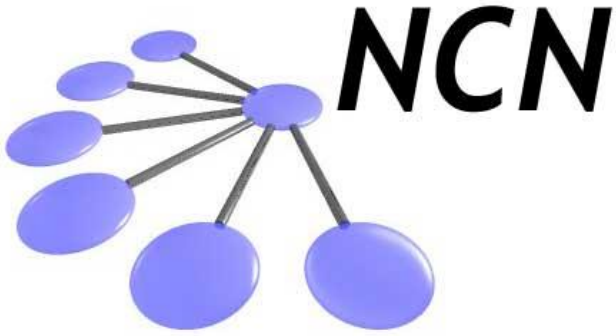
Topological Insulators: Electronic structure, material systems and its applications



PURDUE
UNIVERSITY

Parijat Sengupta
Network for Computational Nanotechnology
Electrical and Computer Engineering
Purdue University

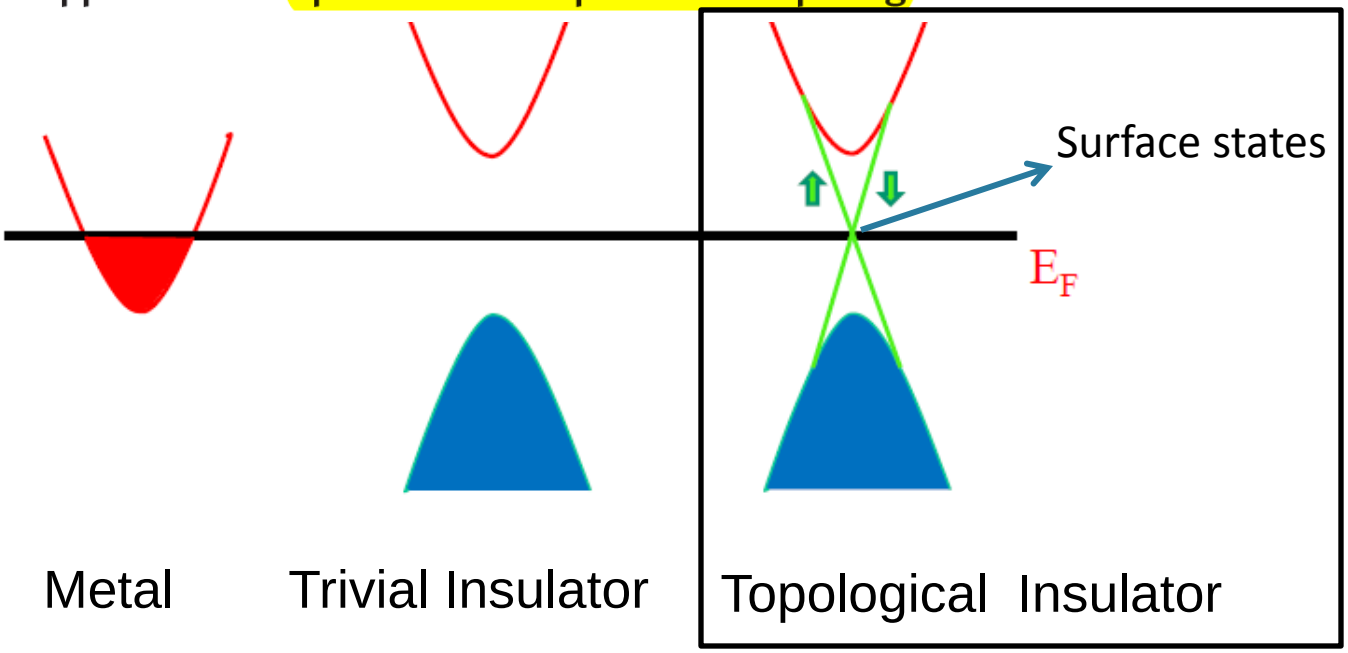
Complete set of slides from my final PhD defense
Advisor : Prof. Gerhard Klimeck

A new addition to the metal-insulator classification

The birth of topological insulators

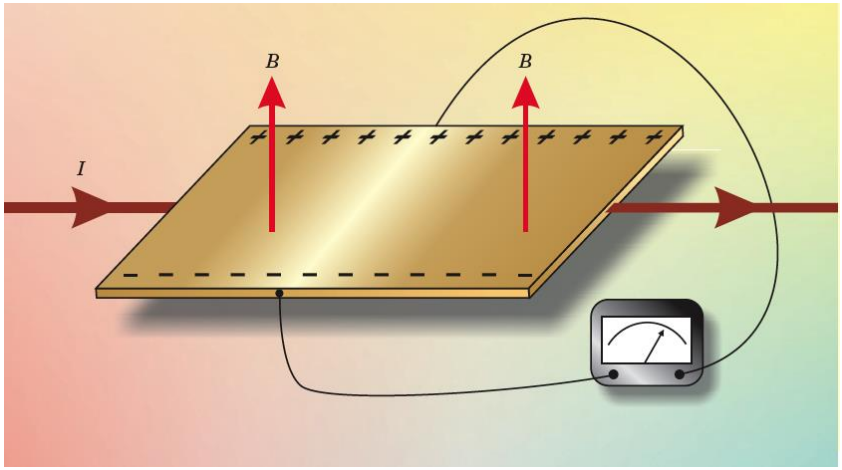
Joel E. Moore[1,2] Nature, Vol. 464, 11 March, 2010

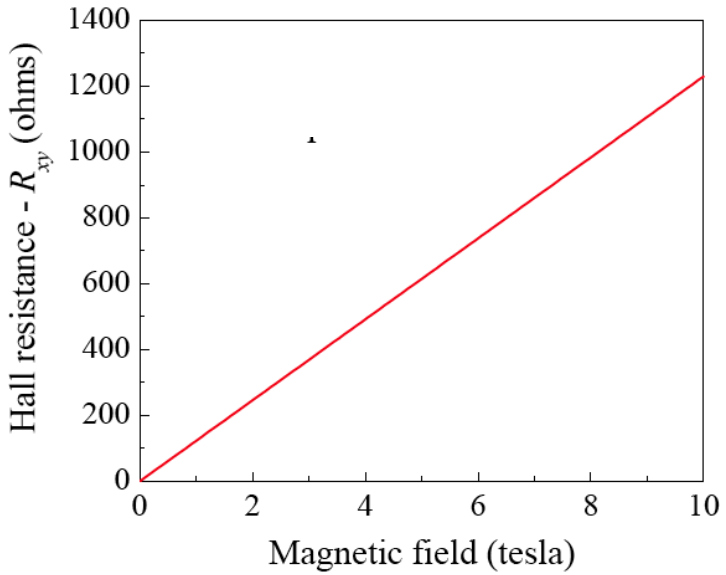
Certain insulators have exotic metallic states on their surfaces. These states are formed by topological effects that also render the electrons travelling on such surfaces insensitive to scattering by impurities. Such topological insulators may provide new routes to generating novel phases and particles, possibly finding uses in technological applications in spintronics and quantum computing.



Tracing the roots of topological insulator

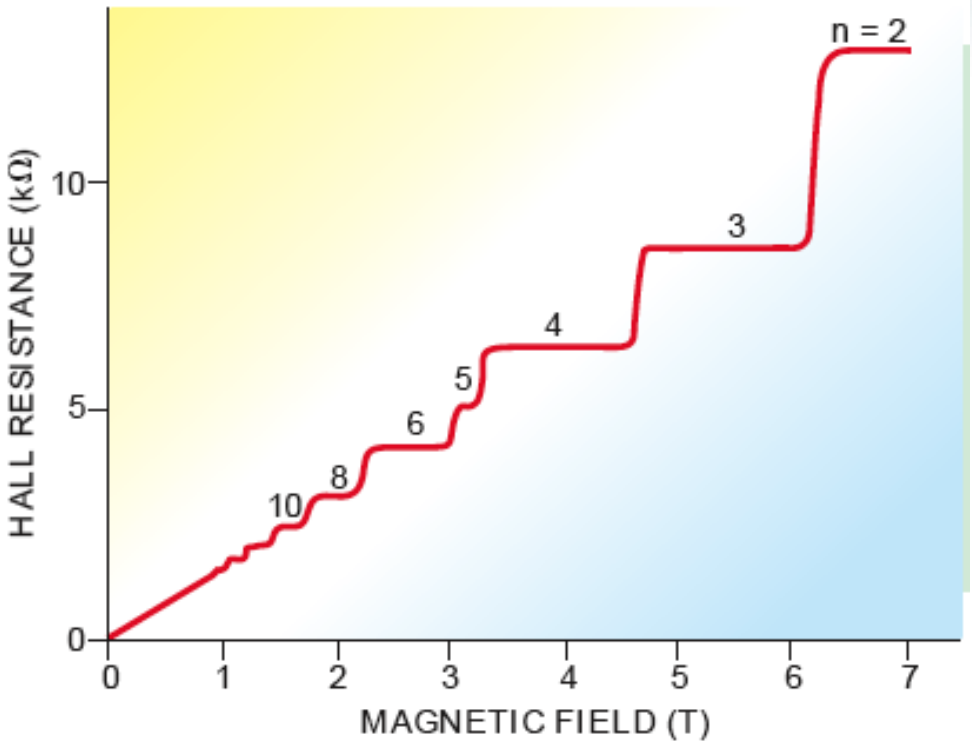
The Hall effect of 1869 is a start point





How does the Hall resistance behave for a 2D set-up under low temperature and high magnetic field (The Quantum Hall Effect) ?

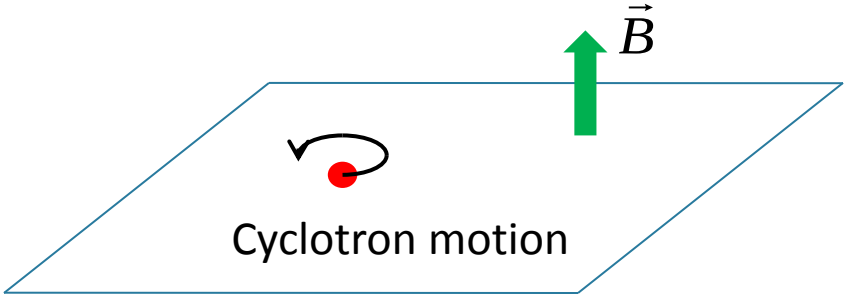
The Quantum Hall Plateau



$$\sigma_{xy} = \frac{ne^2}{h}$$

$$\frac{h}{e^2} = 26k\Omega$$

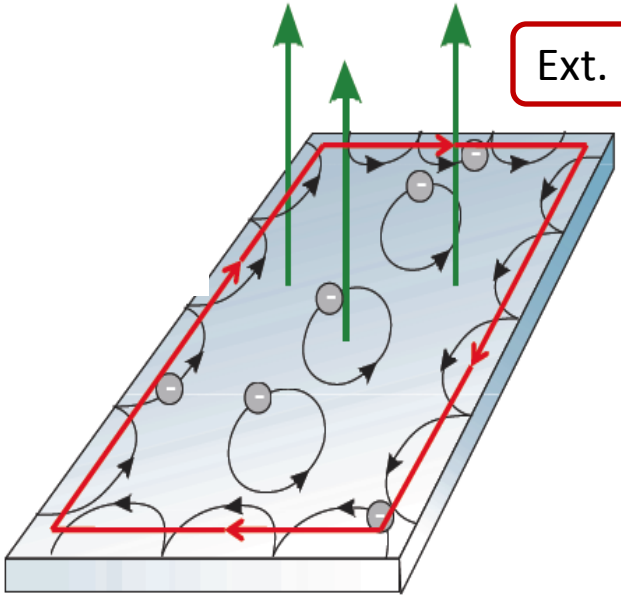
Hall Conductance is quantized



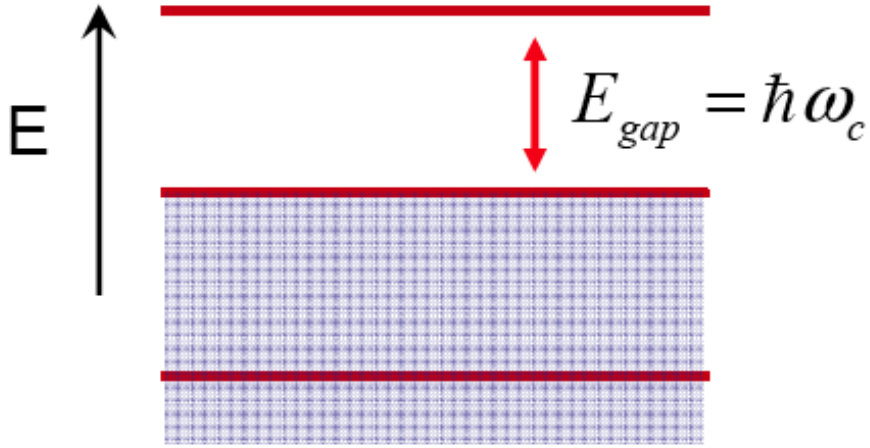
Landau Levels

$$E_n = \hbar\omega_c\left(n+\tfrac{1}{2}\right), \quad \omega_c = \frac{eB}{mc}, \quad n = 0,1,2,\ldots$$

Plateau and the edge states



Skipping orbits along the edge



Landau Levels

Skipping orbits induce a gapless edge mode along the sample boundary

Question: Are edge states possible without external B field ?

