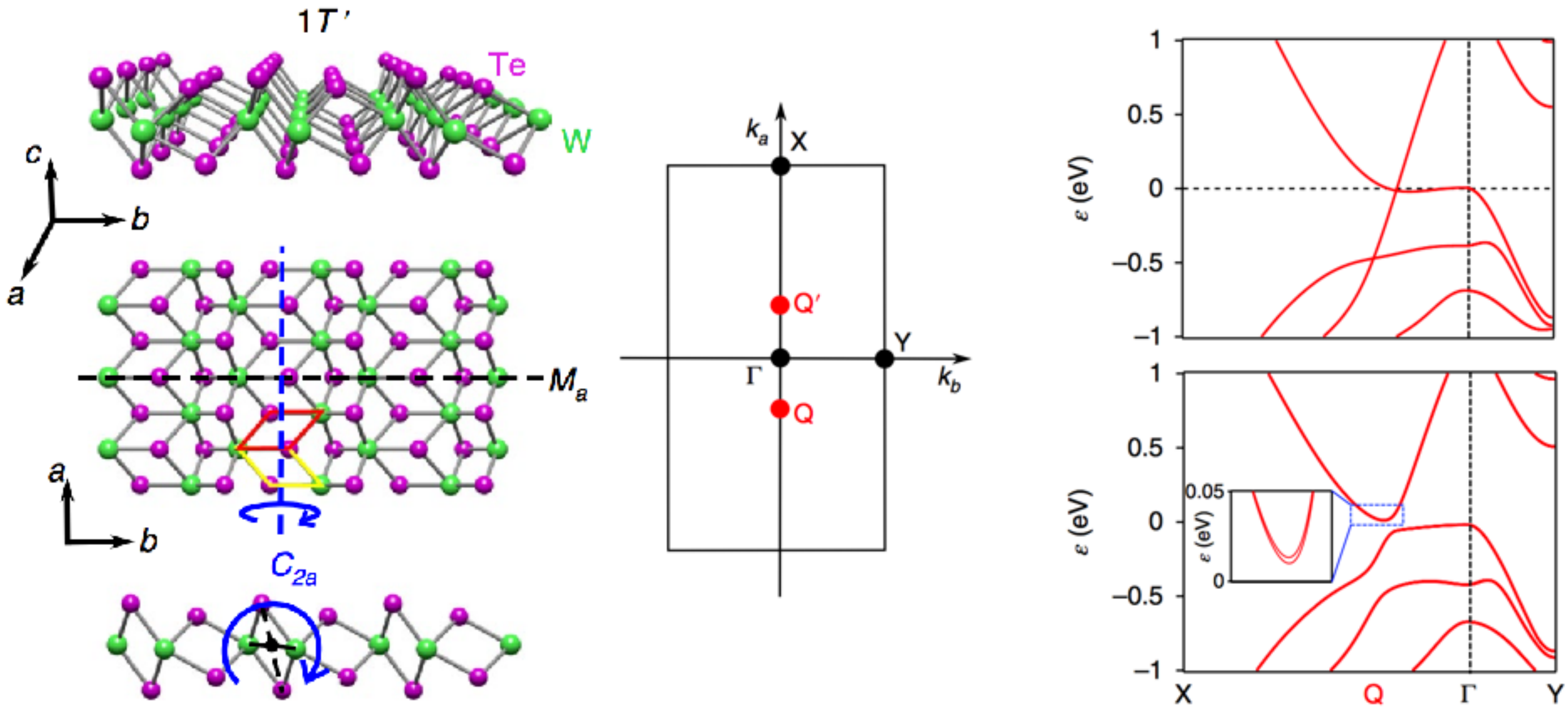






Mirror / screw symmetry

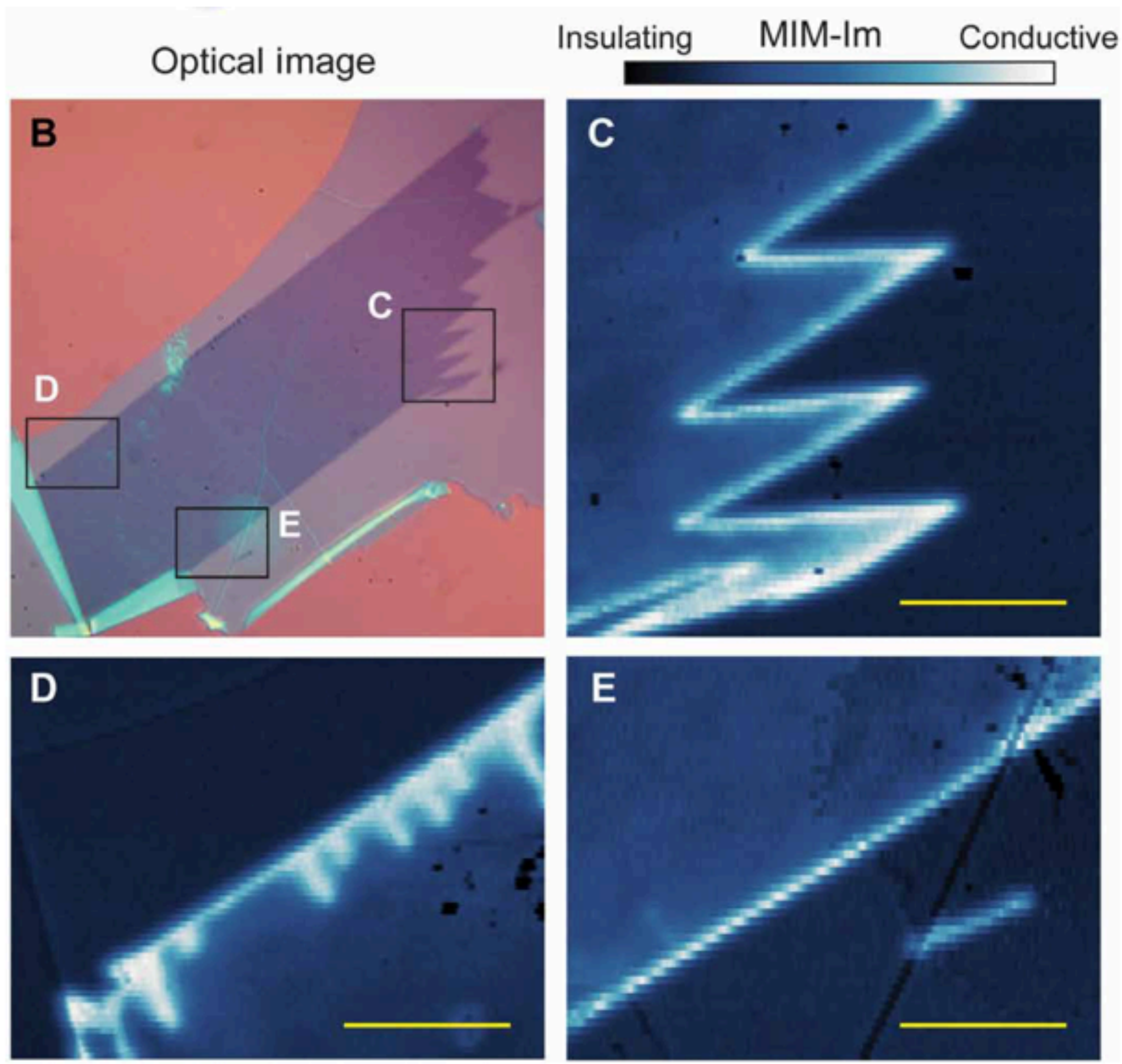
Xu et al., Nature Physics 2018



(Tilted) Dirac cones appear at incommensurate momenta.

