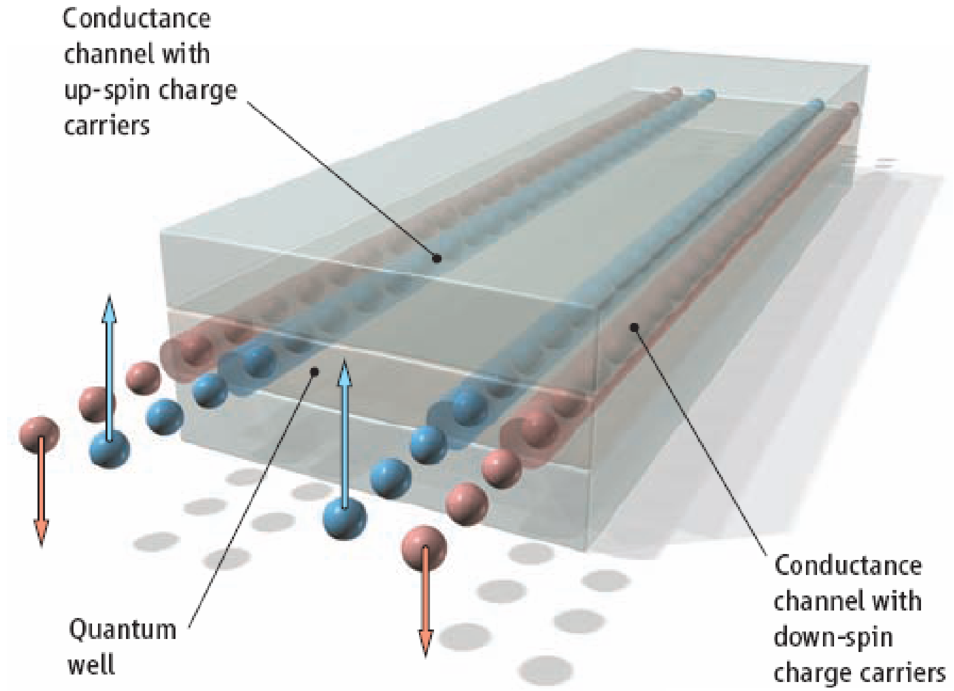
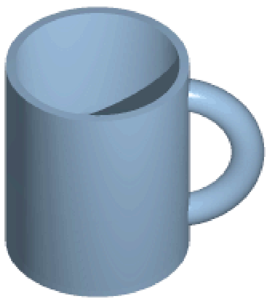
Interacting topological insulators





KITP 2011

Shoucheng Zhang, Stanford University

Colloborators

Stanford group: Xiaoliang Qi, Andrei Bernevig, Congjun Wu, Chaoxing Liu, Taylor Hughes, Sri Raghu, Suk-bum Chung, Joseph Maciejko, Haijun Zhang, Xiao Zhang

Stanford experimentalists: Yulin Chen, Ian Fisher, ZX Shen, Yi Cui, Aharon Kapitulnik, Goldhaber-Gordon...

Wuerzburg colleagues: Laurens Molenkamp, Hartmut Buhmann, Markus Koenig Ewelina Hankiewicz, Bjoern Trauzettle

Tsinghua colleagues: Qikun Xue, Jinfeng Jia, Xi Chen, Bangfen Zhu...

IOP colleagues: Zhong Fang, Xi Dai, ...

Mainz colleagues: Claudia Felser, Juergen Koebler, Stas Chadov,

Overview

Brief introduction

Topological field theory of interacting topological insulators

general definition, topological Mott insulator, fractional TI

Quantized anomalous Hall effect

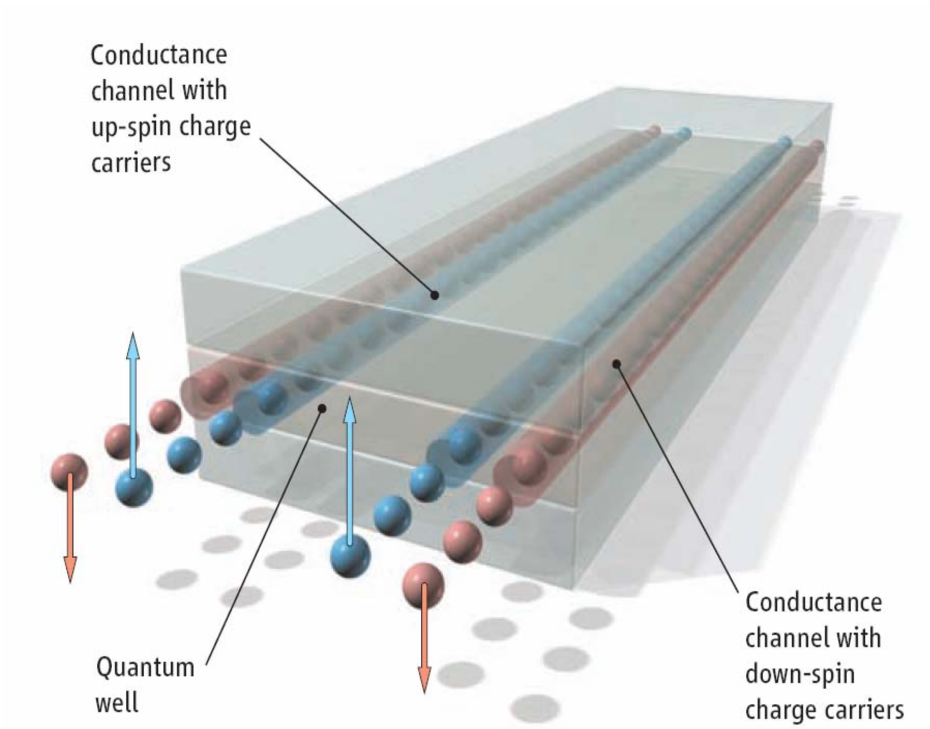
materials candidates

A new class of interacting TIs

binary compound, simple crystal structure, single Dirac cone, insulating bulk!

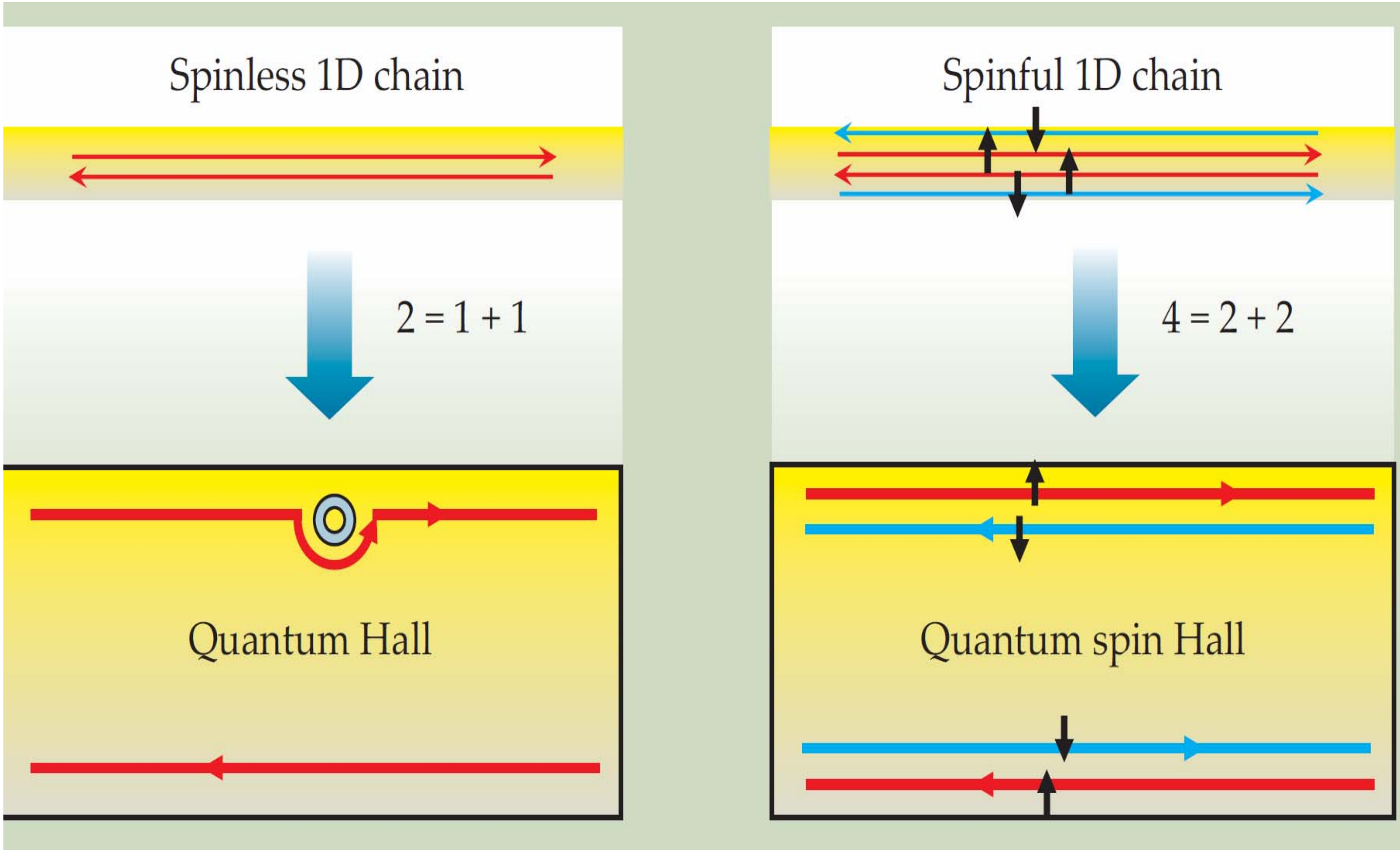
Discovery of the 2D and 3D topological insulator materials

HgTe Theory: Bernevig, Hughes and Zhang, Science **314**, 1757 (2006)
Experiment: Koenig et al, Science **318**, 766 (2007)
BiSb Theory: Fu and Kane, PRB **76**, 045302 (2007)
Experiment: Hsieh et al, Nature **452**, 907 (2008)
Bi2Te3, Sb2Te3, Bi2Se3 Theory: Zhang et al, Nature Physics **5**, 438 (2009)
Bi2Se3 Experiment: Xia et al, Nature Physics **5**, 398 (2009),
Experiment Bi2Te3: Chen et al Science **325**, 178 (2009), Kapitulnik et al
One of the most active fields in CMP!



Schematic of the spin-polarized edge channels in a quantum spin Hall insulator.

Quantum Hall effect and quantum spin Hall effect



HgTe, InAs/GaSb

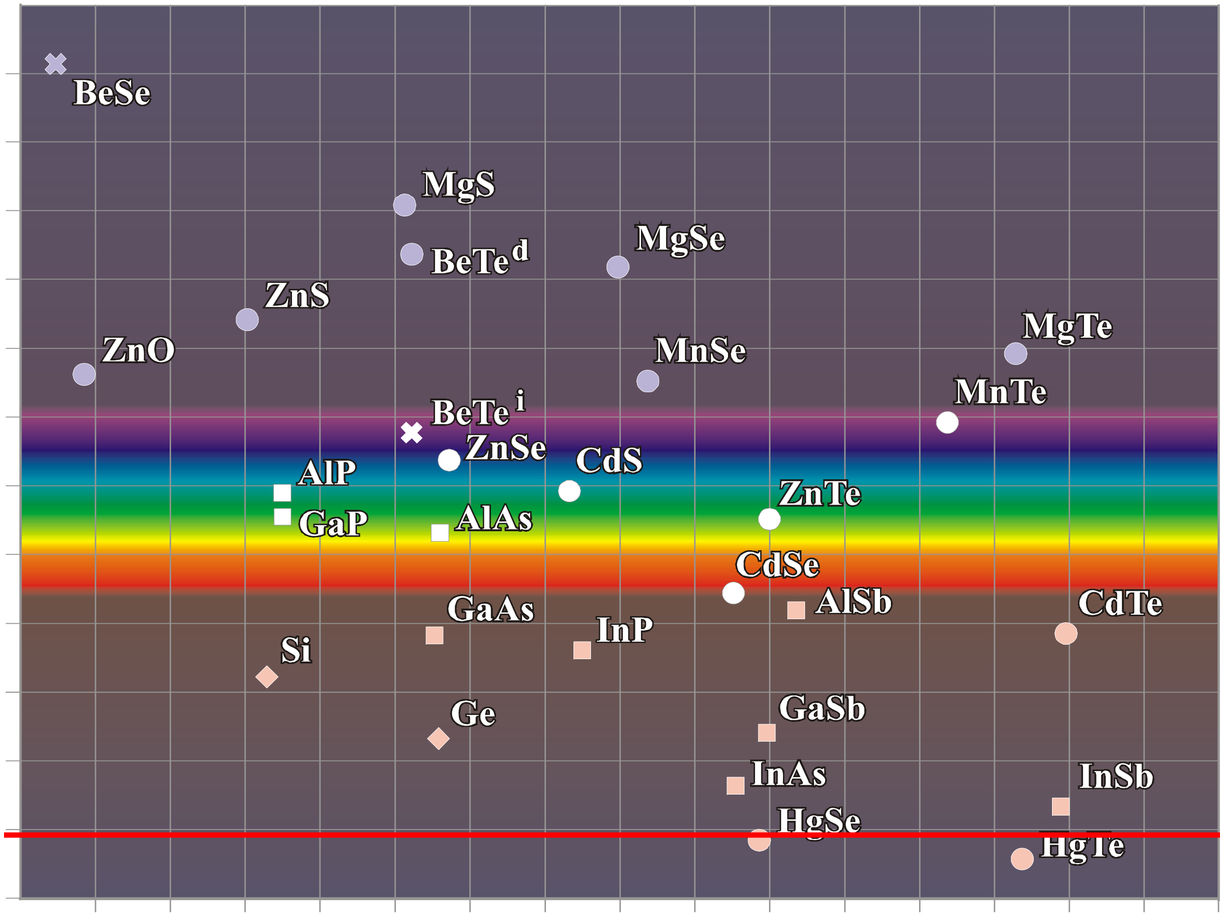
From traffic jam to info-superhighway on chip

Traffic jam inside chips today

Info highways for the chips in the future

Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells

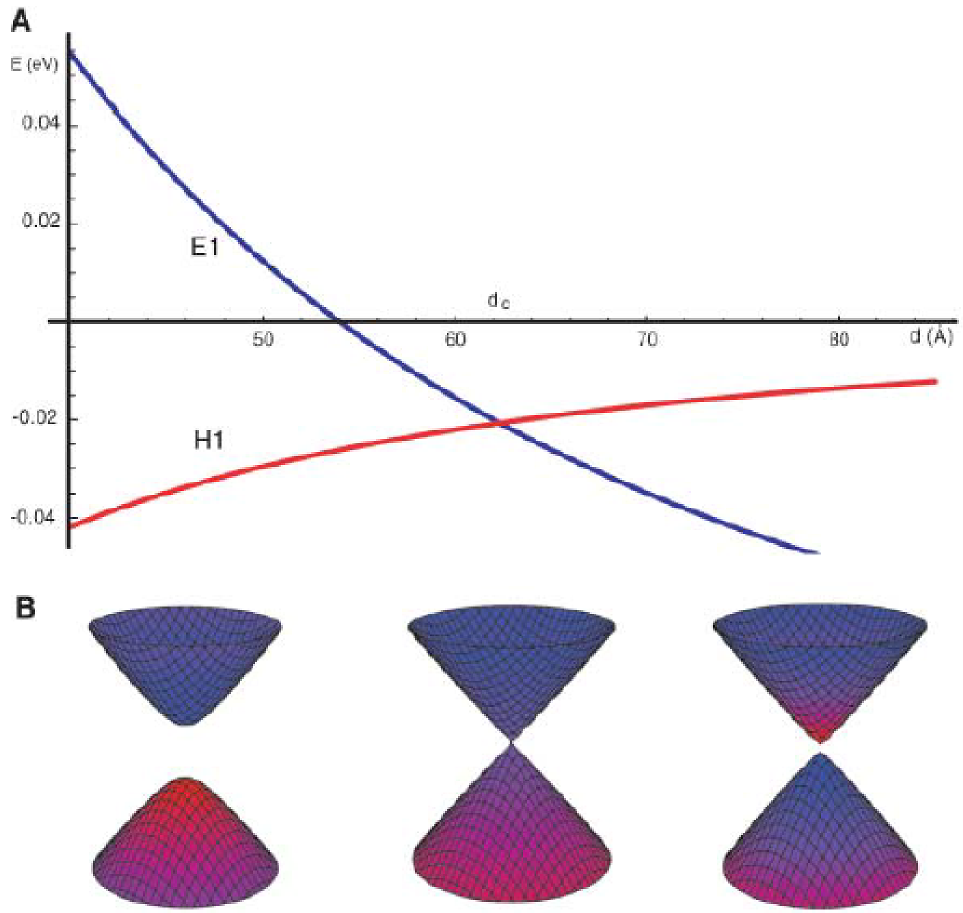
B. Andrei Bernevig,[1,2] Taylor L. Hughes,[1] Shou-Cheng Zhang[1]*



Thanks to many fruitful discussions with Wurzburg colleagues

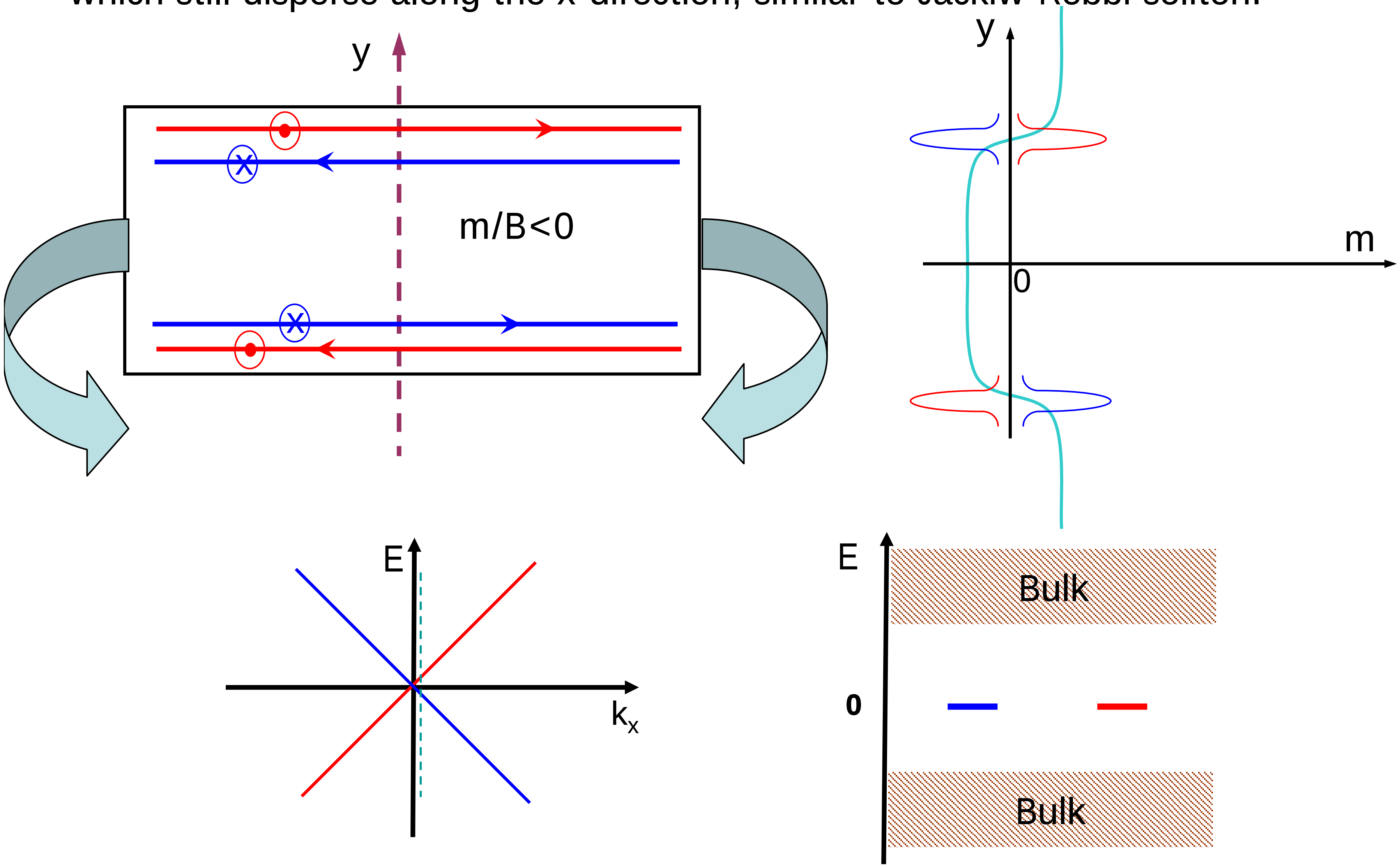
Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells

B. Andrei Bernevig,[1,2] Taylor L. Hughes,[1] Shou-Cheng Zhang[1]*



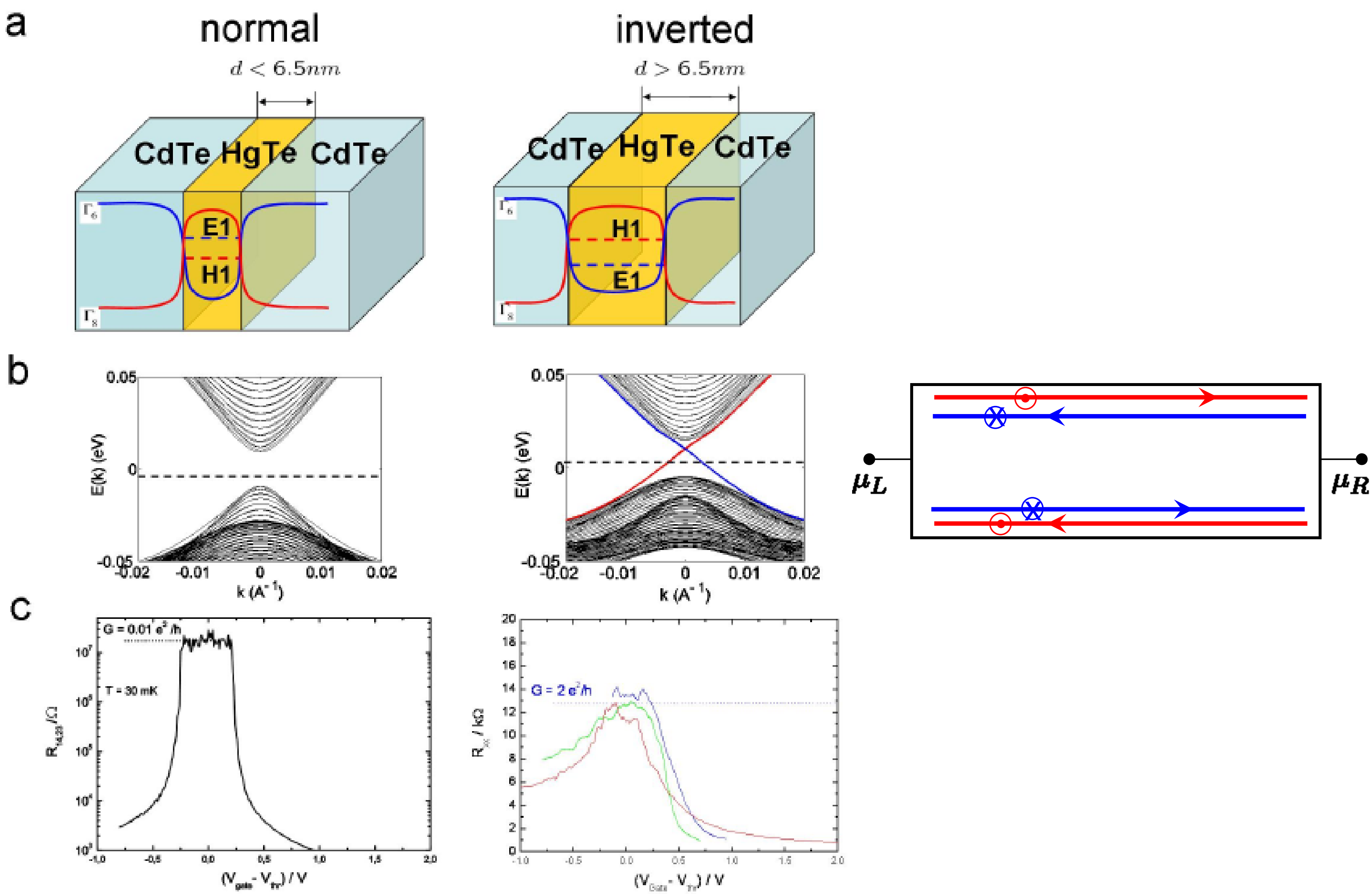
Mass domain wall

Cutting the Hall bar along the y-direction we see a domain-wall structure in the band structure mass term. This leads to states localized on the domain wall which still disperse along the x-direction, similar to Jackiw-Rebbi soliton.



Experimental observation of the QSH edge state

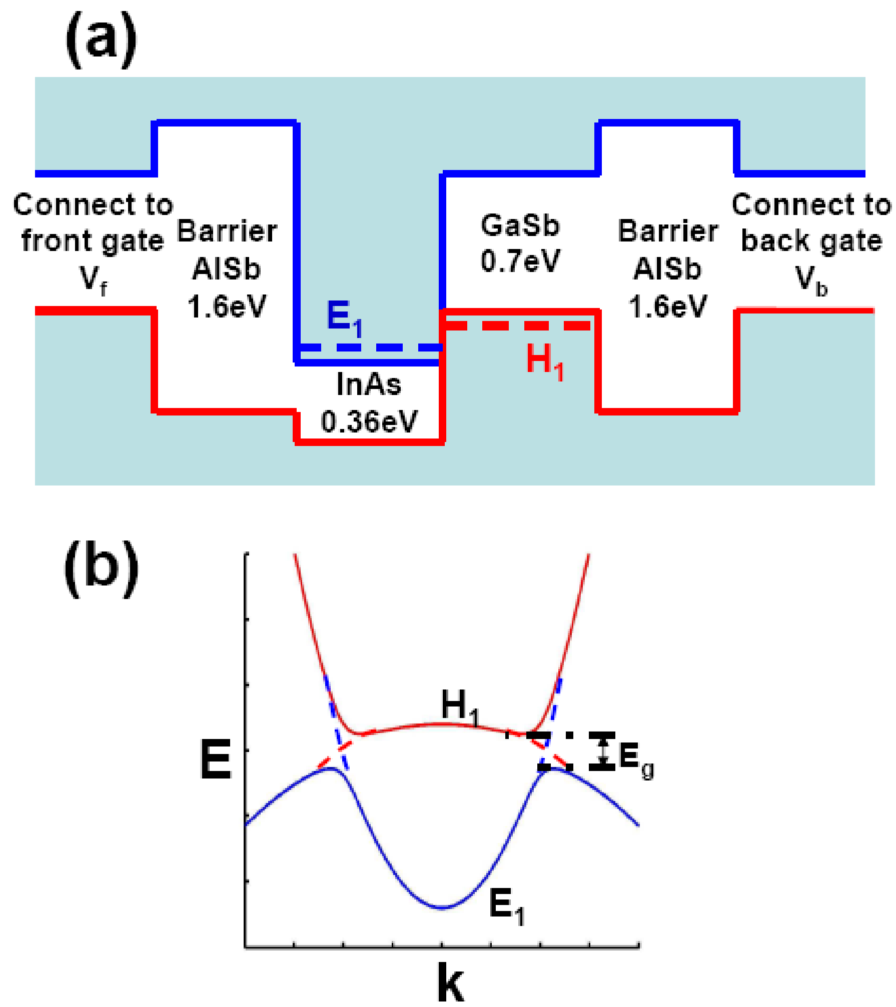
(Konig et al, Science 2007)



QSH state in InAs/GaSb type II quantum wells

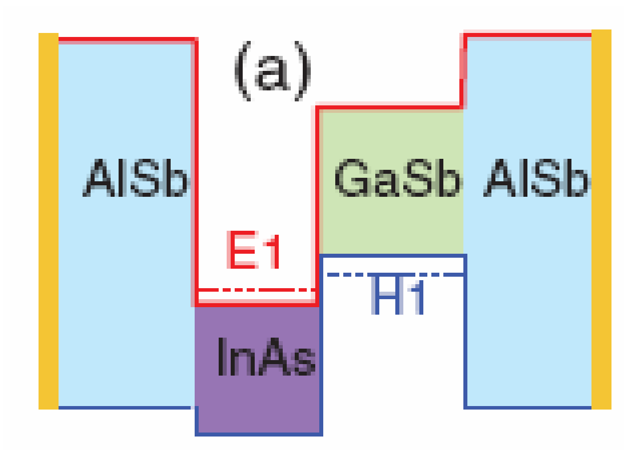
(theoretically predicted by Liu et al PRL 100, 236601 (2008), Zhang group)

- In HgTe, the band inversion occurs intrinsically in the material. However, in InAs/GaSb quantum wells, a similar inversion can occur, since the valance band edge of GaSb lies above the conduction band edge of InAs.
- A small hybridazation gap opens up due to tunneling at the interface.
- Theoretical work show that the QSH can occur in InAs/Gab quantum wells. This material can be fabricated commercially in many places around the world.
- InAs can also be used for superconducting proximity effect.

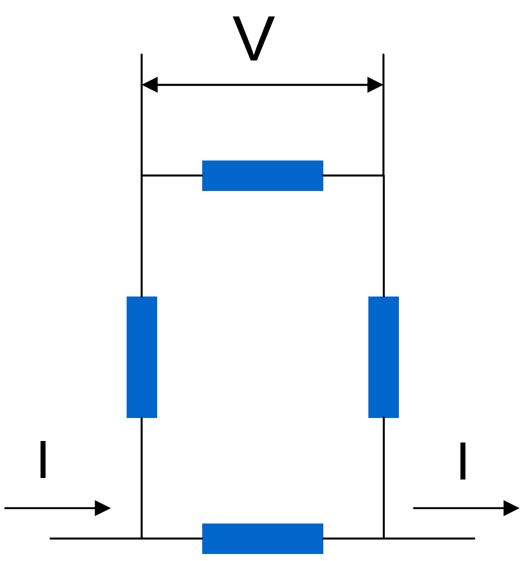


Experiment in InAs/GaSb QWs

- Difficulty: small band gap, (~4meV) and large residual bulk carriers even in the insulating regime.
- Experimental setup:



I. Knez, et al, PRL 107, 136603 (2011)



$R=h/4e^2$

Experiment in InAs/GaSb QWs

- The sample size dependencies of the bulk and edge resistance are different

Bulk contribution $$G_{bulk} = \frac{W}{L}\sigma$$

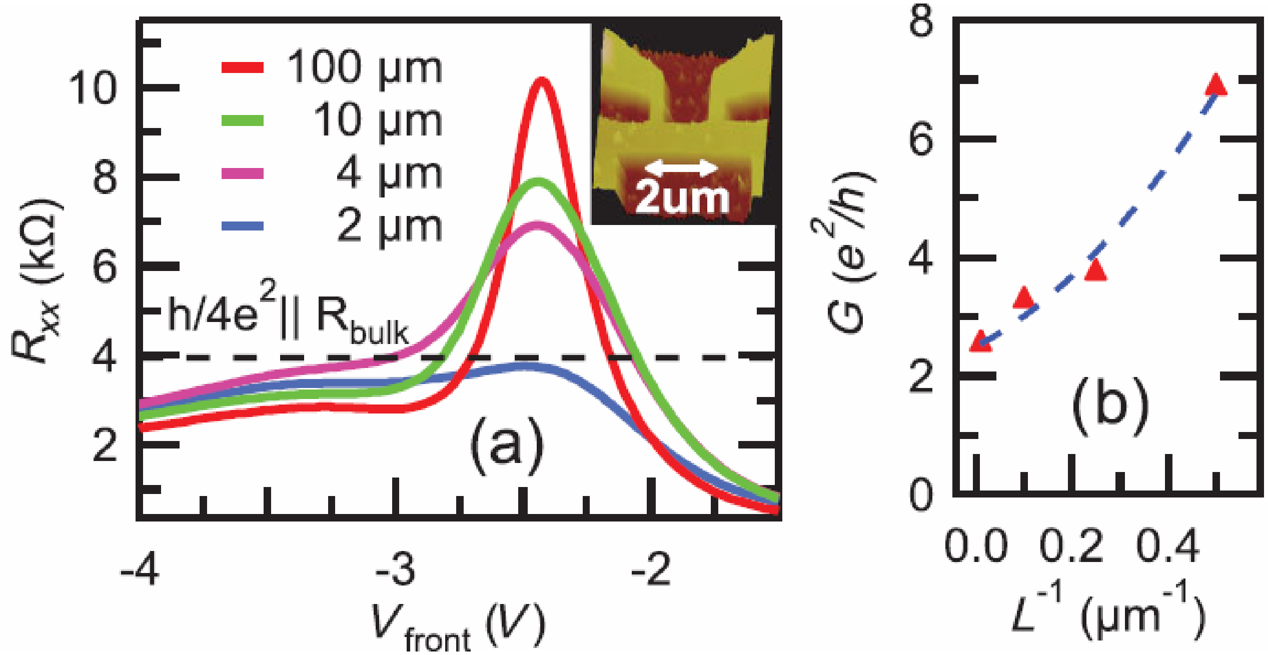
Edge contribution $$G_{edge} = \frac{4e^2}{h}\frac{l_\phi}{L}$$

I. Knez, et al, PRL 107, 136603 (2011), Rui Du group

Size dependence

- Fix W/L, so that bulk contribution is fixed. When L is large, edge contribution is negligible.

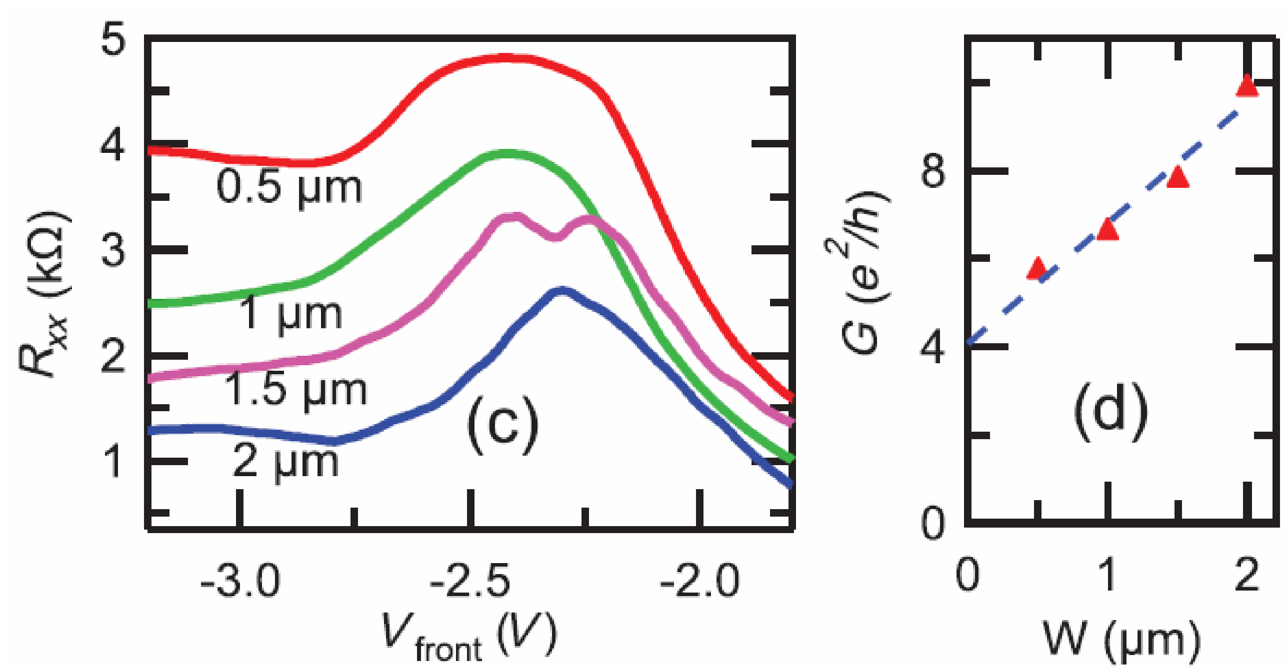
$$G_{bulk} = \frac{W}{L}\sigma \qquad G_{edge} = \frac{4e^2}{h}\frac{l_\phi}{L}$$



I. Knez, et al, PRL 107, 136603 (2011)

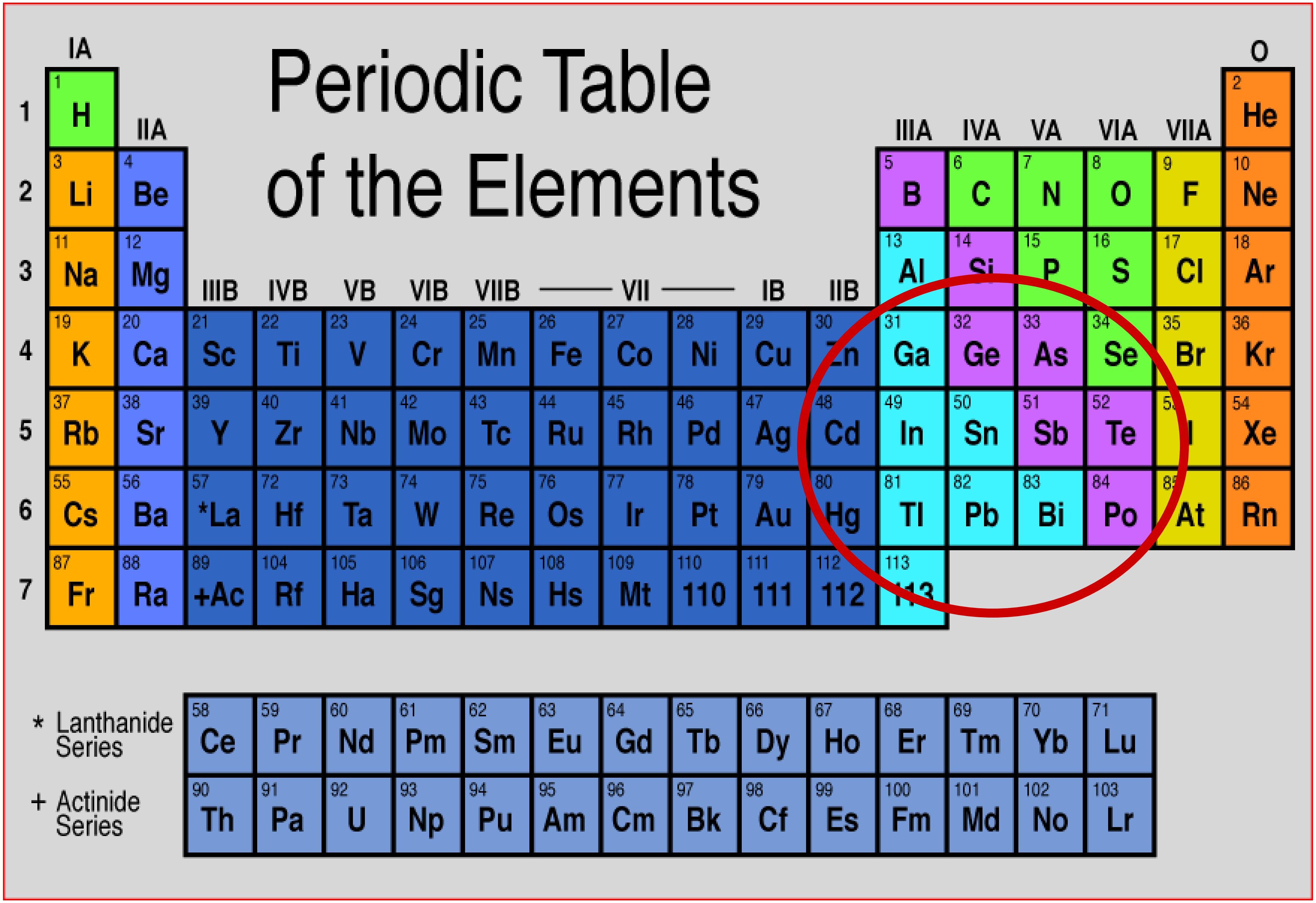
Size dependence

- Fix L, so that edge contribution is fixed. When W is small, bulk contribution is negligible. $G_{bulk} = \frac{W}{L}\sigma$ $G_{edge} = \frac{4e^2}{h}\frac{l_\phi}{L}$

