Room temperature topological insulators

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Julius-Maximilians Universität Würzburg

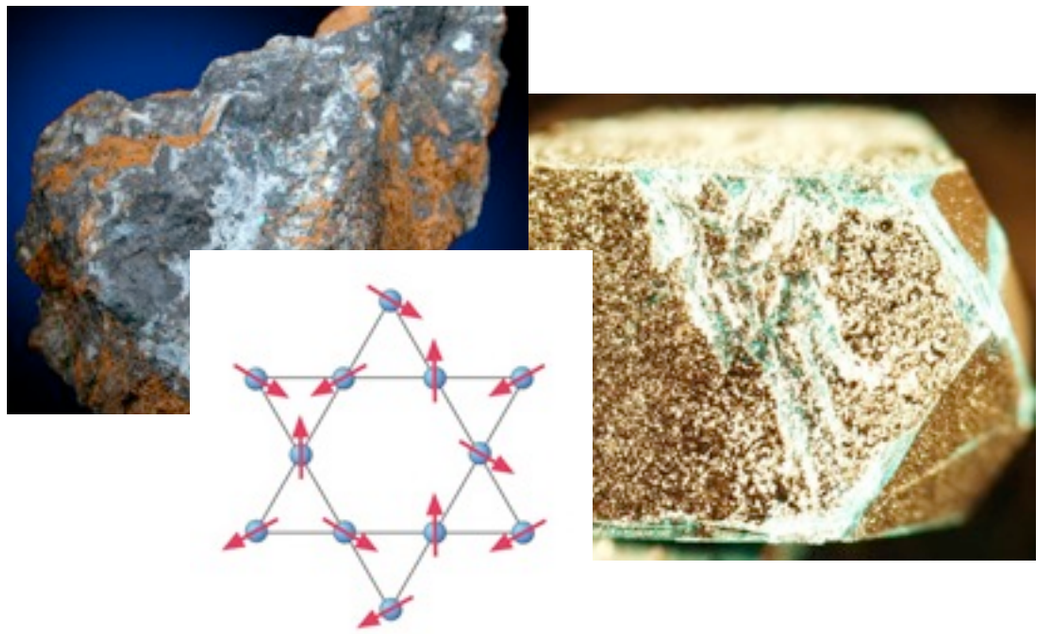
ERC Topolectrics

SFB Tocotronics

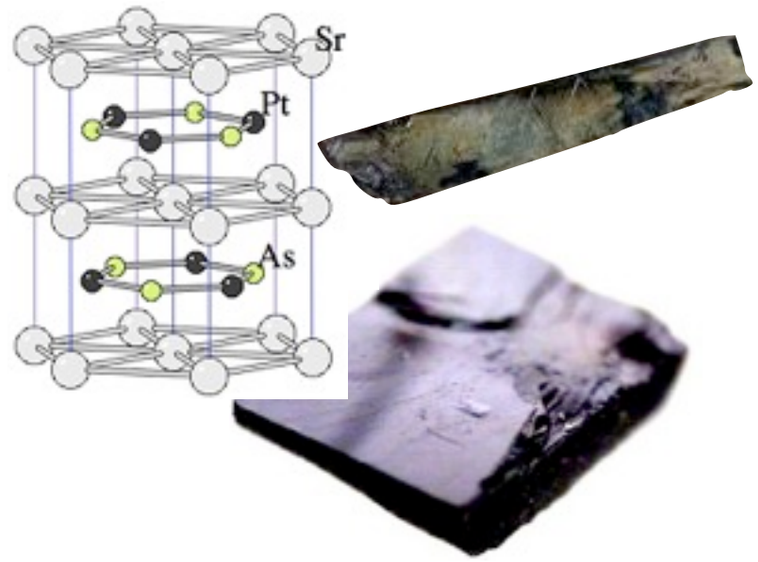
Synquant Workshop, KITP, UC Santa Barbara, Nov. 22 2016

Correlated electron systems

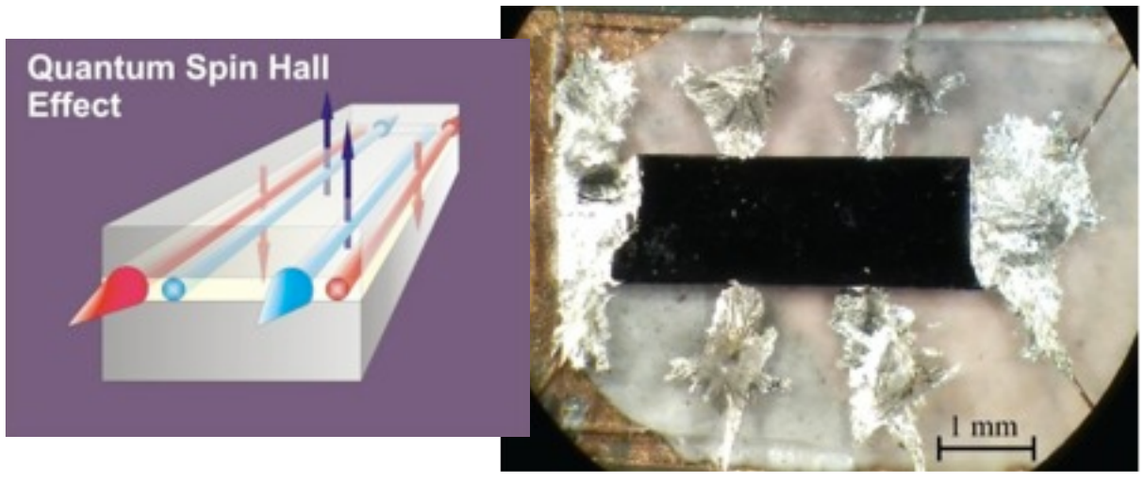
Frustrated Magnetism



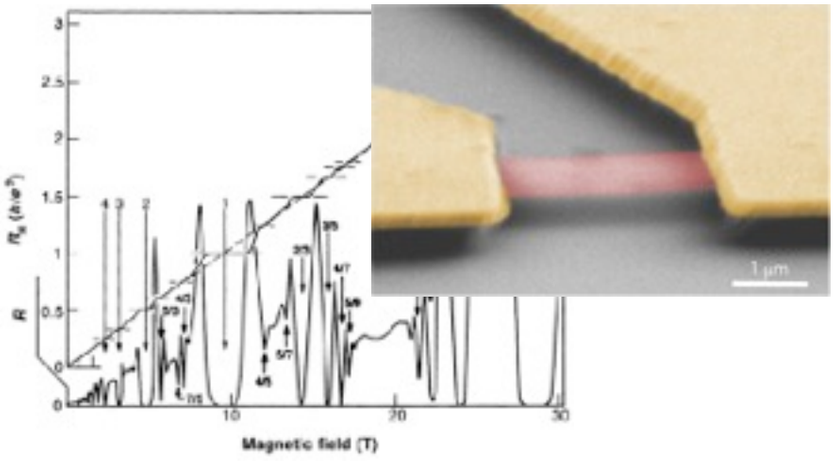
Superconductivity



Spin-orbit Phenomena



Quantum Hall Effect



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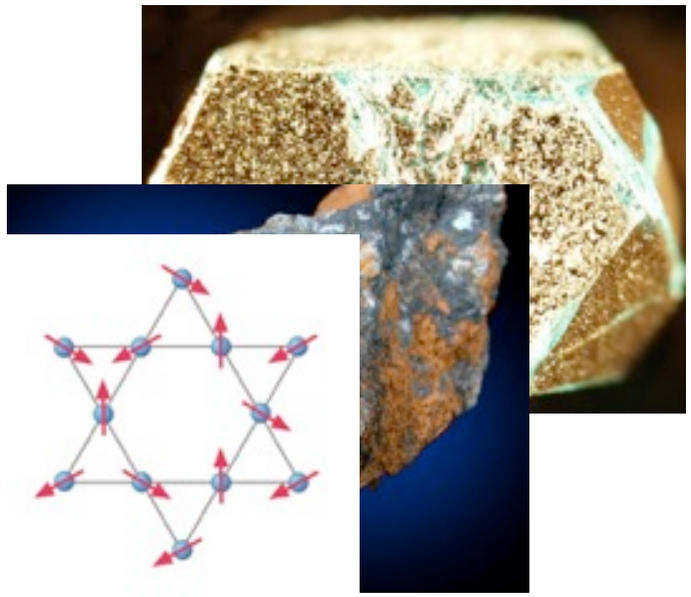
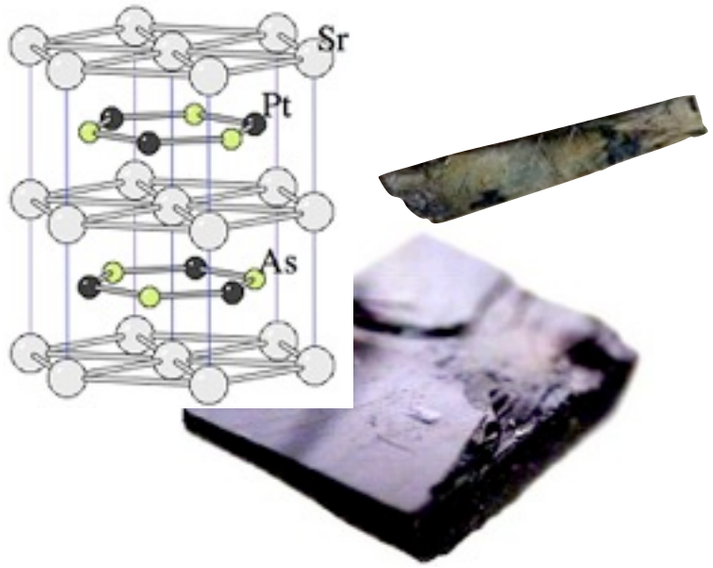


Superconductivity



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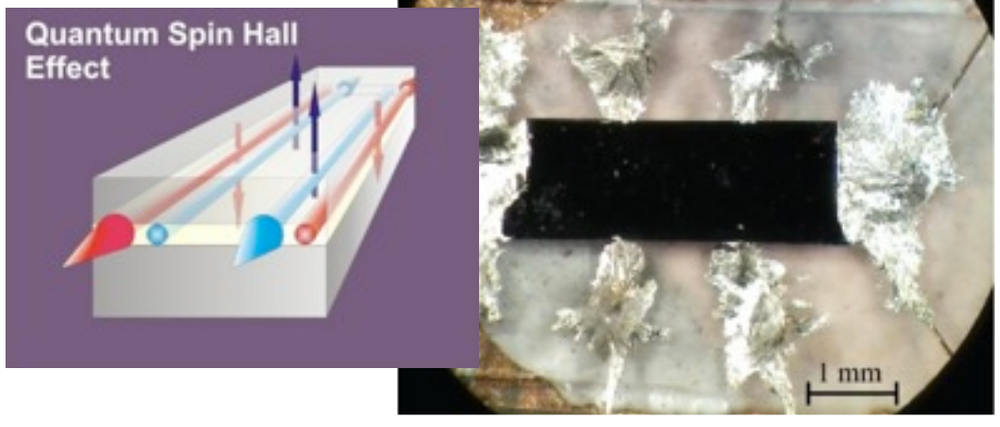
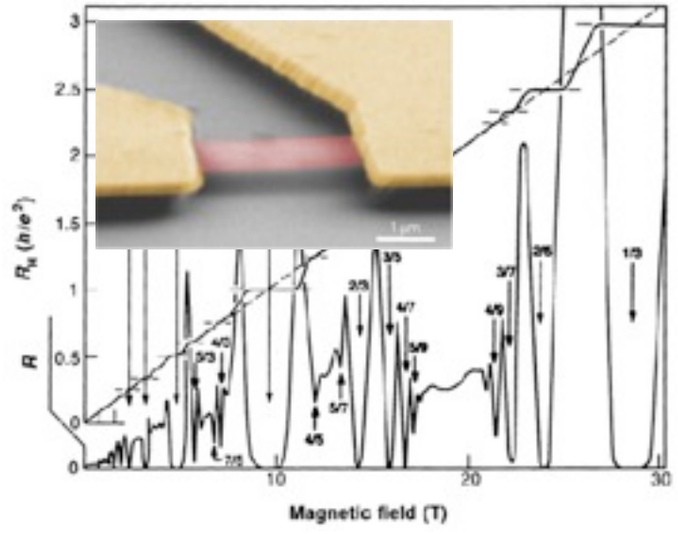


Quantum Hall Effect



Correlated electron systems

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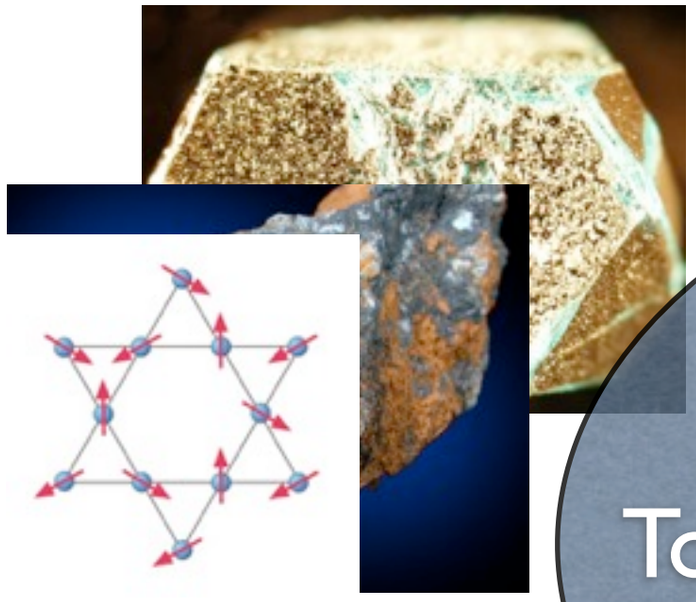

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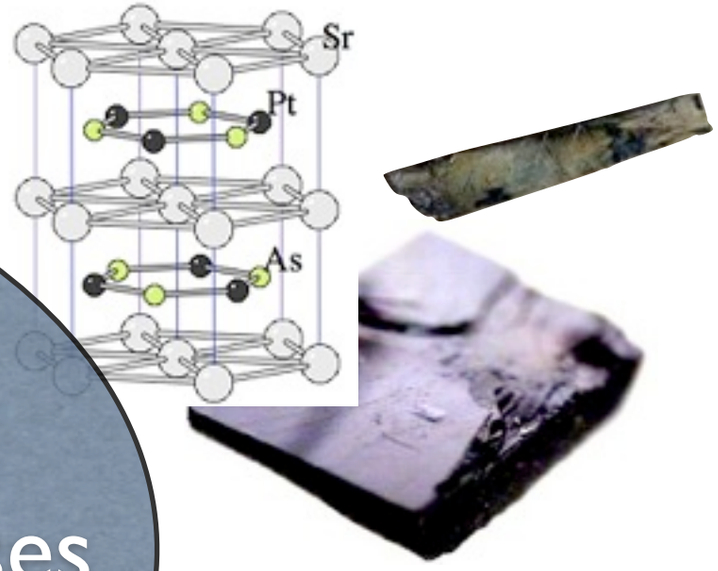
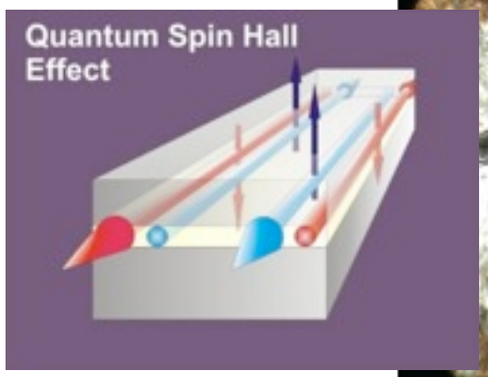
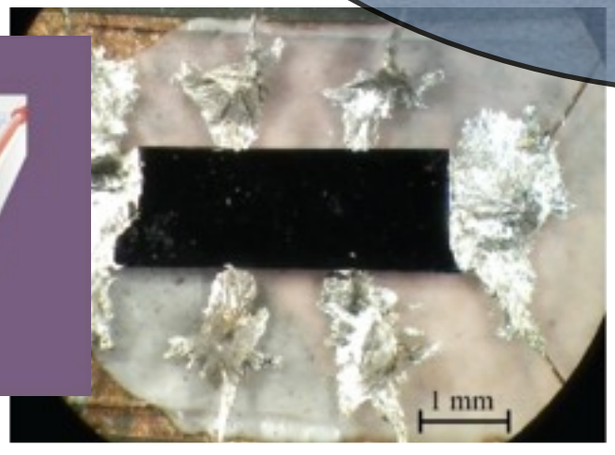