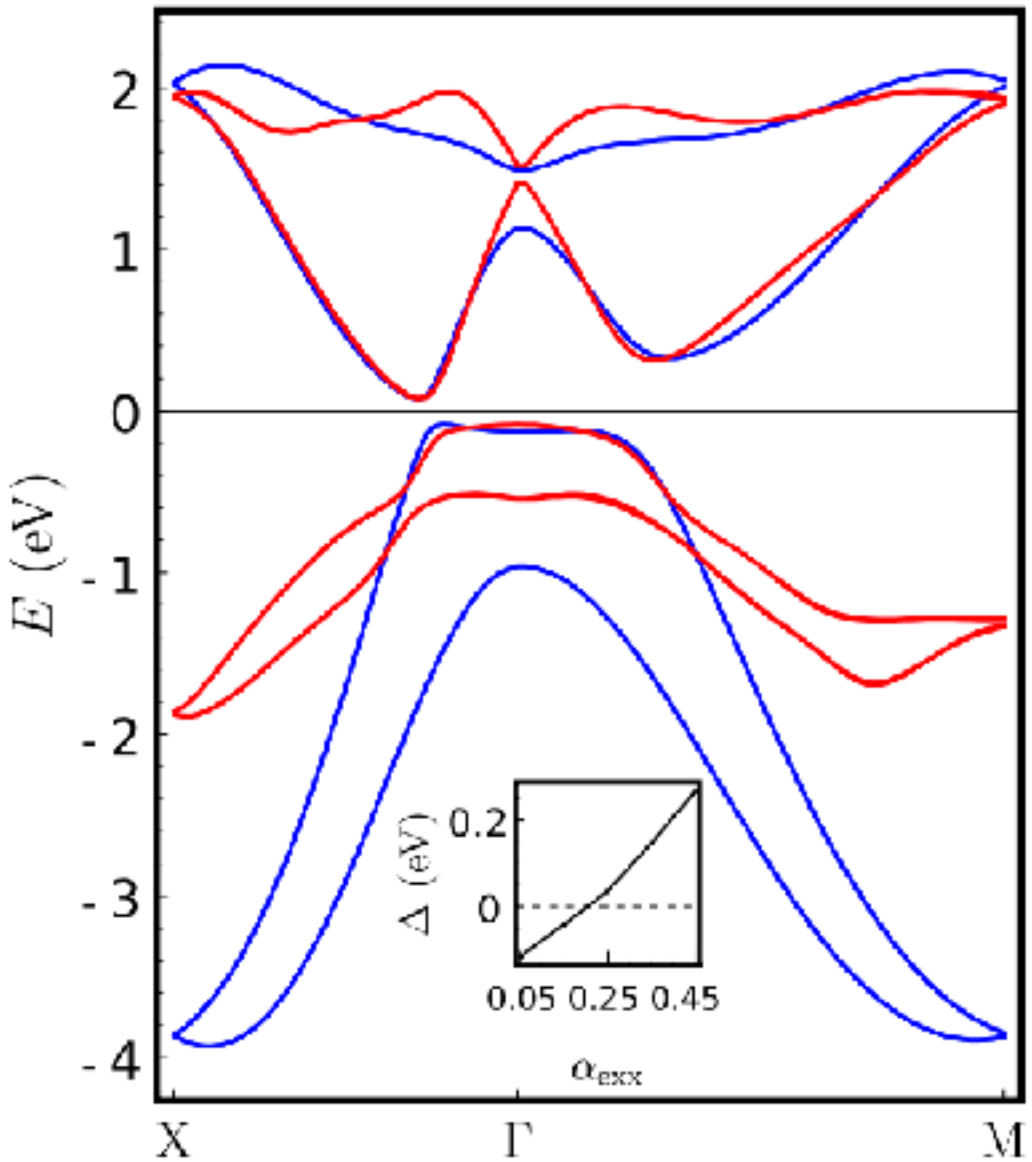
Edge state imaging

Shi et al., Science Advances 2019



Effective model for WTe2

Ok et al., Phys. Rev. B 99, 121105(R) (2019)