Is there a crystal attribute that can substitute an external B field

Spin orbit Interaction : $H_{SO}^{eff} = \lambda(\mathbf{p} \times \nabla V).\mathbf{S}$

Internal B field

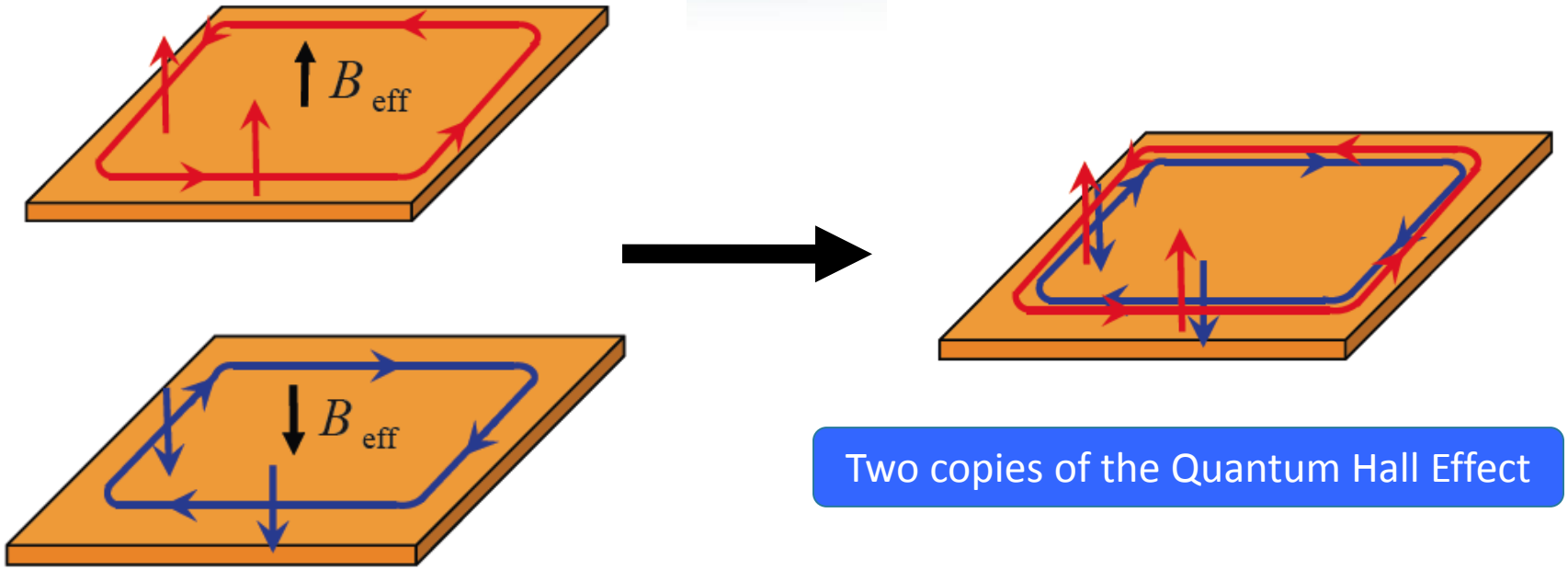
1. Momentum dependent force, analogous to B field
2. Opposite force for opposite spins
3. Energy $\pm\mu B$ depends on electronic spin
4. Spin-orbit strongly enhanced for atoms of large atomic number

Fundamental difference lies under a Time Reversal Symmetric Operation

Time Reversal Symmetry Violation

1. Quantum Hall ☑
2. Intrinsic B field ☒

Quantum Hall effect with spin-dependent B field

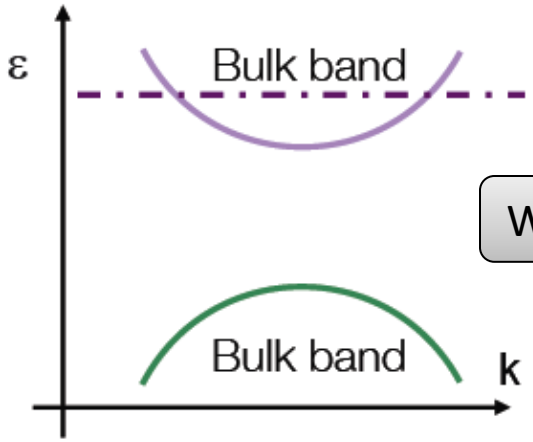


Two copies of the Quantum Hall Effect

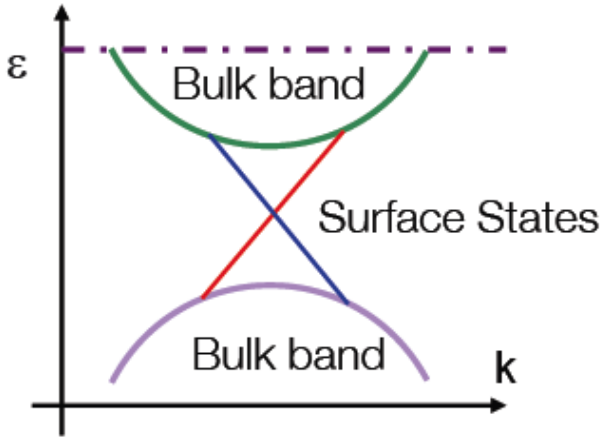
The Quantum Hall effect had skipping orbits induced edge states

What is the counterpart in the case of a spin dependent B field ?

The edge/surface states…



We need to produce this →



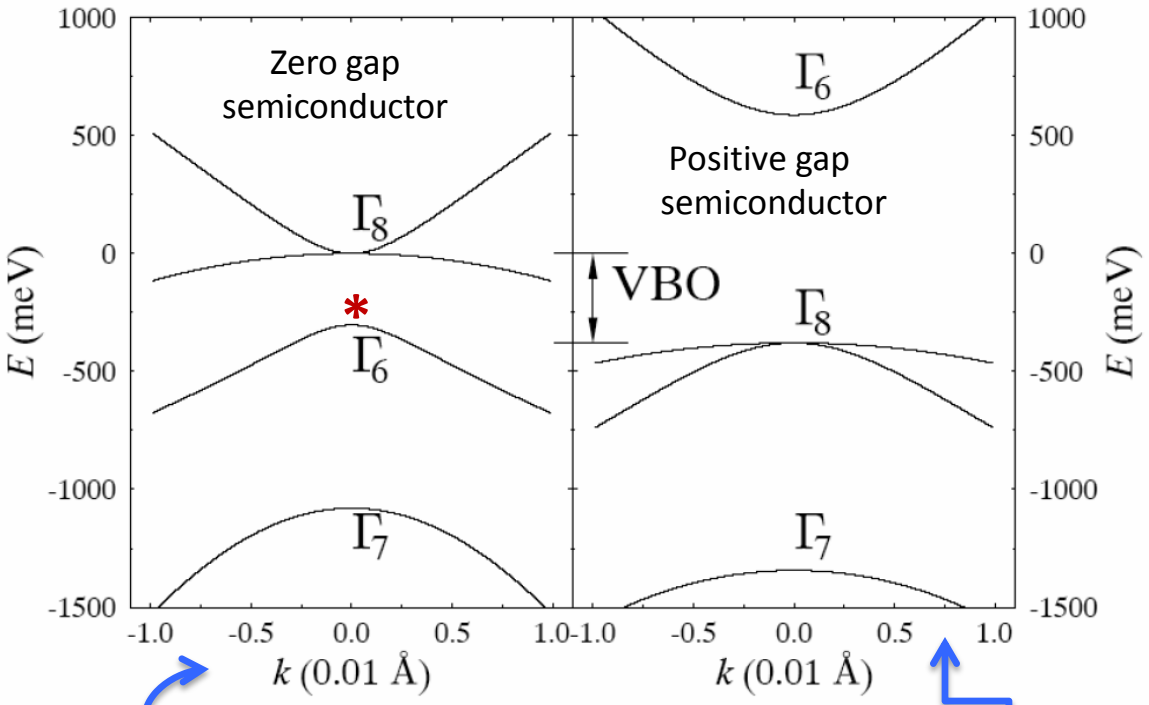
Normal Insulator

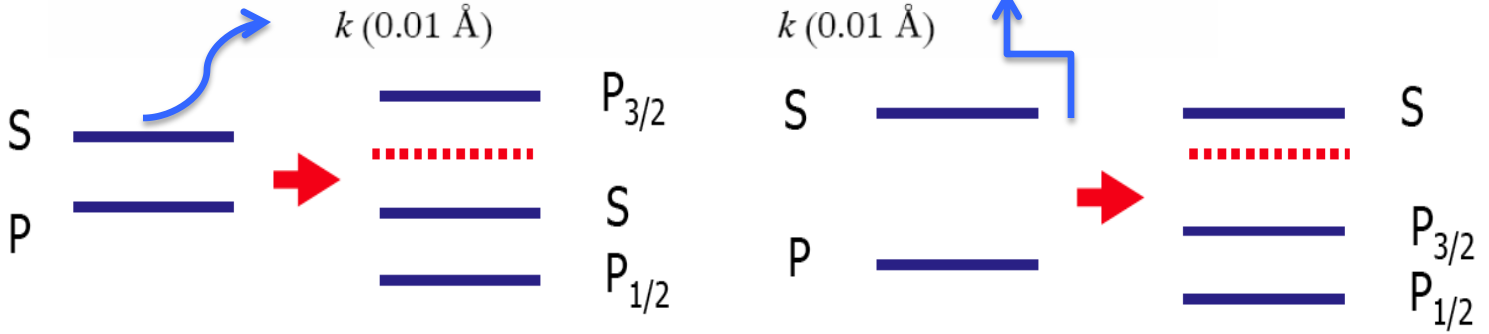
Robust if they are bound to the surface

Every material possesses these surface states but they are fragile to perturbation and disorder

Key question : How to generate a bound surface state ?

Step 1) for bound surface states – A zero gap material

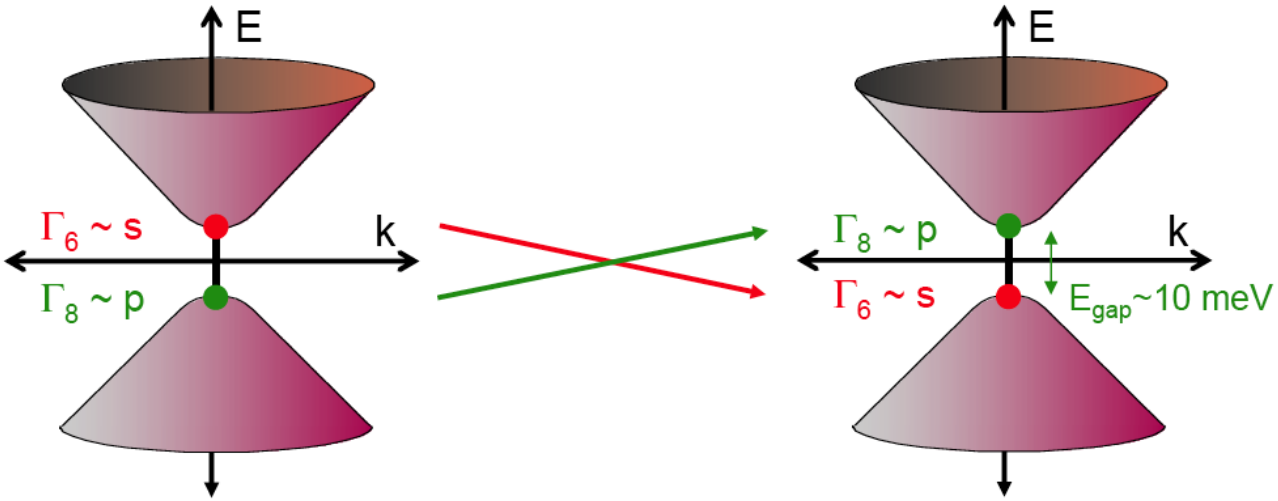




* These notations are valid only for ZB crystals

Step 2) Inversion of the zero gap material

If HgTe is confined – the band gap splits from its zero value to a negative band gap semiconductor

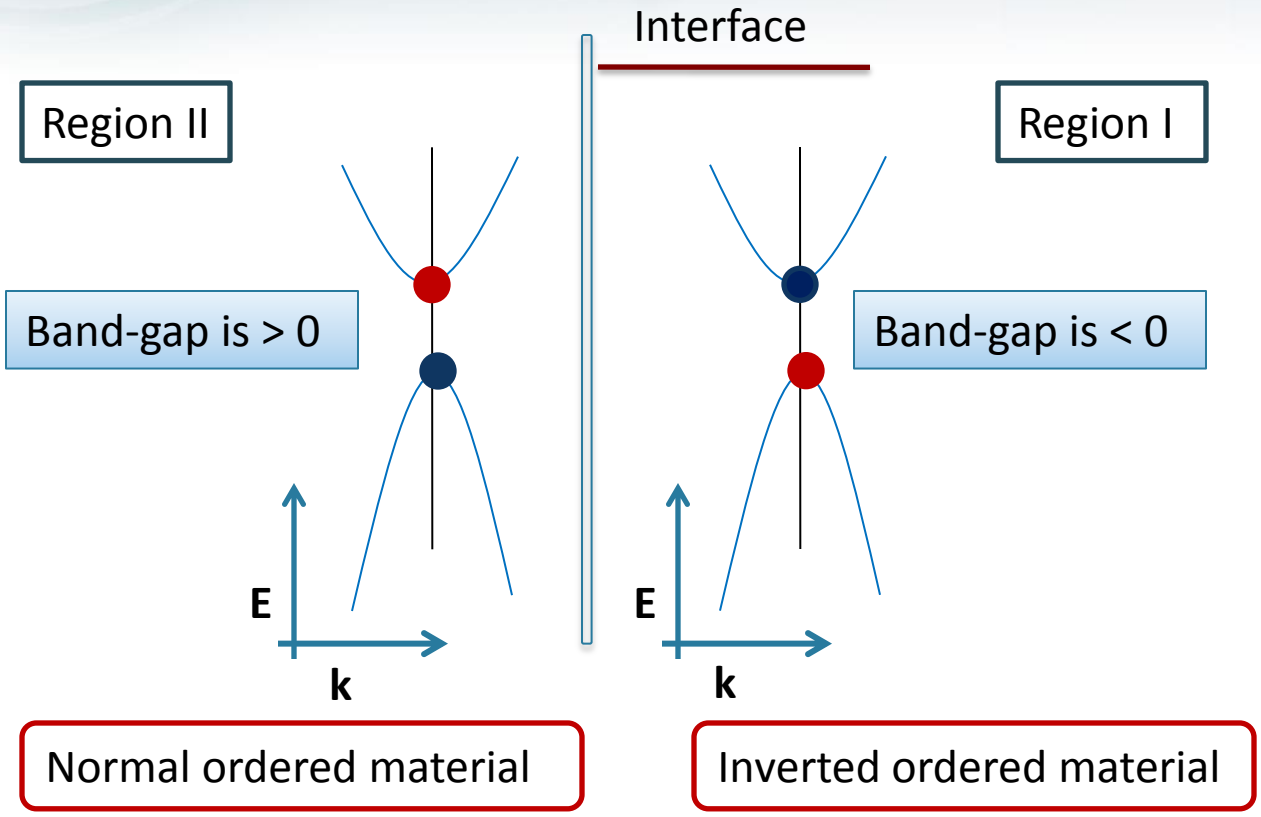


Normal ordered material

Inverted ordered material

Bands of opposite parity (p like band and s like band) interchange their relative positions.