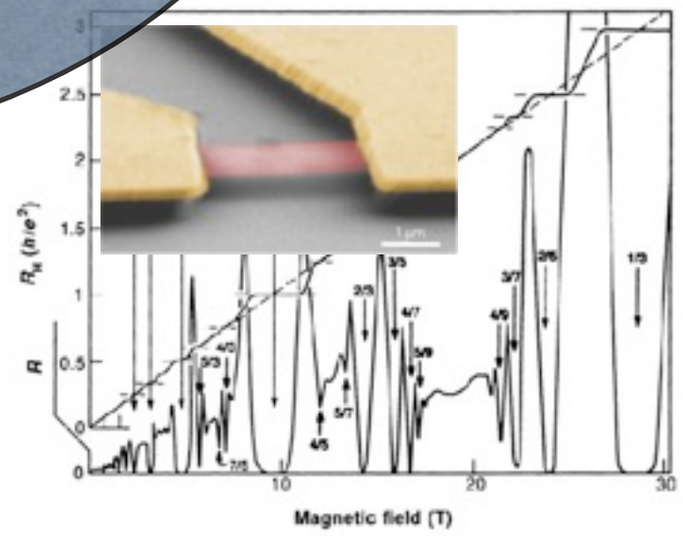
Topological Quantum Phases

Spin-orbit Phenomena





Quantum Hall Effect



Outline

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Topological phases a elevated temperature

- paradigm: quantum Hall effect

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- paradigm: quantum Hall effect

Room temperature QSHE: Bi/SiC(0001)

- low-energy model: substrate renormalization
- experiment: tentative QSHE with 650 meV band gap

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Topological phases a elevated temperature

- paradigm: quantum Hall effect

Room temperature QSHE: Bi/SiC(0001)

- low-energy model: substrate renormalization
- experiment: tentative QSHE with 650 meV band gap

Edge state hierarchy of TCIs: (Pb,Sn)Se

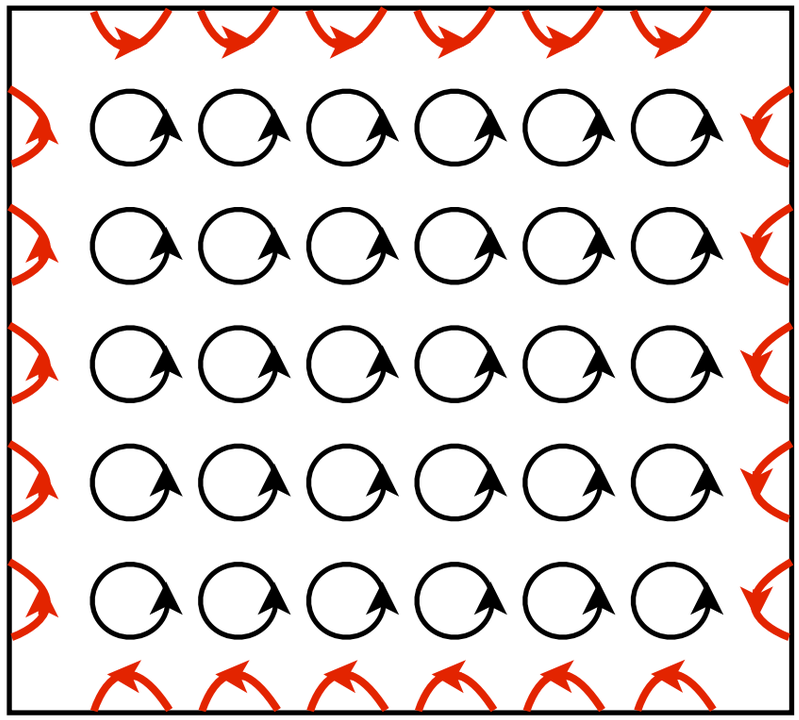
- toy-model: midgap states in a staggered flux lattice
- experiment: 1D non-dispersive DOS along odd-step terraces

Topological phases at elevated temperature

Integer Quantum Hall effect (IQHE)

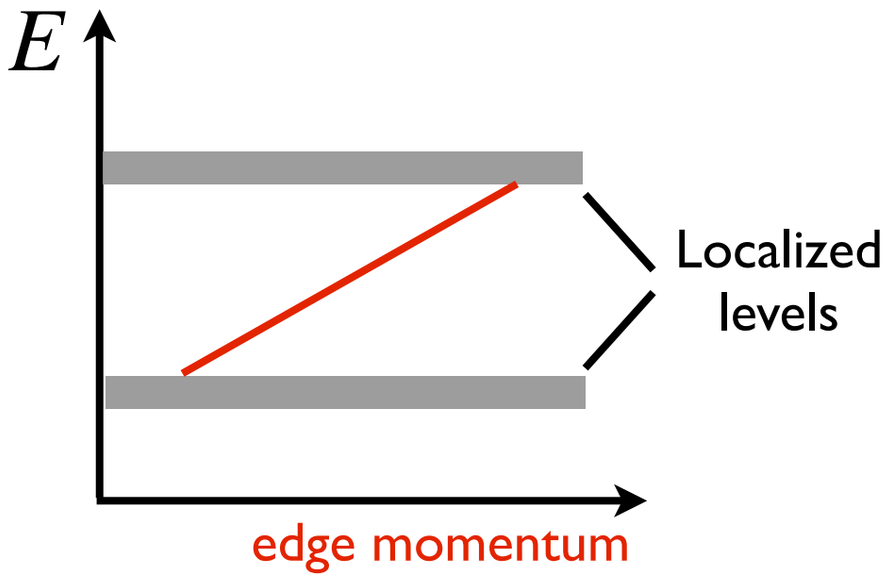
Von Klitzing 1980; Laughlin 1981; Thouless 1982; Haldane 1988

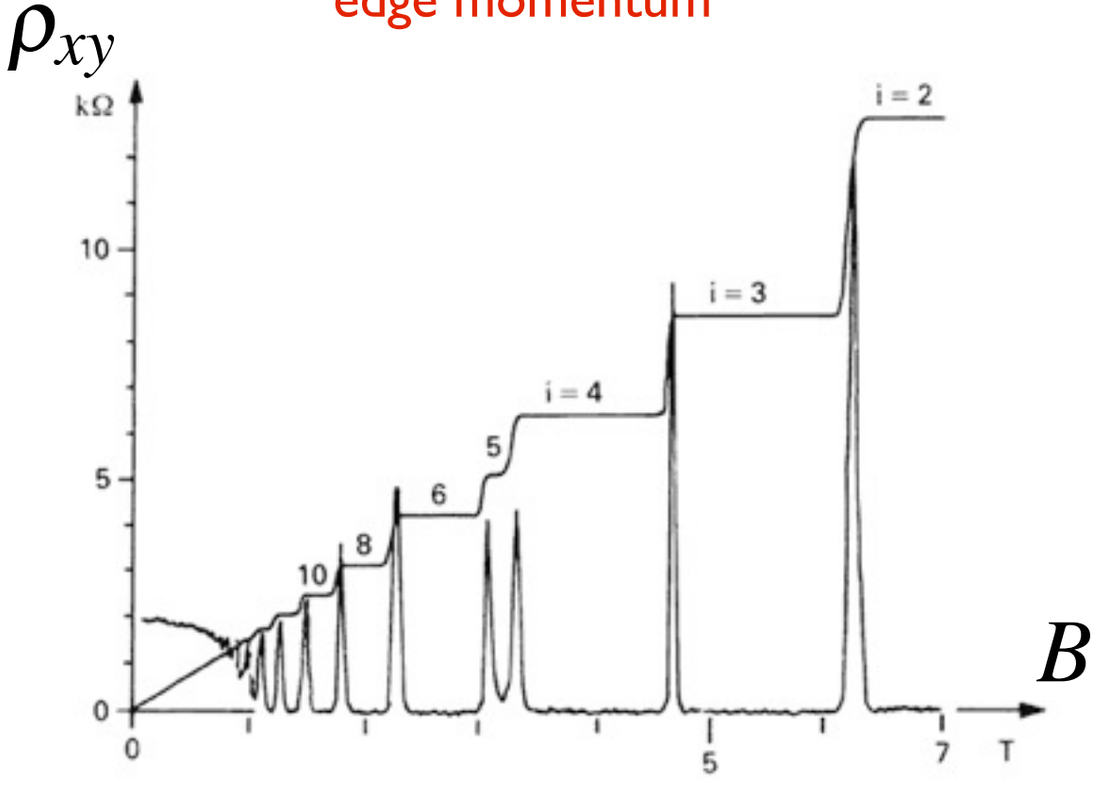
Chiral mode at the edge of the sample



$$\sigma_{xy} = C\frac{e^2}{h}$$

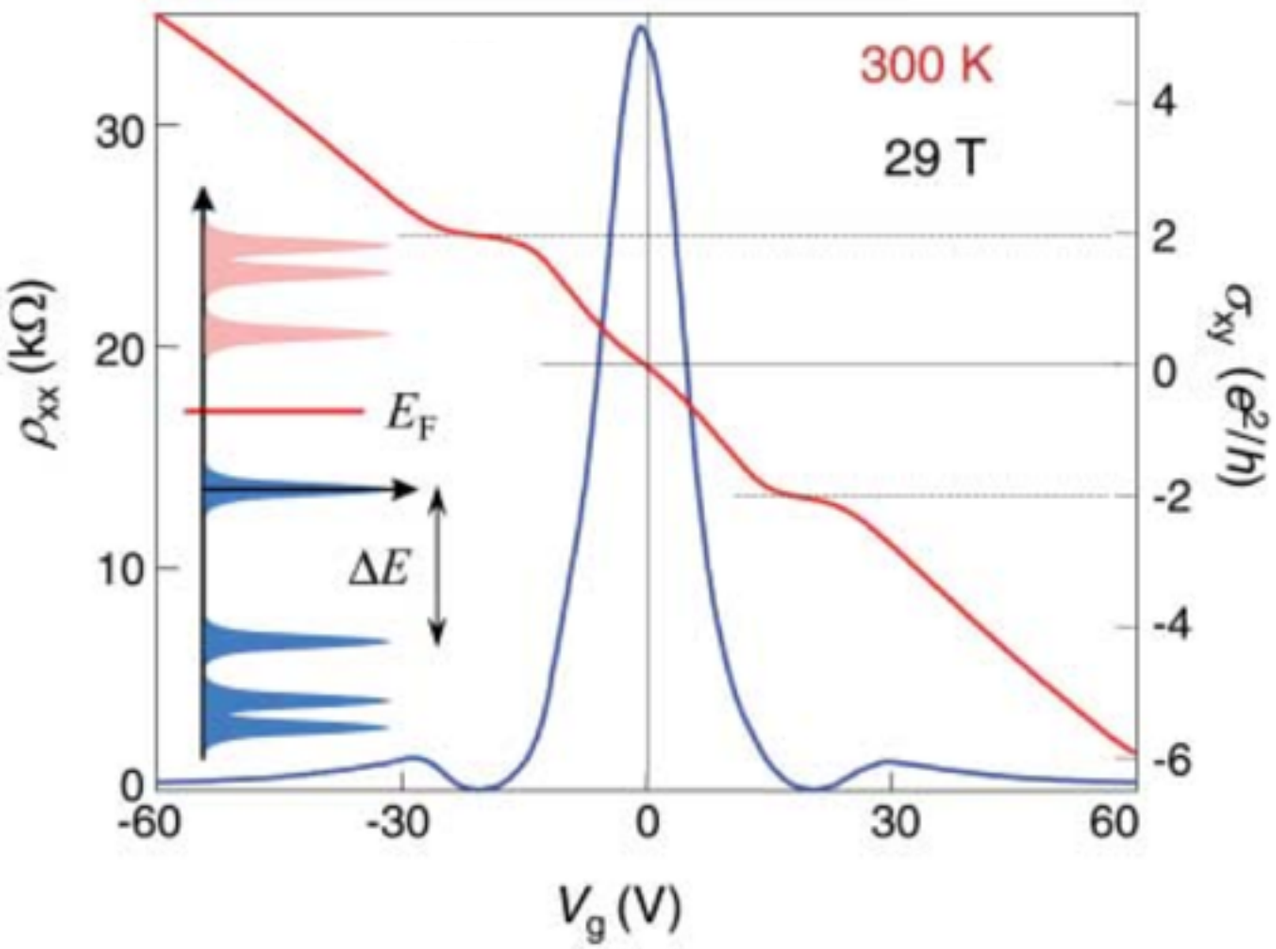
Chern number $C \in \mathbb{Z}$:
topological invariant

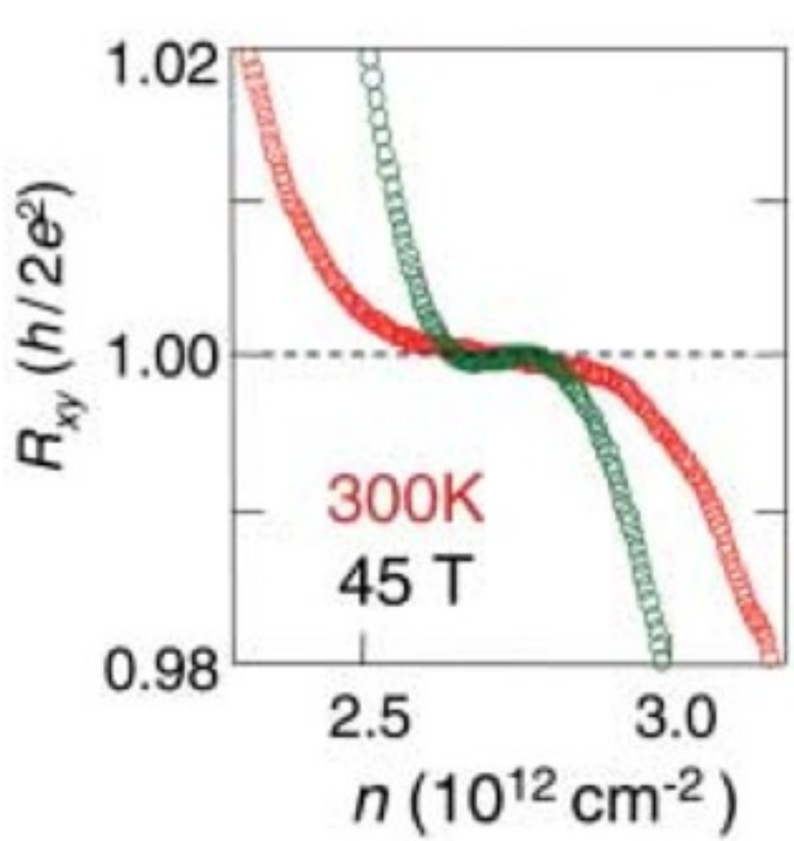




Room-Temperature Quantum Hall Effect in Graphene

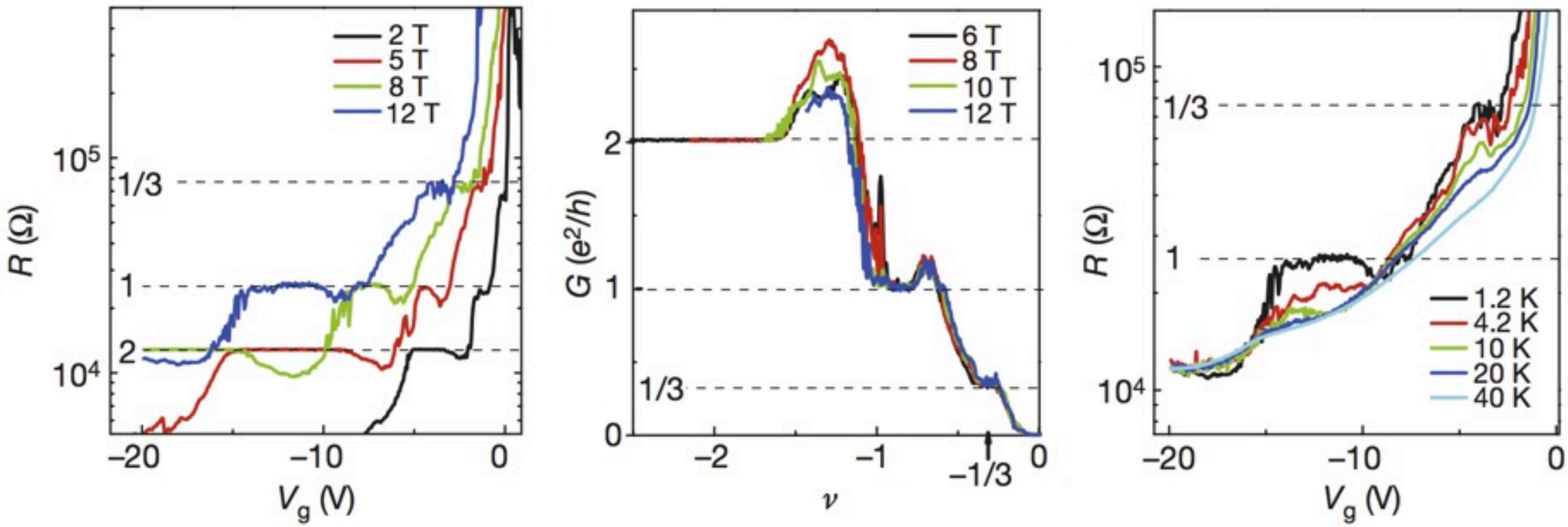
K. S. Novoselov,[1] Z. Jiang,[2,3] Y. Zhang,[2] S. V. Morozov,[1] H. L. Stormer,[2] U. Zeitler,[4] J. C. Maan,[4] G. S. Boebinger,[3] P. Kim,[2*] A. K. Geim[1*]





Fractional quantum Hall effect and insulating phase of Dirac electrons in graphene

Xu Du[1]†, Ivan Skachko[1], Fabian Duerr[1], Adina Luican[1] & Eva Y. Andrei[1]