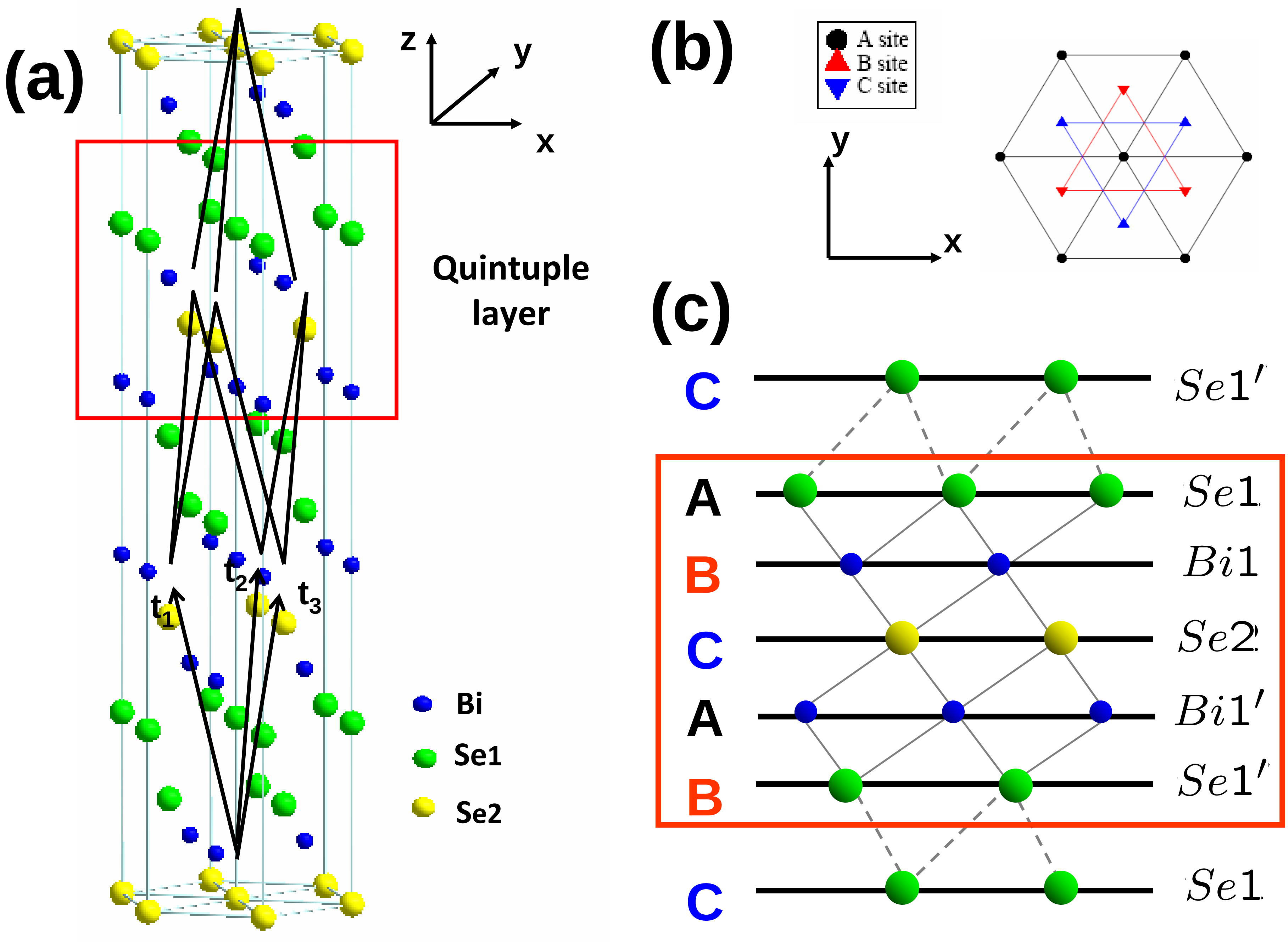


I. Knez, et al, PRL 107, 136603 (2011)

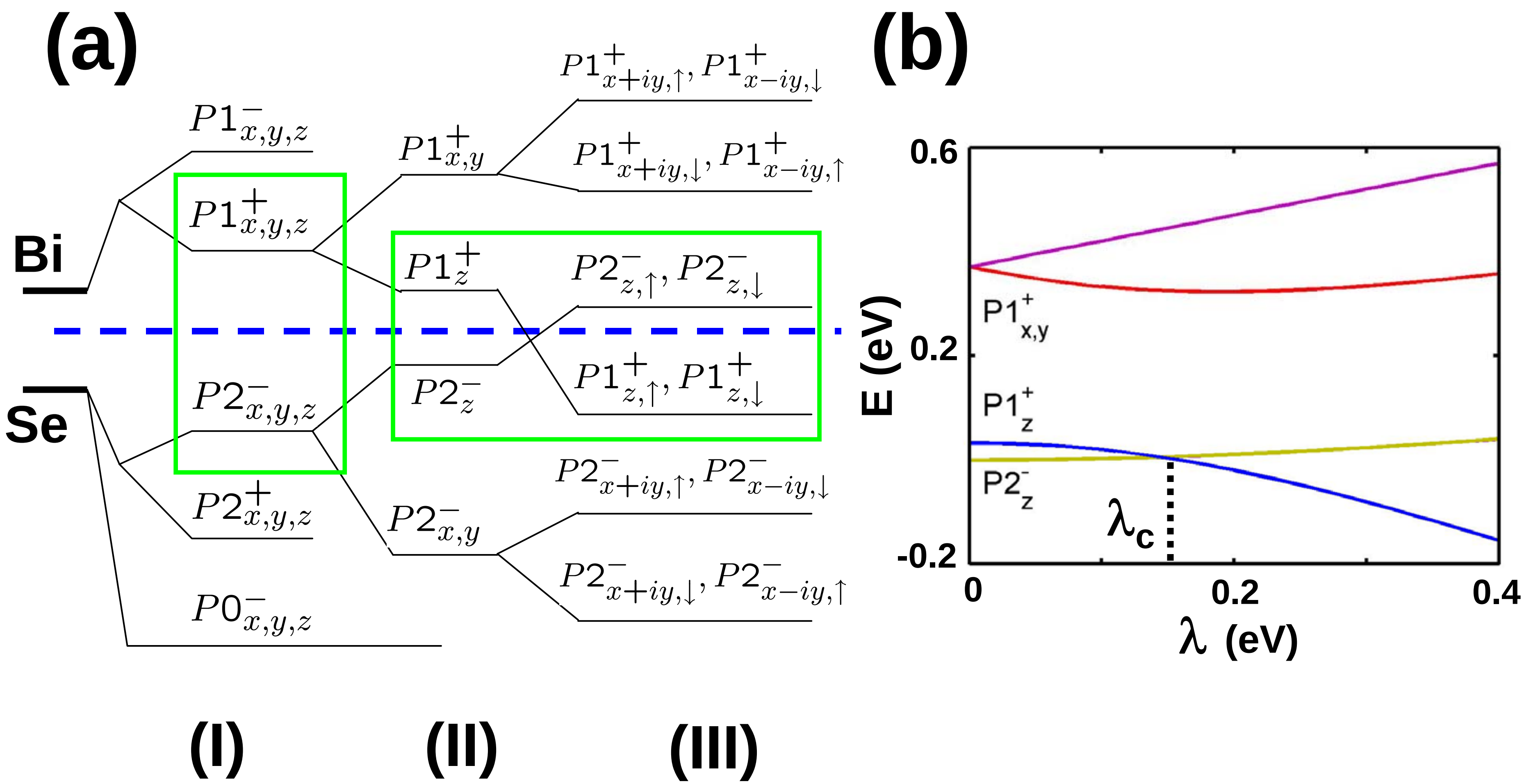
3D topological insulators



3D insulators with a single Dirac cone on the surface

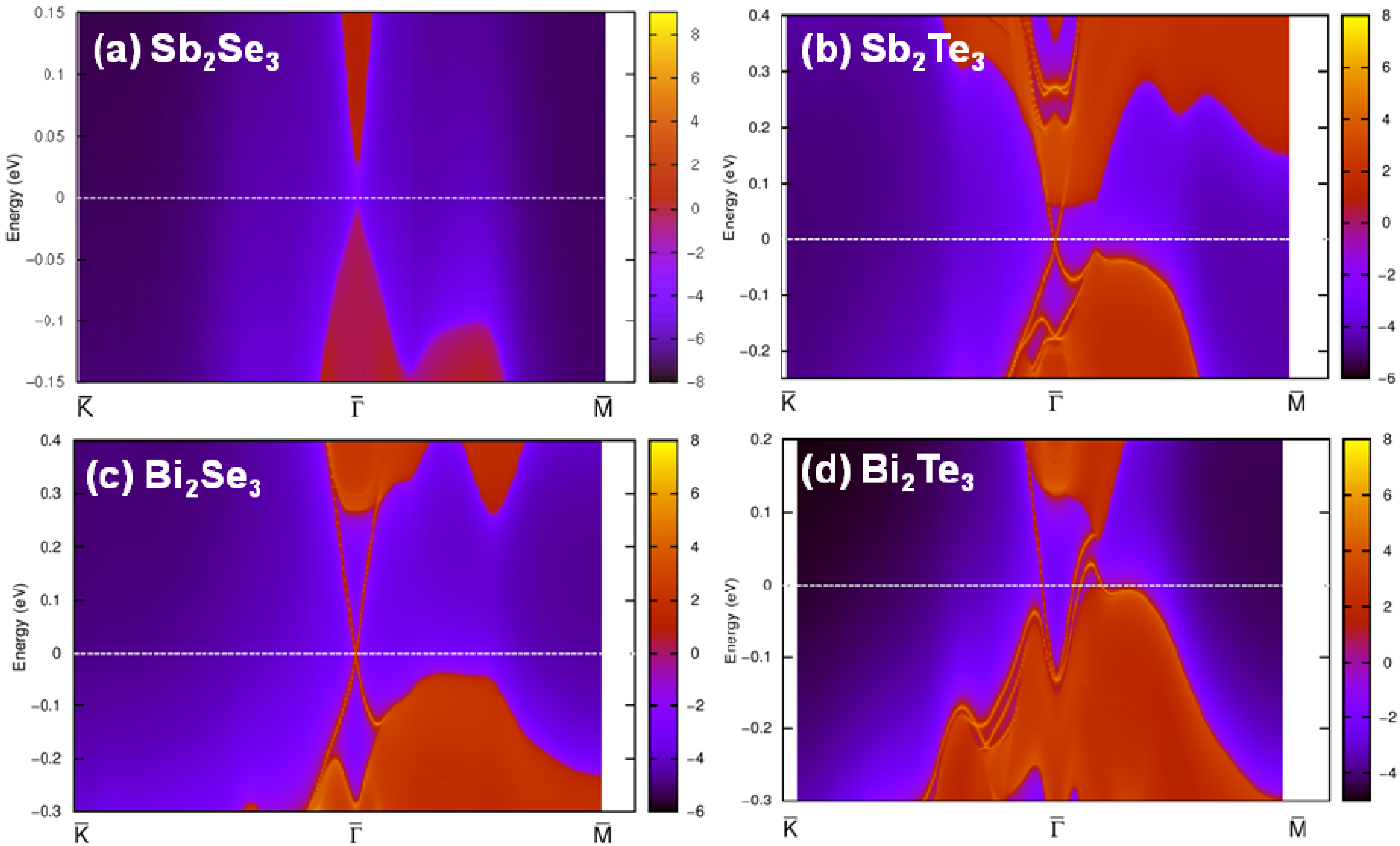


Relevant orbitals of Bi2Se3 and the band inversion

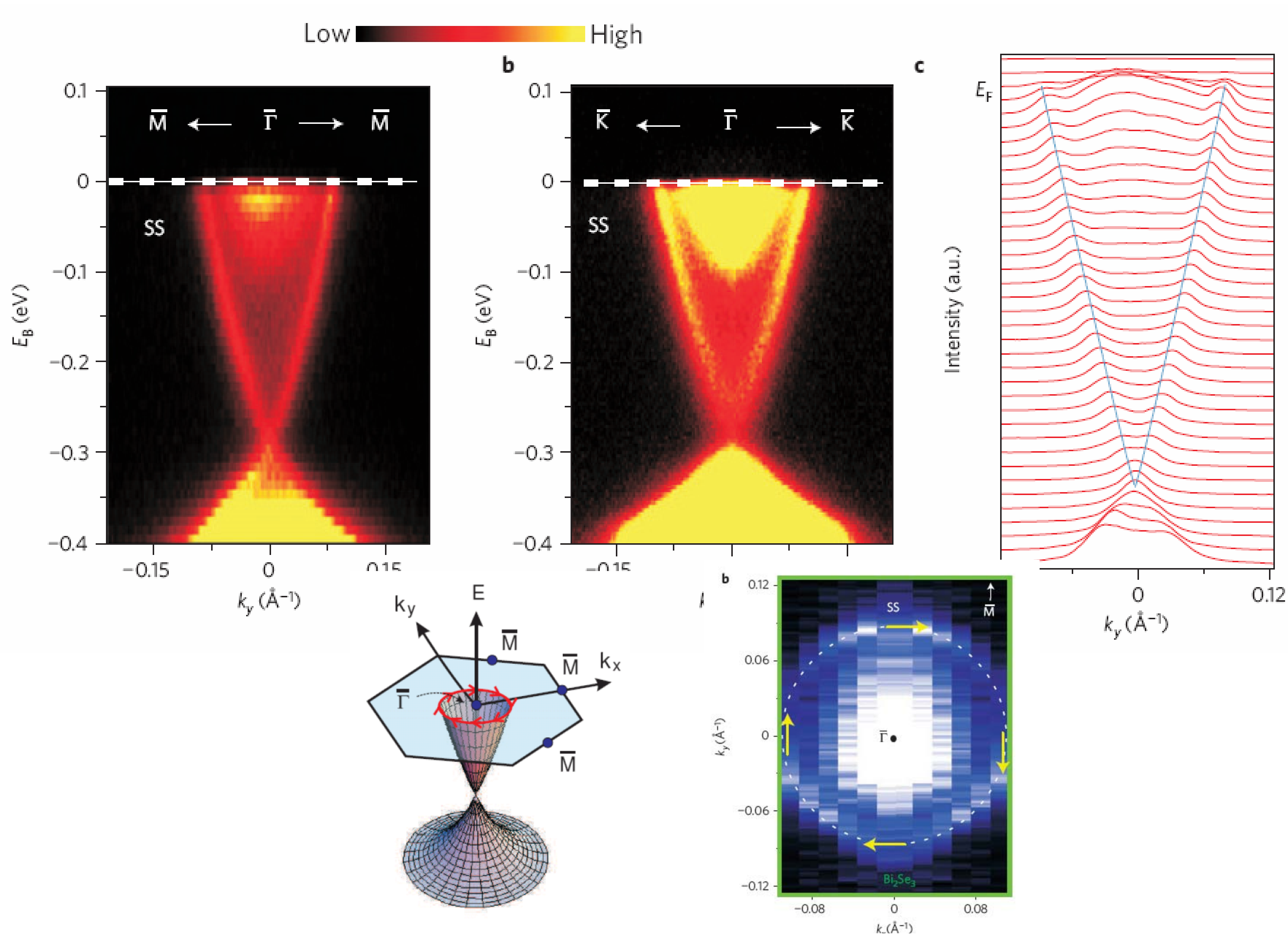


Topological insulators in Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3 with a single Dirac cone on the surface

Haijun Zhang[1], Chao-Xing Liu[2], Xiao-Liang Qi[3], Xi Dai[1], Zhong Fang[1] and Shou-Cheng Zhang[3]*