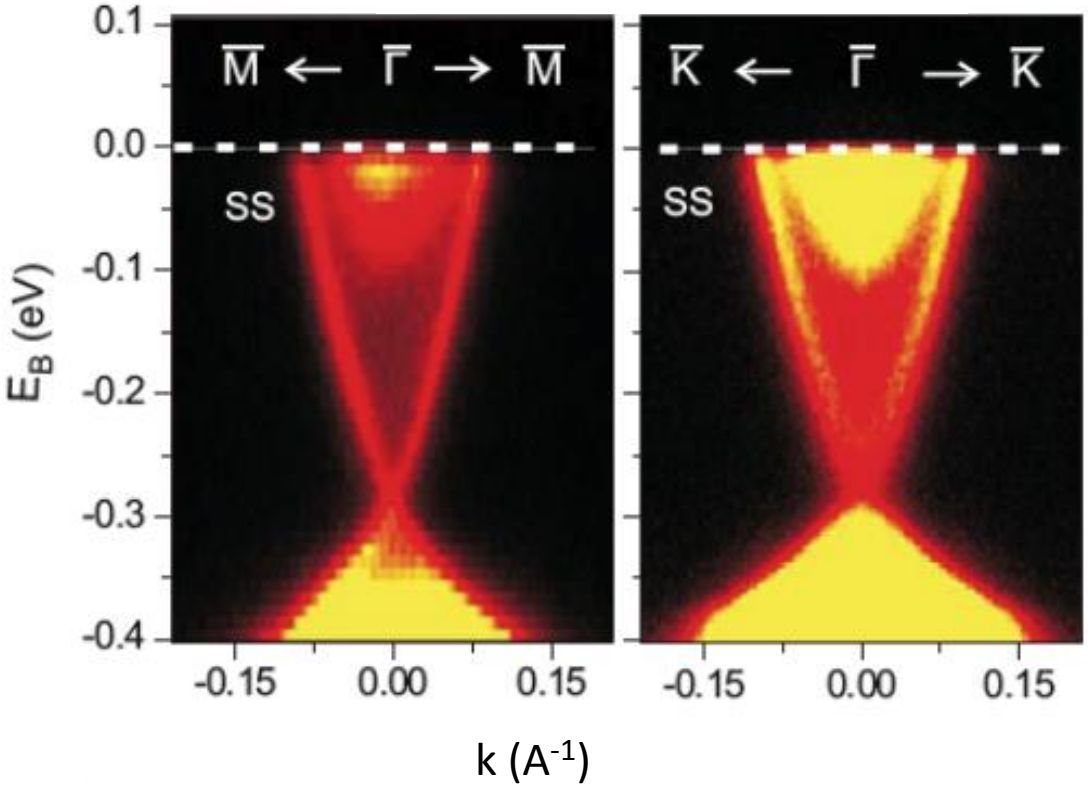
Step 3) Contact with a "normal" band-gap ordered material

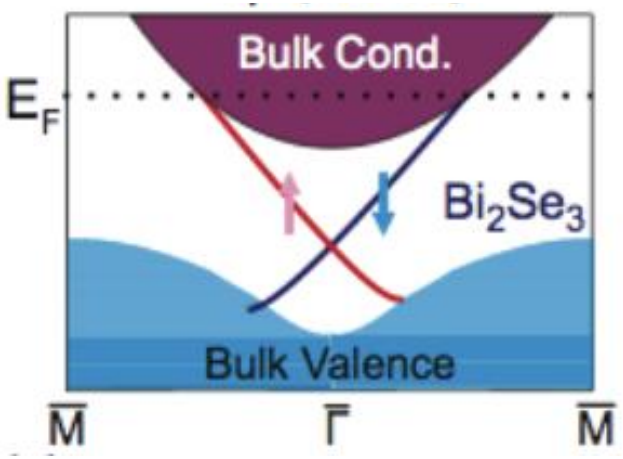


There must be a state that closes the band-gap (band-gap = 0) for a continuous transition from region I to region II

Experimental observations: Surface states of Bi_2Se_3

Surface state are usually probed using ARPES*





Bi_2Se_3 has inverted band order at Γ and is in contact with normal-ordered vacuum

* Angle Resolved Photoemission spectroscopy

The TRIM points

Before we proceed, some basic facts about band structure theory

$E(\vec{k},\uparrow) = E(-\vec{k},\uparrow)$ Space Inversion symmetry (1)

$E(\vec{k},\uparrow) = E(-\vec{k},\downarrow)$ Time reversal symmetry (2)

If both space inversion and time reversal symmetry are simultaneously fulfilled, then the following holds

$E(\vec{k},\uparrow) = E(\vec{k},\downarrow)$ Spin degeneracy occurs at the same $\vec{k}$ point (3)

There are certain special points on the Brillouin zone where equation (3) is always true

Such points are known as **T**ime **R**eversal **I**nvariant **M**omenta Points (TRIM)

TRIM points

On the surface Brillouin zone which is 2D, there are four TRIM points

$$(0,0), (\pi, 0), (0, \pi), (\pi, \pi)$$

Let us pick $(\pi, 0)$ to prove that it ***is*** TRIM

Step 1 : Does space inversion symmetry hold ?

$(\pi, 0) \xrightarrow{\text{yields}} (-\pi, 0)$: Separated in k-space by 2π

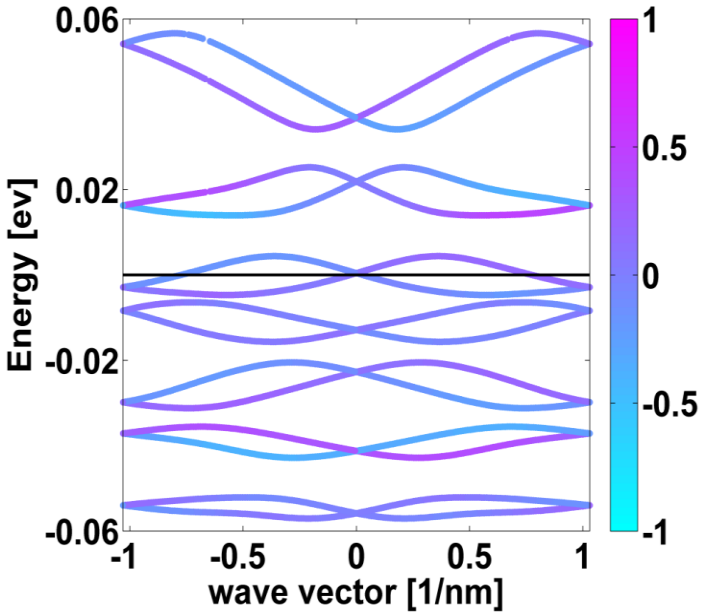
Bloch's theorem tells that points separated by 2π are equivalent

$\therefore$ $(\pi, 0)$ and $(-\pi, 0)$ are space inversion symmetric

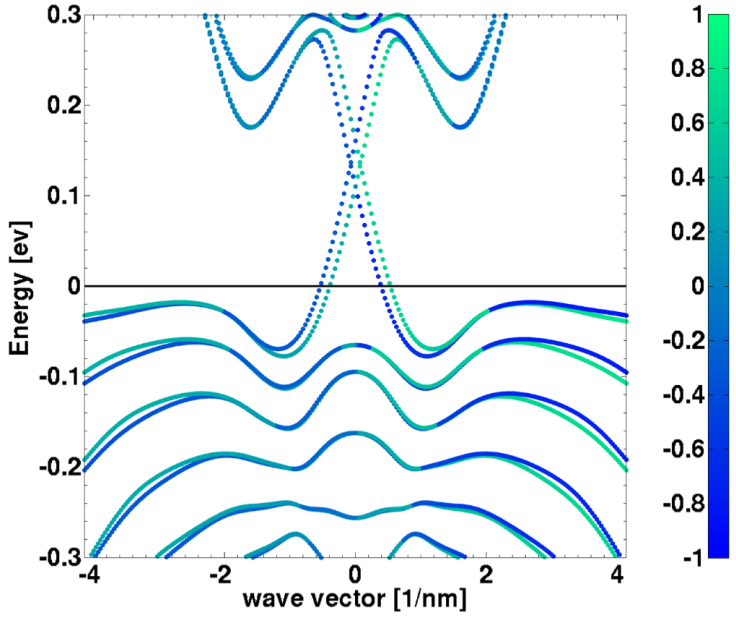
Time reversal symmetry holds in general → $(\pi, 0)$ is TRIM!

How does the band structure appear at the TRIM points ?

Trivial Insulator



Topological Insulator



Energy bands are time reversed pairs which are degenerate at $k = 0$ and $k = \pi$

This degeneracy is a fundamental degeneracy that cannot be removed!

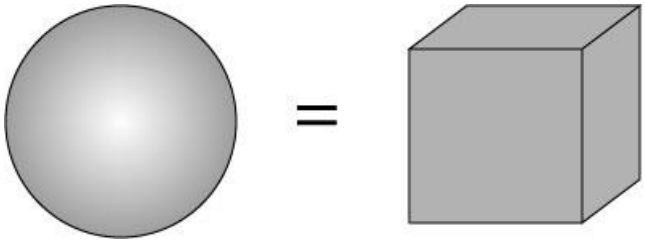
Energy bands are time reversed pairs which are degenerate at $k = 0$ and $k = \pi$

Time reversed pairs of conduction and valence energy bands also meet at $k = 0$ since it is a point of inversion : Fundamental degeneracy !

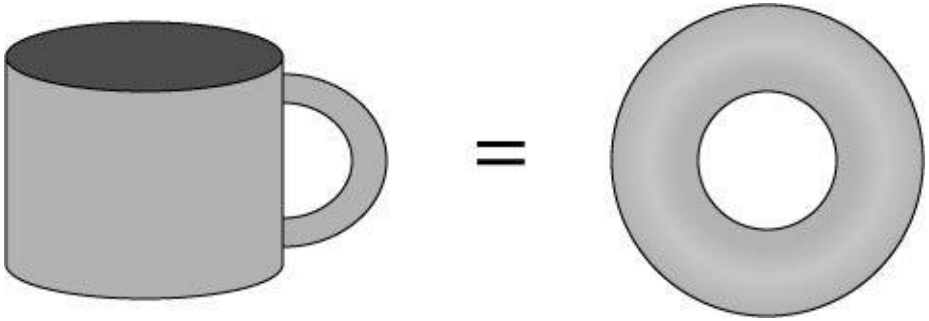
Topology

The key concept is of smooth deformation :

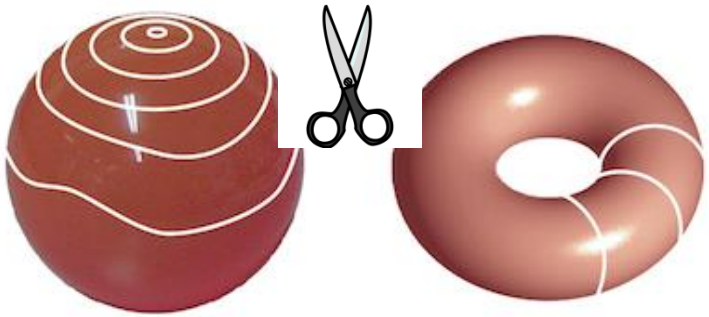
Sphere can be transformed in to an cuboid



A coffee mug in to a donut



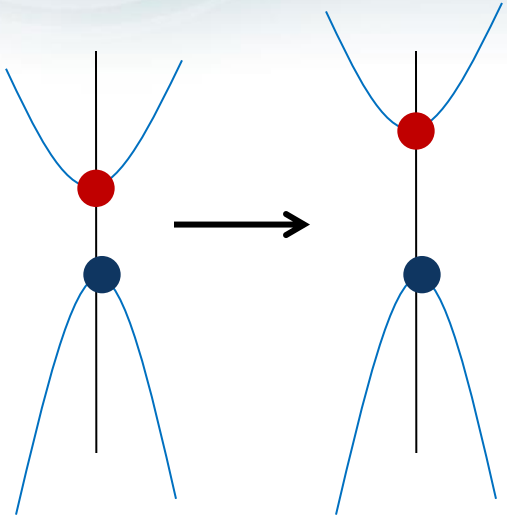
But a sphere cannot be transformed in to a donut without scooping material out of it!



Sphere and donut belong to two different classes

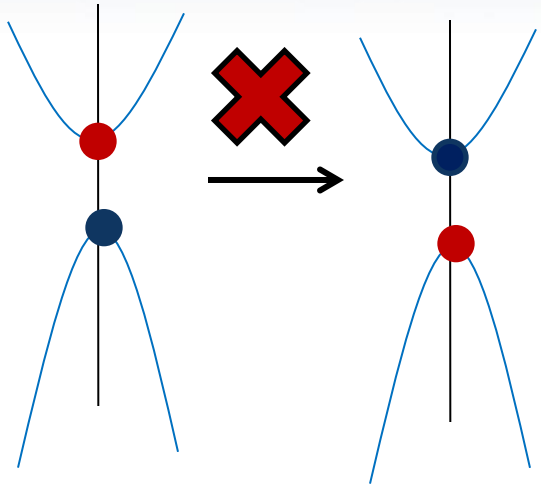
Topology is the property of something that doesn't change when you bend it or stretch it as long as you don't break anything.

Topology and electron bands



Cond band

Valence band



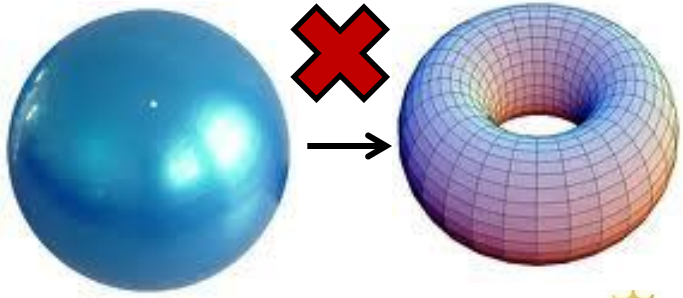
Band-gap > 0 is preserved

Smooth deformation

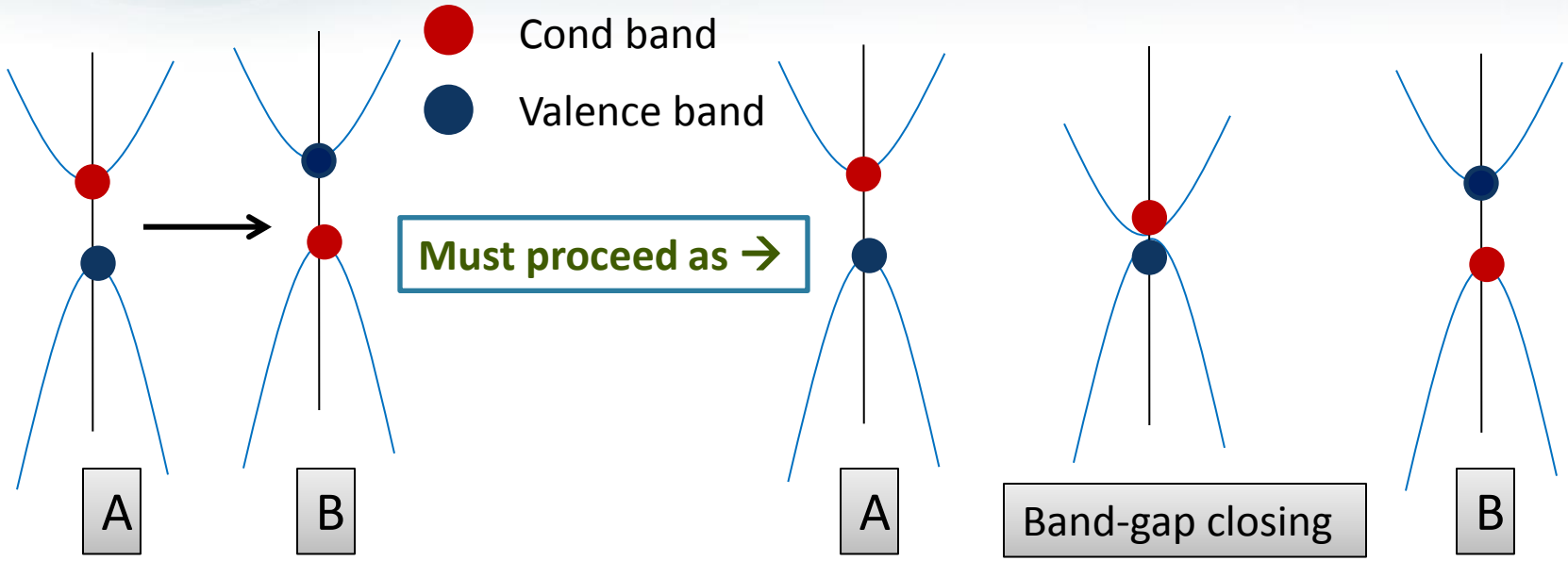
Band-gap changes from + to -

Not a smooth deformation

Positive band-gap and negative band-gap material belong to two different topological classes!