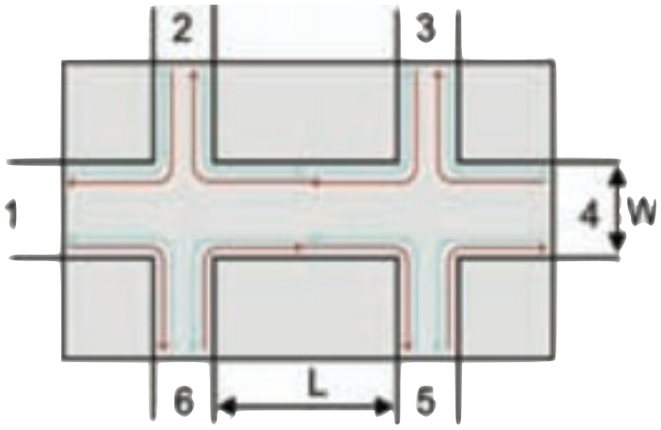


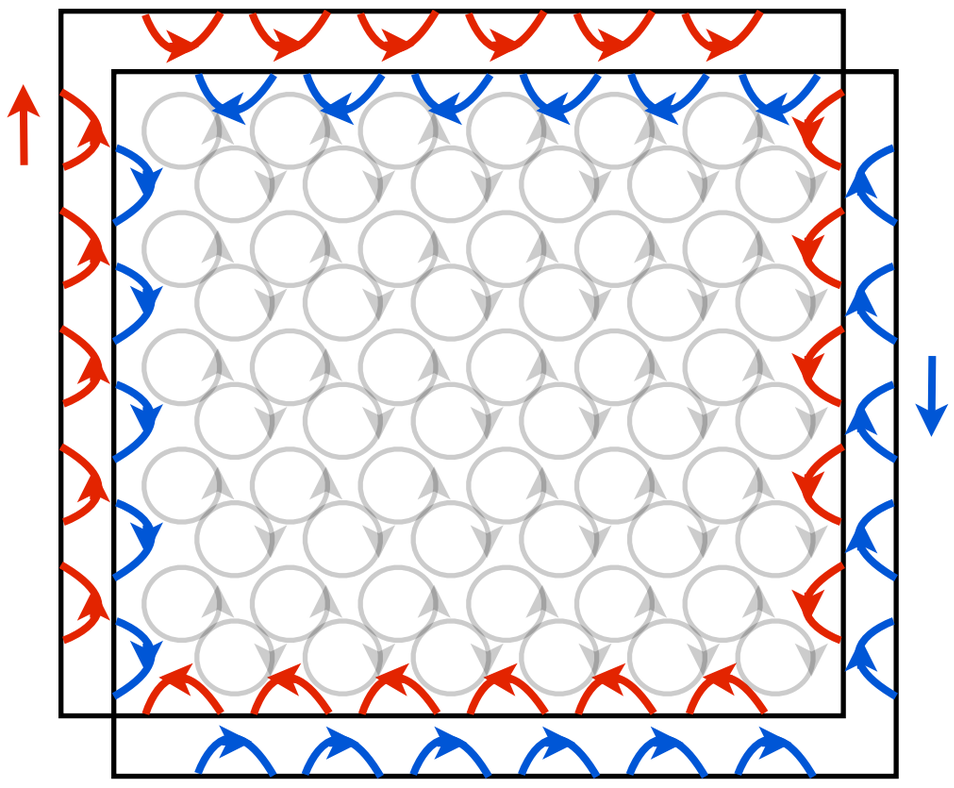
Quantum spin Hall effect

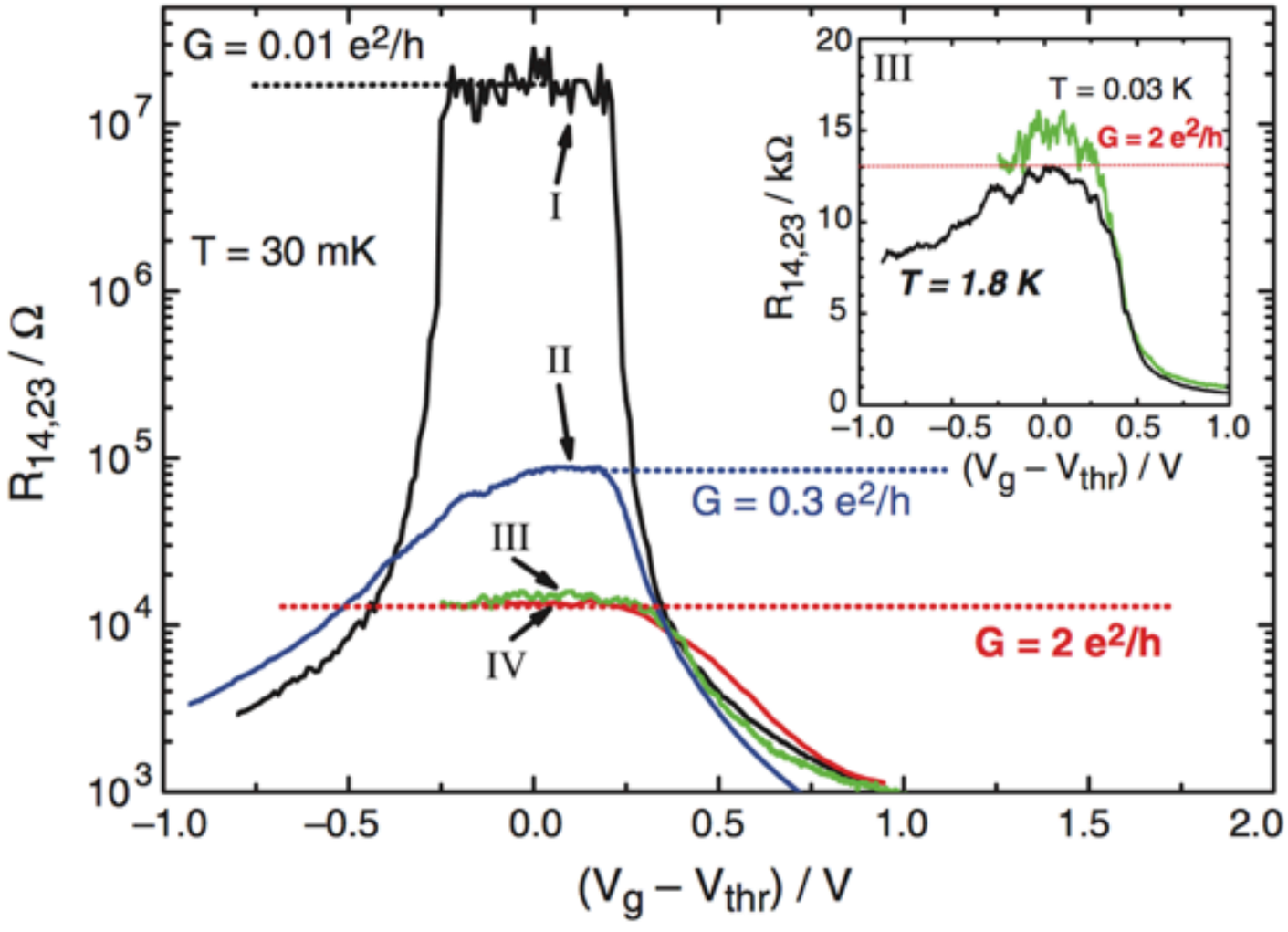
Quantum spin Hall effect in HgTe

König et al. (Molenkamp group), Science 2007

Time-reversed counterpropagating edge modes



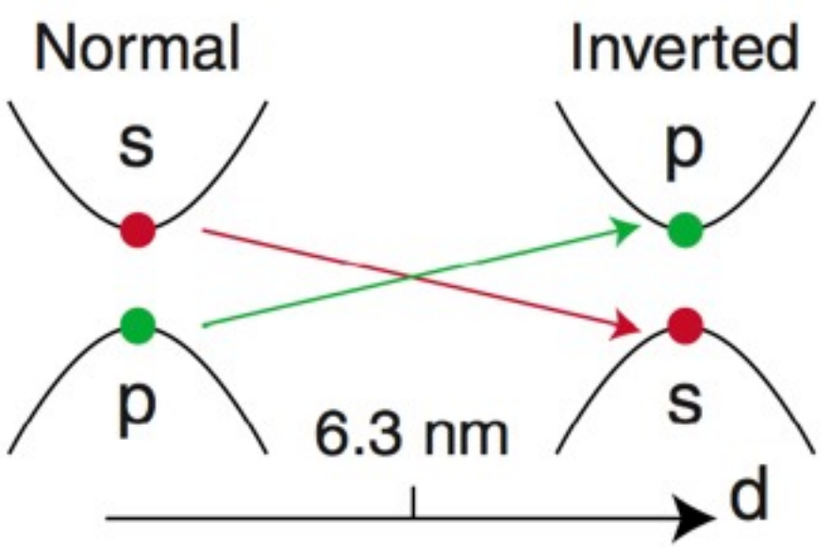


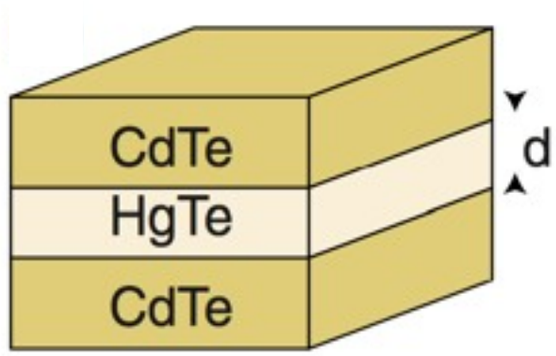


Mechanisms of QSHE

Band inversion

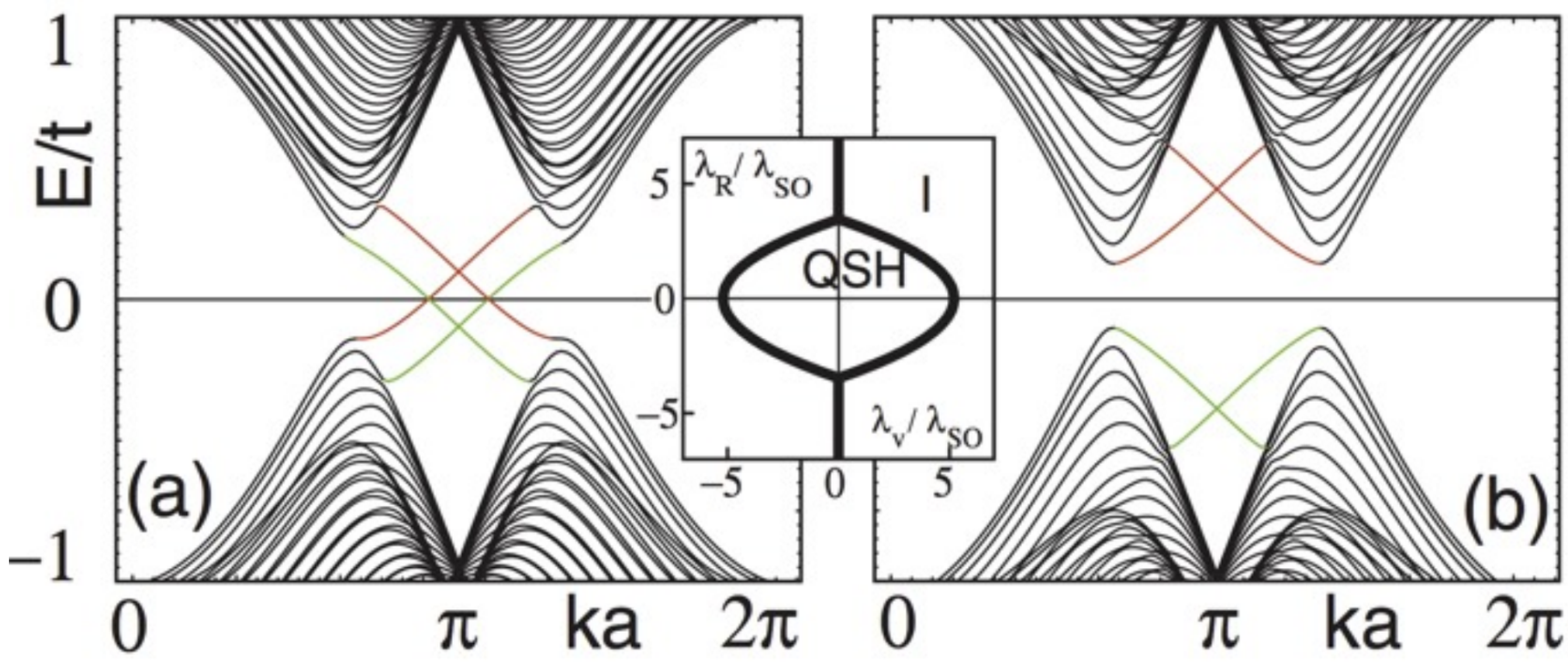
Bernevig, Hughes, Zhang, Science 2006





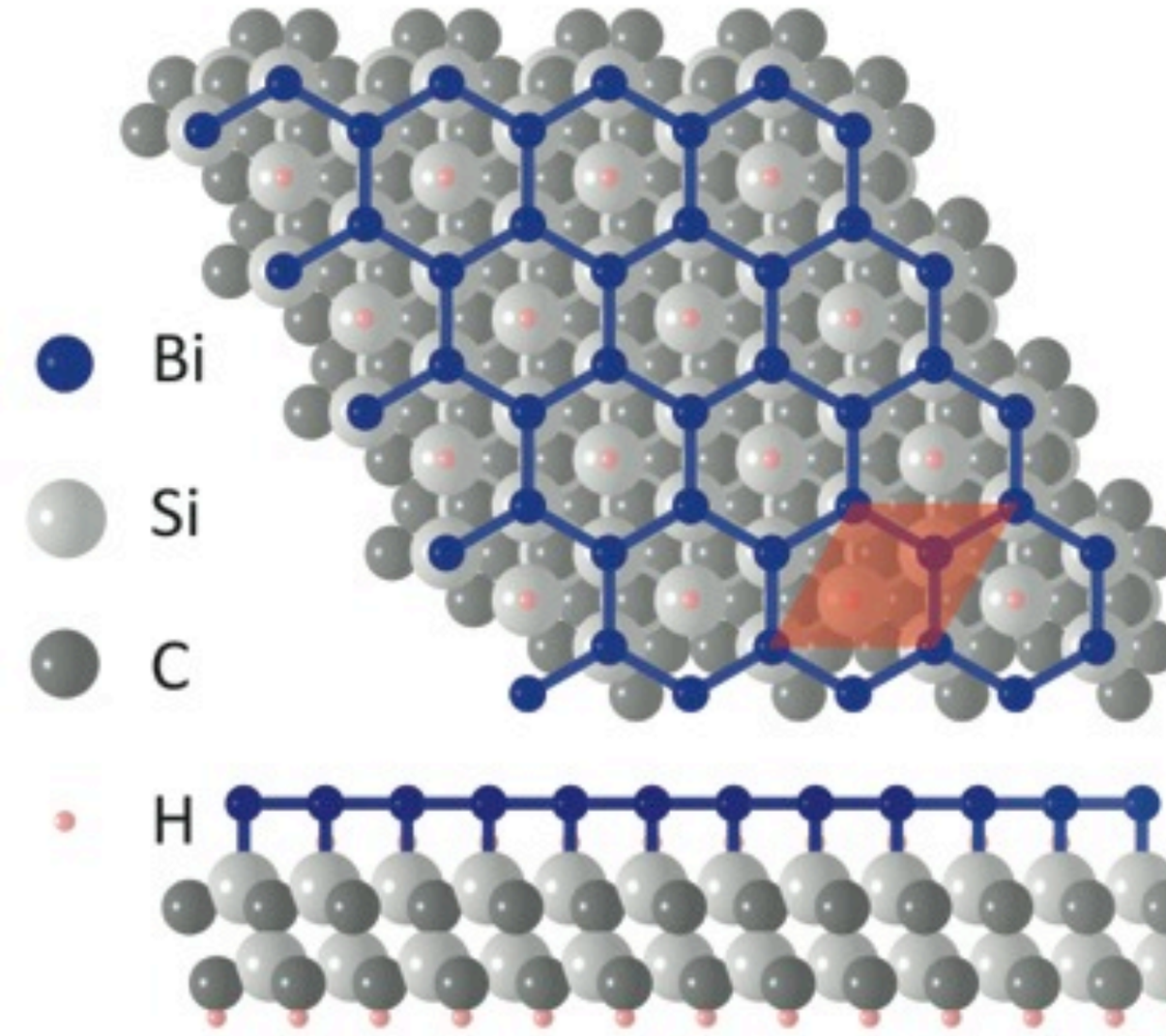
Dirac electron mass due to SOC

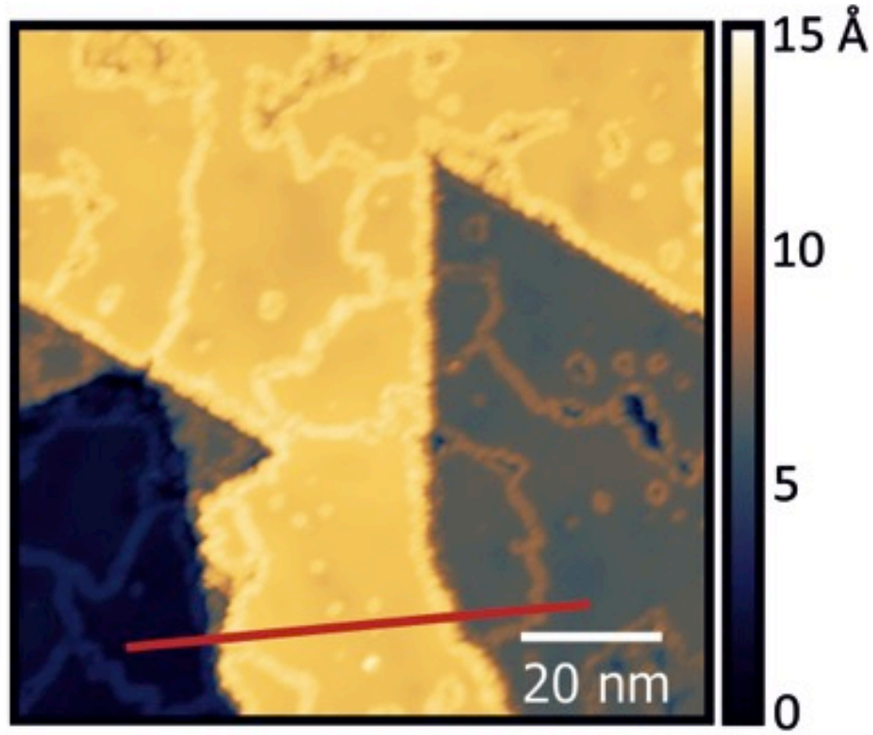
Kane & Mele PRL 2005

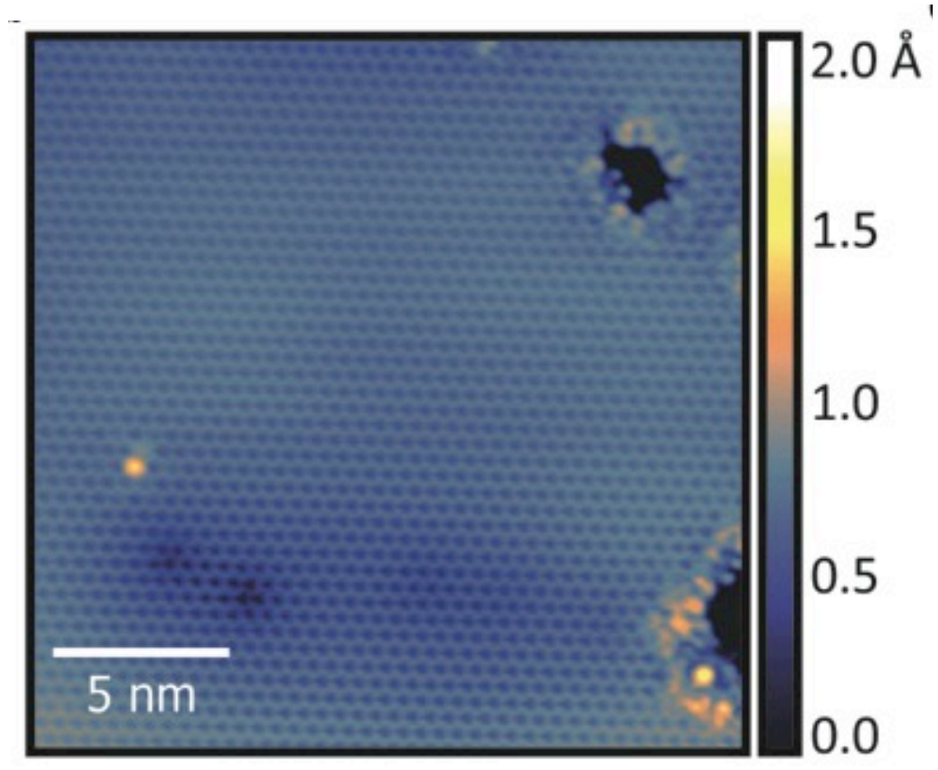


Room temperature QSHE: Bi/SiC(0001)

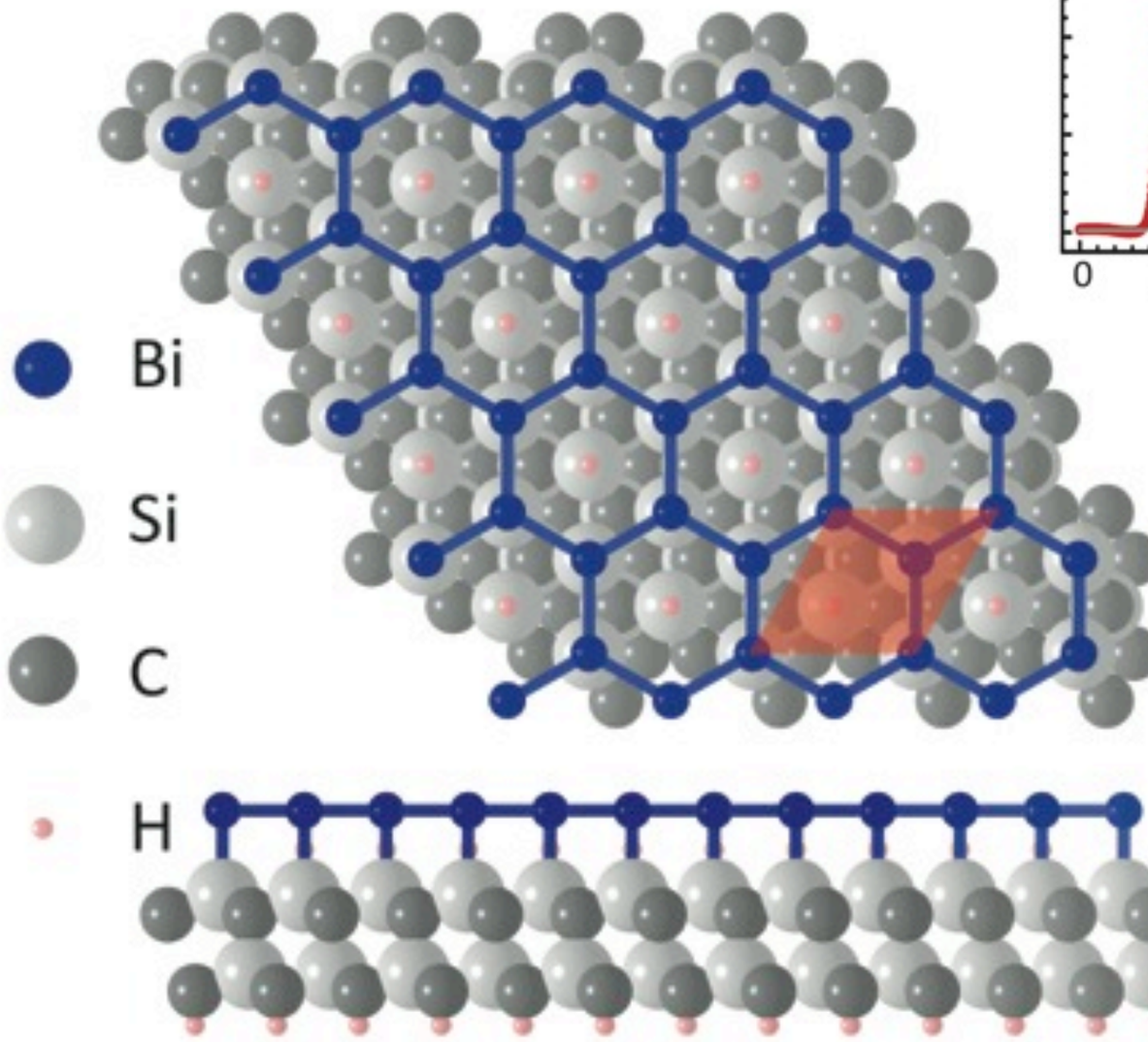
Bi/SiC(0001) monolayer-substrate compound