$$\mathcal{H}(\boldsymbol{k}) = \mathcal{H}_0(\boldsymbol{k}) + \mathcal{H}_{\text{int}}^{\text{SOC}} + \mathcal{H}_{\text{R}}^{\text{SOC}}$$

$$\mathcal{H}_0(\boldsymbol{k}) = \sigma_0 \otimes \begin{pmatrix} \epsilon_d(\boldsymbol{k}) & 0 & \tilde{t}_d g_{k_x} e^{ik_y} & \tilde{t}_0 f_{k_x} \\ 0 & \epsilon_p(\boldsymbol{k}) & -\tilde{t}_0 f_{k_x} & \tilde{t}_p g_{k_x} \\ \tilde{t}_d g^*_{k_x} e^{-ik_y} & -\tilde{t}_0 f^*_{k_x} & \epsilon_d(\boldsymbol{k}) & 0 \\ \tilde{t}_0 f^*_{k_x} & \tilde{t}_p g^*_{k_x} & 0 & \epsilon_p(\boldsymbol{k}) \end{pmatrix}$$

$$\mathcal{H}_{\text{int}}^{\text{SOC}} = V \sigma_2 \rho_3 \tau_2$$

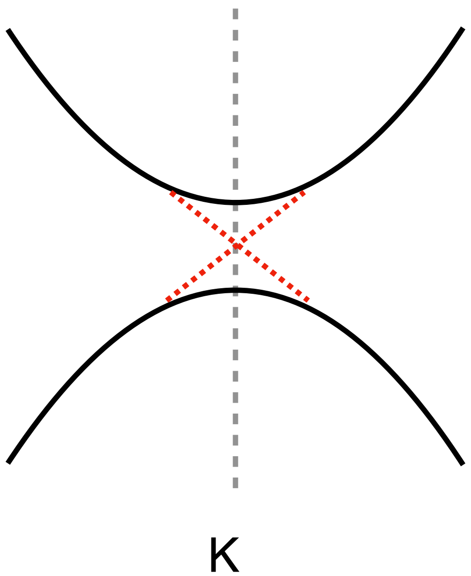
$$\mathcal{H}_{\text{R}}^{\text{SOC}} = \sigma_2 \rho_0 \tau_2$$

Effective 8-band model retains all microscopic symmetries.

Custodial glide symmetry in WTe2

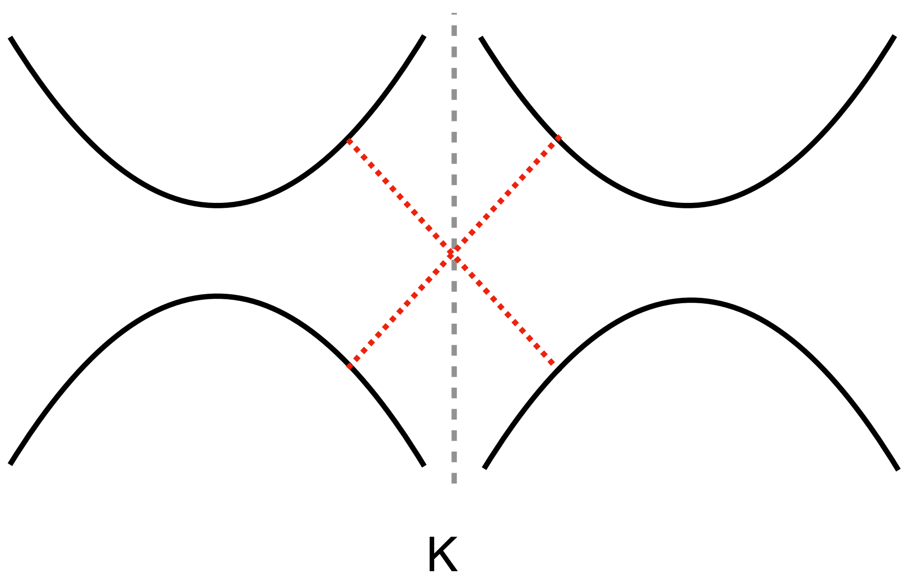
Ok et al., Phys. Rev. B 99, 121105(R) (2019)

The glide symmetry in WTe2 allows for Dirac cone centers away from the high symmetry points and a large direct gap at the edge support.