Topology and electron bands



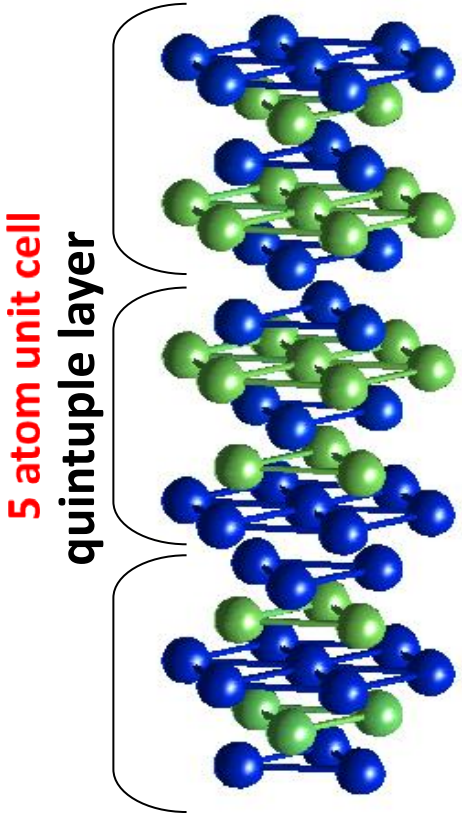
Two topologically inequivalent classes A and B cannot be continuously deformed in to one another. A connection state must be present.

Which compounds exhibit topological insulator behaviour?

Naturally available topological insulators

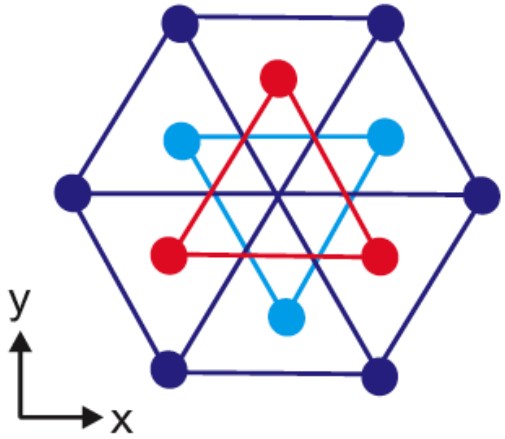
Bi_2Te_3 , Bi_2Se_3 , Sb_2Te_3 are topological insulators: Robust states on the surface under room temperature conditions

Bi_2Te_3



Quintuple layer ordered as Te(1) - Bi(1) -Te(2) - Bi(1) - Te(1)

Inequivalent **Te** atom serves as centre of inversion



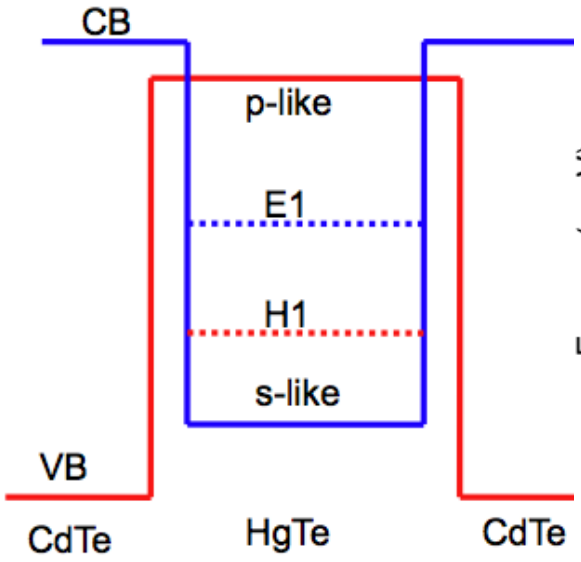
These belong to the class of 3D topological insulators

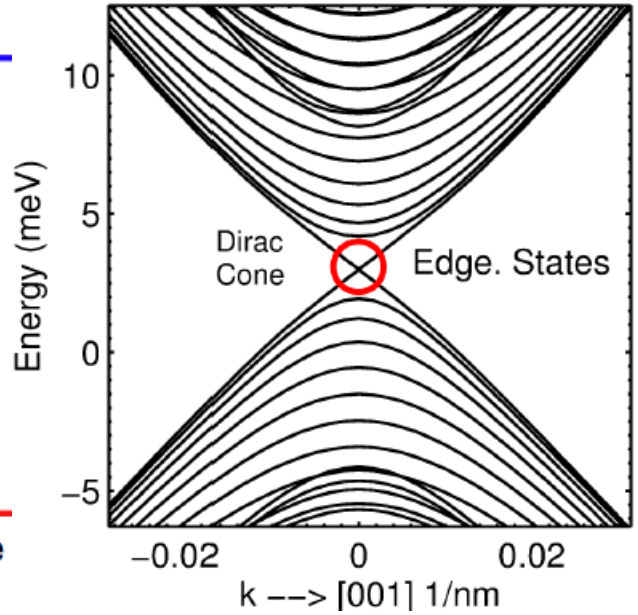
Engineered topological insulators

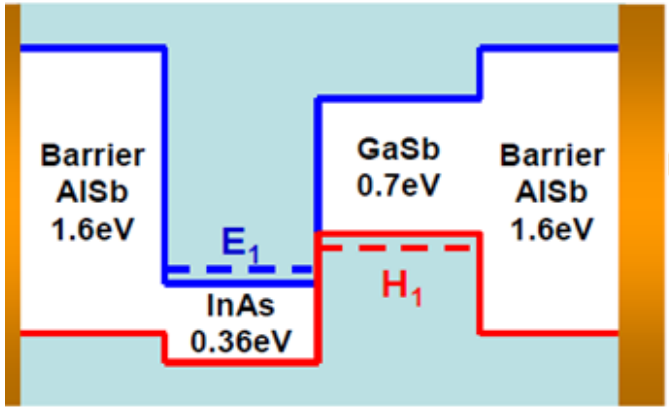
Topological insulators with protected states on the edge of a quantum well

CdTe/HgTe/CdTe quantum well heterostructure (zinc-blende)

GaSb/InAs quantum well heterostructure (zinc-blende)



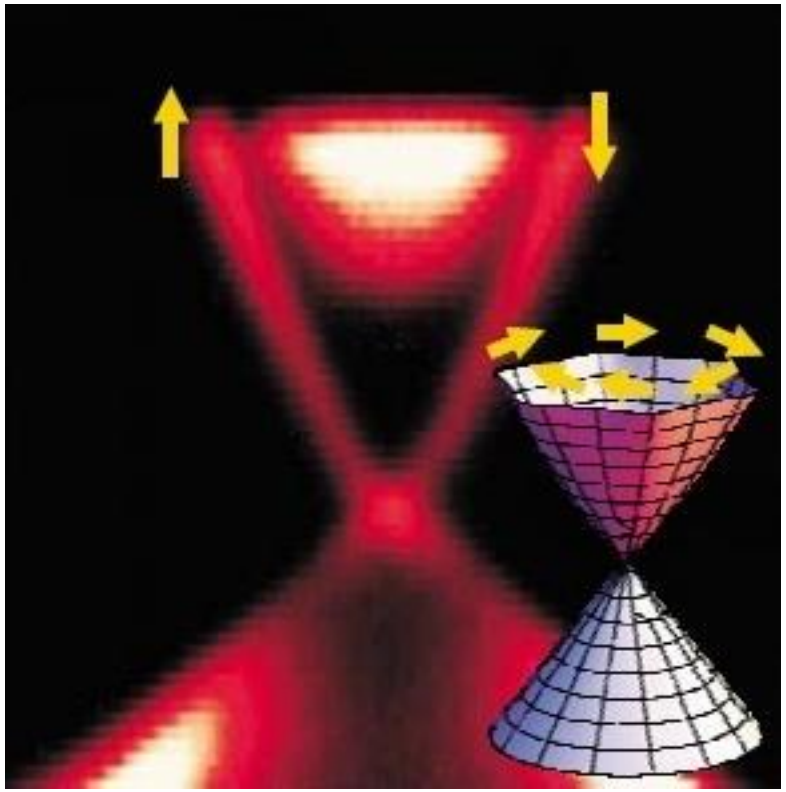




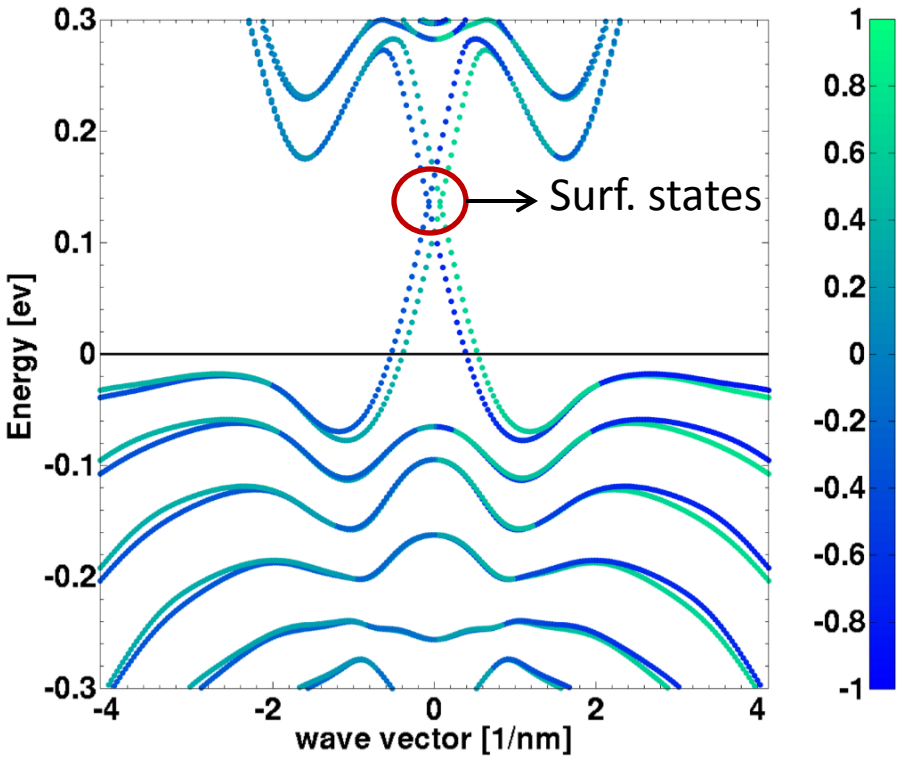
These are known as 2D topological insulators

Numerical modeling of 3D topological insulators

Dispersion obtained through ARPES*



$sp^3d^5s^*$ tight binding calculation

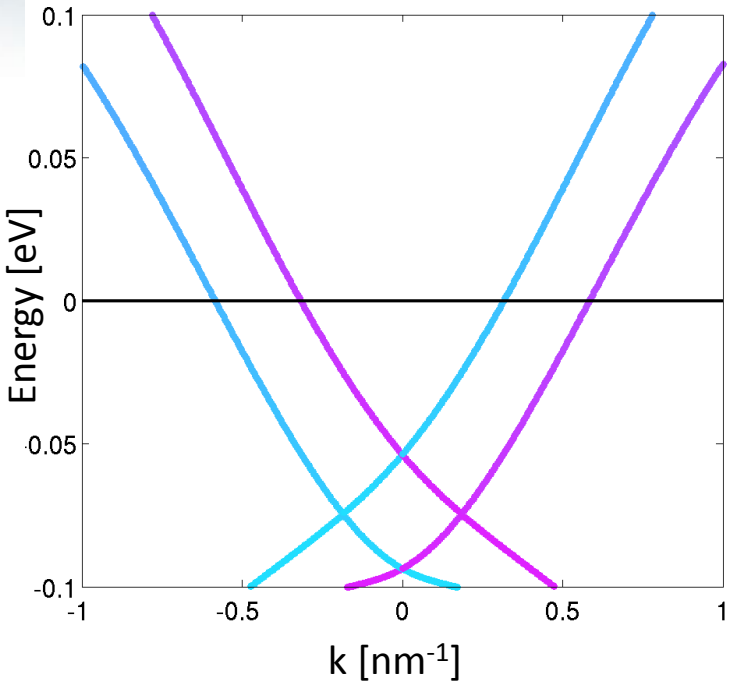


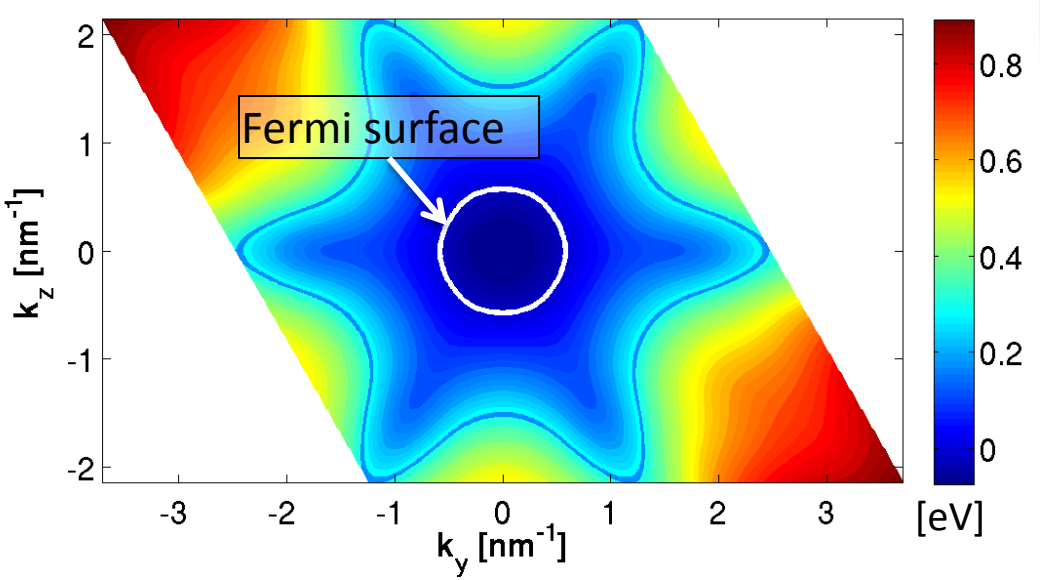
Six quintuple layer (~6.0 nm) Bi_2Te_3 quantum well