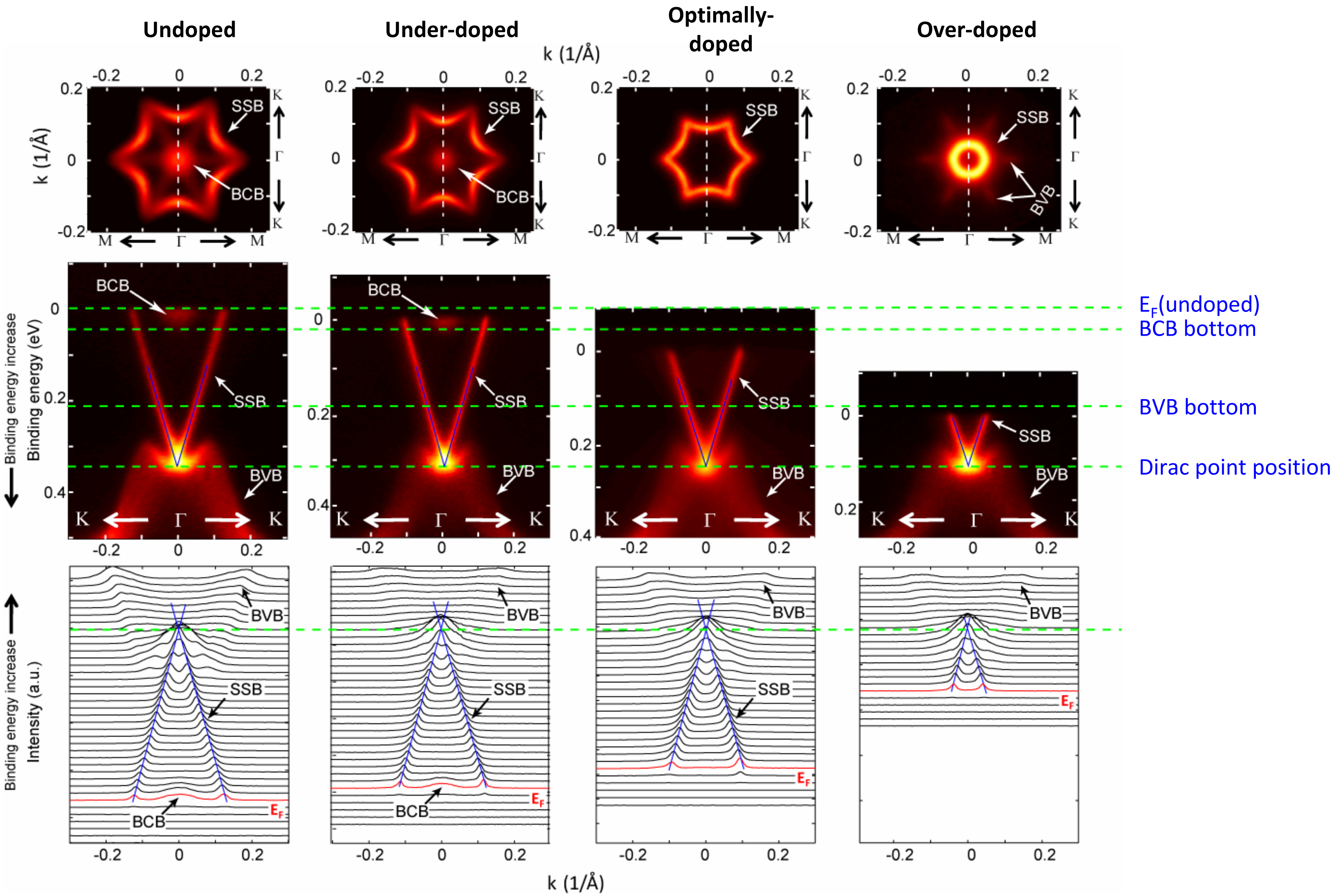


Arpes experiment&theory on Bi2Se3 surface states,
Hasan group

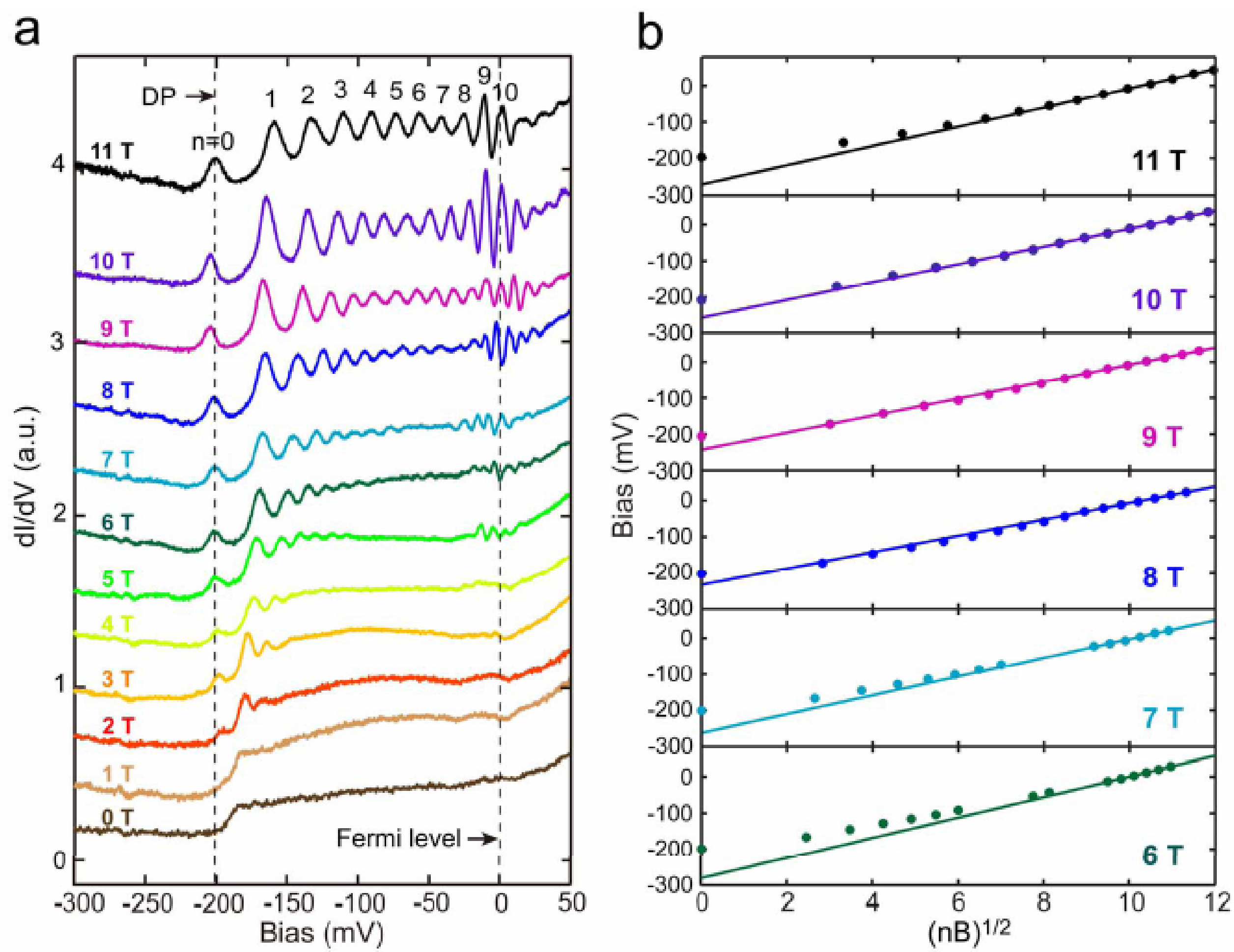


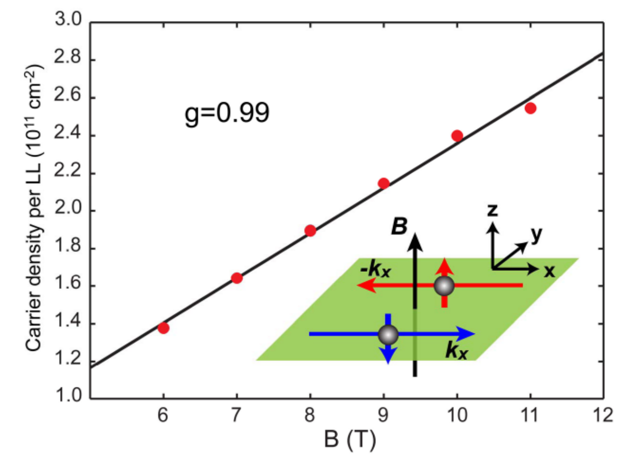
Arpes experiment on Bi2Te3 surface states, Shen group

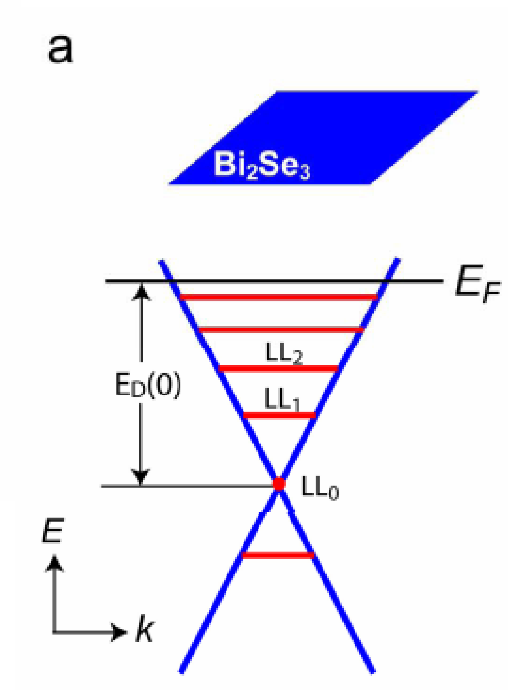
Doping evolution of the FS and band structure



Surface Landau levels, Xue group, Hanaguri group







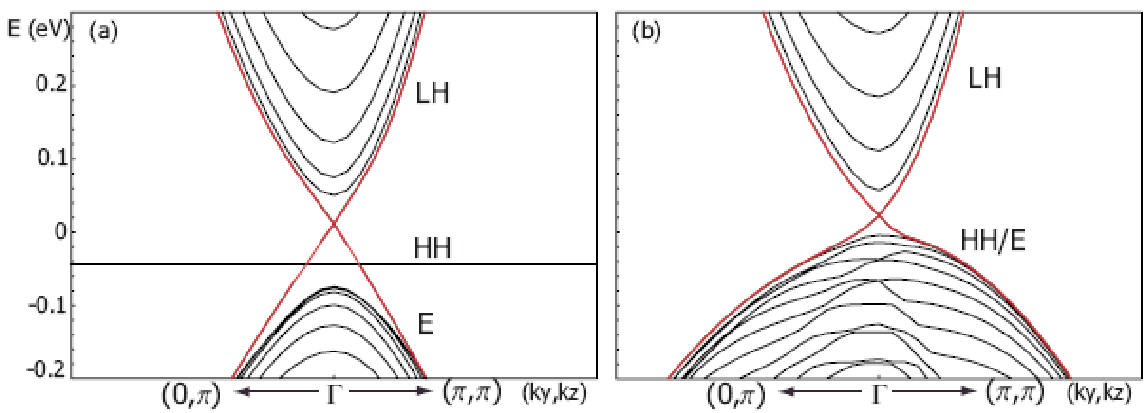
Clean 3D Topological Insulator HgTe

PHYSICAL REVIEW B **77**, 125319 (2008)

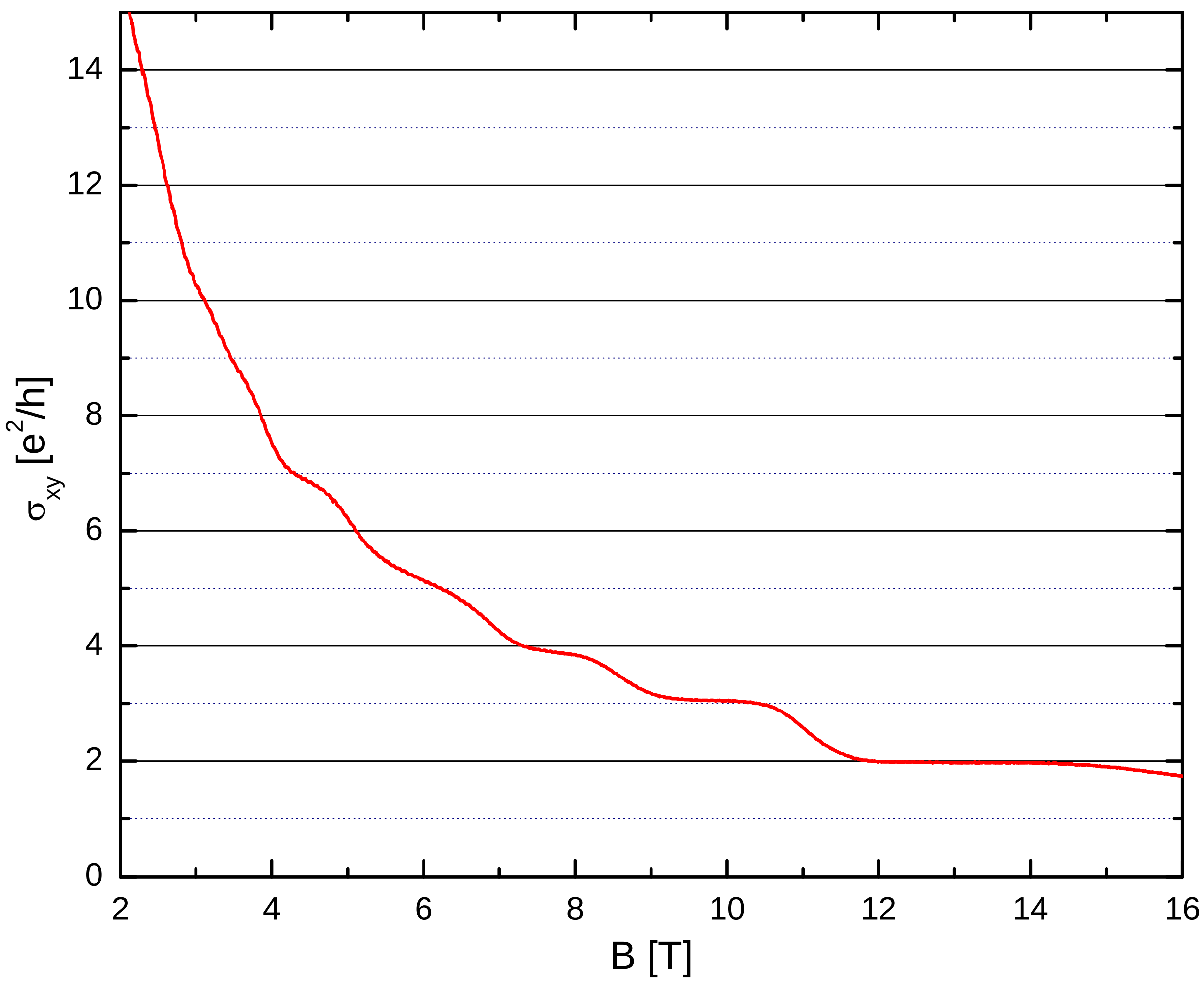
Helical edge and surface states in HgTe quantum wells and bulk insulators

Xi Dai,[1,2] Taylor L. Hughes,[3] Xiao-Liang Qi,[3] Zhong Fang,[1] and Shou-Cheng Zhang[3]
[1]*Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China*
[2]*Department of Physics, University of Hong Kong, Pokfulam Road, Hong Kong*
[3]*Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA*
(Received 10 May 2007; revised manuscript received 27 December 2007; published 14 March 2008)

The quantum spin Hall (QSH) effect is the property of a new state of matter which preserves time reversal, has an energy gap in the bulk, but has topologically robust gapless states at the edge. Recently, the QSH state has been theoretically predicted and experimentally observed in HgTe quantum wells [B. A. Bernevig *et al.*, Science **34**, 1757 (2006); M. Konig *et al.*, *ibid.* **318**, 766 (2007)]. In this work, we start from realistic tight-binding models and demonstrate the existence of the helical edge states in HgTe quantum wells and calculate their physical properties. We also show that three-dimensional HgTe is a topological insulator under uniaxial strain and show that the surface states are described by single-component massless relativistic Dirac fermions in 2+1 dimensions. Experimental predictions are made based on the quantitative results obtained from rea



Quantized 2D QHE in 3D HgTe with strain (Molenkamp et al)



Topological insulators: starting a new family

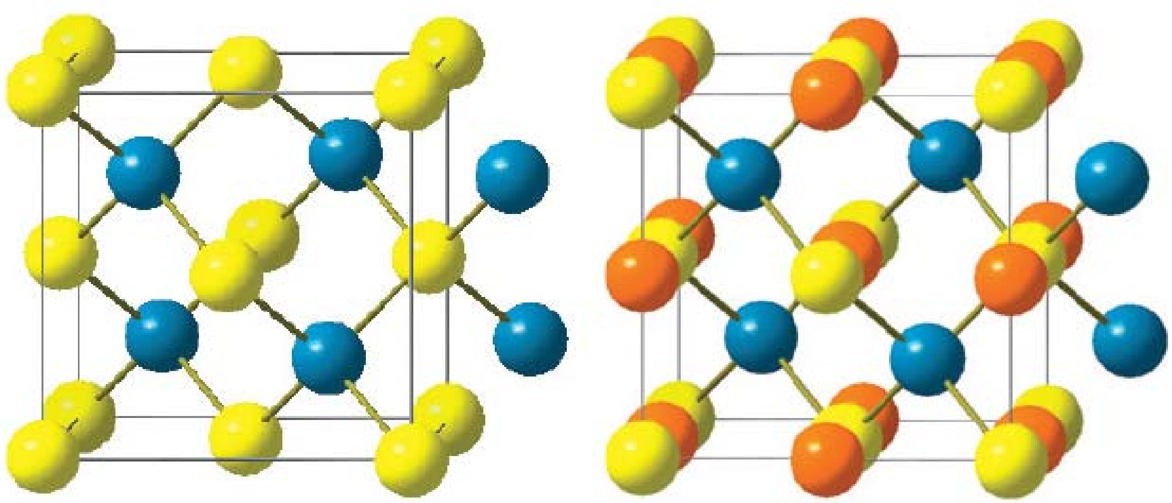
nature materials

LETTERS

PUBLISHED ONLINE: 30 MAY 2010 | DOI: 10.1038/NMAT2770

Tunable multifunctional topological insulators in ternary Heusler compounds

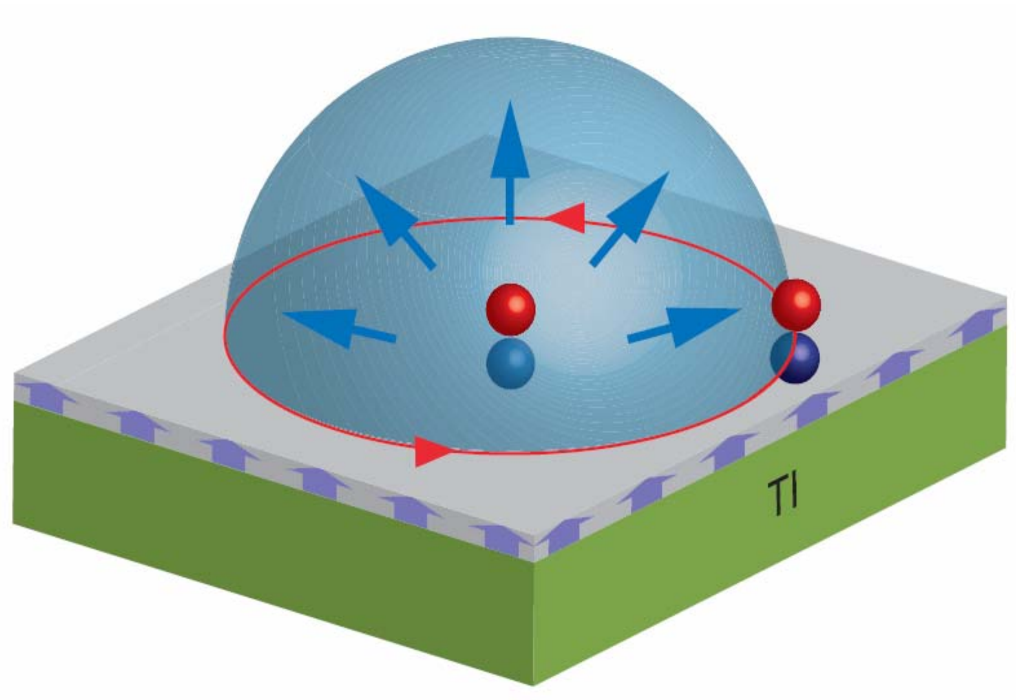
Stanislav Chadov[1], Xiaoliang Qi[2,3], Jürgen Kübler[4], Gerhard H. Fecher[1], Claudia Felser[1]* and Shou Cheng Zhang[3]*



General theory of topological insulators

- Topological field theory of topological insulators. Generally valid for interacting and disordered systems. Directly measurable physically. Quantized magneto-electric effect (Qi, Hughes and Zhang)

$$S_0 = \frac{1}{8\pi}\int d^3x dt \left(\varepsilon \mathbf{E}^2 - \frac{1}{\mu}\mathbf{B}^2\right)$$



- For a periodic system, the system is time reversal symmetric only when

$\theta=0$ => trivial insulator

$\theta=\pi$ => non-trivial insulator

$$S_\theta = \left(\frac{\theta}{2\pi}\right)\left(\frac{\alpha}{2\pi}\right)\int d^3x dt \mathbf{E}\cdot\mathbf{B}$$

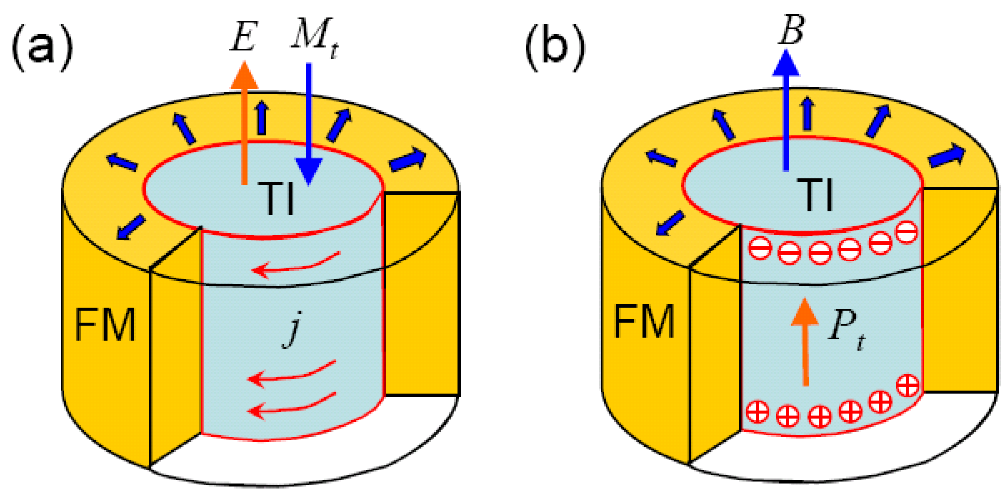
$$\alpha = \frac{e^2}{\hbar c}$$

- Topological band theory based on Z2 topological band invariant of single particle states.
(Fu, Kane and Mele, Moore and Balents, Roy)

$$S_\theta = \frac{\theta}{2\pi}\frac{\alpha}{16\pi}\int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} = \frac{\theta}{2\pi}\frac{\alpha}{4\pi}\int d^3x dt \partial^\mu (\epsilon_{\mu\nu\rho\sigma} A^\nu \partial^\rho A^\tau)$$

The Topological Magneto-Electric (TME) effect

- Equations of axion electrodynamics predict the robust TME effect.