$$\xi = \hbar v_{\mathrm{D}} / \Delta_{\mathrm{d}}$$

bulk edge



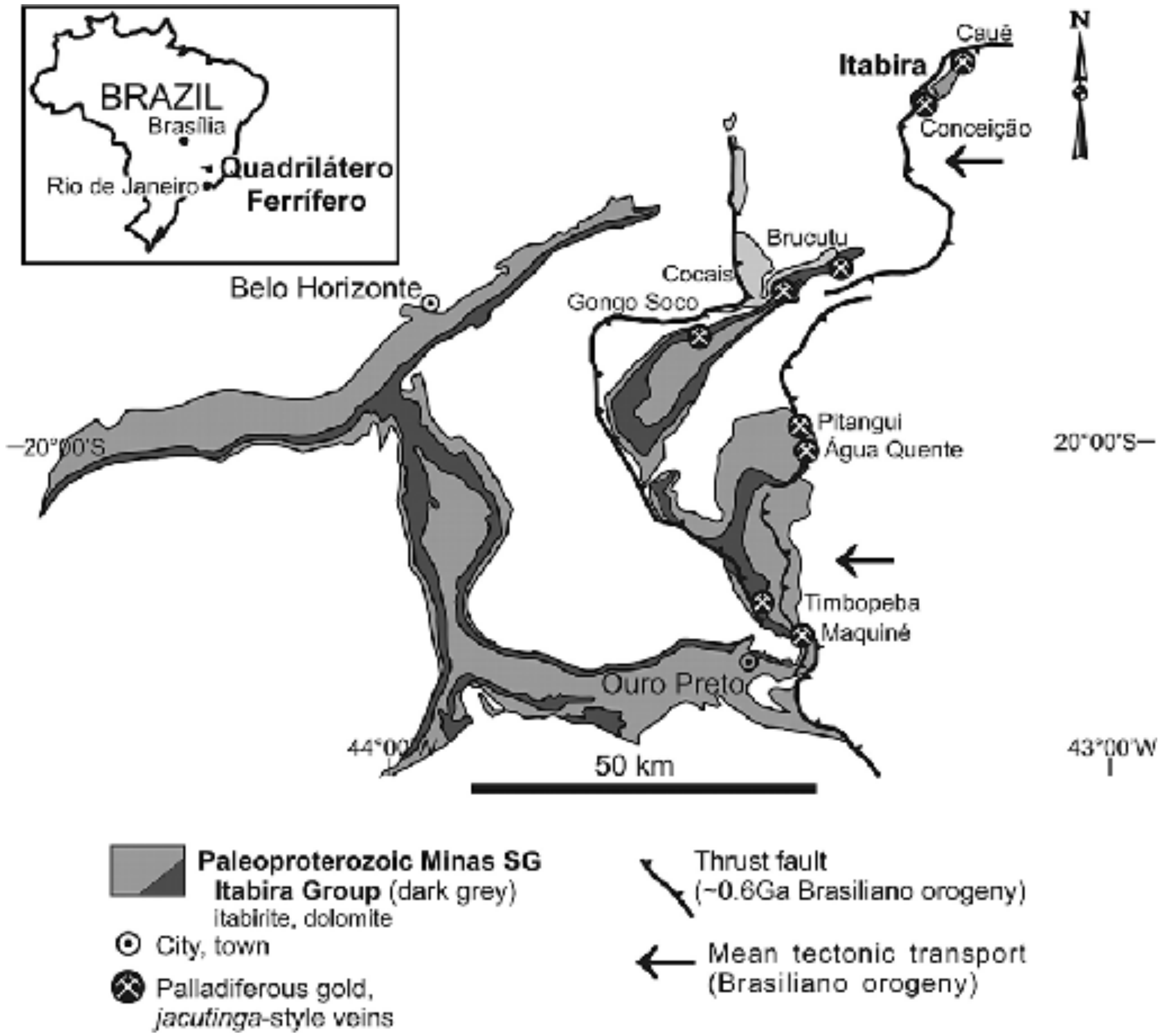
Strong 1D confinement of edge channels reduces coupling to bulk states.

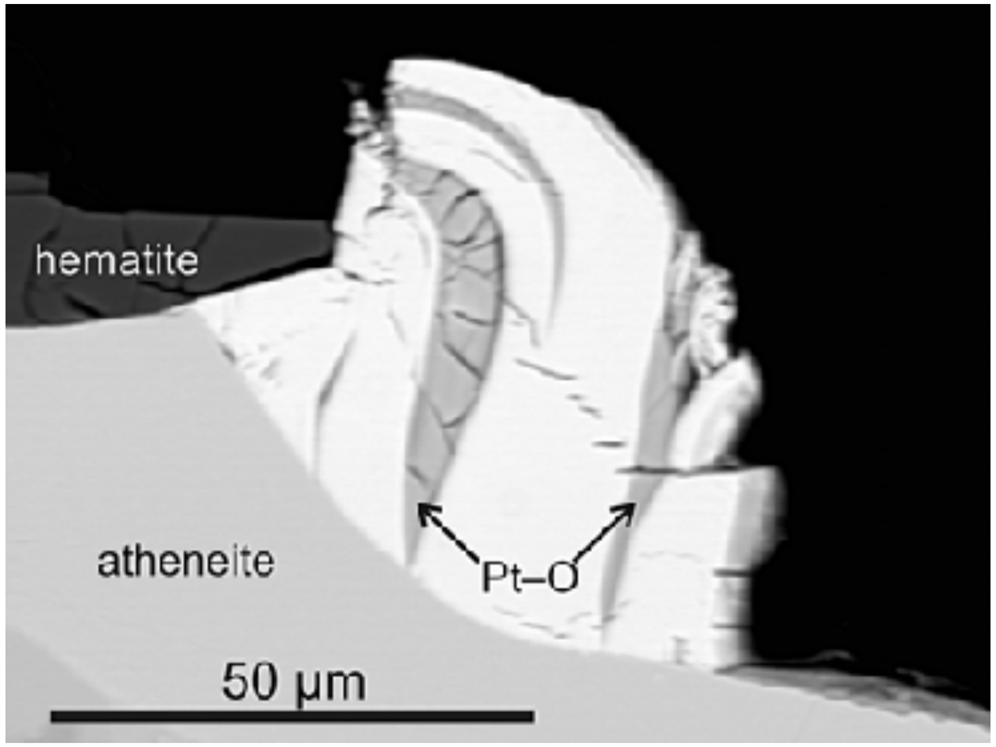
Optimizing the QSHE edge is not identical to just maximizing the 2d bulk gap.