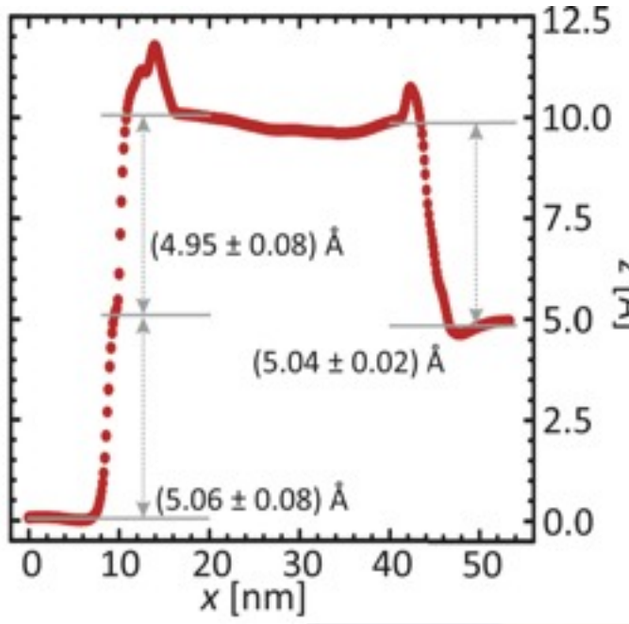


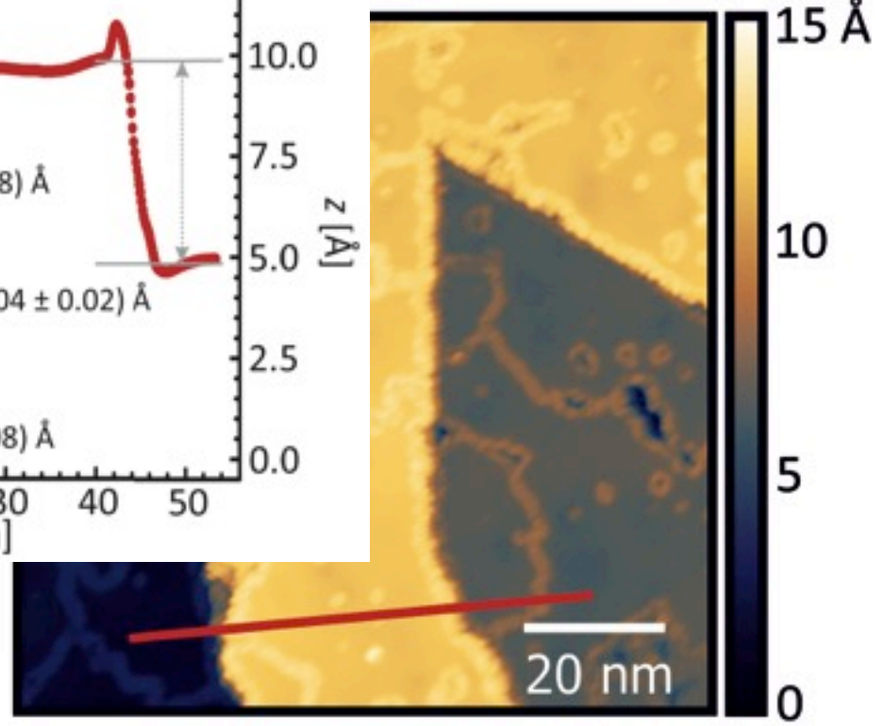


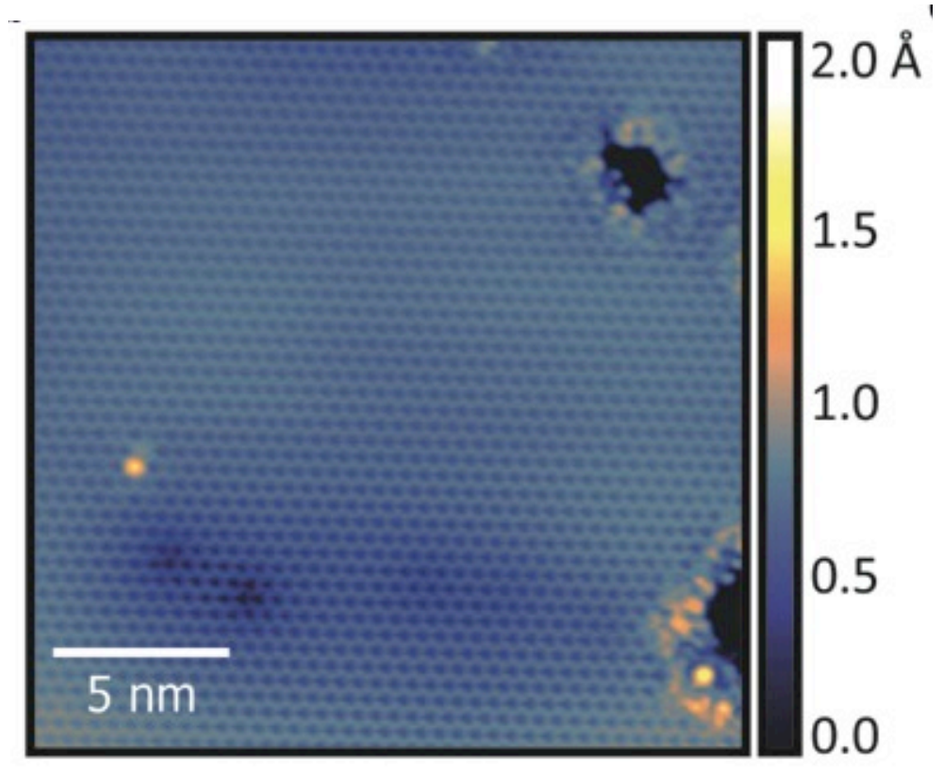


Bi/SiC(0001) monolayer-substrate compound

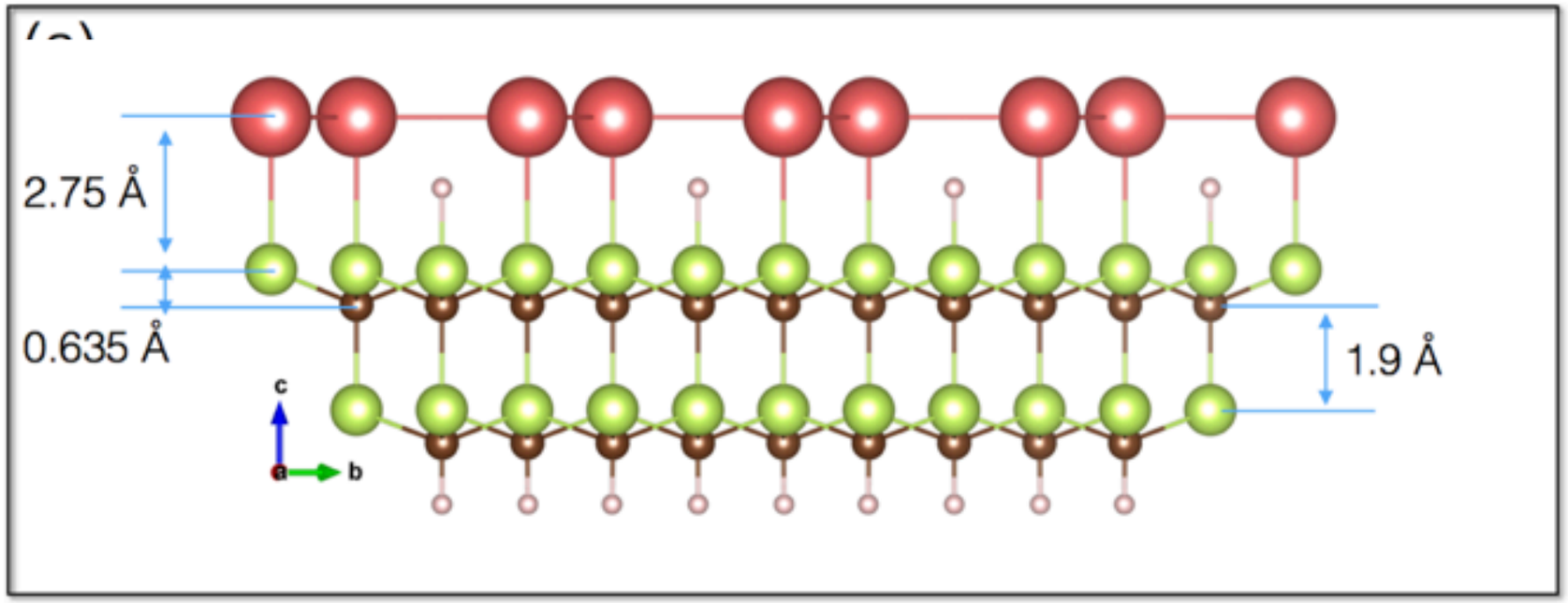


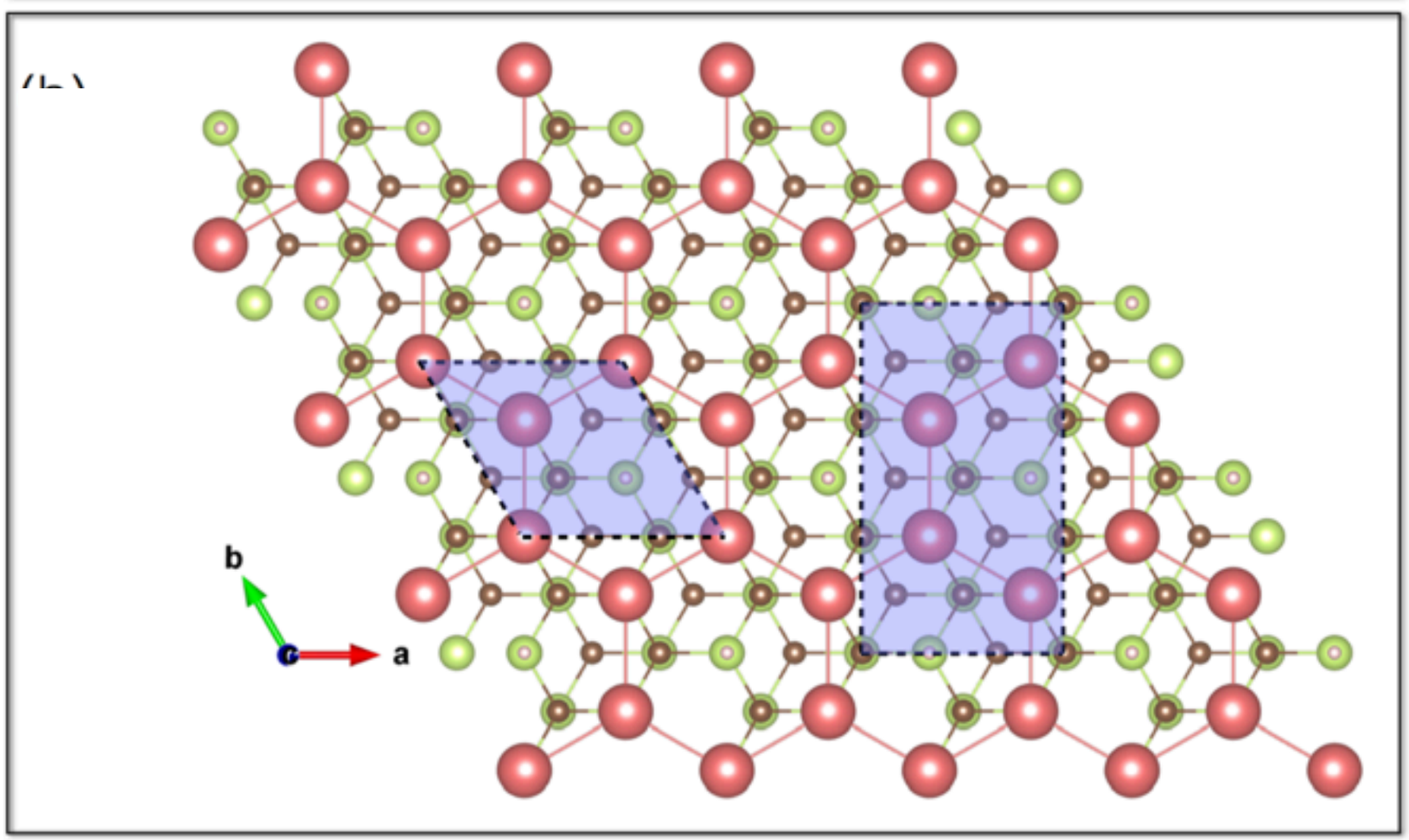






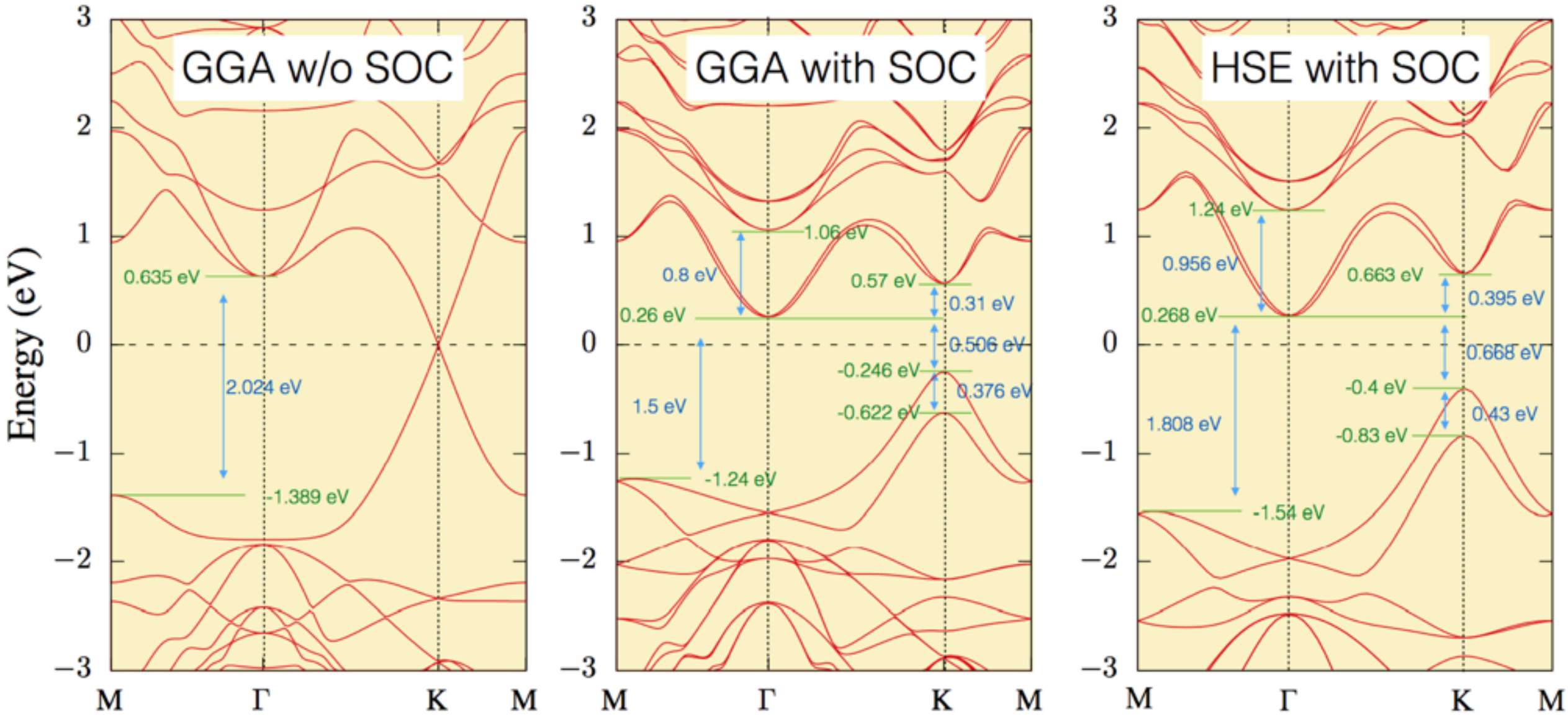