Stable surface states (SS) in the mid-gap region

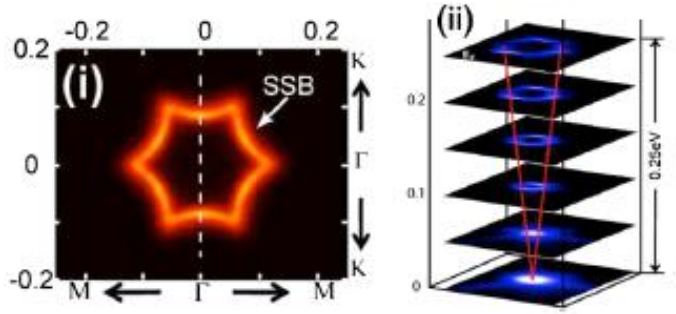
Rev of Mod. Phys, Vol 82, Oct-Dec 2010

Validation: Reproducing experimental Fermi surface warping



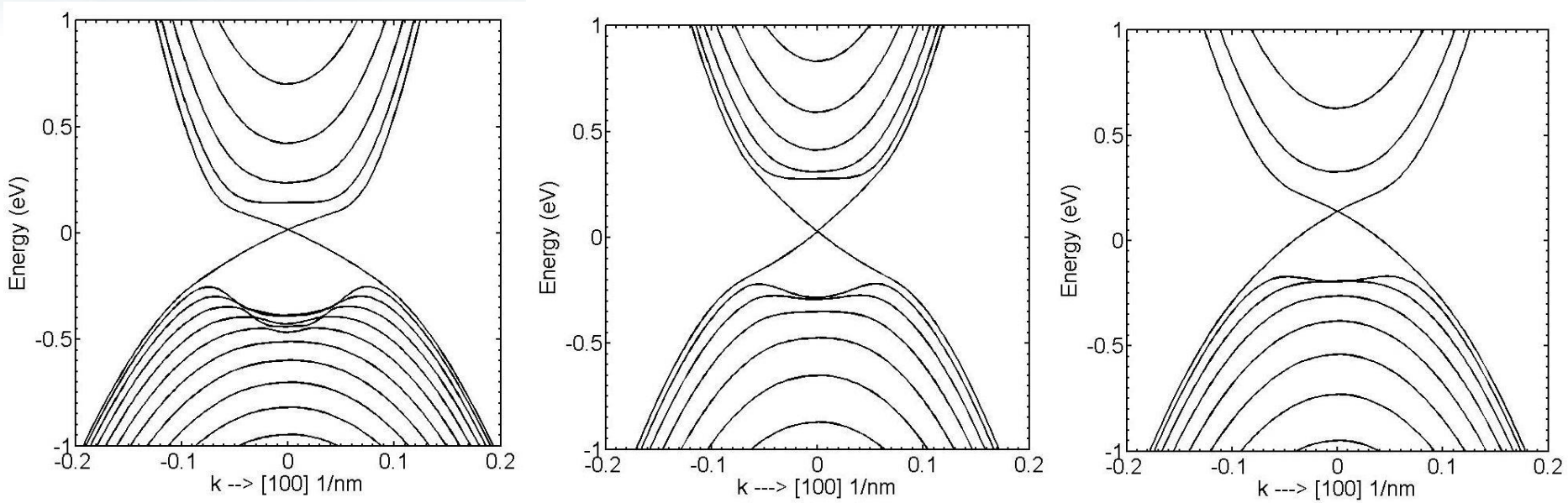


Similar warping of iso-energetic Bi_2Te_3 surfaces has been observed in ARPES measurements.



Numerical calculations performed with 20-band tight binding model

Surface states in a six quintuple layered quantum well (6.0 nm)



Bi_2Te_3 Bi_2Se_3 Sb_2Te_3

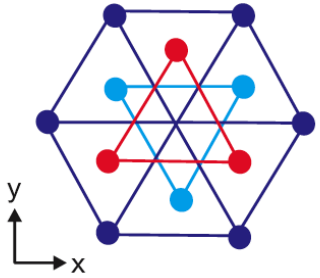
Band structure of 3D topological insulators with 4-band k.p model*

How do k.p calculations compare to tight binding?

Hamiltonian for the surface state

The surface states are characterized by a linear Hamiltonian given as

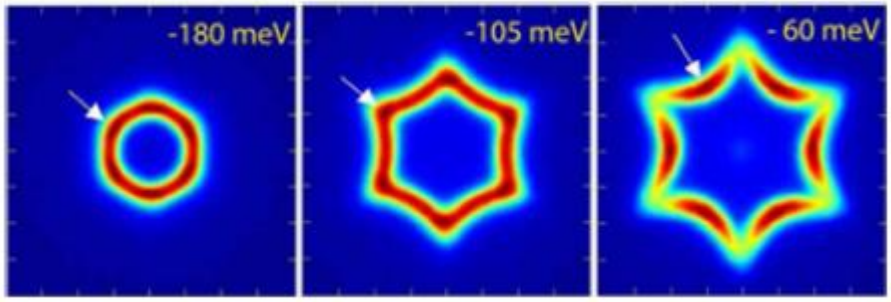
$$\hbar v_f(\sigma_x p_y - \sigma_y p_x)$$



The next higher order term that satisfies C_{3v} symmetry must be k^3

$$\hbar v_f(\sigma_x p_y - \sigma_y p_x) + \lambda(k_+^3 + k_-^3)\sigma_z$$

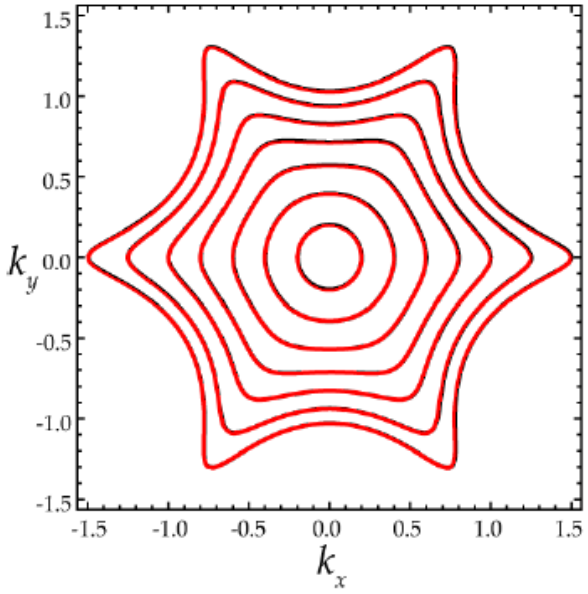
What this means is that as we move away from the Γ point, higher order terms dominate→ Experimentally proven through ARPES*



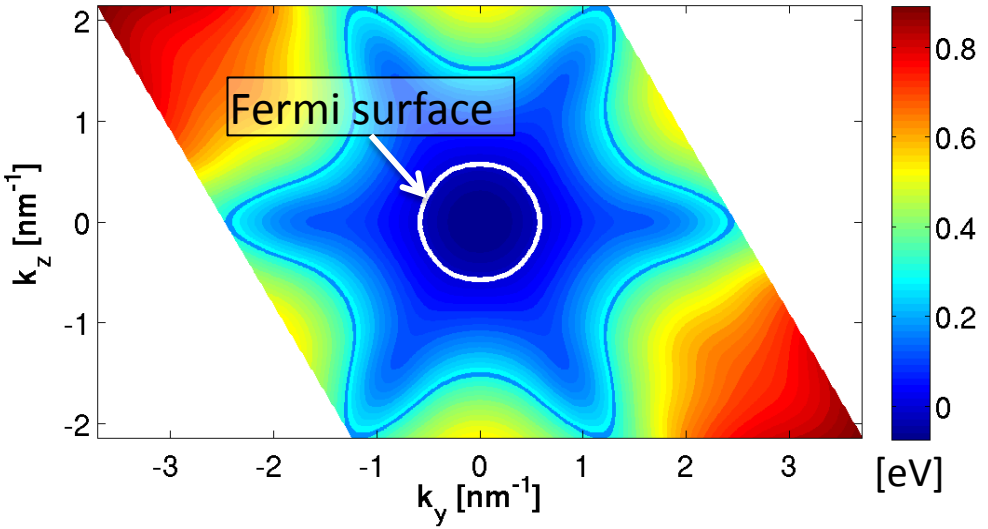
*Physical Review Letters, 104(1):016401, Jan 2010

Comparing k.p to tight binding for 3D TIs

Energy contour with modified k.p that includes higher order k^3 terms



Energy contour with 20-band tight binding



k.p can correctly predict energies close to the Γ point. Full crystal symmetry absent!

$sp^3d^5s^*$ tight binding gives correct Fermi-surface warping → Full symmetry (including higher order terms) included in the Hamiltonian

Common electronic structure trait in 2D and 3D TIs

Both 2D and 3D TIs are narrow band-gap compounds with high spin-orbit coupling

Spin-orbit coupling induces band inversion necessary for a TI

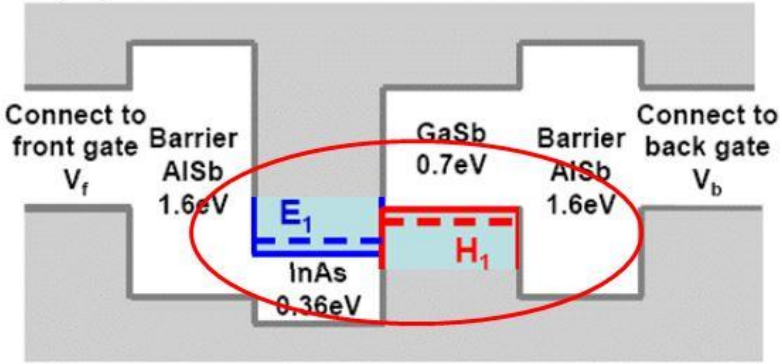
Question : Any other intrinsic mechanism like so-coupling that can invert bands?

Evidence for Helical Edge Modes in Inverted InAs/GaSb Quantum Wells

Ivan Knez and Rui-Rui Du
Department of Physics and Astronomy, Rice University, Houston, TX 77251-1892

Gerard Sullivan
Teledyne Scientific and Imaging, Thousand Oaks, CA 91630

We present an experimental study of low temperature electronic transport in the hybridization gap of inverted InAs/GaSb composite quantum wells. Electrostatic gate is used to push the Fermi level into the gap regime, where the conductance as a function of sample length and width is measured. Our analysis shows strong evidence for the existence of helical edge modes proposed by Liu et al [Phys. Rev. Lett., 100, 236601 (2008)]. Edge modes persist inspite of sizable bulk conduction and show only a weak magnetic field dependence - a direct consequence of gap opening away from zone center.



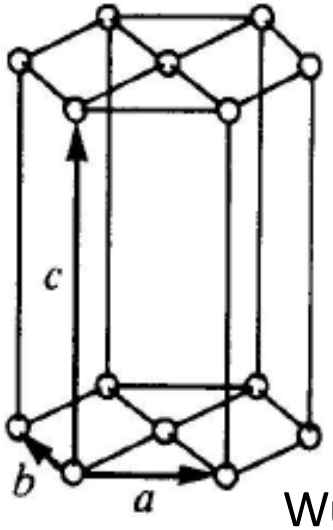
Broken gap devices yield inverted band order

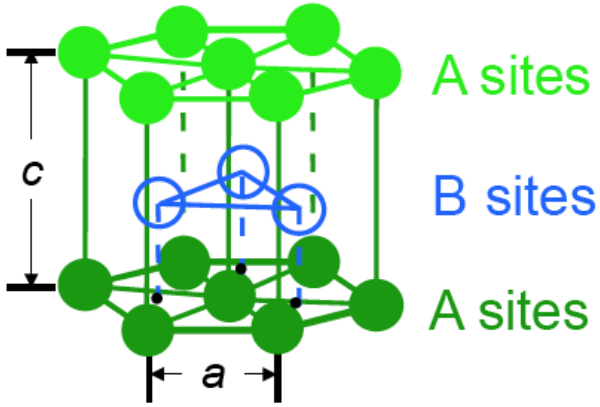
Is there any other crystal attribute that can invert bands?

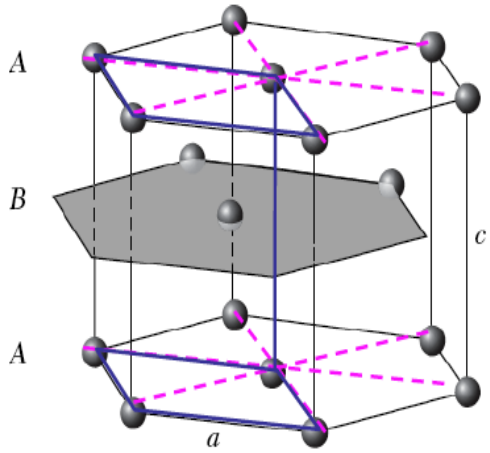
Spin-orbit coupling which inverts bands is effectively an internal magnetic field

Question: Can electric field similarly invert bands?