Jacutingaite mineral Pt_2HgSe_3

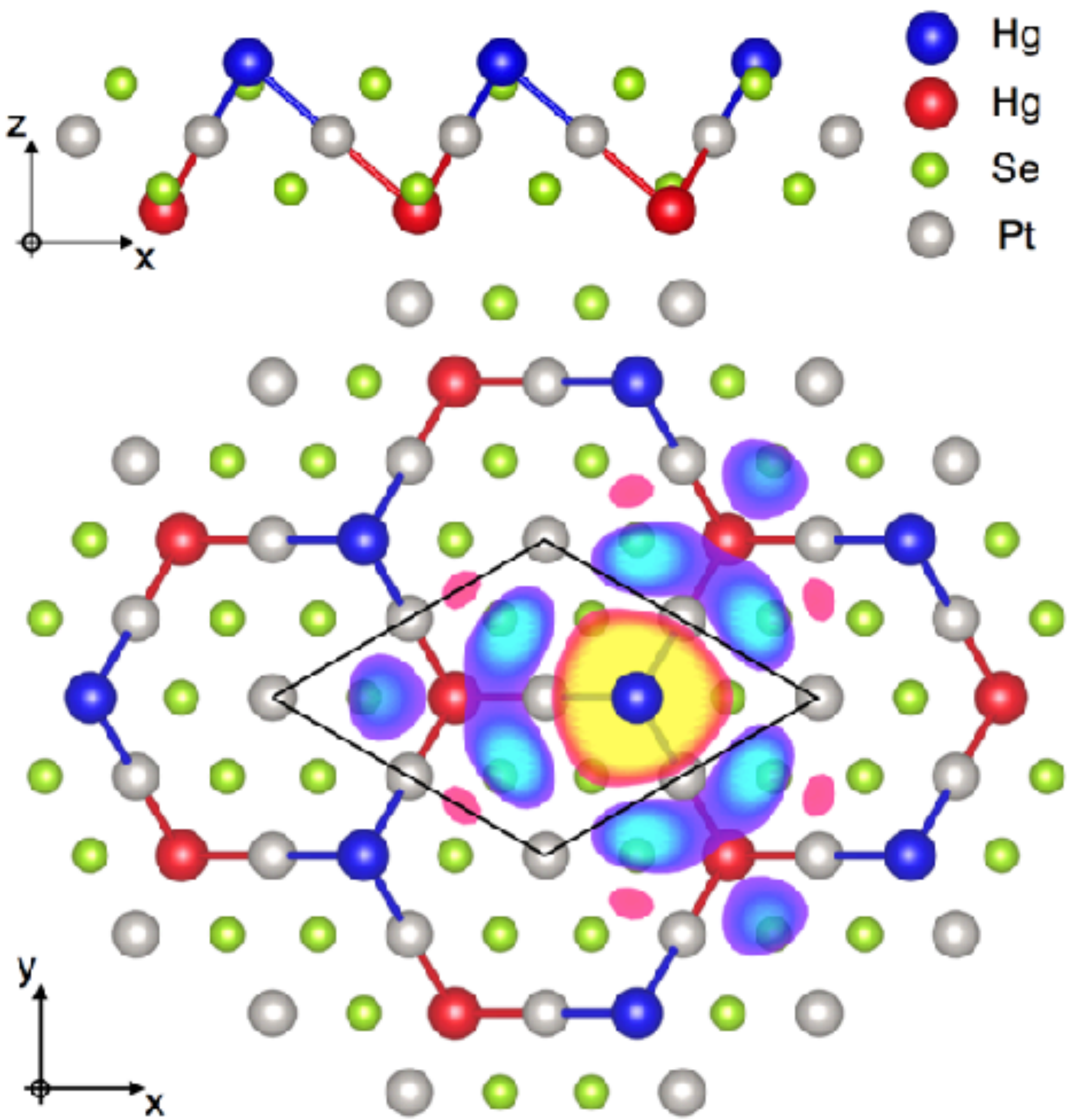
Experimental discovery

Vymazalova et al., The Canadian Mineralogist 50, 431 (2012).