Theoretical compound modelling



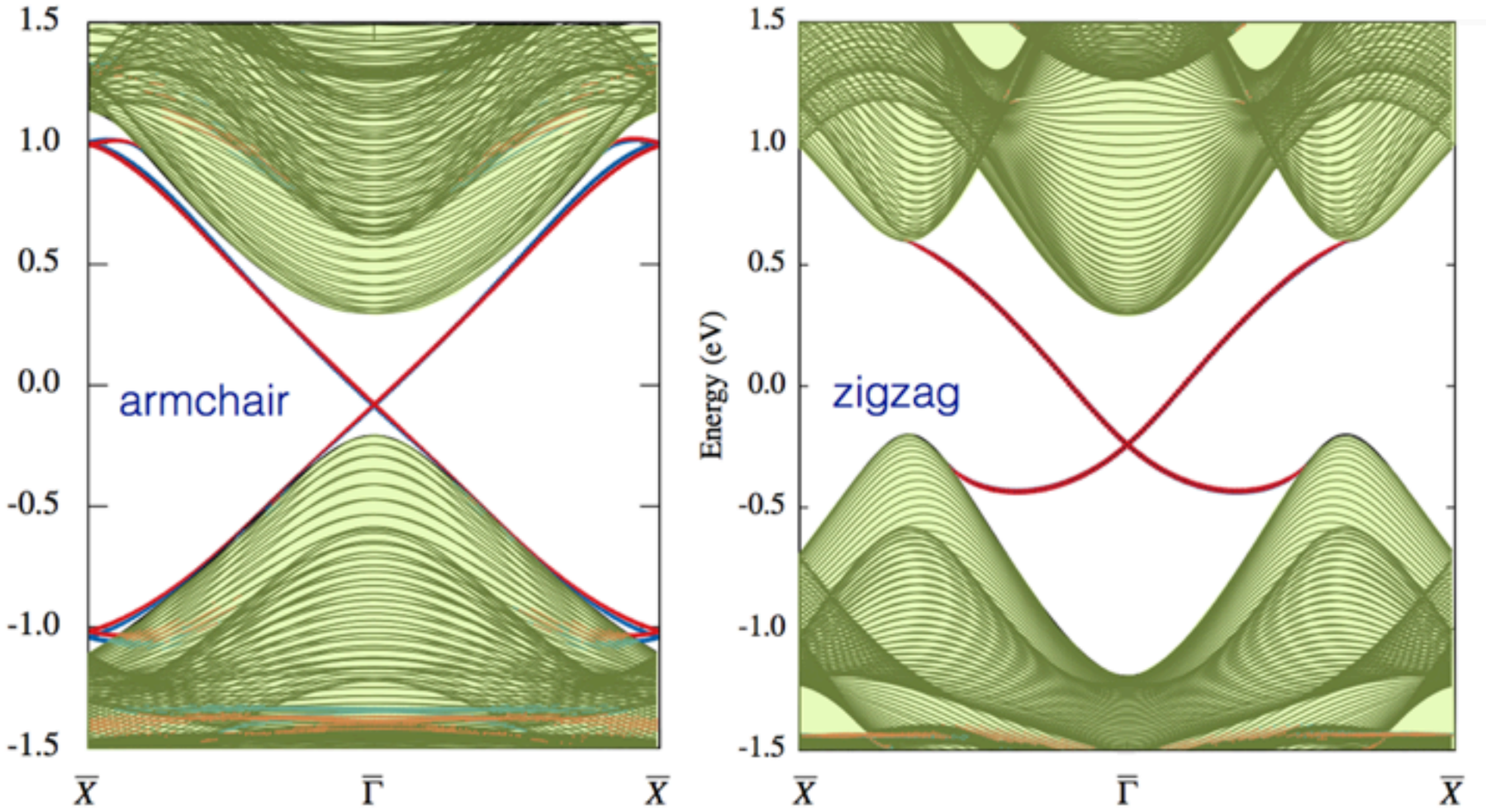


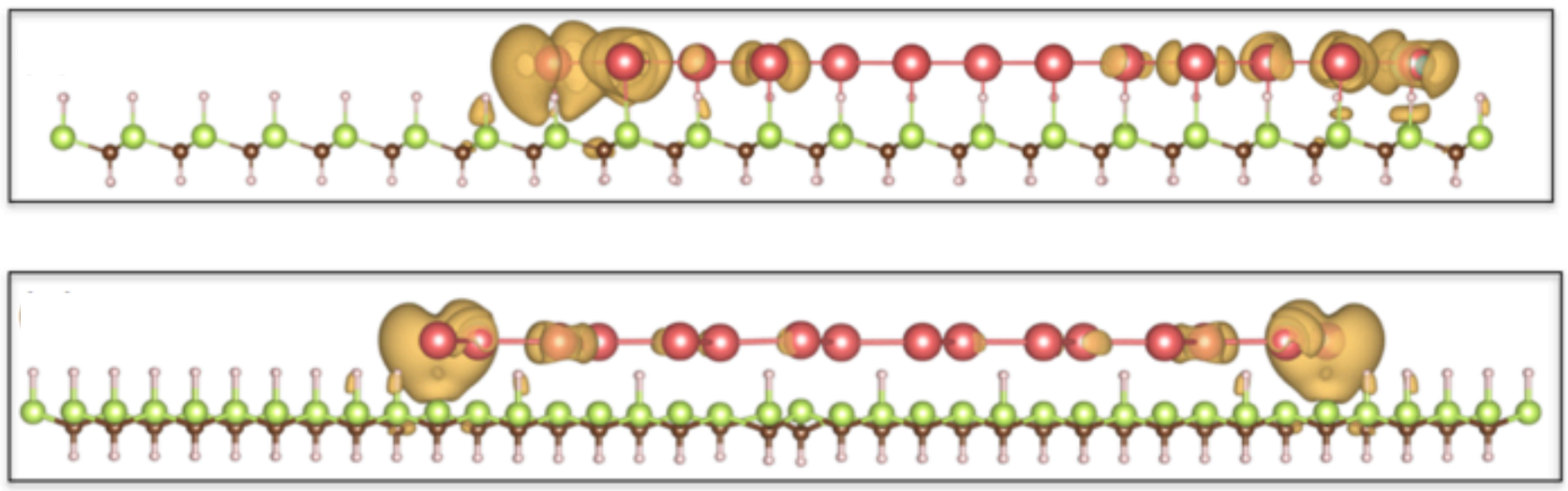
Electronic structure

indication from DFT: SOC opens large gap at the K point



Edge states





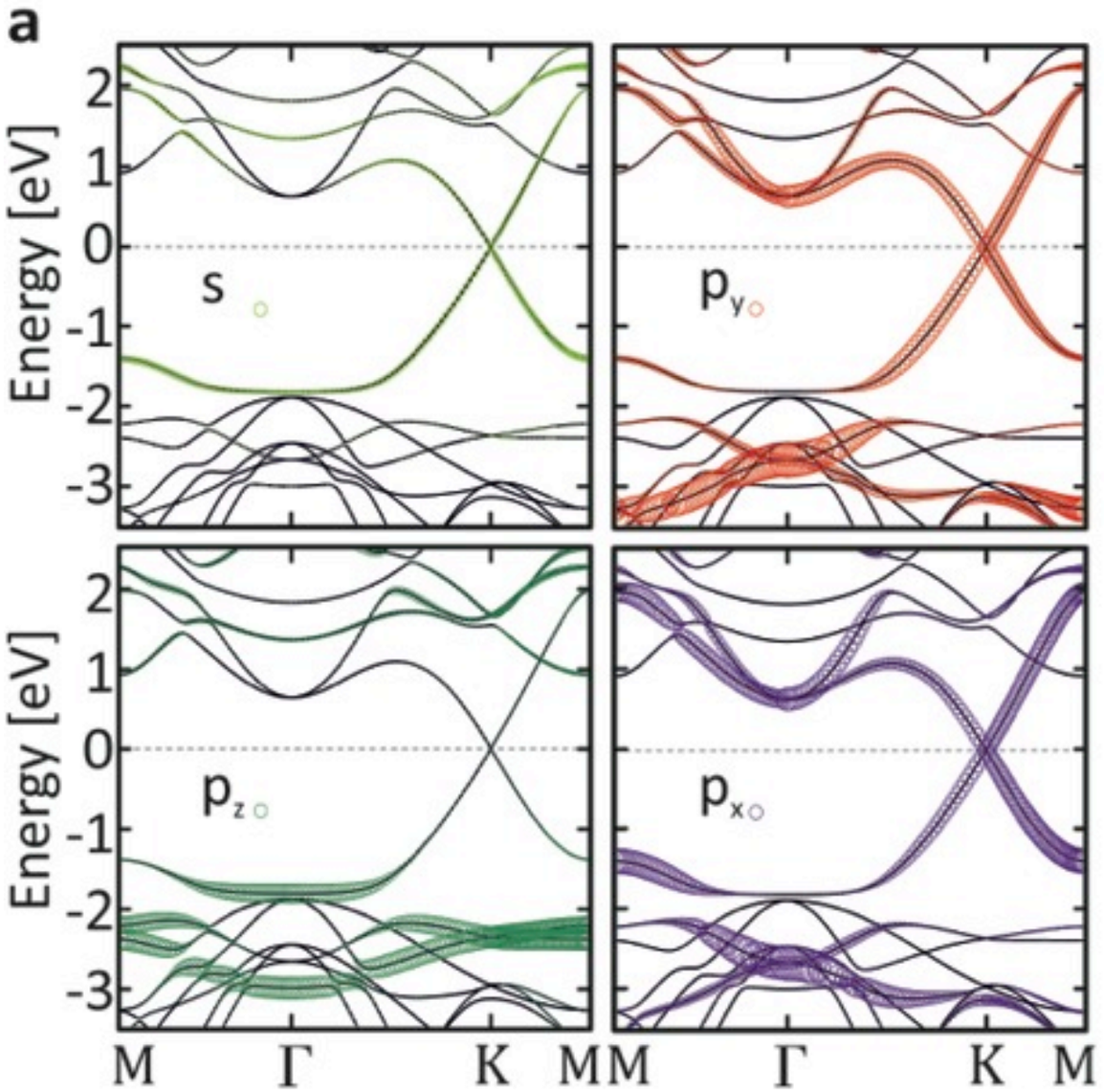
Band structure analysis w/o spin-orbit coupling