Commonly used wurtzite-based nitride crystals are moderate ferroelectrics→
Possesses an internal polarization (electric) field : A crystal property



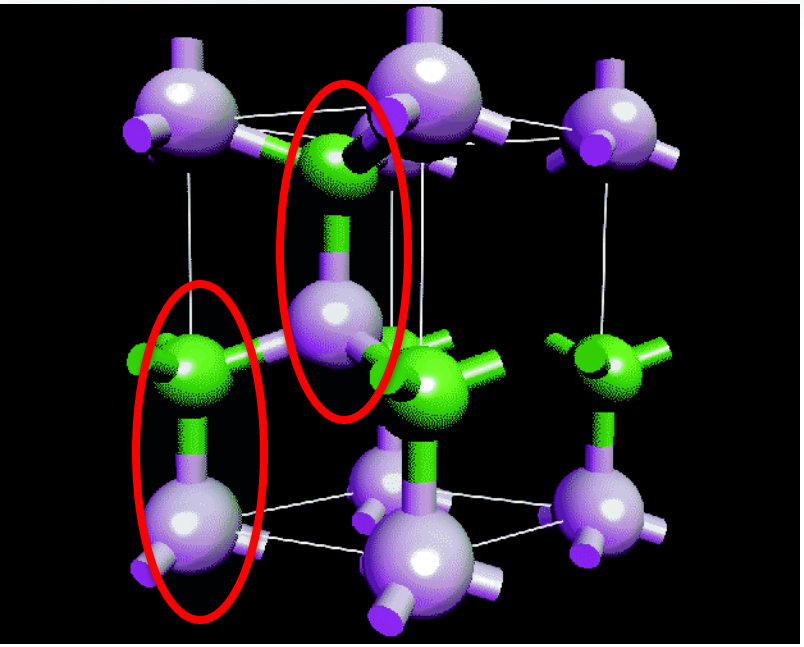




Wurtzite belongs to hexagonal crystal lattice system with two inter-penetrating hcp lattices

c/a = $(8/3)^{1/2}$ → This ratio has curious properties

Spontaneous polarization in Wurtzite crystal

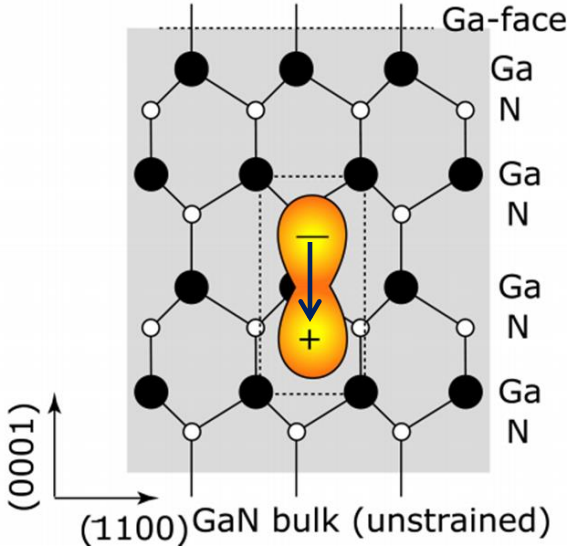


Unit Cell of Wurtzite XN

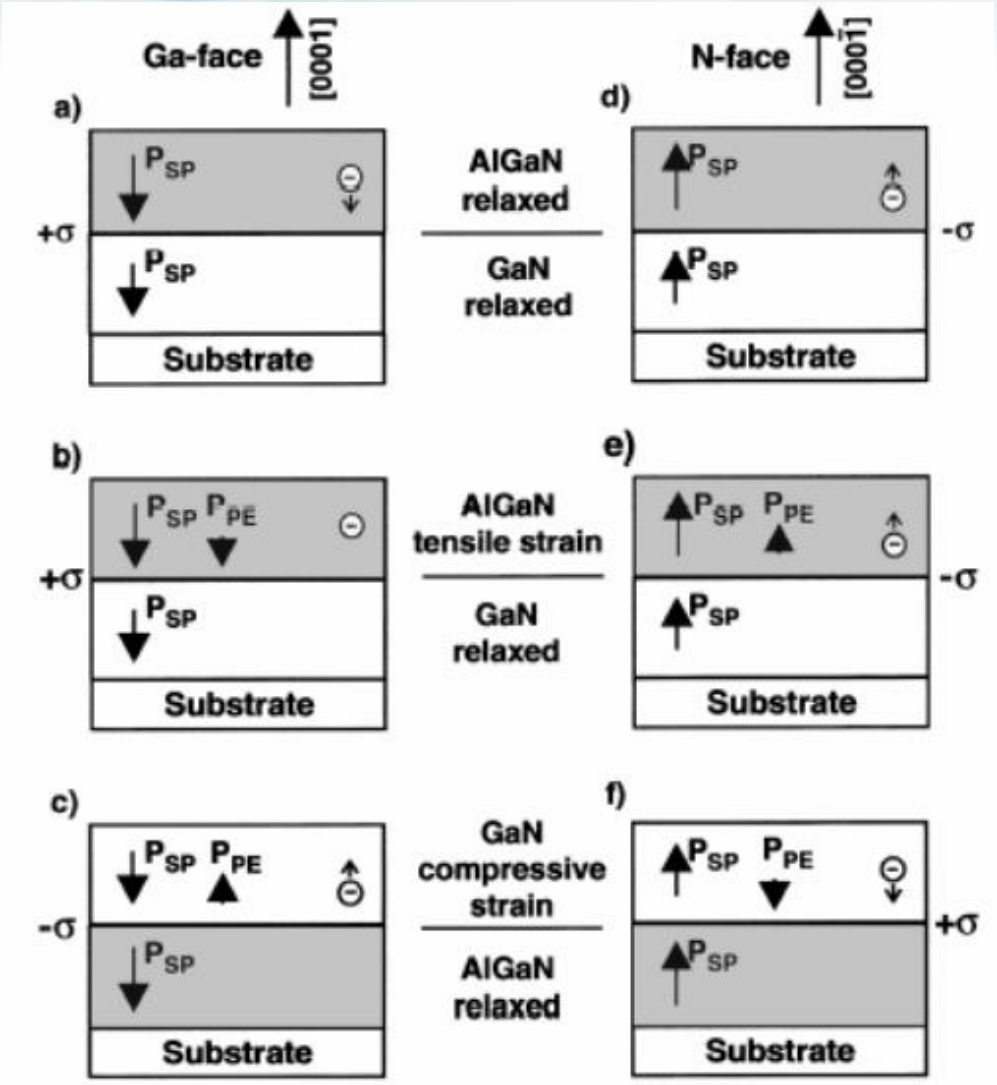
Purple = X (Al, Ga, In) Green = N

Spontaneous Polarization due to crystal asymmetry in wurtzite

- In ideal wurtzite crystal the c/a ratio = $(8/3)^{1/2}$
- In real wurtzite crystal this ratio is altered
  - The X-N (X = Al, Ga, In) bond along c-axis is deformed leading to a net dipole moment
- The dipoles cancel in bulk but remain at the surface



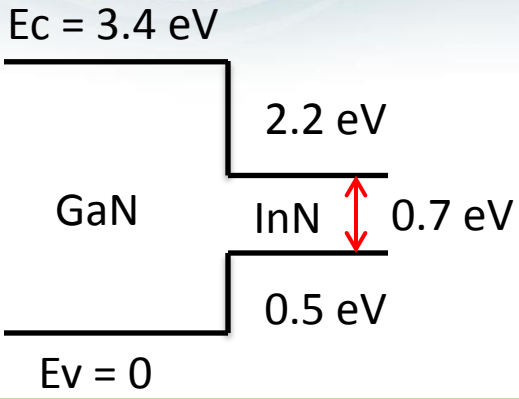
Schematic showing operation of internal E-field in nitrides*



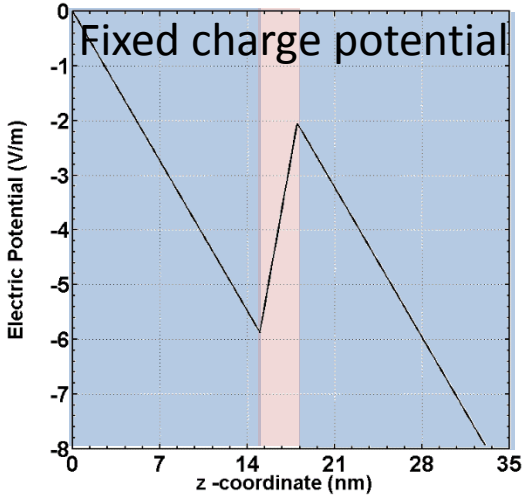
1. To invert the band order internal electric field must be maximized
2. Piezoelectric field is stronger than spontaneous polarization
3. A strong piezo field needs a large strain
4. InN grown on GaN has large strain (~11 % lattice mismatch)
5. InN is a narrow band-gap material

*Journal of Applied Phys. Vol.85, 3222 (1999)

The GaN-InN-GaN system



Straddling : Type-I heterojunction



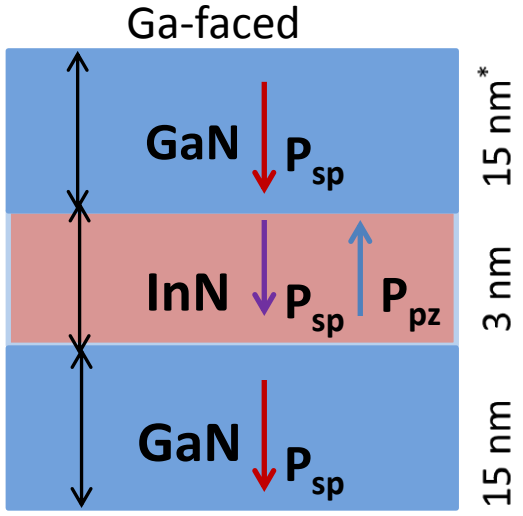
Potential drop in InN well = 3.827 V

GaN and InN are lattice mismatched by ~11 %

Large piezoelectric constants result in strong internal electric field

Spontaneous polarization is closely matched → Less significant

GaN is relaxed. InN is biaxially strained (compressive)



Spontaneous and piezoelectric polarization field

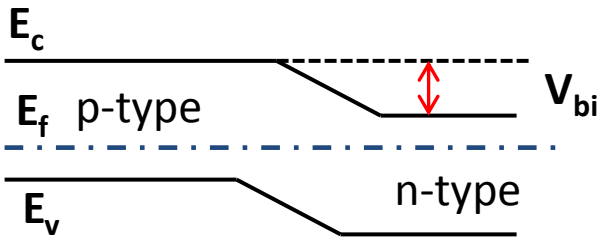
GaN/InN/GaN produces large built-in fields

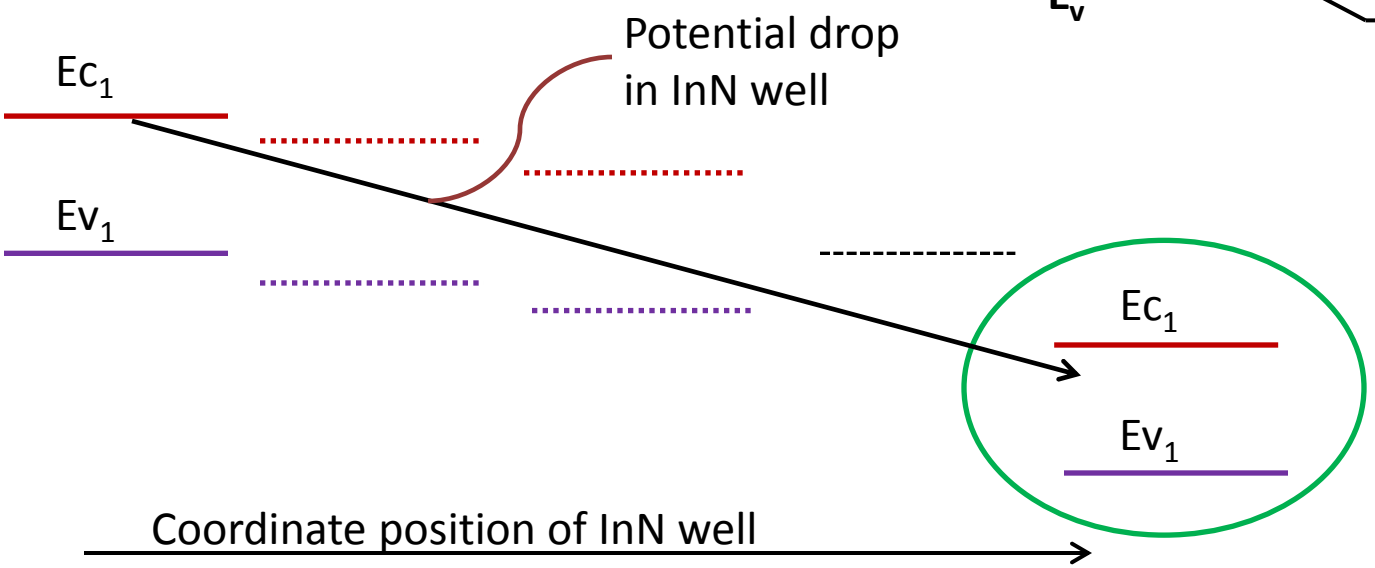
What can this large electric field do?

The large electric field alters the position of the band edges

For instance: Gradient of band edges due to built-in electric field of a p-n junction

Similar trend for the band-edge position of the InN region

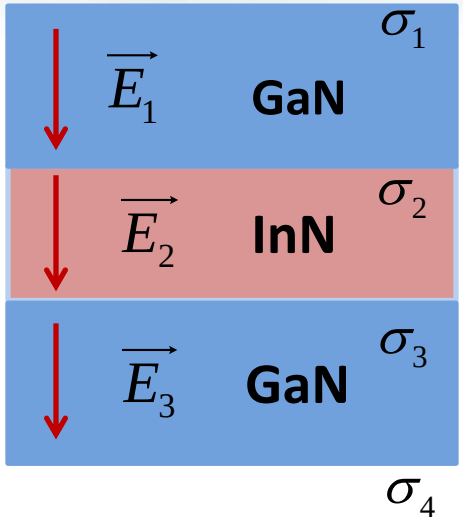




The conduction band edge has fallen below the valence band edge

Creation of a broken-gap heterostructure

8-band k.p electronic structure calculations



$$H = H_{(8x8)} + V_{sp+pz} + H_{strain}$$

H = Eff. Hamiltonian

Strain is computed with the Bir-Pikus def. potentials

$$\varepsilon_1 \vec{E}_1 = \sigma_1 \qquad \sigma_1 = \sigma_{sp}(GaN)$$

$$\varepsilon_2 \vec{E}_2 - \varepsilon_1 \vec{E}_1 = \sigma_2 \qquad \sigma_2 = -\sigma_{sp}(GaN) + \sigma_{sp}(InN) + \sigma_{pz}$$

$$\varepsilon_1 \vec{E}_3 - \varepsilon_2 \vec{E}_2 = \sigma_3 \qquad \sigma_3 = -\sigma_2$$