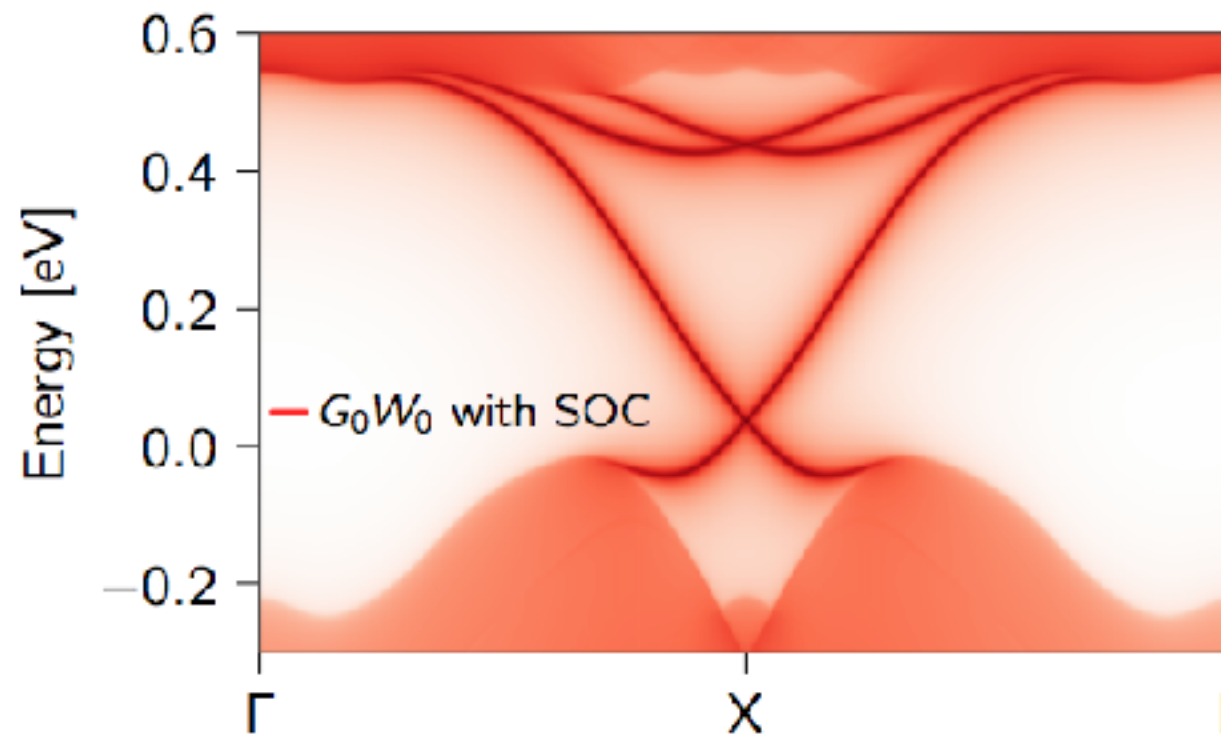




Crystal structure and QSHE



Marrazzo et al., PRL 2018

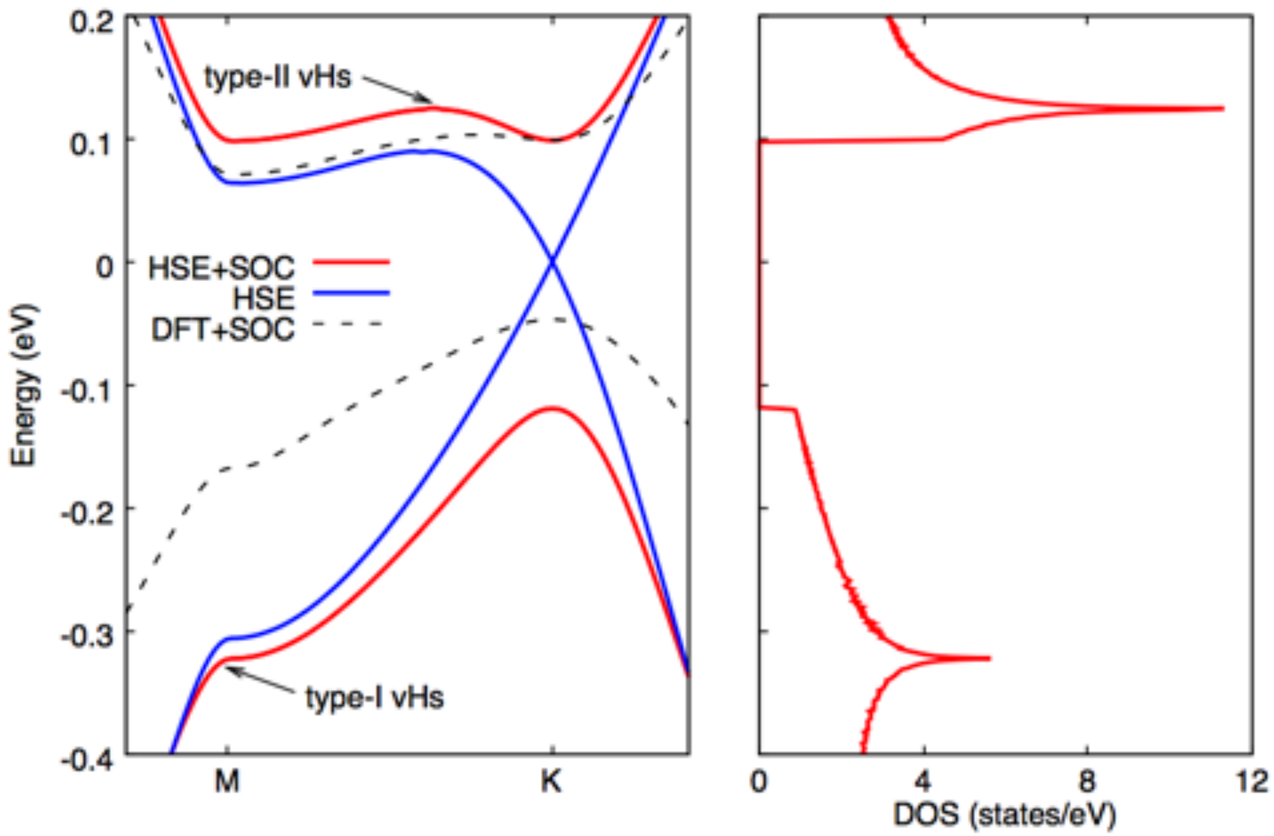