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

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

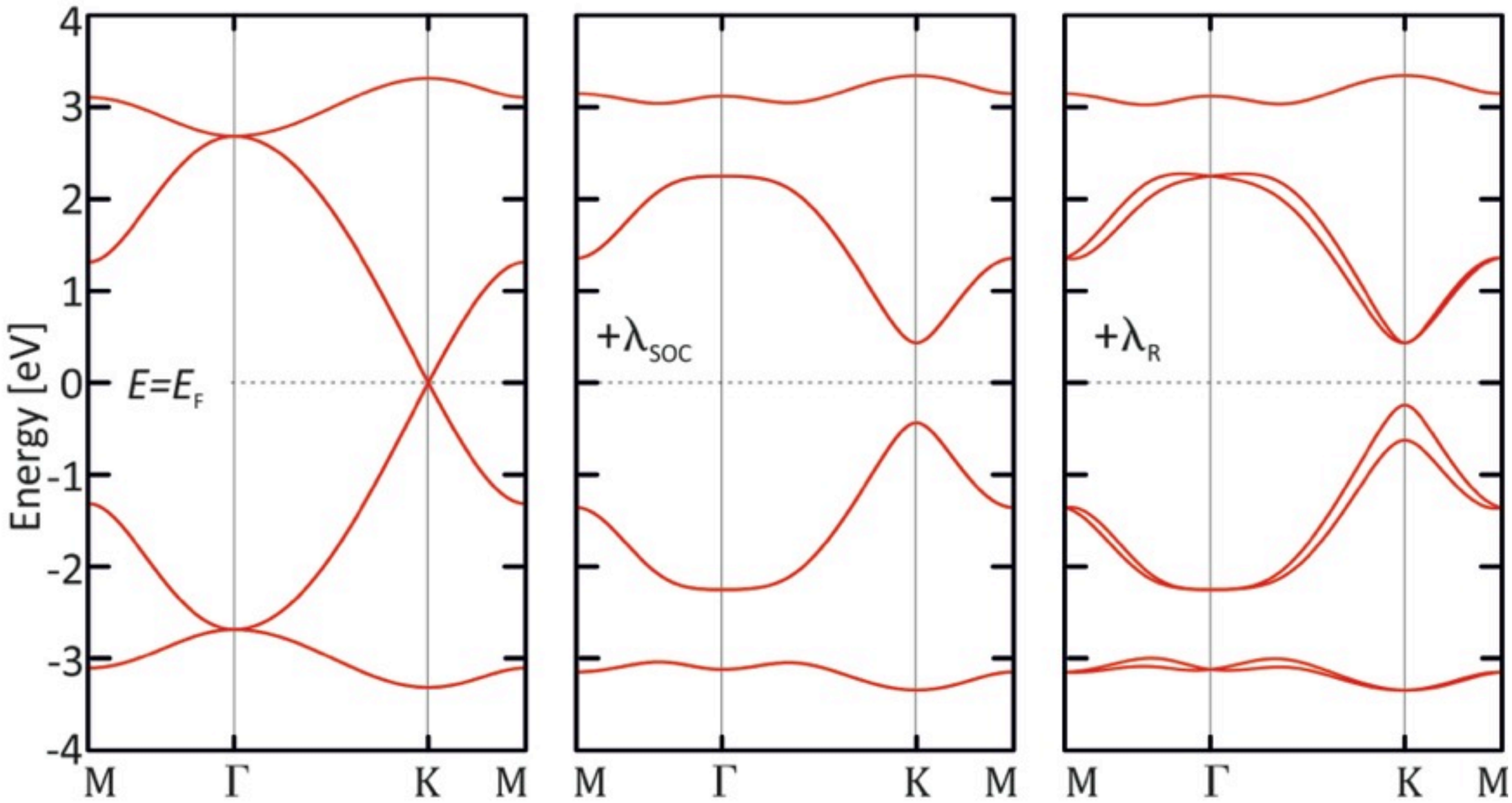
$$H^{\sigma\sigma}_{\text{eff}} = \begin{pmatrix} H^{\sigma\sigma}_{\uparrow\uparrow} & H^{\sigma\sigma}_{\uparrow\downarrow} \\ H^{\sigma\sigma}_{\downarrow\uparrow} & H^{\sigma\sigma}_{\downarrow\downarrow} \end{pmatrix}$$

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

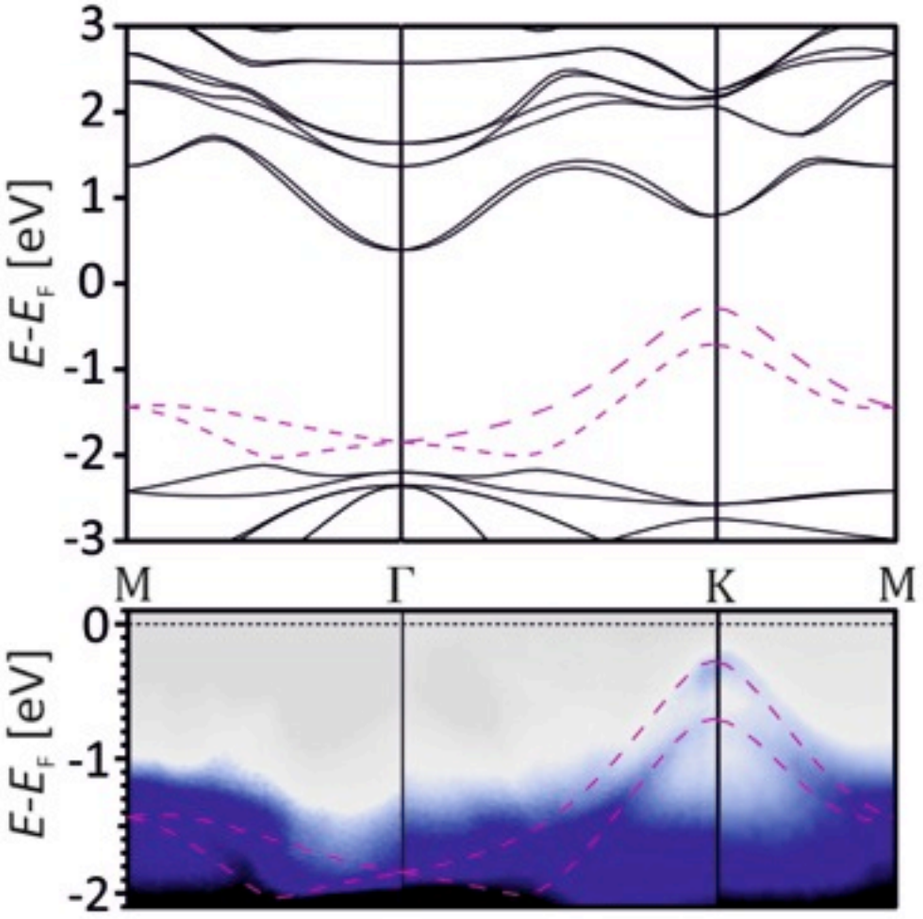
$$H^{\sigma\sigma}_{\uparrow\downarrow} = (H^{\sigma\sigma}_{\downarrow\uparrow})^\dagger = \lambda_{\text{R}} \begin{pmatrix} 0 & 0 & m_1 & m_2 \\ 0 & 0 & m_2 & m_3 \\ m_4 & m_5 & 0 & 0 \\ m_5 & m_6 & 0 & 0 \end{pmatrix}$$

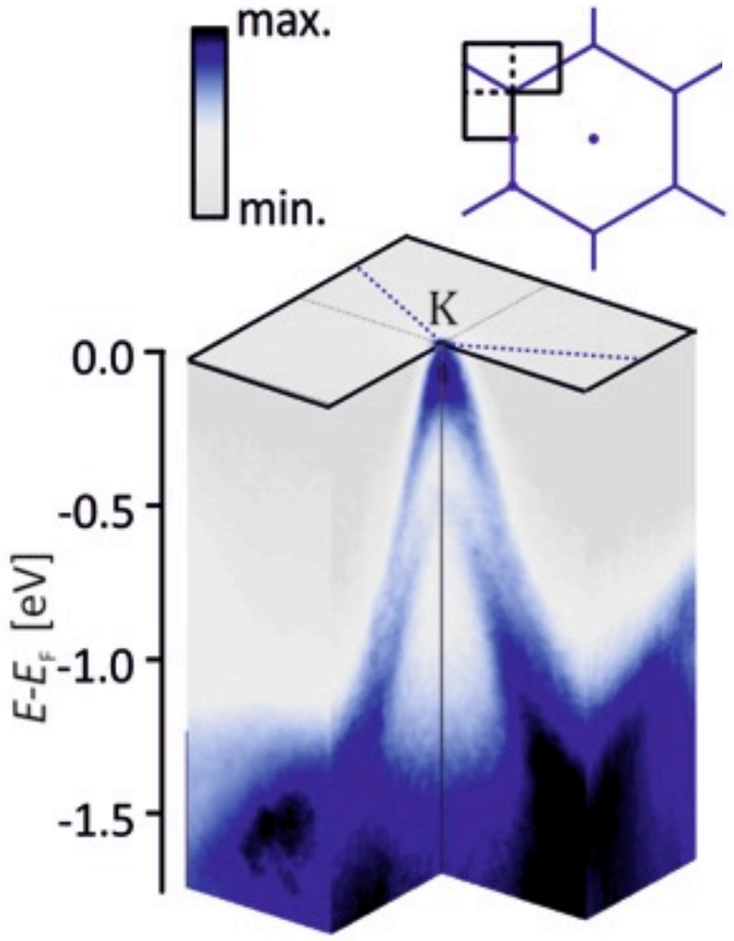
Effective model with SOC

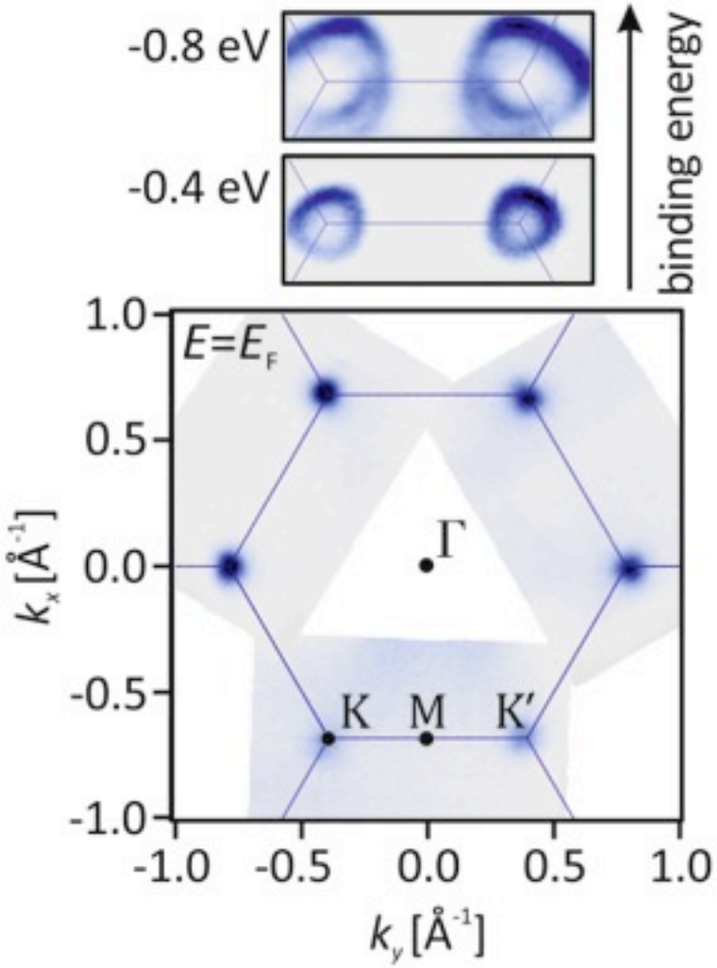
$$H_{\mathrm{eff}}^{\sigma\sigma} = H_0^{\sigma\sigma} + \lambda_{\mathrm{SOC}} H_{\mathrm{SOC}}^{\sigma\sigma} + \lambda_{\mathrm{R}} H_{\mathrm{R}}^{\sigma\sigma}$$