4 π M=α θ/2π **E**

4 π P=α θ/2π **B**

$$
\begin{aligned}
\nabla \cdot \mathbf{D} &= 4\pi\rho \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{E} &= -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \times \mathbf{H} &= \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} \\
\mathbf{D} &= \mathbf{E} + 4\pi\mathbf{P} - 2P_3\alpha\mathbf{B} \\
\mathbf{H} &= \mathbf{B} - 4\pi\mathbf{M} + 2P_3\alpha\mathbf{E}
\end{aligned}
$$

Qi, Hughes and SCZ, PRB 2008

- $P_3=\theta/2\pi$ is the electro-magnetic polarization, microscopically given by the CS term over the momentum space. Change of P_3=2nd Chern number!

$$
P_3(\theta_0) = \int d^3k \mathcal{K}^\theta
$$

$$
= \frac{1}{16\pi^2}\int d^3k \epsilon^{\theta ijk}\,\mathrm{Tr}\left[\left(f_{ij} - \frac{1}{3}[a_i, a_j]\right)\cdot a_k\right]
$$

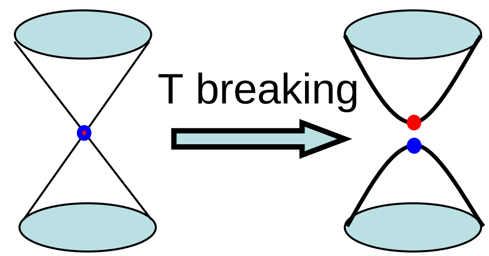
θ term with open boundaries

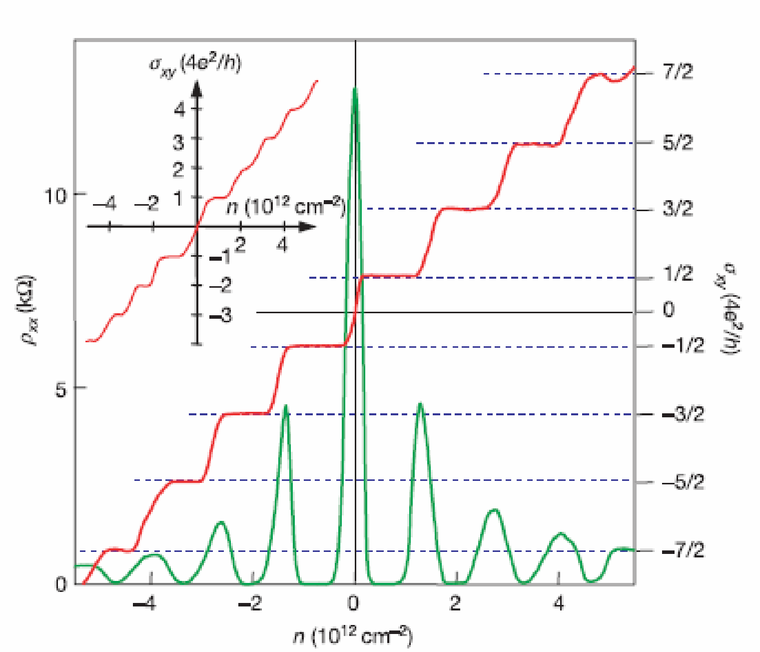
• θ=π implies QHE on the boundary with $\sigma_{xy} = \frac{1}{2}\frac{e^2}{h}$

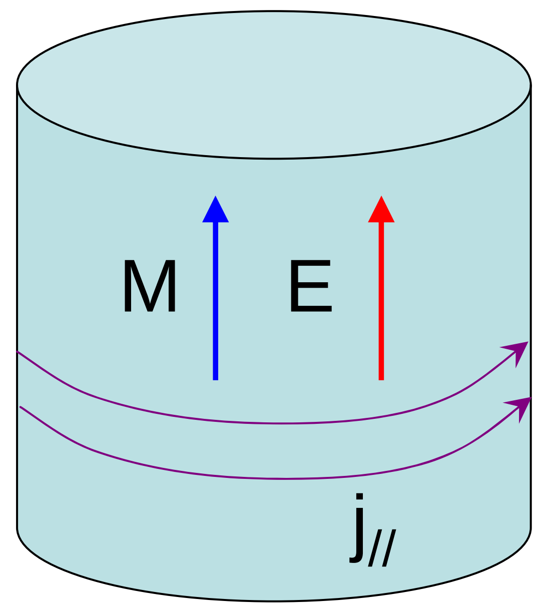
$$S_\theta = \frac{\theta}{2\pi}\frac{\alpha}{16\pi}\int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} = \frac{\theta}{2\pi}\frac{\alpha}{4\pi}\int d^3x dt \partial^\mu (\epsilon_{\mu\nu\rho\sigma} A^\nu \partial^\rho A^\tau)$$

• For a sample with boundary, it is only insulating when a small T-breaking field is applied to the boundary. The surface theory is a CS term, describing the half QH.

• Each Dirac cone contributes $\sigma_{xy}=1/2e^2/h$ to the QH. Therefore, θ=π implies an odd number of Dirac cones on the surface!

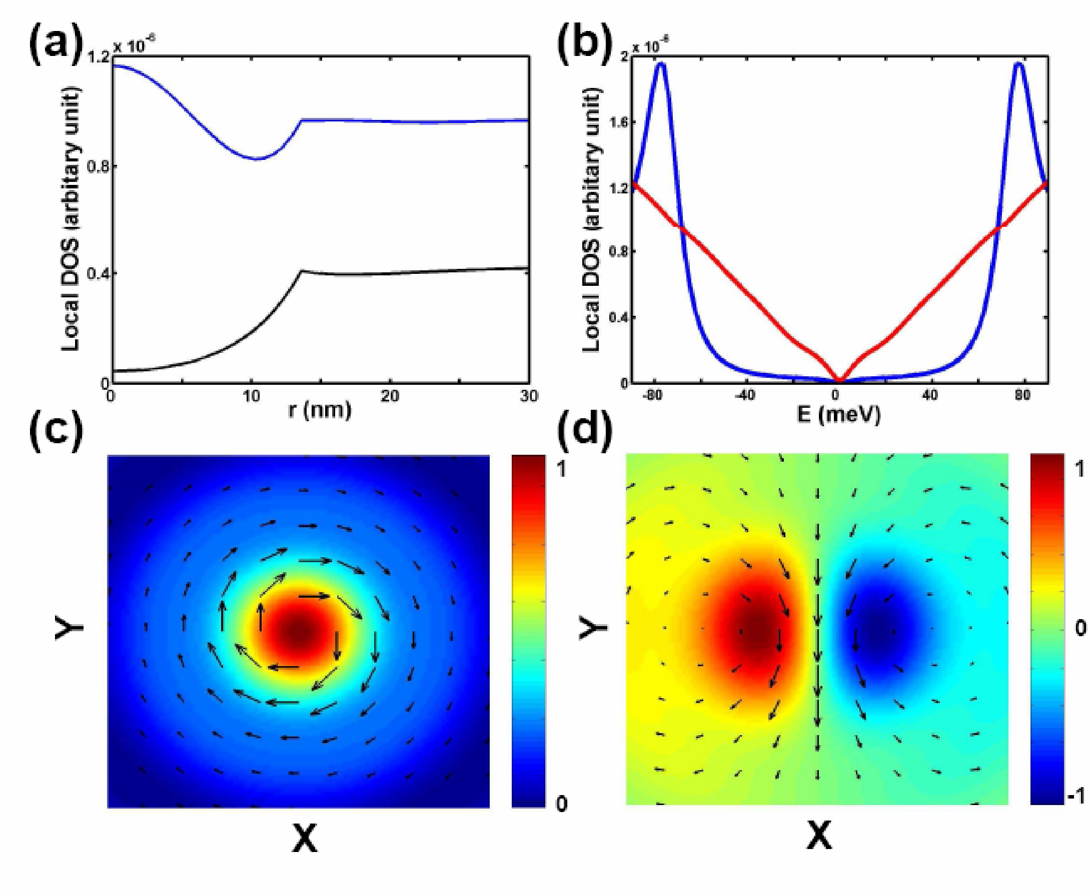


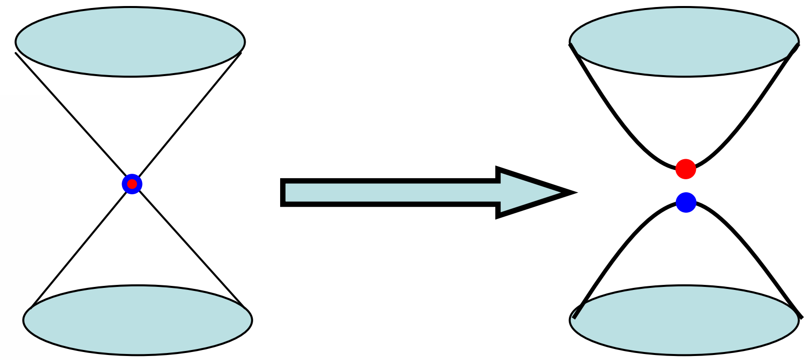


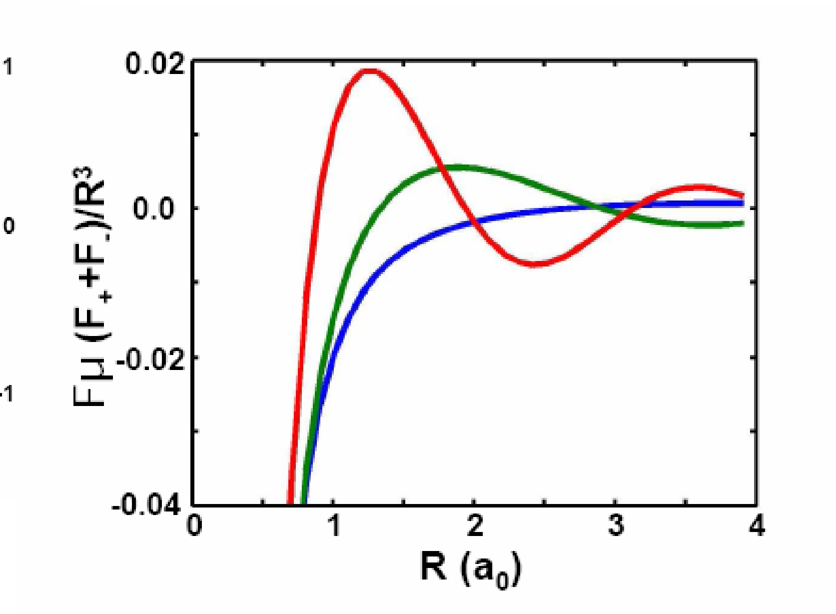


• Surface of a TI = ¼ graphene

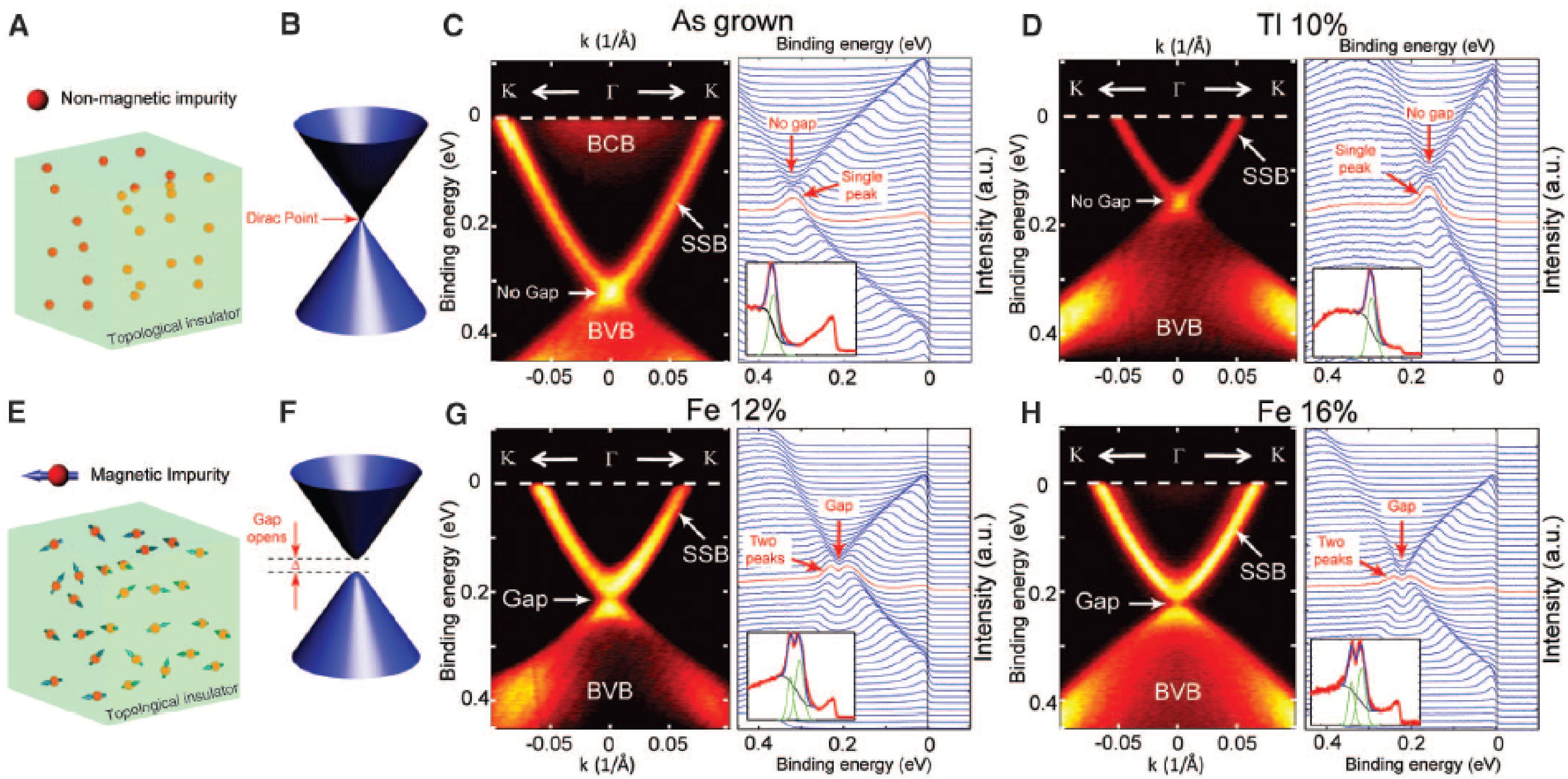
RKKY coupling of the surface states (Liu et al, PRL 2009)



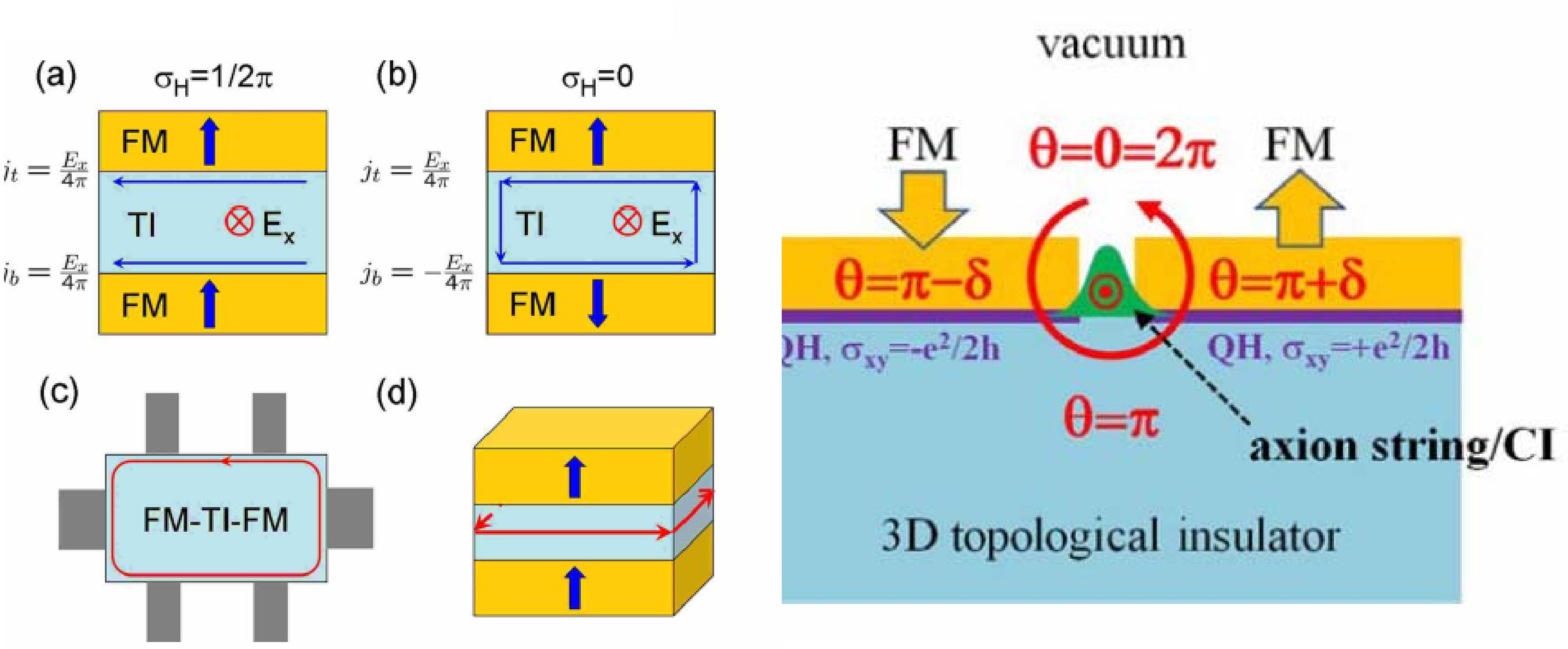




Arpes experiment observes gap at the Dirac point in magnetically doped samples $(BiFe)_2Se_3$ (Chen et al, Science 2010, and experiments from Princeton)



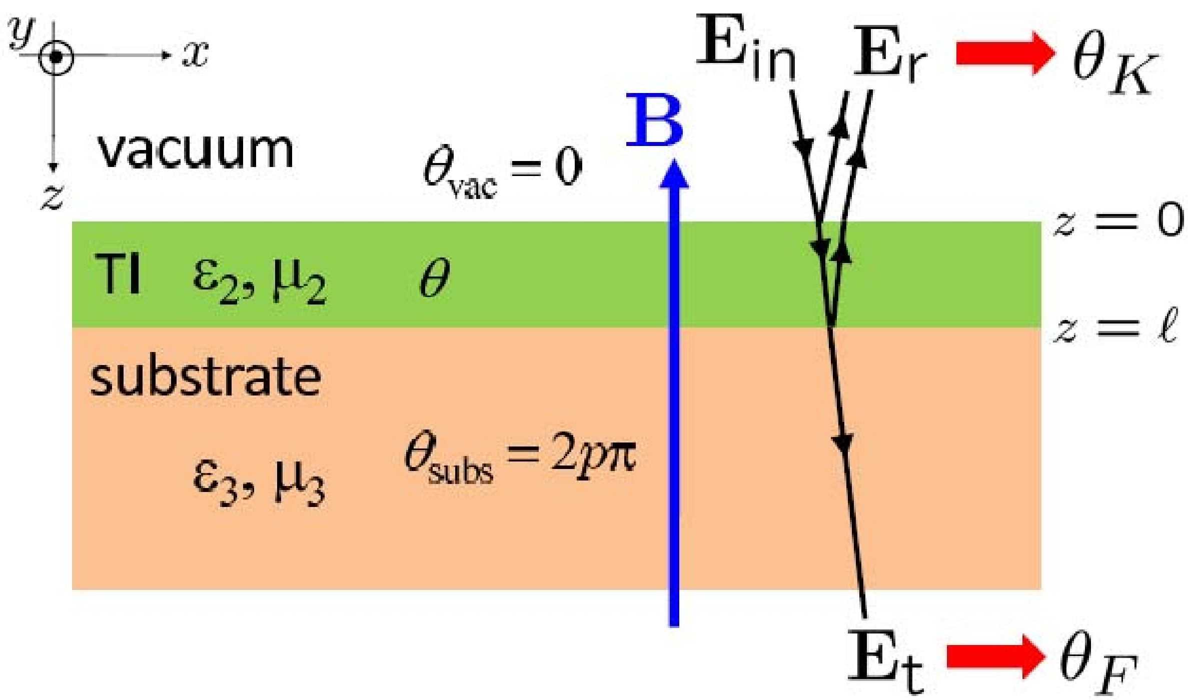
Applications of topological insulators



Qi, Hughes and SCZ, PRB 2008, proposed the chiral state on the topological surface with a magnetic domain wall. This proposal forms a basis for interconnect devices.