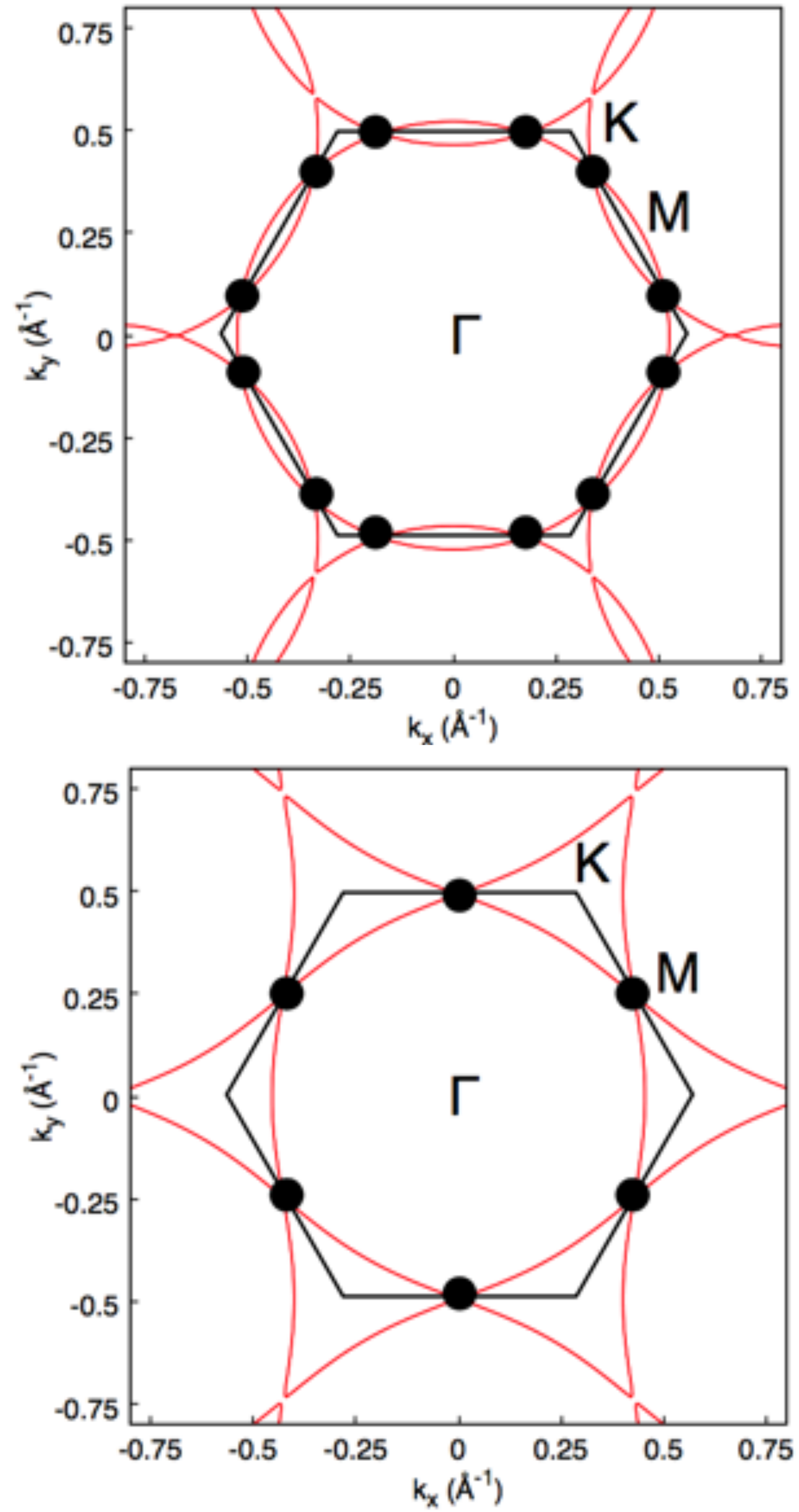
$$\Delta \sim 1.5\lambda_{\mathrm{SOC}}$$

Jacutingaite features strong n.n.n. hybridization and hence an ideal Kane Mele realization