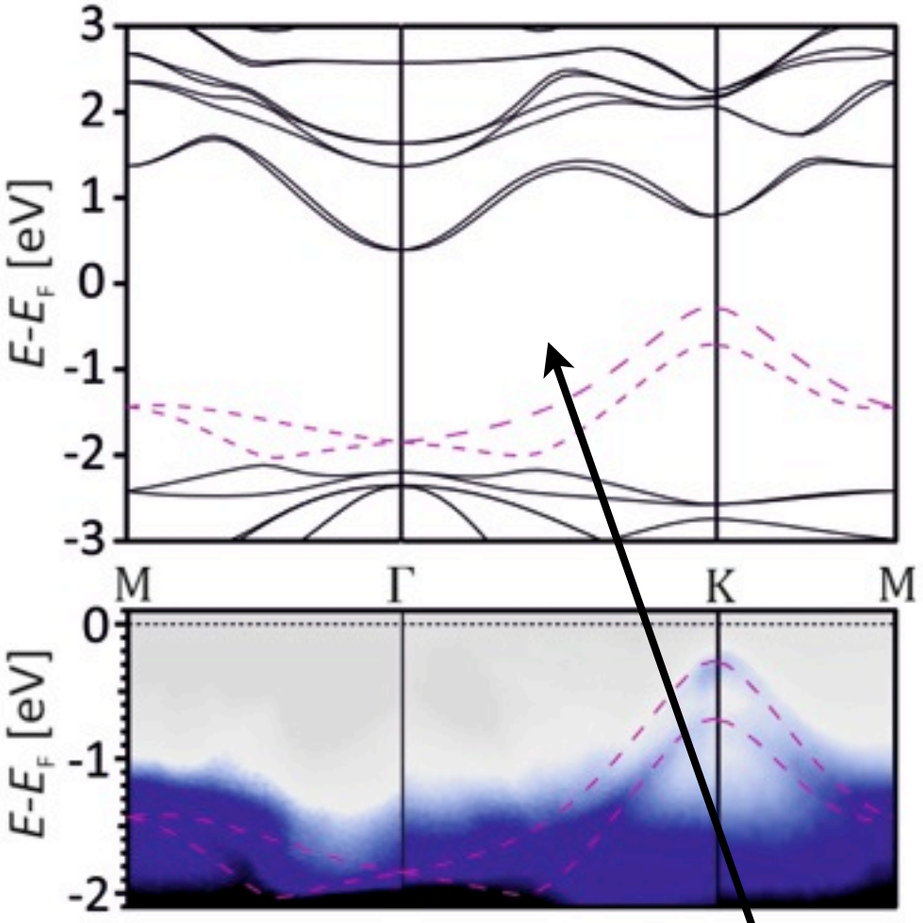
Theory vs. ARPES

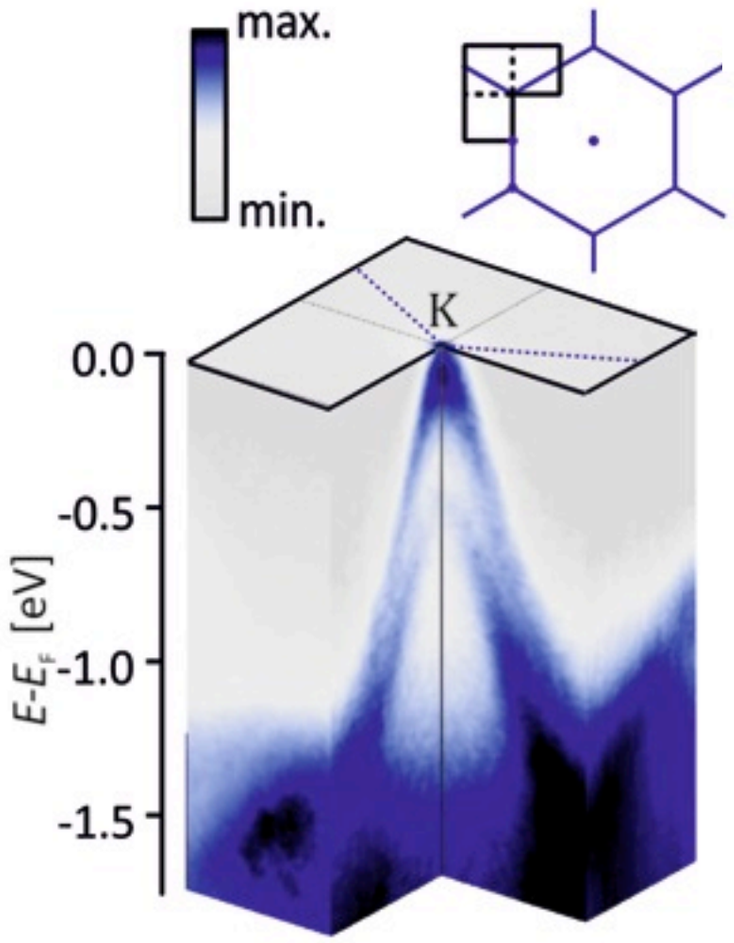


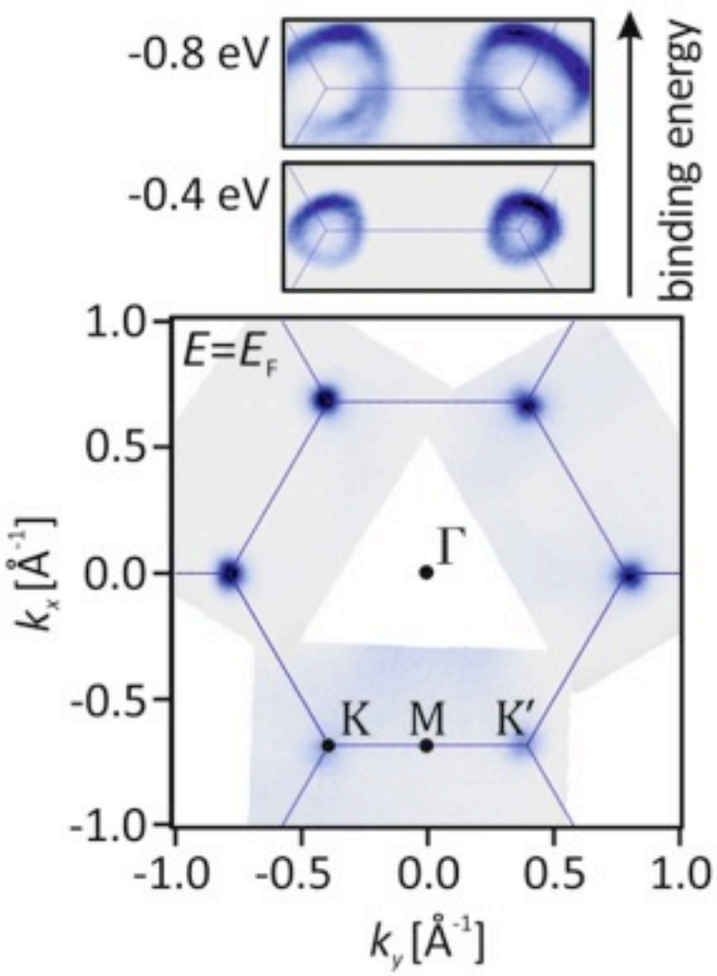




Theory vs. ARPES

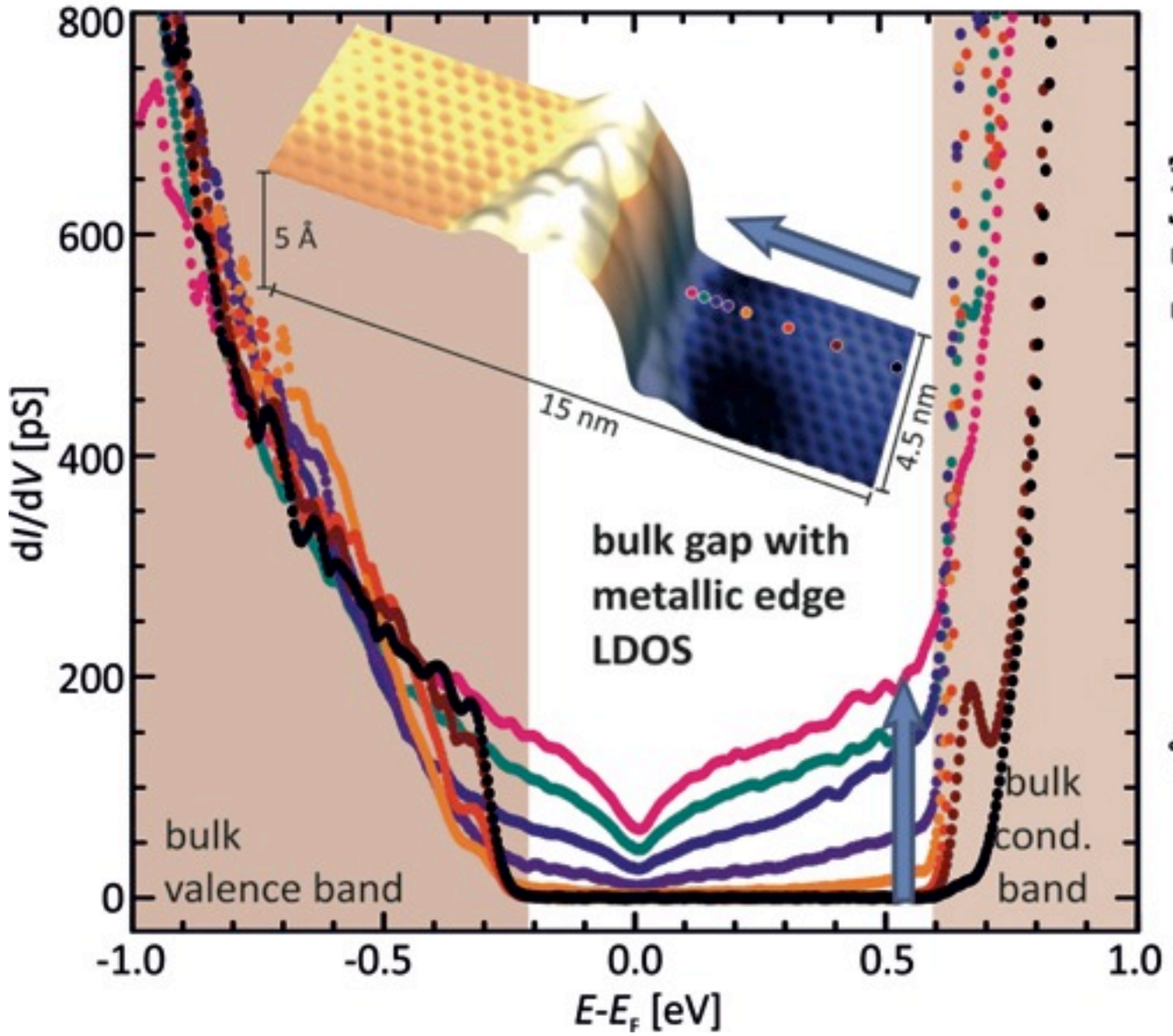


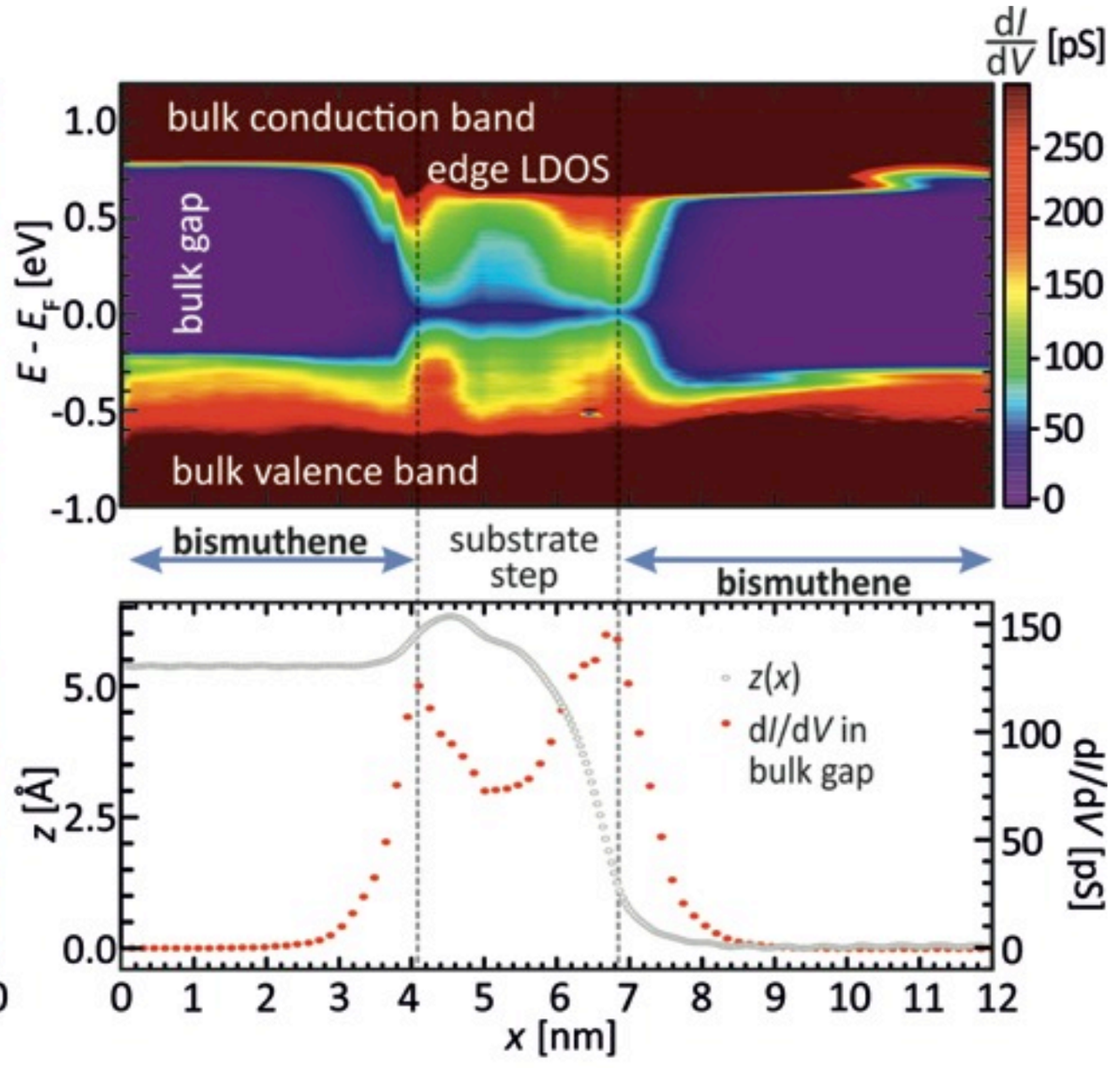




band gap: 0.67 eV!