Low frequency Faraday/Kerr rotation

(Qi, Hughes and Zhang, PRB78, 195424, 2008, Zhang group 2010, MacDonald group 2010)



Adiabatic

Requirement:

$$\hbar\omega \ll E_g$$

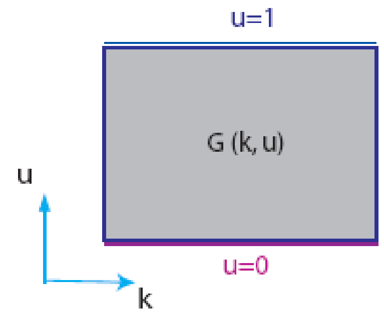
(surface gap)

$$\frac{\cot \theta'_F + \cot \theta'_K}{1 + \cot^2 \theta'_F} = \alpha p, \qquad p \in \mathbb{Z}.$$

Universal quantization in units of the fine structure constant!

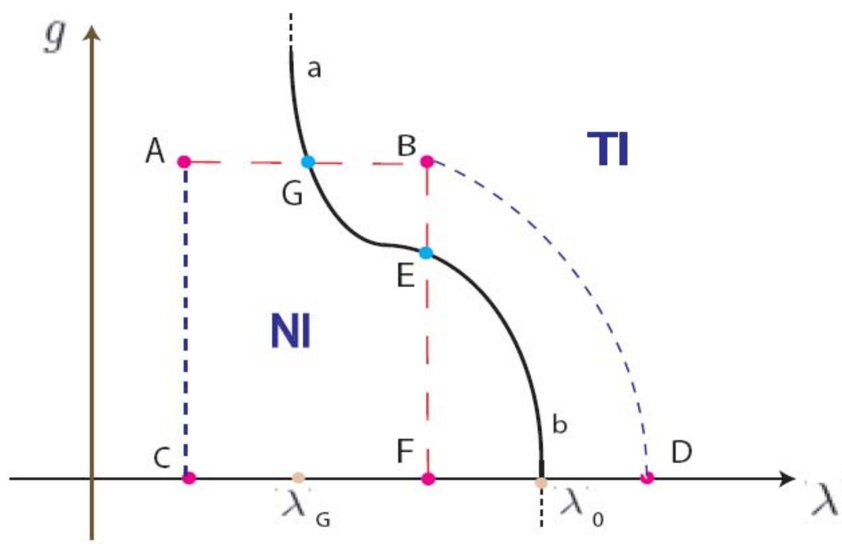
Generalization to general interacting TI (Wang, Qi, SCZ, PRL 2010)

$$P_3 = \frac{\pi}{6}\int_0^1 du \int \frac{d^4k}{(2\pi)^4} \mathrm{Tr}\,\epsilon^{\mu\nu\rho\sigma}[G\partial_\mu G^{-1} G\partial_\nu G^{-1}$$
$$\times G\partial_\rho G^{-1} G\partial_\sigma G^{-1} G\partial_u G^{-1}]$$



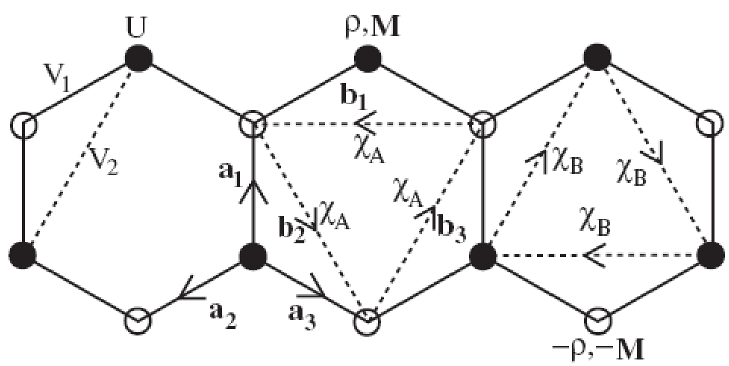
- Topological order parameter for generally interacting TI
- Experimentally measurable through the topological magneto-electric effect
- WZW extension u introduces integer ambiguity of P3
- P3 is topologically quantized to be integer or half-integer
- Also applies to disordered systems, see Li et al, Groth et al.

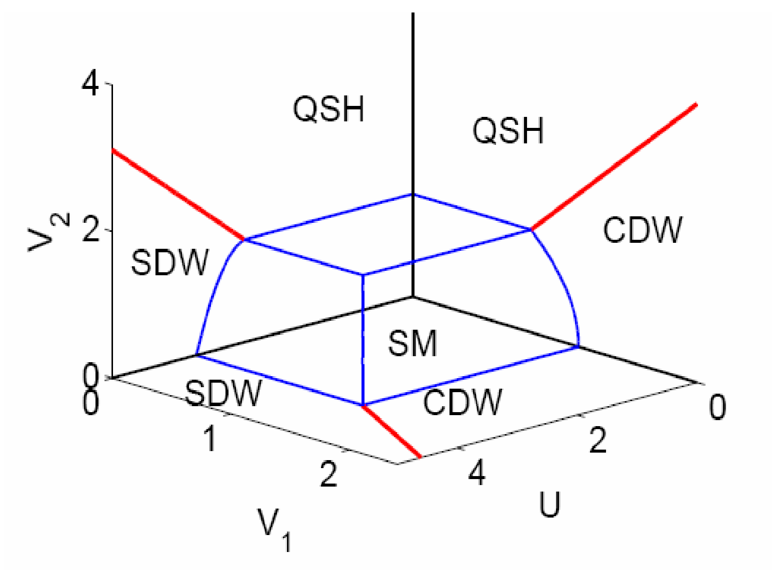
$$\pi_5(\mathrm{GL}(n,\mathrm{C})) = \mathbb{Z}$$



Topological Mott insulators

- Dynamic generation of spin-orbit coupling can give rise to TMI (Raghu et al, PRL 2008).
- Interplay between spin-orbit coupling and Mott physics in 5d transition metal Ir oxides, Nagaosa, SCZ et al PRL 2009, Balents et al, Franz et al.
- Topological Kondo insulators (Sun, Galetski, Coleman et al)





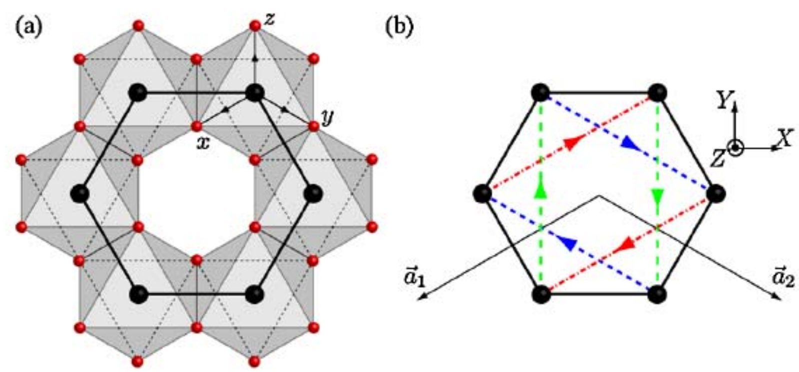


FIG. 1 (color online). (a) The honeycomb lattice of Ir atoms in Na_2IrO_3 viewed from the c axis. A large black circle shows an Ir atom surrounded by six O atoms (red small circles). (b) The transfer integrals on the honeycomb lattice. A black solid line shows $-t$, while blue short-dashed, red dash-dotted, and green long-dashed arrows indicate $it'\sigma_x$, $it'\sigma_y$, $it'\sigma_z$, respectively.

Fractional topological insulators (Maciejko et al, PRL 2010)

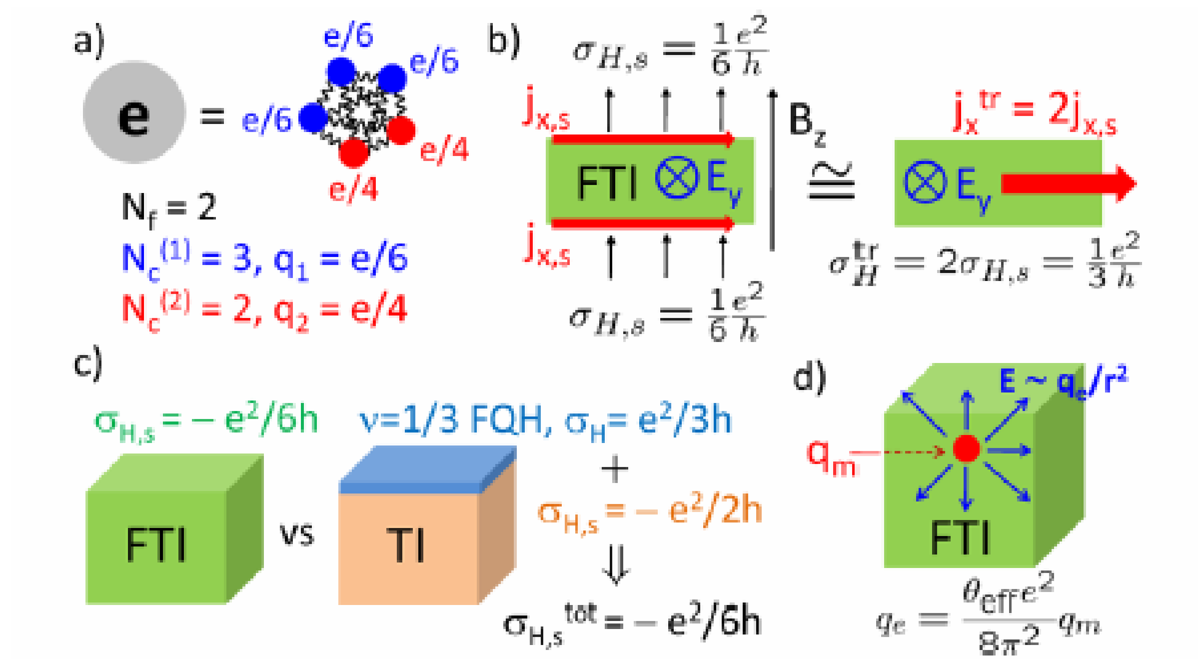
PRL **105**, 246809 (2010) PHYSICAL REVIEW LETTERS week ending 10 DECEMBER 2010

Fractional Topological Insulators in Three Dimensions

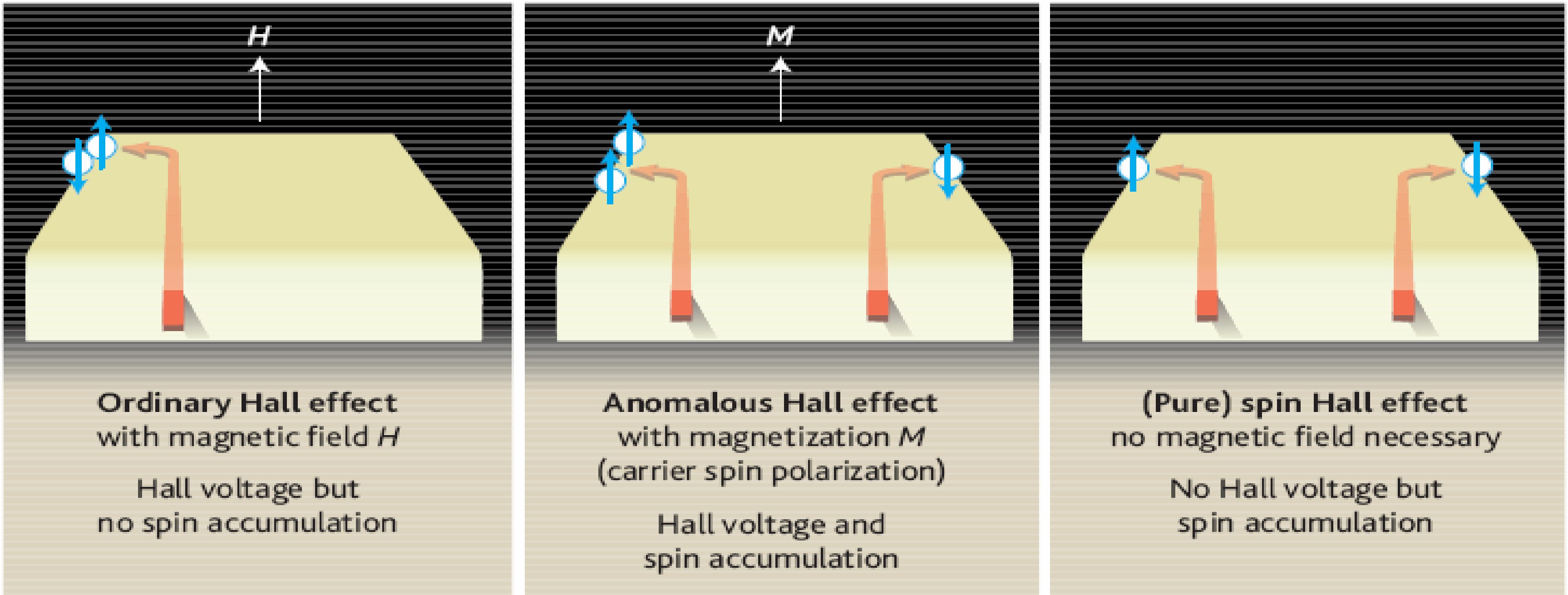
Joseph Maciejko,[1] Xiao-Liang Qi,[2,1] Andreas Karch,[3] and Shou-Cheng Zhang[1]

$$S_\theta = \frac{\theta}{2\pi}\frac{\alpha}{16\pi}\int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} = \frac{\theta}{2\pi}\frac{\alpha}{4\pi}\int d^3x dt \partial^\mu(\epsilon_{\mu\nu\rho\sigma} A^\nu \partial^\rho A^\tau)$$

$$\sigma_{H,s} = \frac{p}{q}\frac{e^2}{2h}, \qquad p, q \text{ odd.}$$



Completing the table of Hall effects



Hall **1879**	**Anomalous Hall** **1889**	**Spin Hall** **2004**
QHE **1980**	**QAHE** **2011?**	**QSHE** **2006/2007**

Theoretical prediction of the quantized AHE state

Quantum Anomalous Hall Effect in $Hg_{1-y}Mn_yTe$ Quantum Wells

Chao-Xing Liu,[1,2] Xiao-Liang Qi,[2] Xi Dai,[3] Zhong Fang,[3] and Shou-Cheng Zhang[2]
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(Received 20 February 2008; published 1 October 2008)

The quantum Hall effect is usually observed when a two-dimensional electron gas is subjected to an external magnetic field, so that their quantum states form Landau levels. In this work we predict that a new phenomenon, the quantum anomalous Hall effect, can be realized in $Hg_{1-y}Mn_yTe$ quantum wells, without an external magnetic field and the associated Landau levels. This effect arises purely from the spin polarization of the Mn atoms, and the quantized Hall conductance is predicted for a range of quantum well thickness and the concentration of the Mn atoms. This effect enables dissipationless charge current in spintronics devices.

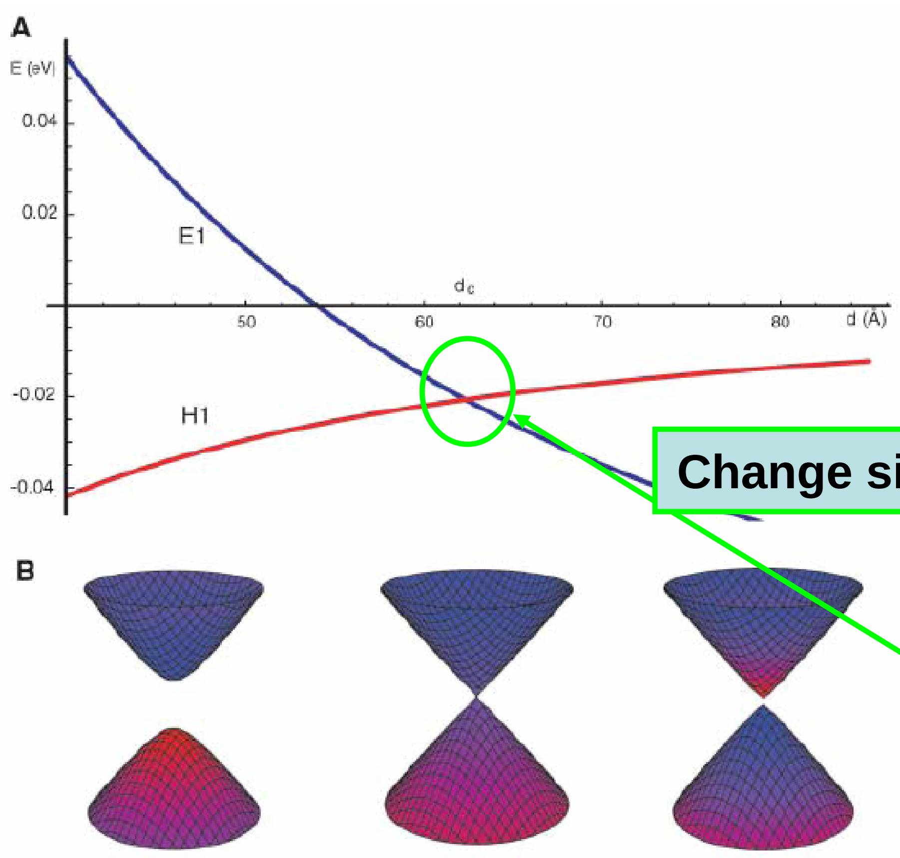
Quantized Anomalous Hall Effect in Magnetic Topological Insulators

Rui Yu,[1] Wei Zhang,[1] Hai-Jun Zhang,[1,2] Shou-Cheng Zhang,[2,3] Xi Dai,[1]* Zhong Fang[1]*

The anomalous Hall effect is a fundamental transport process in solids arising from the spin-orbit coupling. In a quantum anomalous Hall insulator, spontaneous magnetic moments and spin-orbit coupling combine to give rise to a topologically nontrivial electronic structure, leading to the quantized Hall effect without an external magnetic field. Based on first-principles calculations, we predict that the tetradymite semiconductors Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 form magnetically ordered insulators when doped with transition metal elements (Cr or Fe), in contrast to conventional dilute magnetic semiconductors where free carriers are necessary to mediate the magnetic coupling. In two-dimensional thin films, this magnetic order gives rise to a topological electronic structure characterized by a finite Chern number, with the Hall conductance quantized in units of e^2/h (where e is the charge of an electron and h is Planck's constant).

Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells

B. Andrei Bernevig,[1,2] Taylor L. Hughes,[1] Shou-Cheng Zhang[1]*



Change sign

Keep in mind there is two-fold degeneracy due to the time reversal symmetry

$$H_0(k) = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix},$$

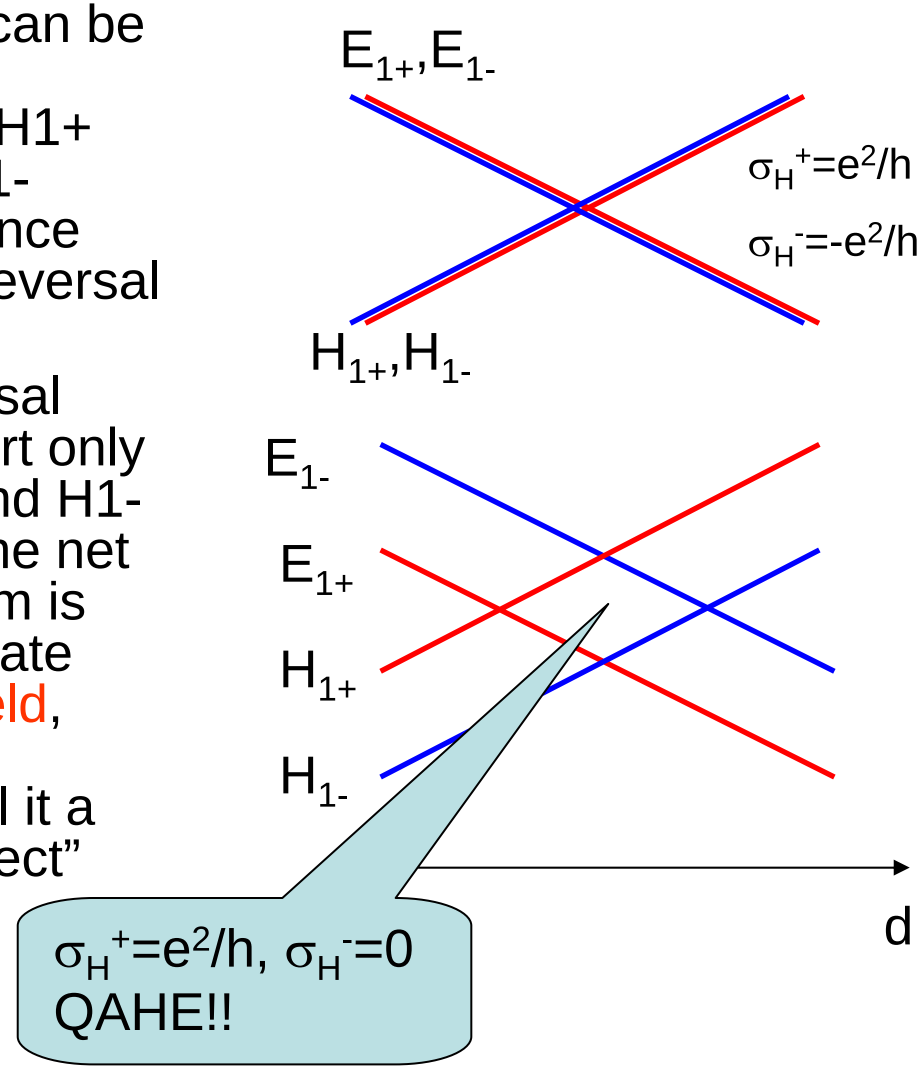
$$h(k) = \begin{pmatrix} \epsilon_k + \mathcal{M}(k) & Ak_+ \\ Ak_- & \epsilon_k - \mathcal{M}(k) \end{pmatrix}$$

$$\epsilon_k = C_0 + C_2 k^2,$$

$$\mathcal{M}(k) = M_0 + M_2 k^2.$$

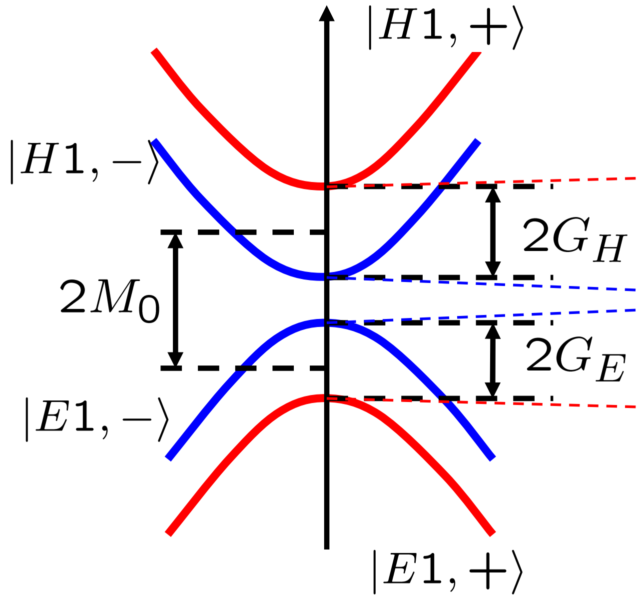
From QSHE to QAHE

- The quantum spin Hall effect can be understood as having Hall conductance $\sigma_H = e^2/h$ for E1+,H1+ bands and $\sigma_H = -e^2/h$ for E1-,H1- bands. The two Hall conductance cancels, as required by time reversal symmetry.
- If we can break the time reversal symmetry, it's possible to invert only E1+ and H1+, but keep E1- and H1- in the normal region, so that the net Hall conductance of the system is e^2/h. This is a quantum Hall state without ORBITAL magnetic field, which is an extreme case of anomalous Hall effect. We call it a "Quantum Anomalous Hall effect" (QAHE).



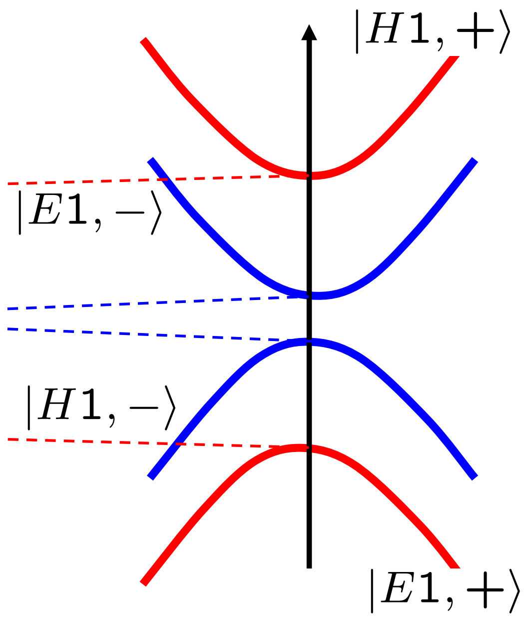
Understanding from edge states: QAH

Small spin splitting, $\sigma_H=0$

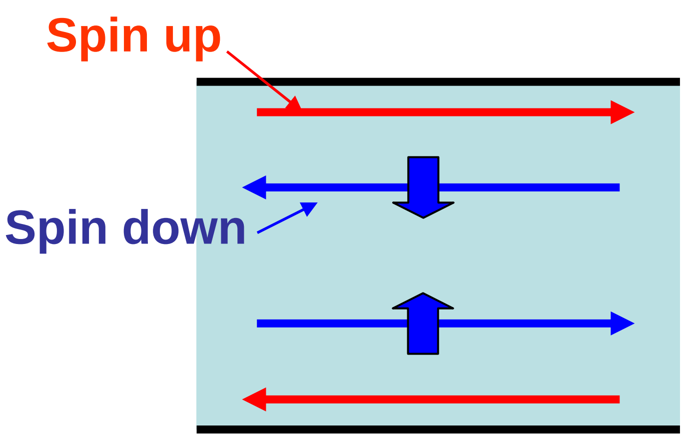


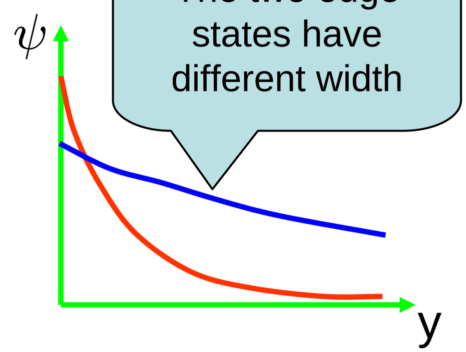
Further increase $|G_H|$ and $|G_E|$

Large splitting, $\sigma_H=e^2/h$

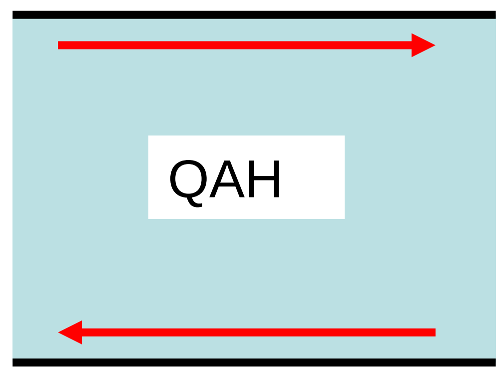


Note that G_E and G_H have opposite sign

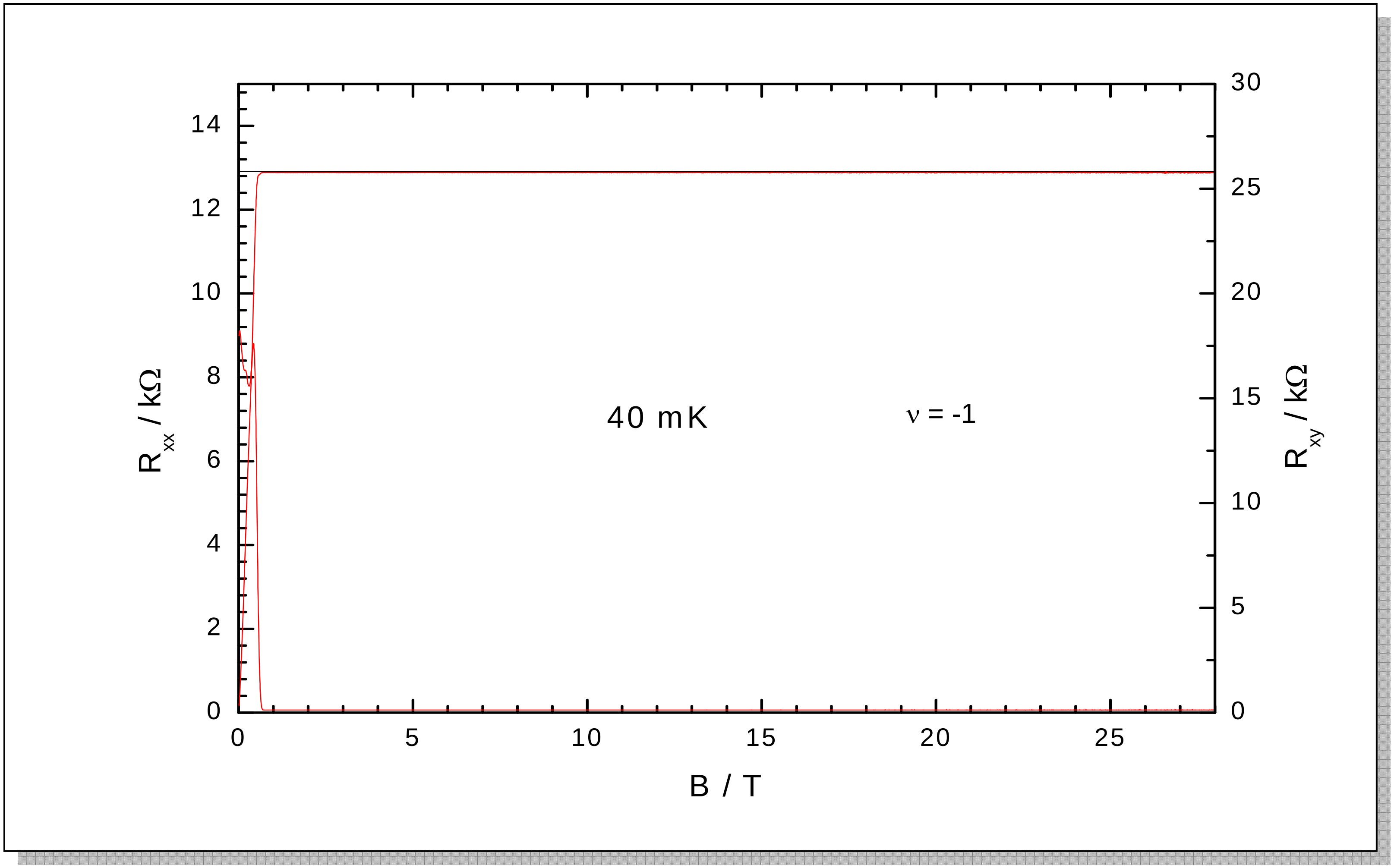




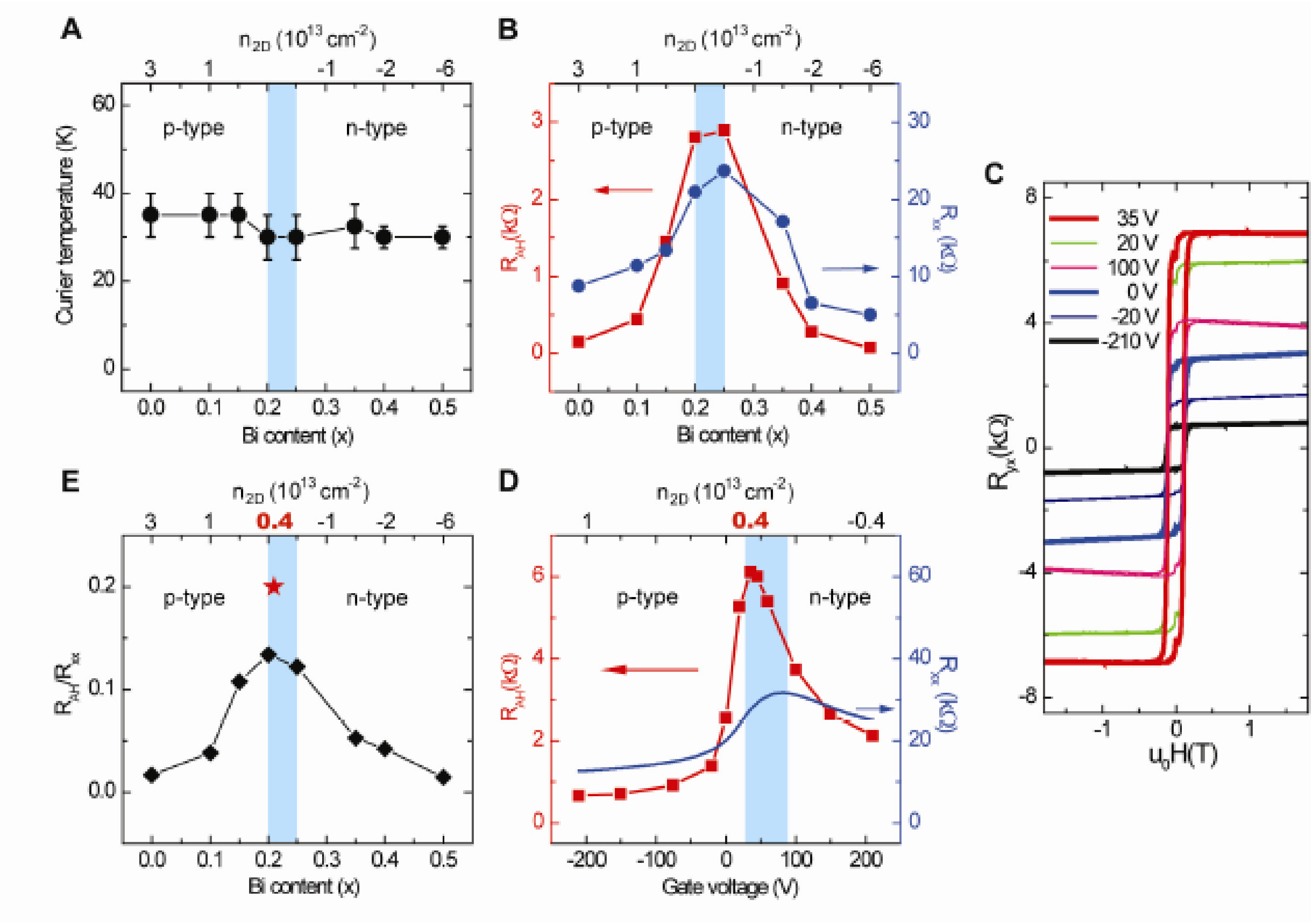
The two edge states have different width



QAH in HgMnTe (Wurzburg experiment)

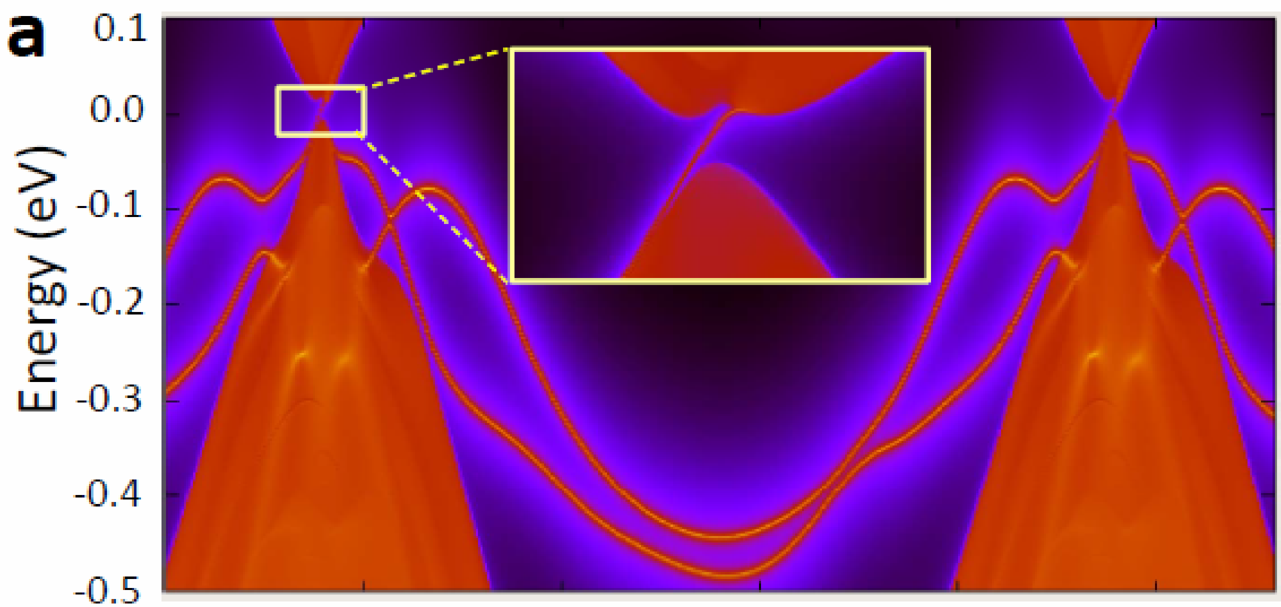


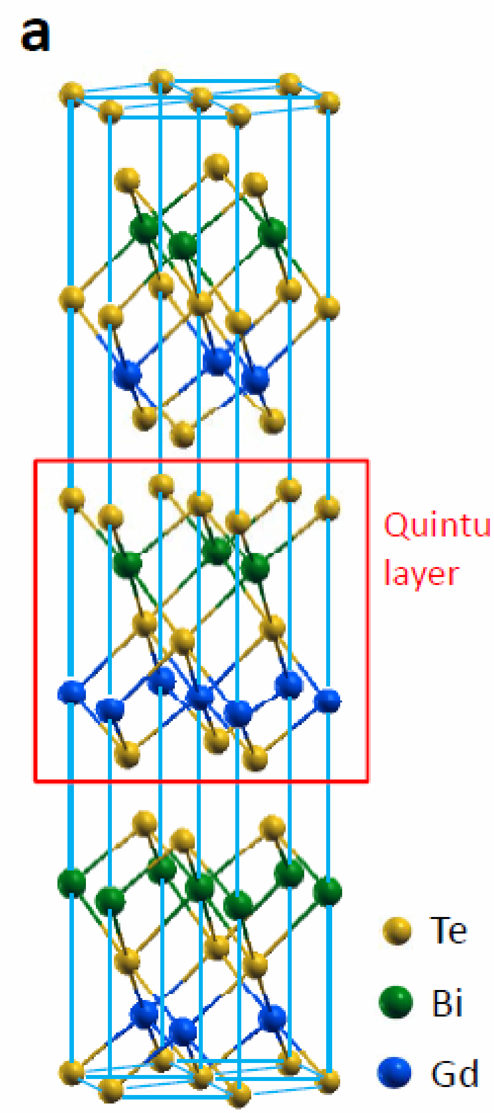
QAH in CrSb2Te3? (Tsinghua/IOP experiment)