Doping dependence of jacutingaite

X. Wu et al., PRB 100, 041117(R) (2019)

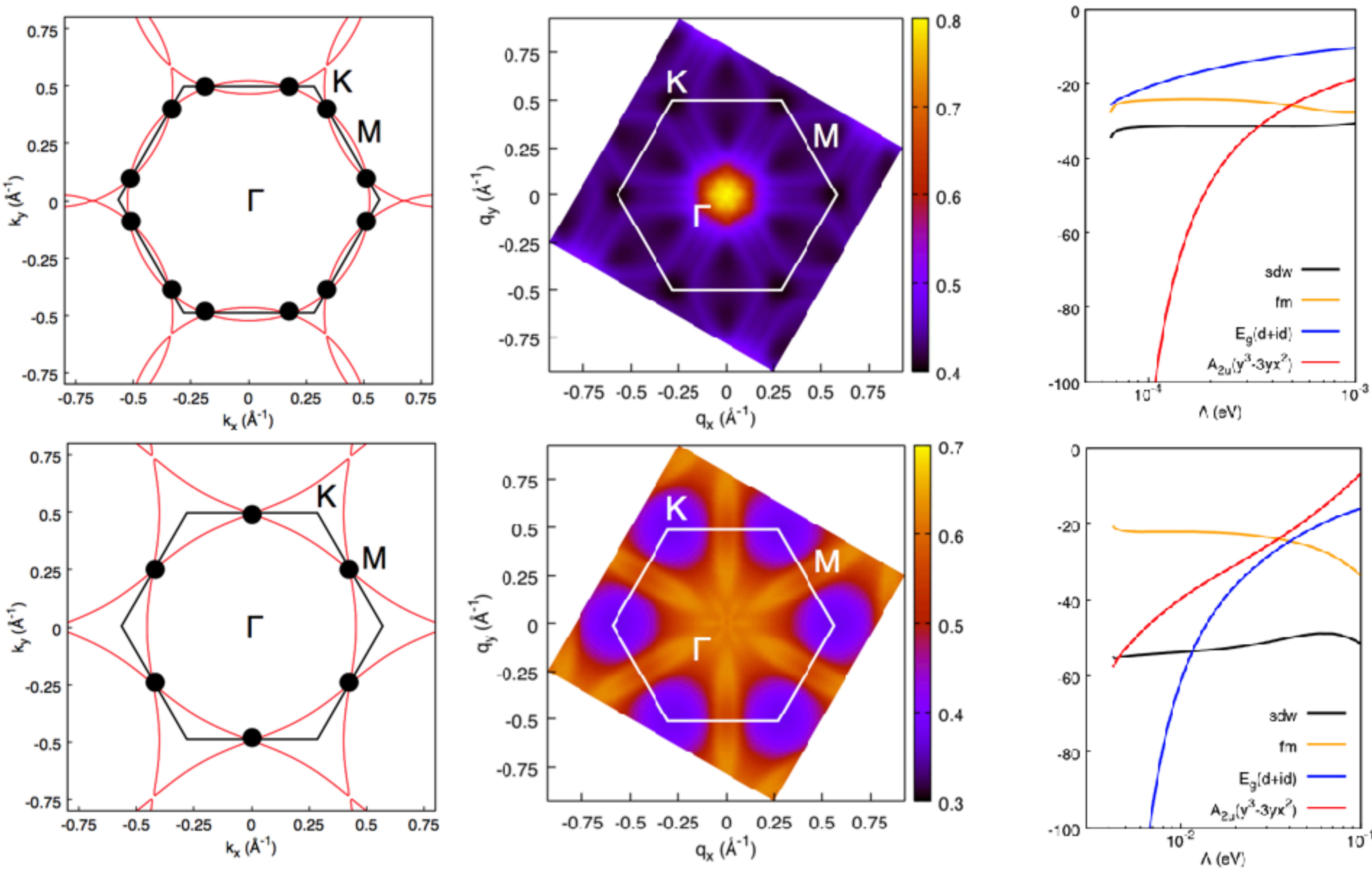




Doping jacutingaite yields access to type I and type II van Hove singularities

Superconductivity in doped jacutingaite

X. Wu et al., PRB 100, 041117(R) (2019)



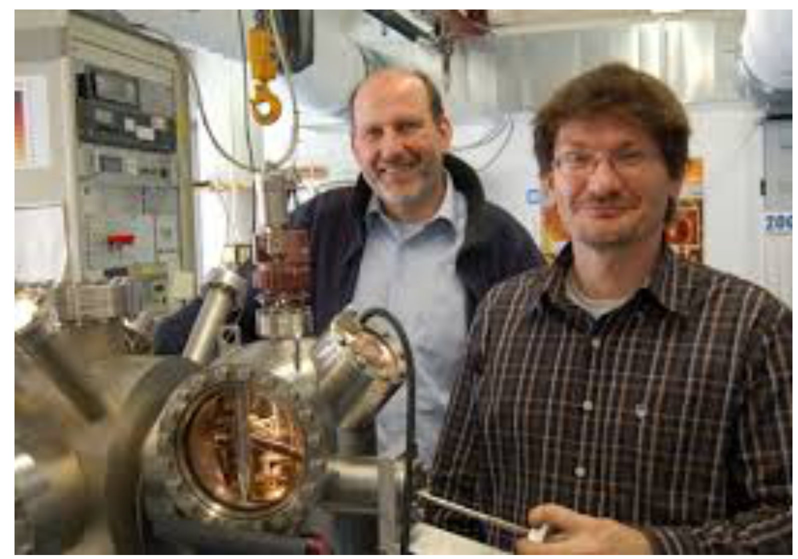
Collaborators

WTe2

UNIVERSITAS TURICENSIS

Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

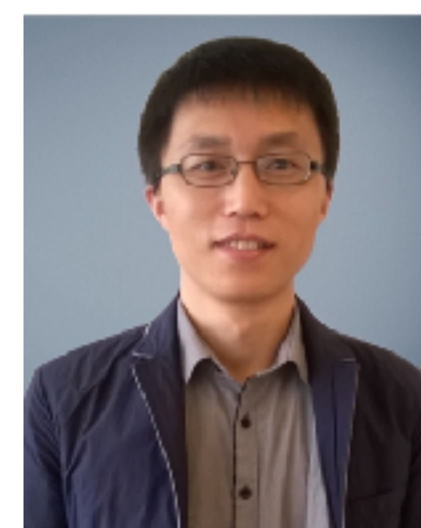
Bi/SiC



ep4

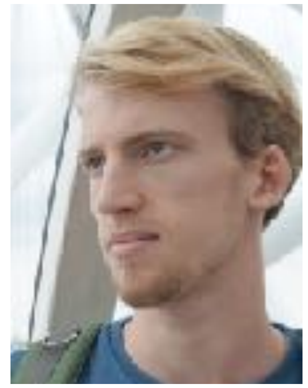
UNIVERSITY OF CALIFORNIA SAN DIEGO

上海科技大学
ShanghaiTech University



Research team and references







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