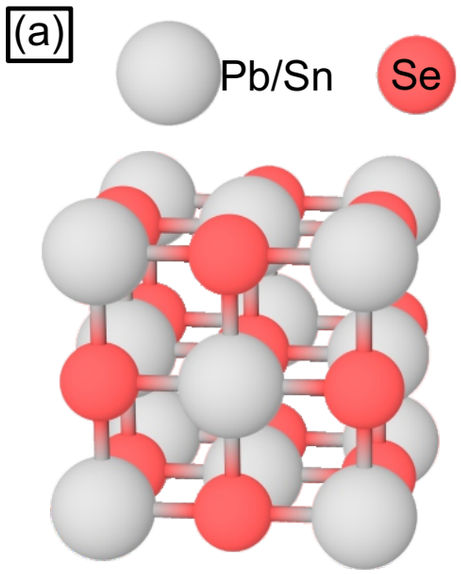
Local edge state spectroscopy

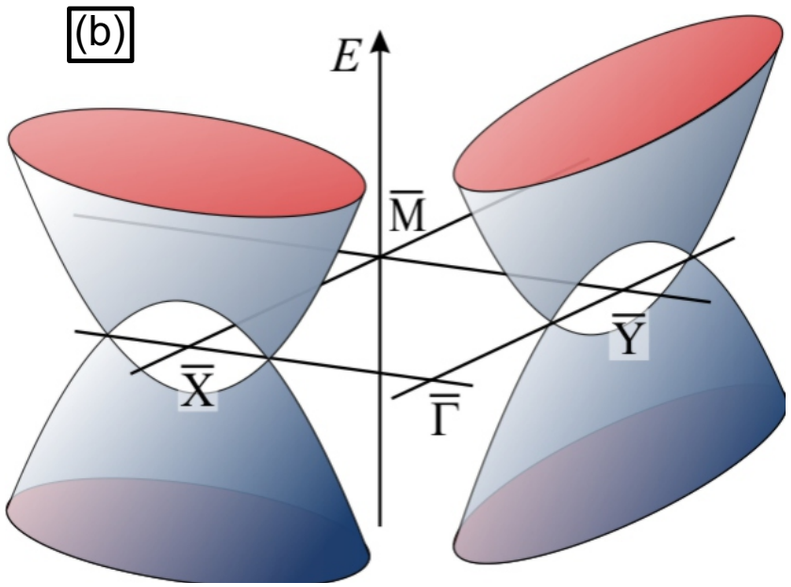


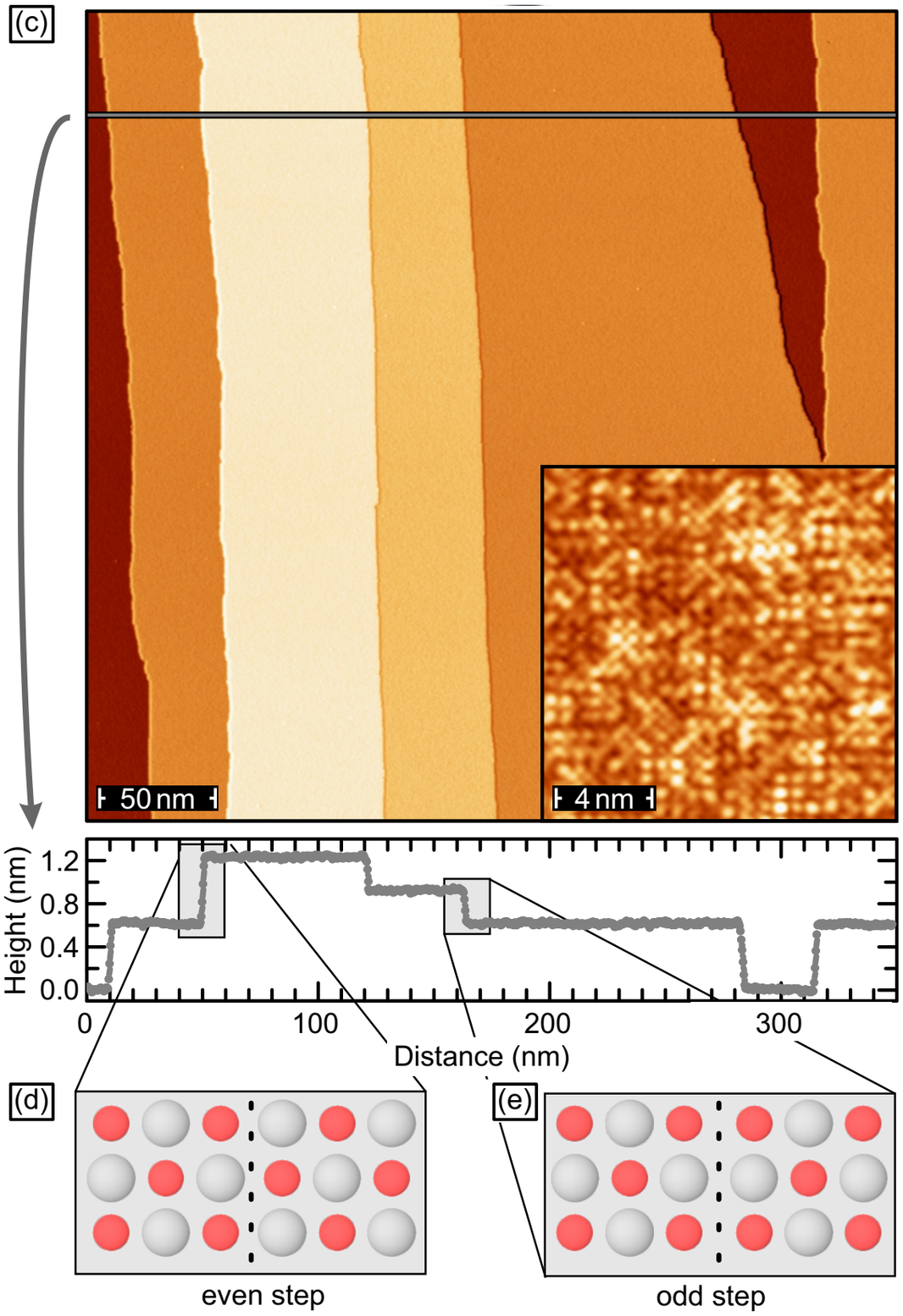


Midgap states at 1D TCI step edges: (Pb,Sn)Se

Step edges on topological crystalline insulators



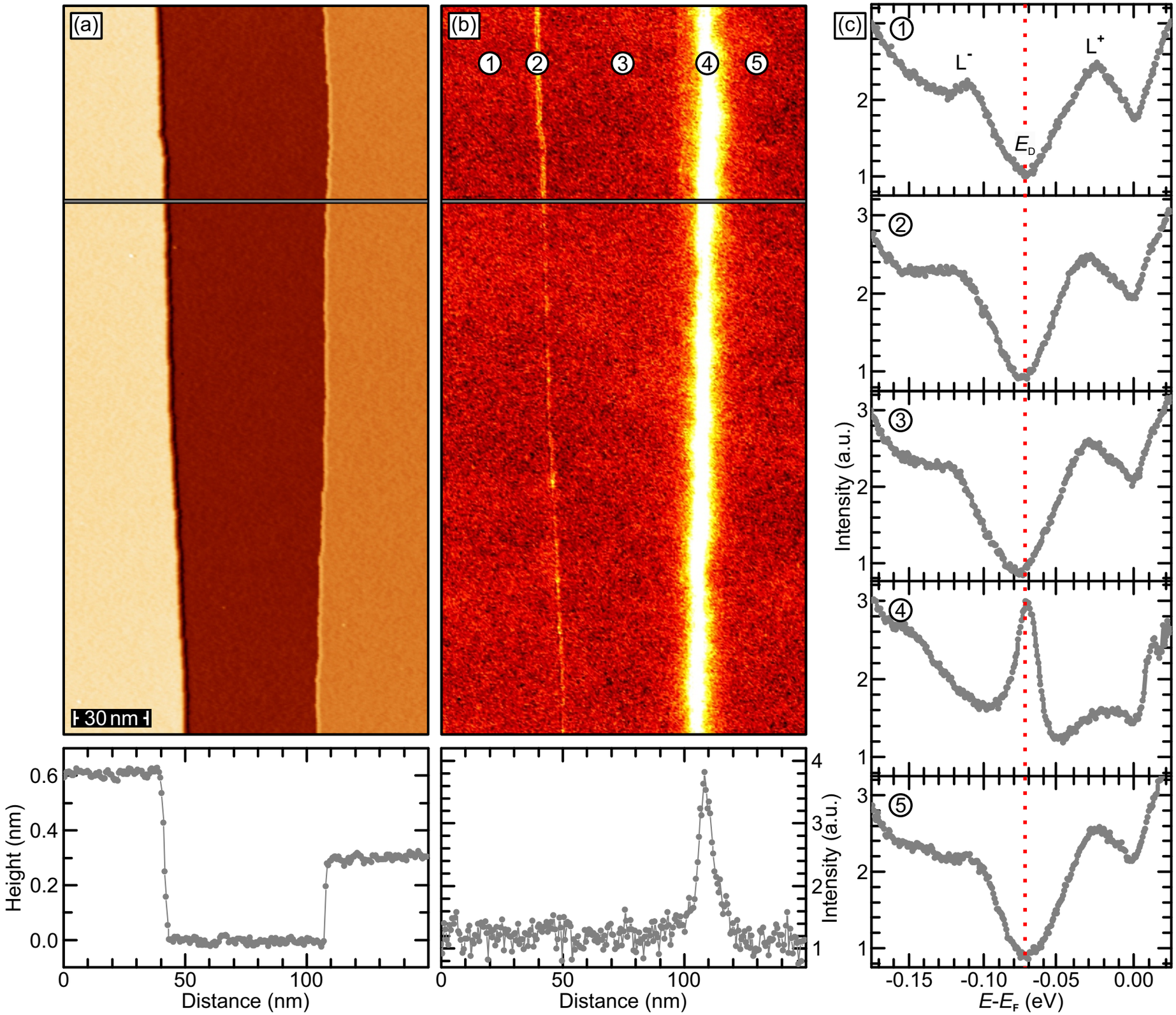




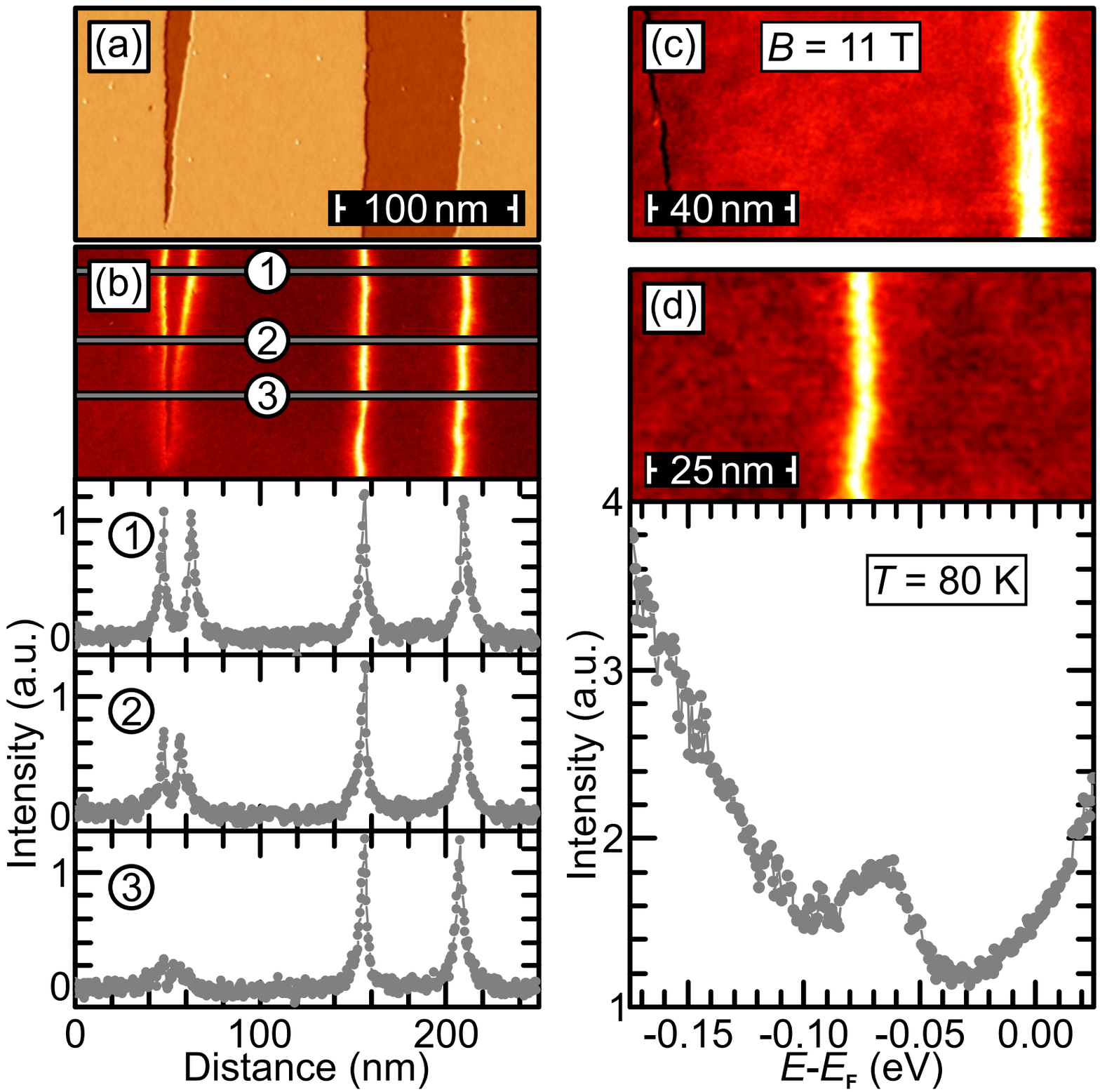
employ STM to analyze step edges on (Pb,Sn)Se surfaces

pick a (0,1) step edge orientation and distinguish even from odd steps

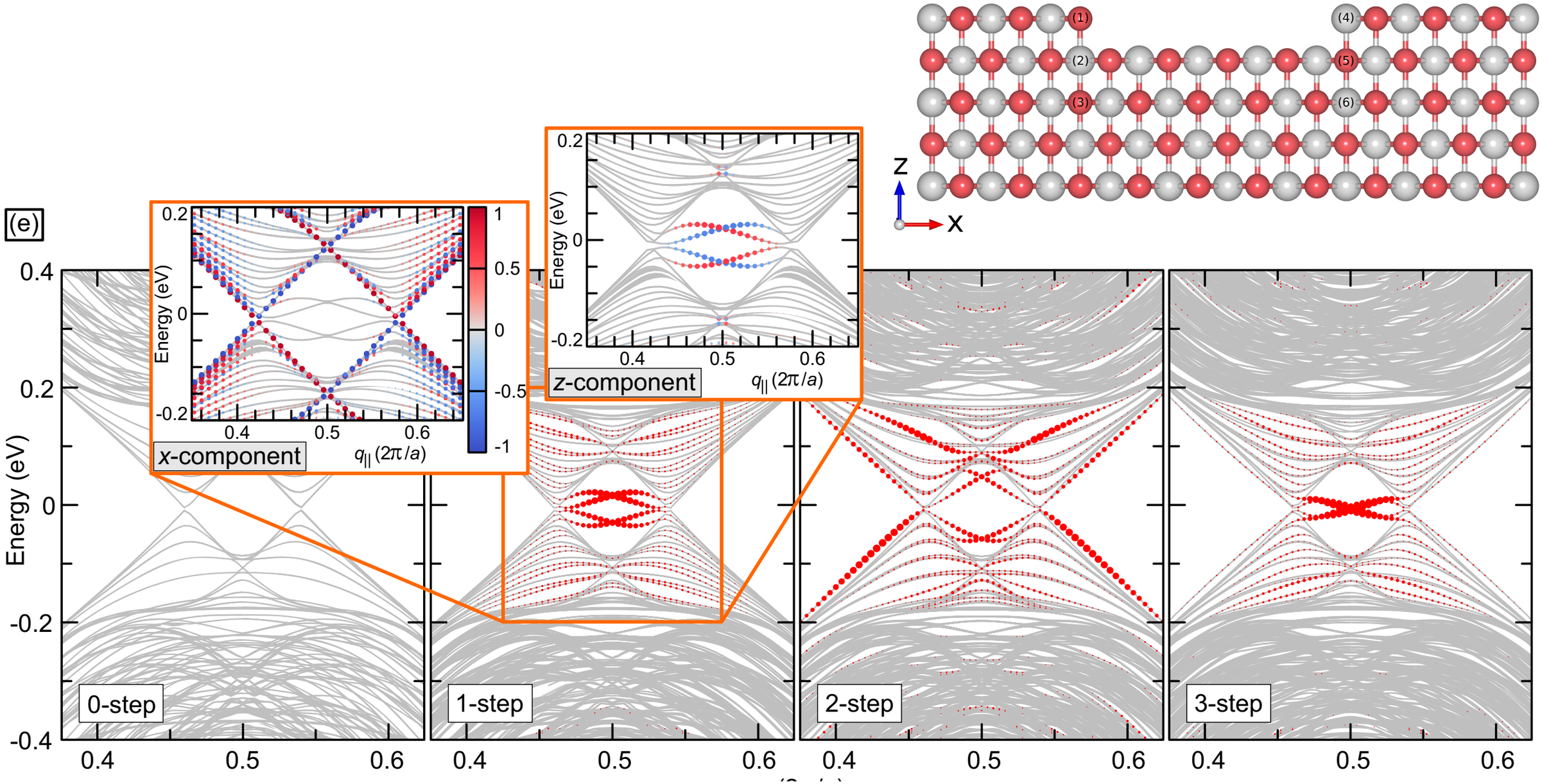
Large 1D DoS only at odd step widths!



Merging step edges



Atomistic approach: DFT



empirical confirmation: 1D DoS only at odd step edges

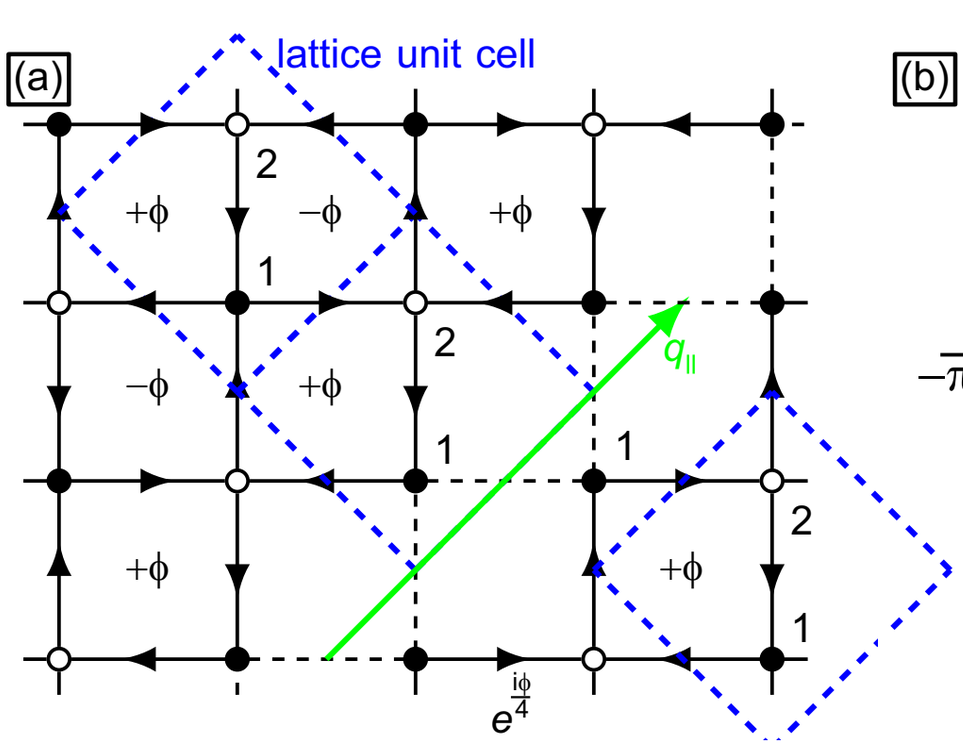
remainder dispersive features are likely to stem from finite size and equal sublattice hybridization

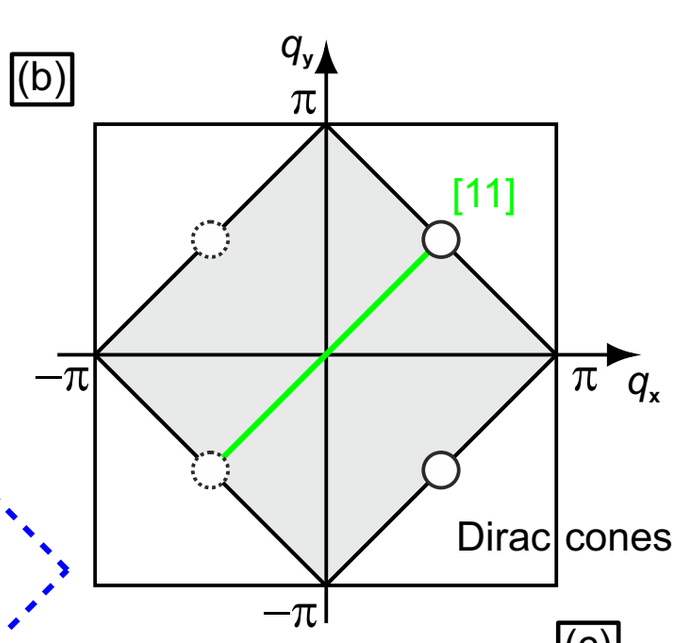
Microscopic explanation: toy model

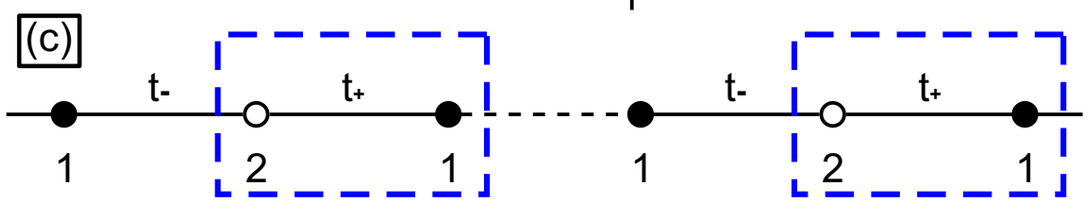
The phenomenon is related to a generalization of the Su-Schrieffer-Heeger model to two spatial bulk dimensions

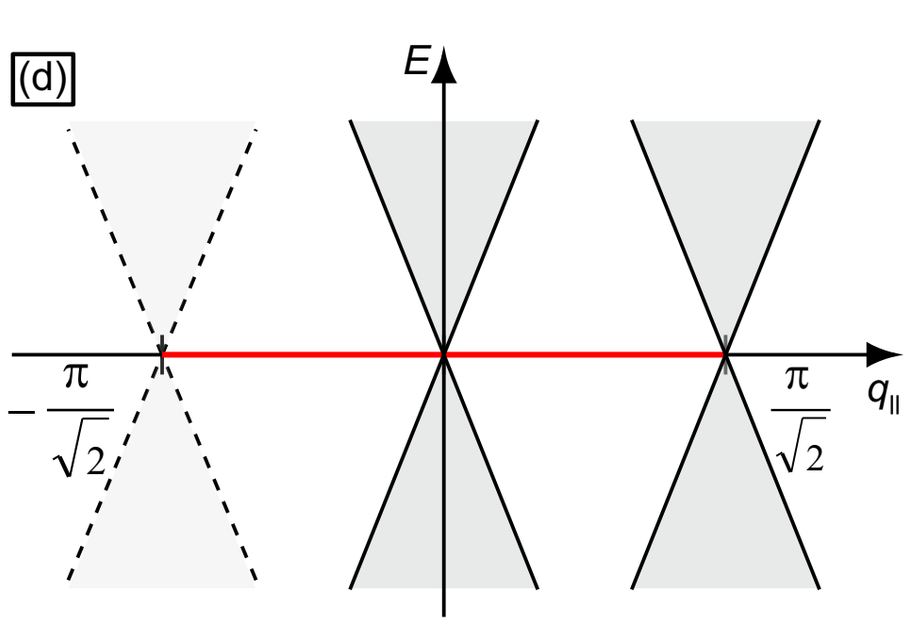
Minimal 2D toy model: staggered flux lattice features 1D SSH midgap states

Details matter: Chirality of dirac cones, edge projection etc.

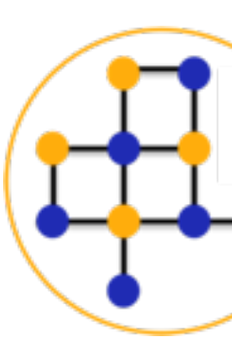








Research team and references



F. Reis et al., *Bismuthene on an SiC Substrate: A Candidate for a New High-Temperature Quantum Spin-Hall Paradigm*, arXiv:1608.00812, under review.

P. Sessi et al., *Robust spin-polarized midgap states at step edges of topological crystalline insulators*, to appear in Science.