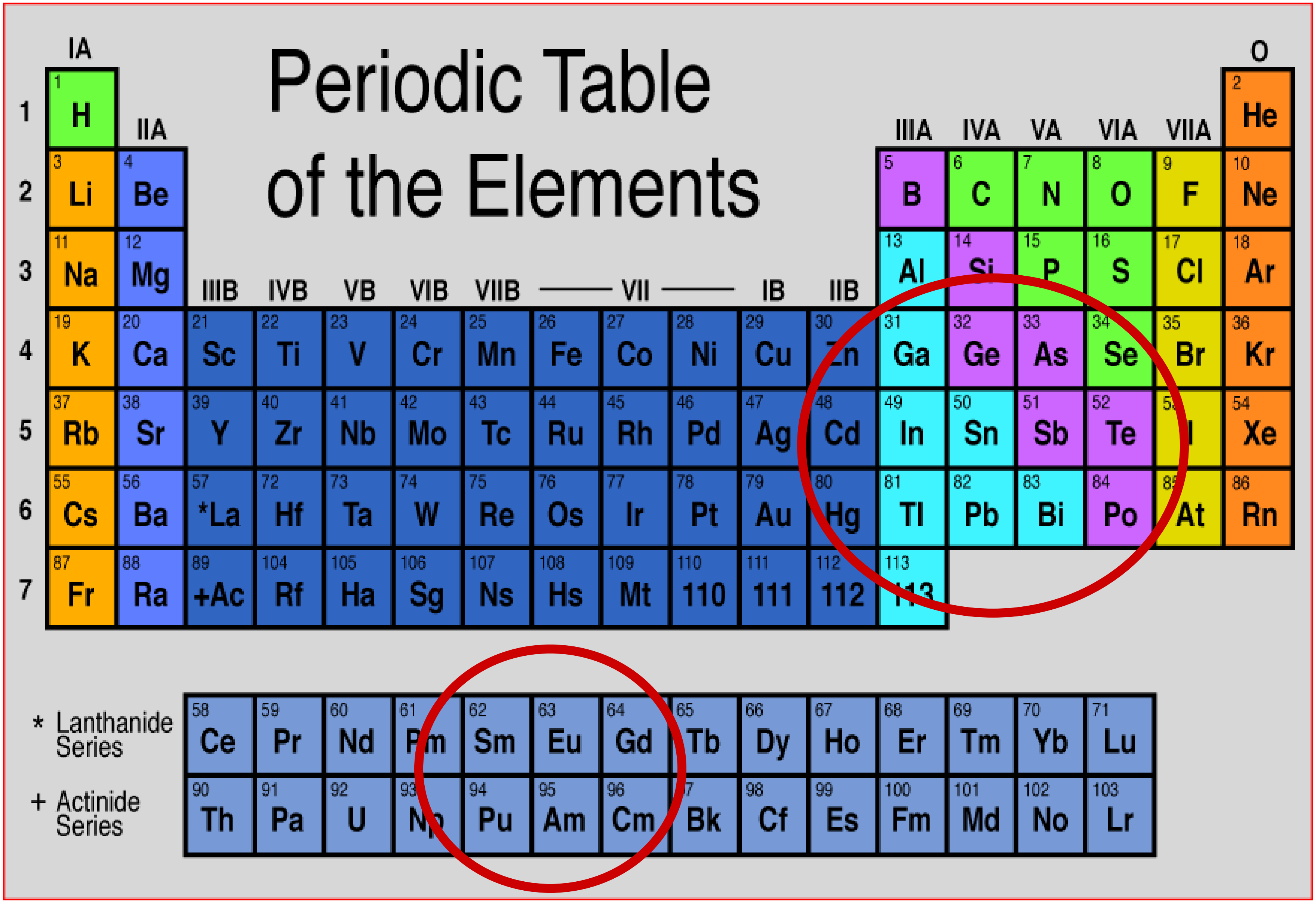
Quantum Anomalous Hall Effect in Magnetic Topological Insulator $GdBiTe_3$

Hai-Jun Zhang, Xiao Zhang & Shou-Cheng Zhang

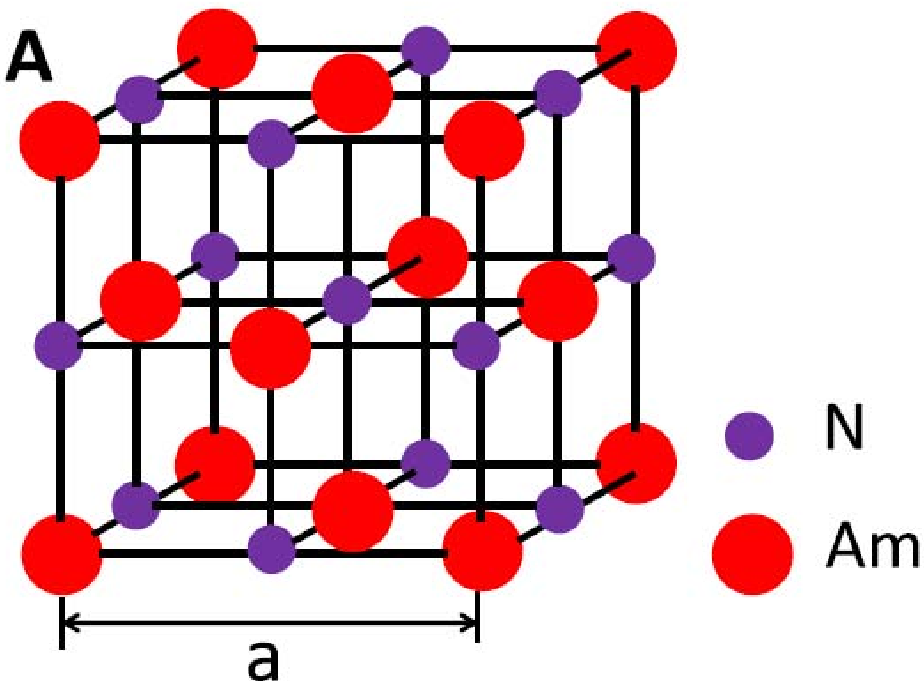


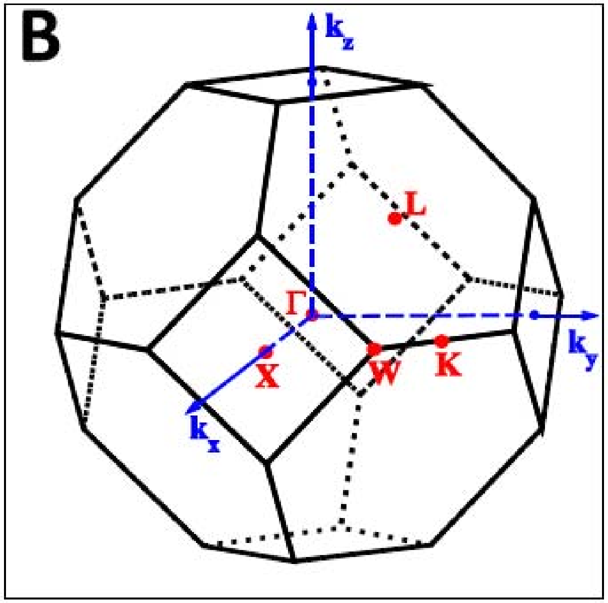


Search for interacting topological insulators



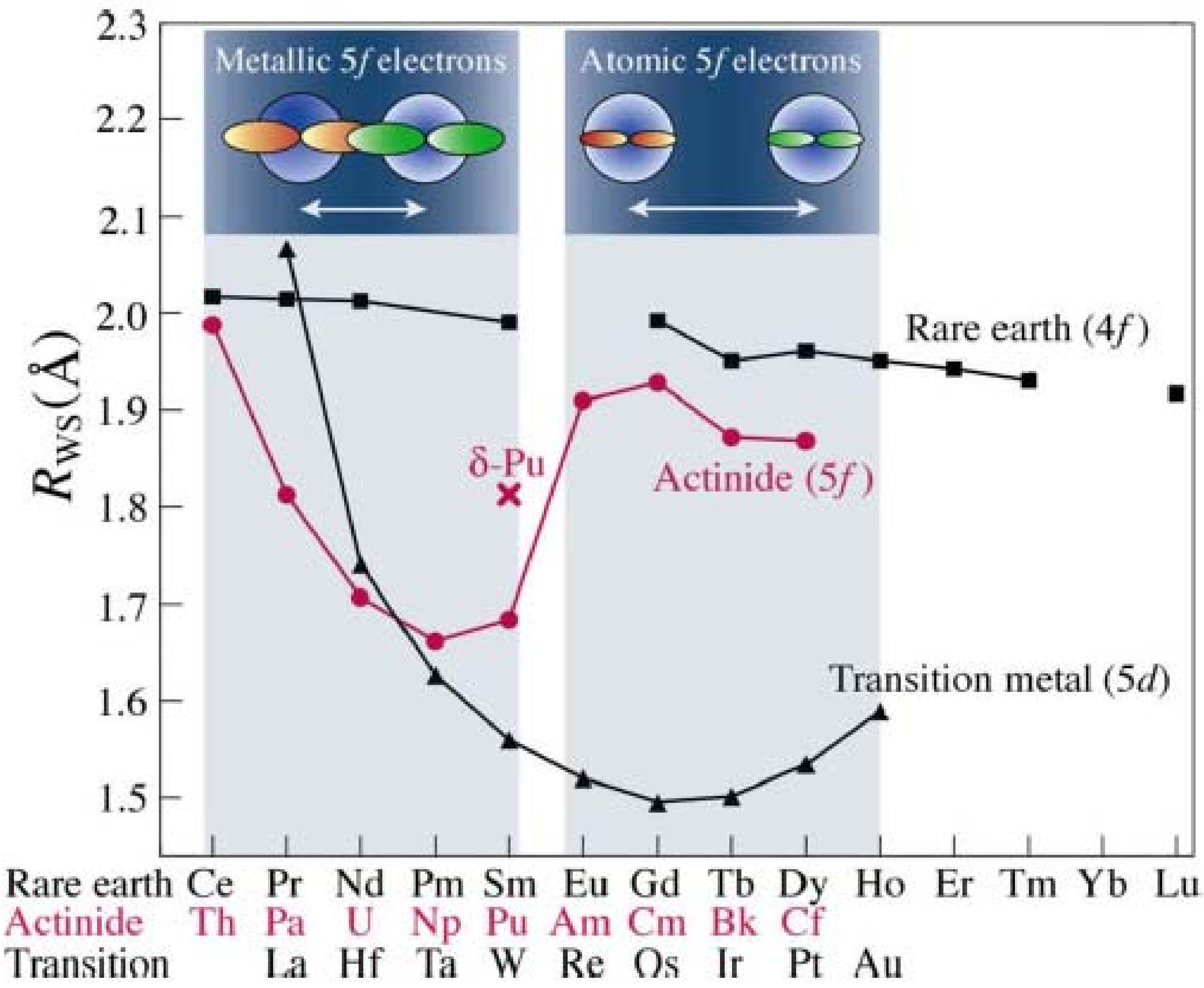
Theoretical prediction of interacting topological Mott insulator





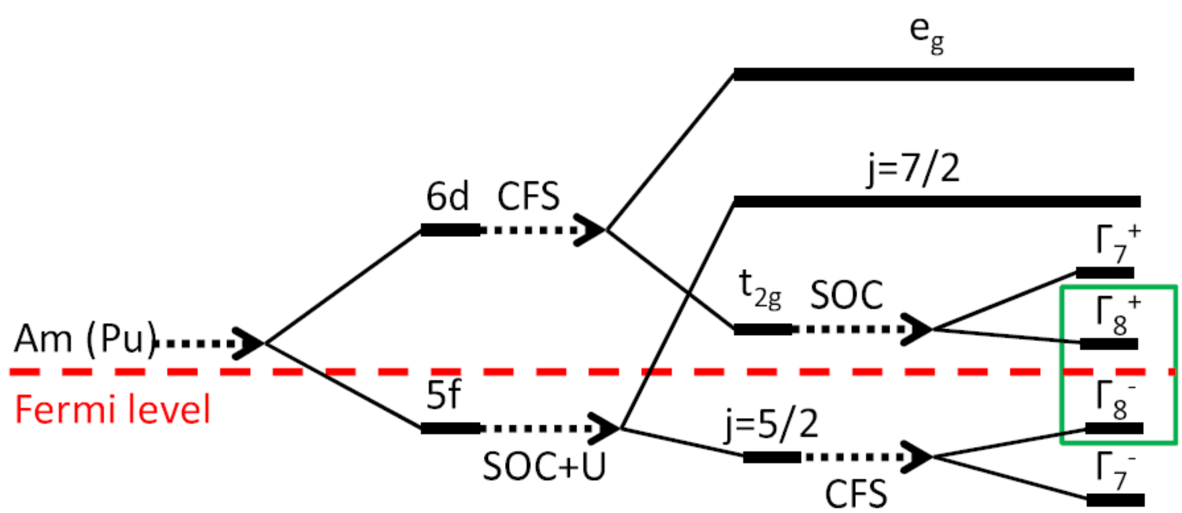
- Actinide based topological Mott insulator.
- Binary compound with a simple Rocksalt crystal structure.
- Strong ionic bonding, insulating bulk, no DOS at E_f!
- Coulomb, SOC and bandwidth comparable scale of 1-2 eV.
- Long life time, ^{241}Am, T=430y, ^{243}Am, T=7300y.

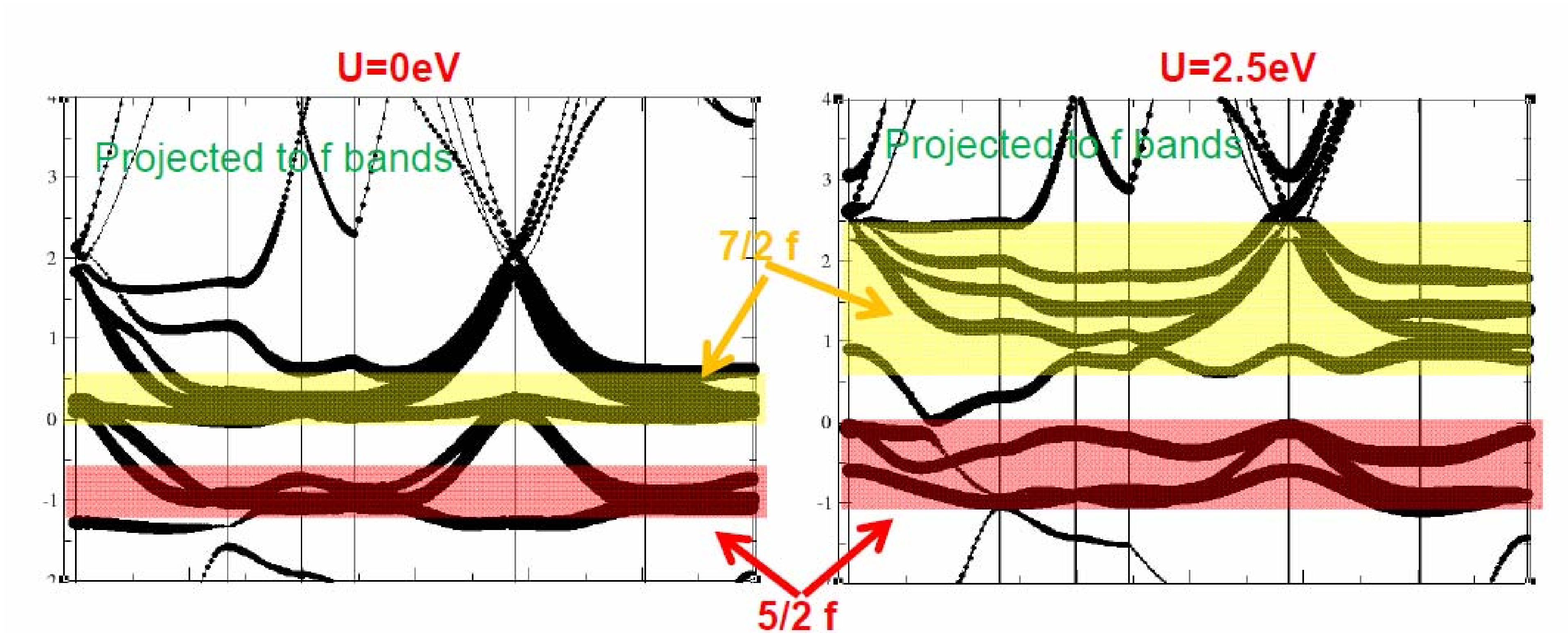
Boundary between itinerant and localized 5f orbitals



- Am $5f^7\ 6d^0\ 7s^2$ => Am^{3+} in AmN, with $5f^6\ 6d^0\ 7s^0$ with filled J=5/2 shell
- Pu $5f^6\ 6d^0\ 7s^2$ => Pu^{2+} in PuTe, with $5f^6\ 6d^0\ 7s^0$ with filled J=5/2 shell

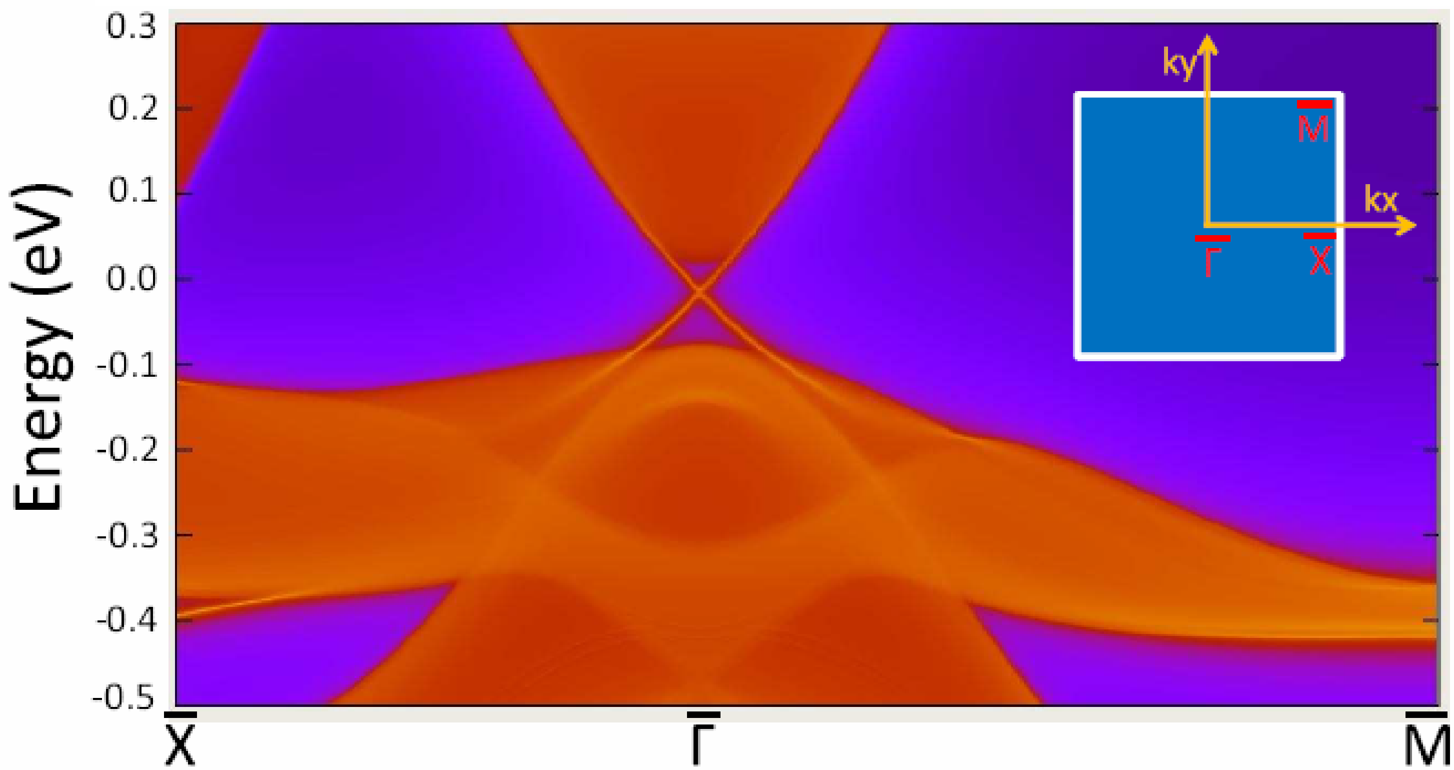
Electronic structure





Single Dirac cone on the surface

	E_g	Γ	$3X$	$4L$	Tot.
AmN	0.100eV	−	+	−	−
AmP	0.085eV	−	+	−	−
AmAs	0.080eV	−	+	−	−
AmSb	0.055eV	−	+	−	−
AmBi	0.040eV	−	+	−	−
PuSe	???	−	+	−	−
PuTe	0.178eV	−	+	−	−



Conclusion

- Topological insulator is a new state of quantum matter.

- Material properties can be predicted and designed.

- Frontiers of the field:
  - Improved material properties
  - New topological insulators
  - Magnetic monopoles and Majorana fermions
  - Topological superconductors
  - Quantized anomalous Hall effect
  - Strongly correlated topological insulators

- Reviews:
  - Qi+Zhang, Physics Today
  - Moore, Nature
  - Hasan and Kane, RMP colloquium
  - Qi+Zhang, RMP, full article:

  •Rev. Mod. Phys. 83, 1057 (2011)