σ_i = Interface charge

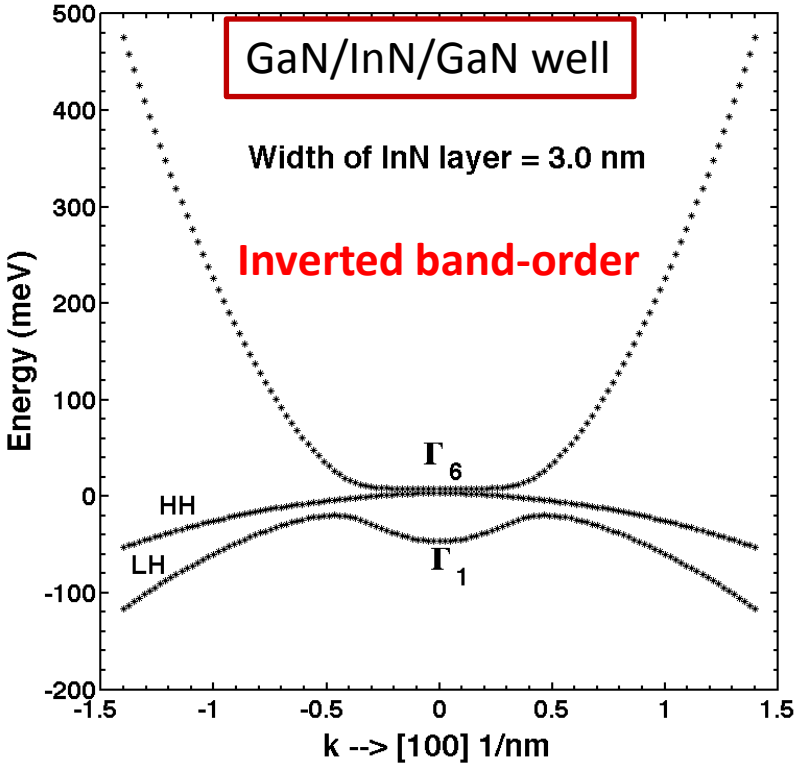
$$\sigma_4 = -\sigma_1$$

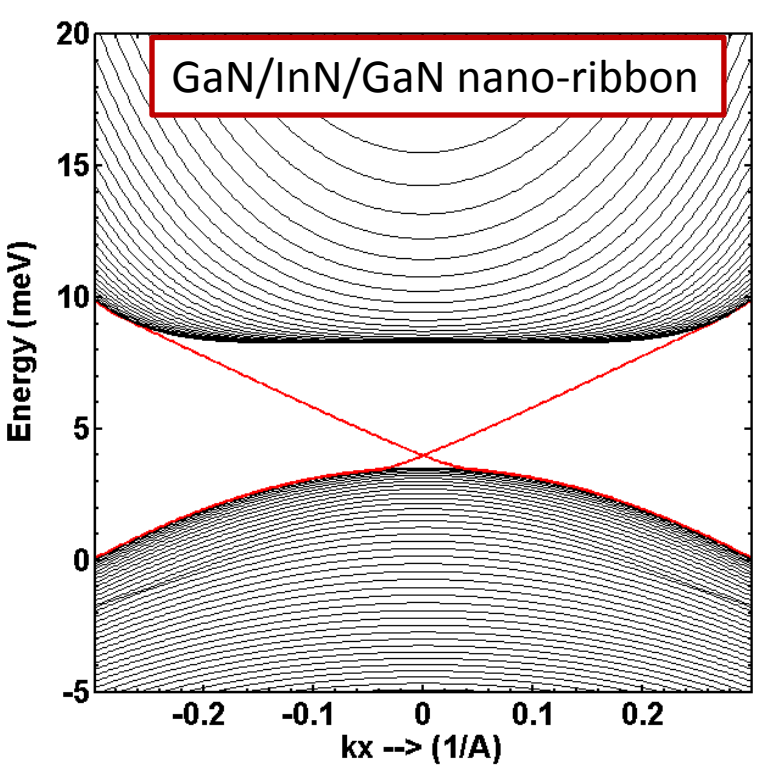
Electric field outside the structure is set to zero

- Geometry Construction
- Structure Relaxation
- Strain
- Electrostatics
- Hamiltonian Construction
- Eigen Solver
- Single Particle Energies

ε_1 and ε_2 are dielectric const. of GaN and InN respectively

Band profile of the GaN/InN/GaN heterostructure



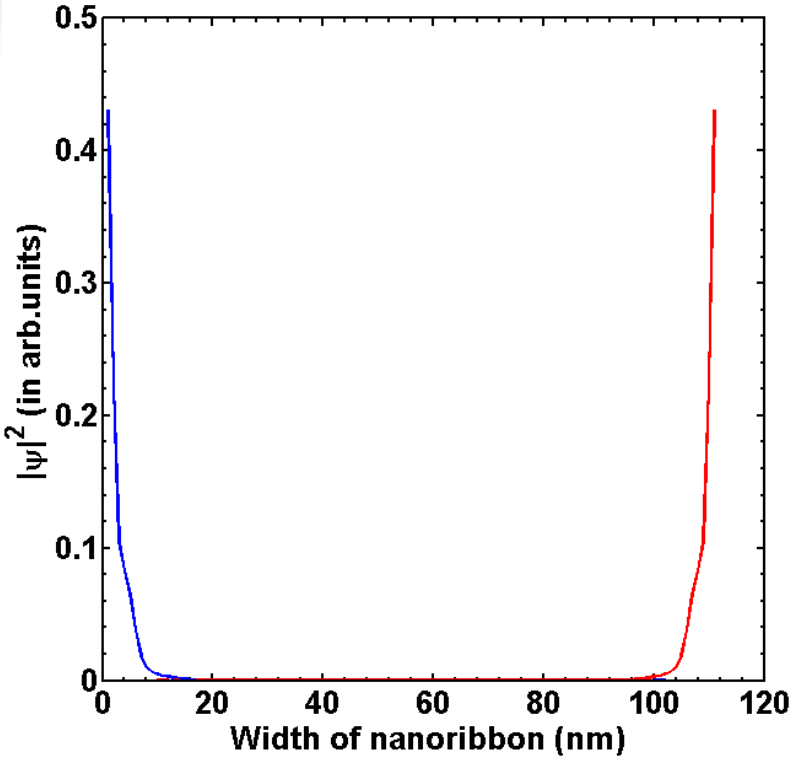


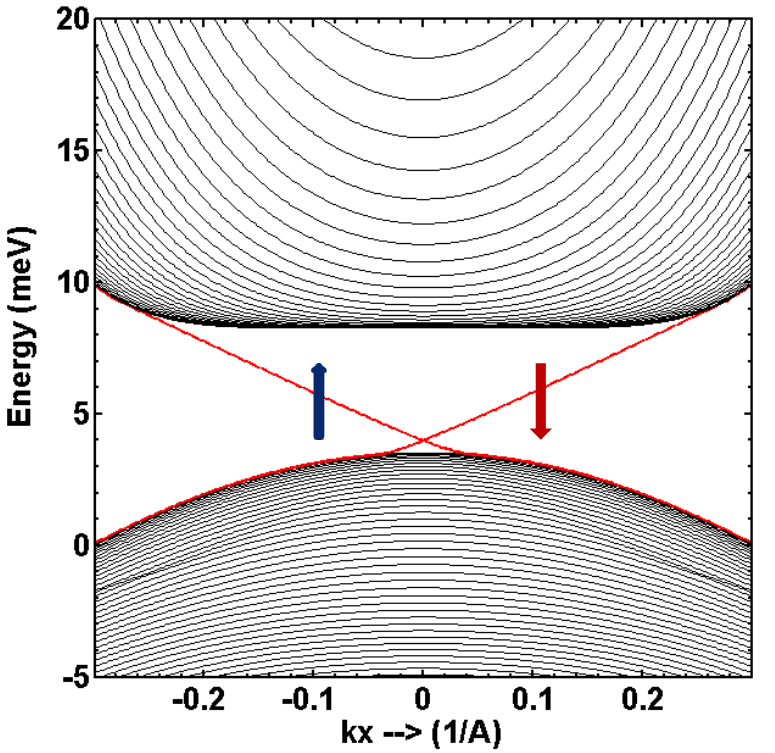
In a normal-ordered nitride in wurtzite phase : *Γ_1 is energetically placed over Γ_6* at the Γ point

Mid-gap linearly dispersing states → Signature of a Topological Insulator

Topological insulator states obtained by constructing a nano-ribbon of width 100 nm from inverted quantum well on left

Wave function of the surface states





Mid-gap states localized at the surface

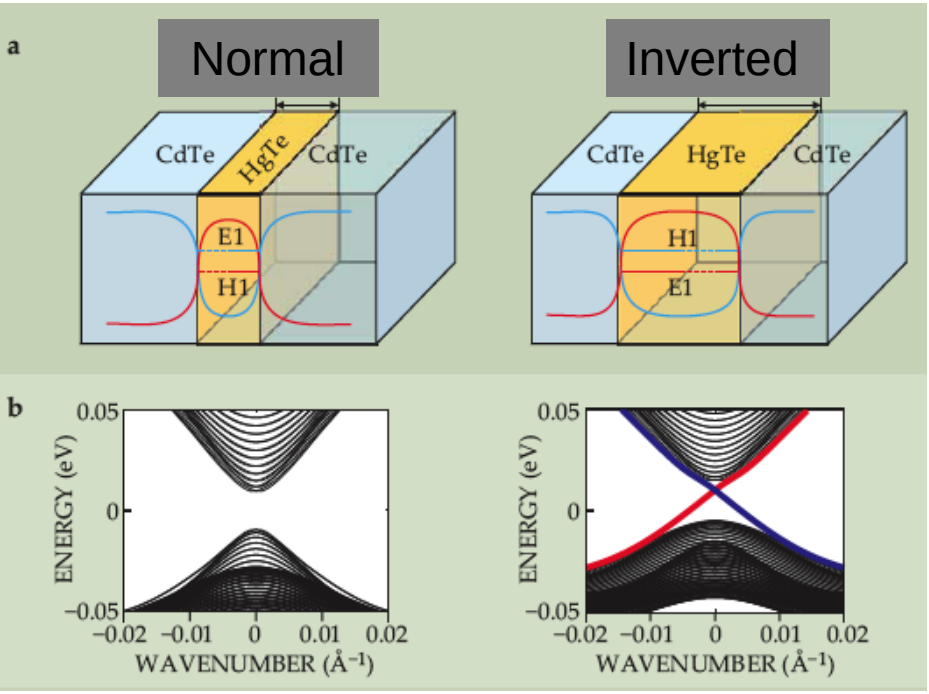
Spin-polarization of bands along z-axis

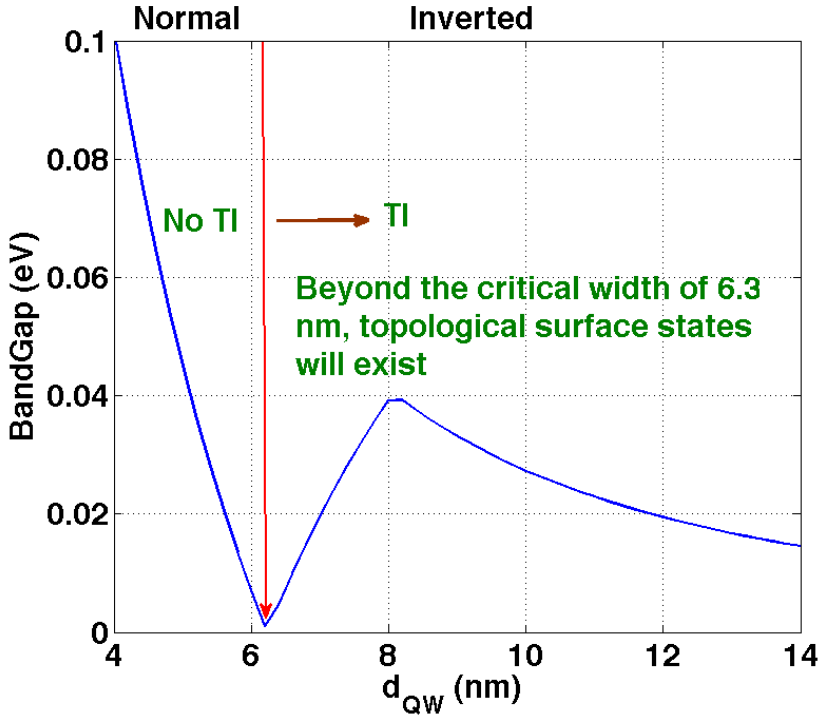
Zero spin-component along x and y axes.
Spin perpendicularly locked to momentum

Another geometry dependent TI is CdTe/HgTe quantum well

Science
AAAS

Quantum Spin Hall Insulator State in HgTe Quantum Wells
Markus König, *et al.*
Science **318**, 766 (2007);
DOI: 10.1126/science.1148047





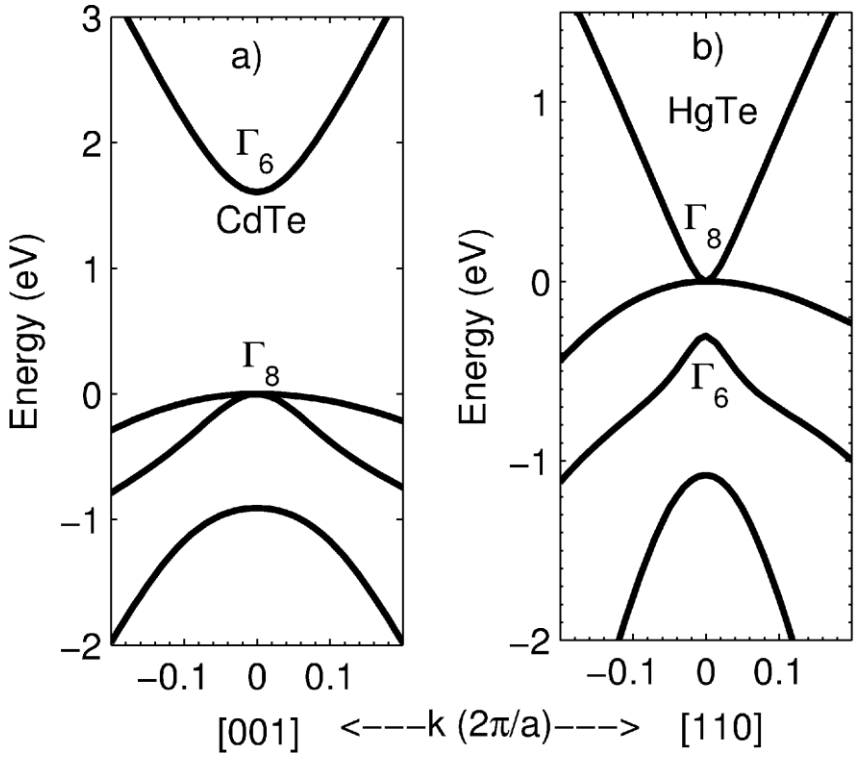
- Quantum well heterostructure (QW) is truncated to form a ribbon
- Bound states exist on the ribbon/edge

The CdTe/HgTe/CdTe quantum well

CdTe/HgTe/CdTe quantum well heterostructure is a 2D topological insulator:

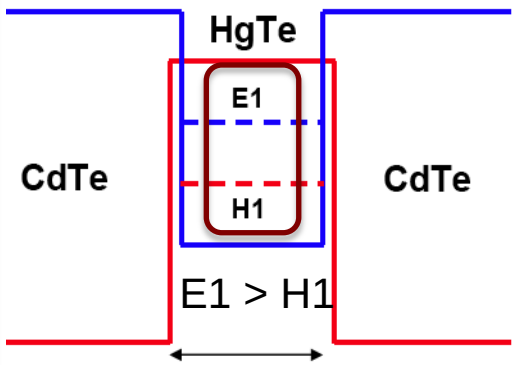
HgTe has inverted band structure and placed adjacent to **CdTe** which is normal band order

Bulk band structure of HgTe and CdTe

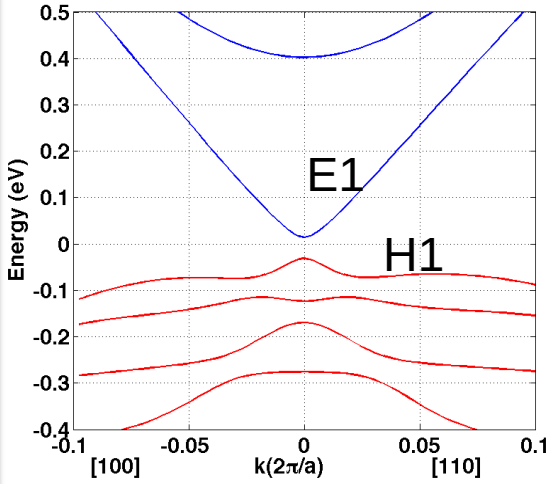


Phase Transition in 2D TI (8 band k.p calculations)

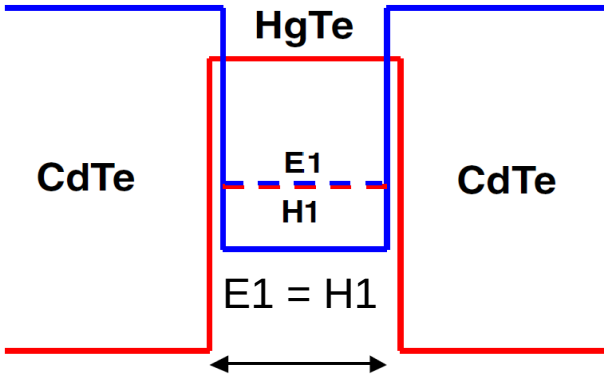
w < 6.3 nm



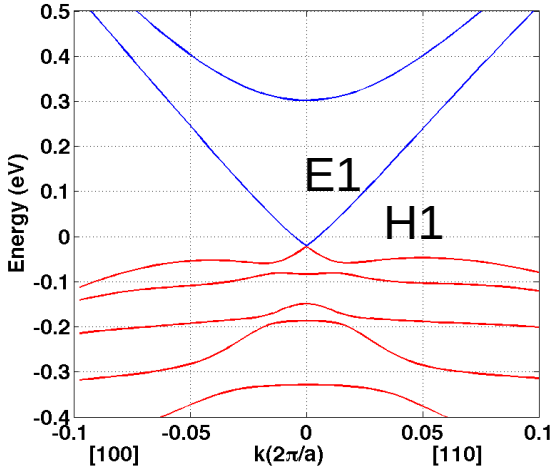
Normal



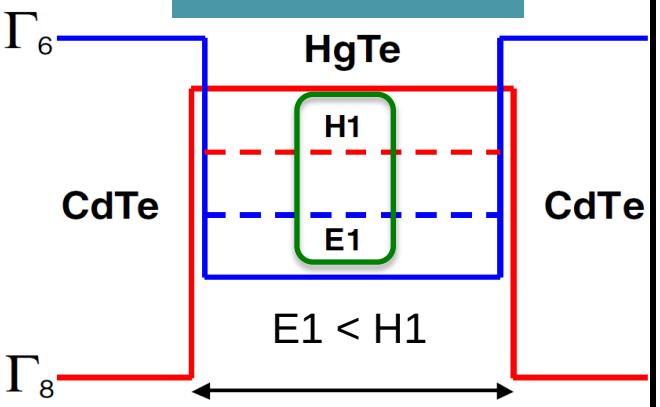
w = 6.3 nm



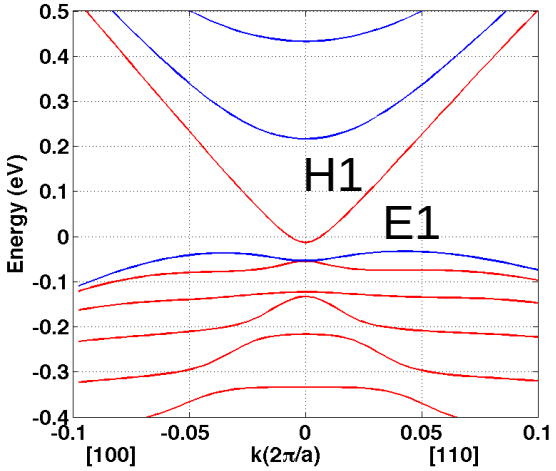
Zero-Gap



w > 6.3 nm

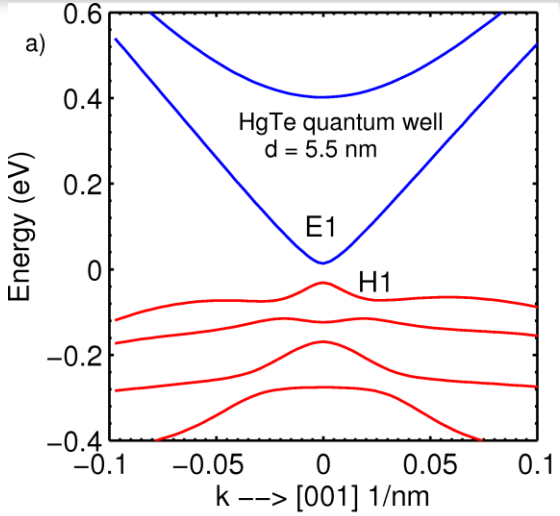


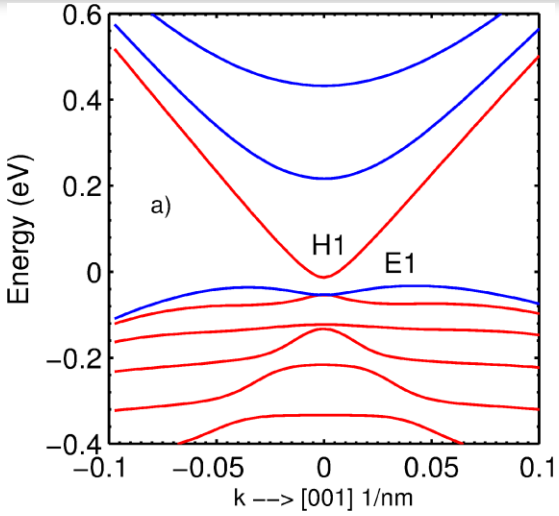
Inverted

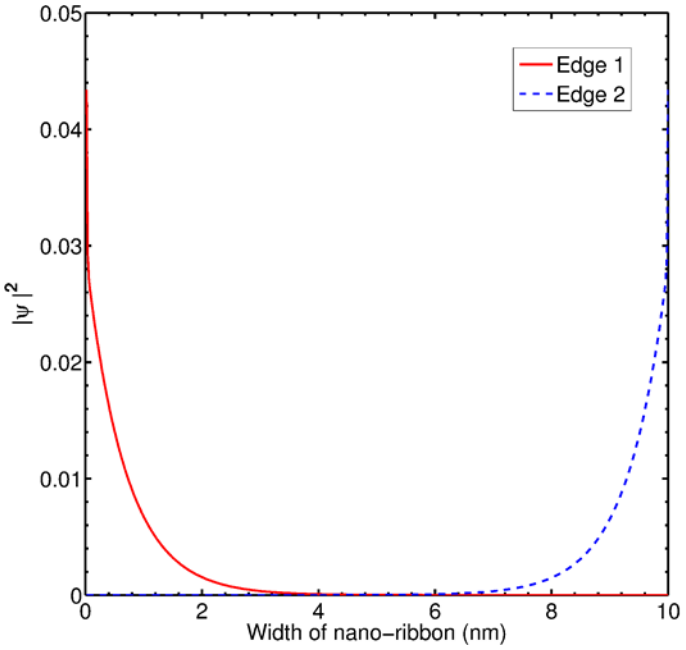


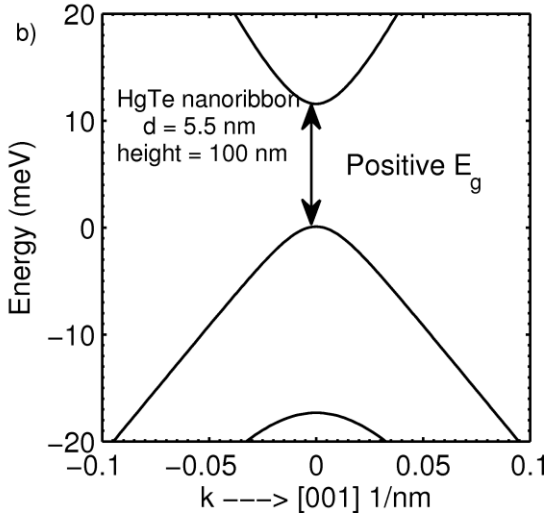
E1 : Electron Band ; H1 : Hole Band ; w : Quantum well width

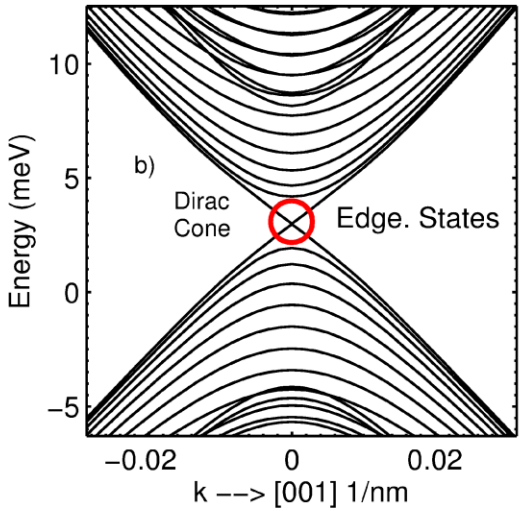
Inverted bulk gives edge/surface states











Amplitude of edge wave function decays in the bulk

Gapped states

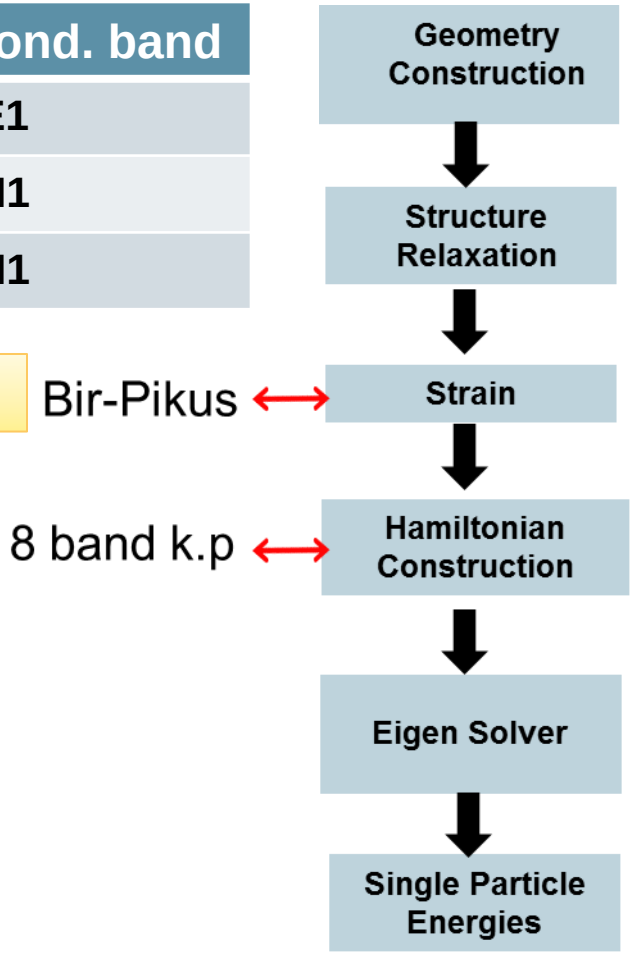
Gapless states

Typical dimensions of a CdTe-HgTe 2D TI

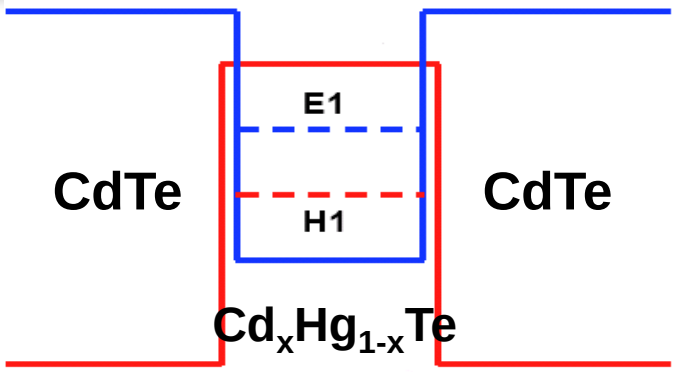
HgTe well	Highest val. band	Lowest cond. band
$d_{QW} < d_C$	H1	E1
$8.2\ nm > d_{QW} > d_C$	E1	H1
$d_{QW} > 8.2nm$	H2	H1

Is the critical width tunable under external influences?

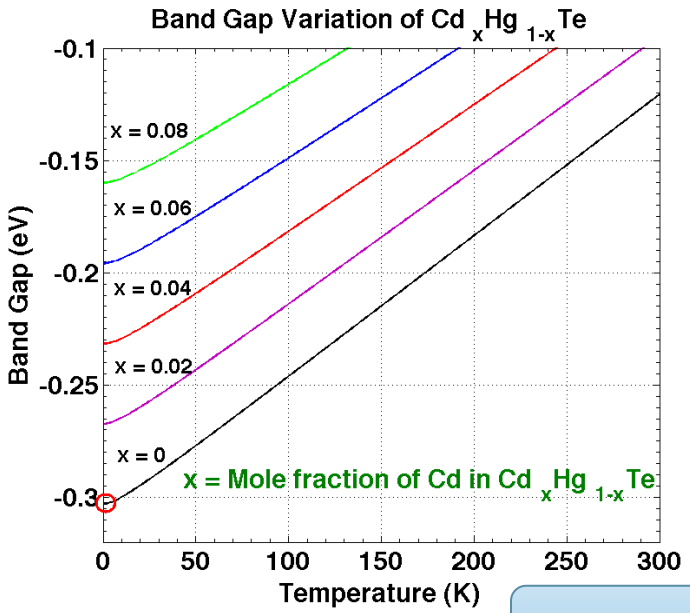
- Well composition
- Changeable barrier potential
- Temperature
- Electric field
- Effective masses of electrons and holes



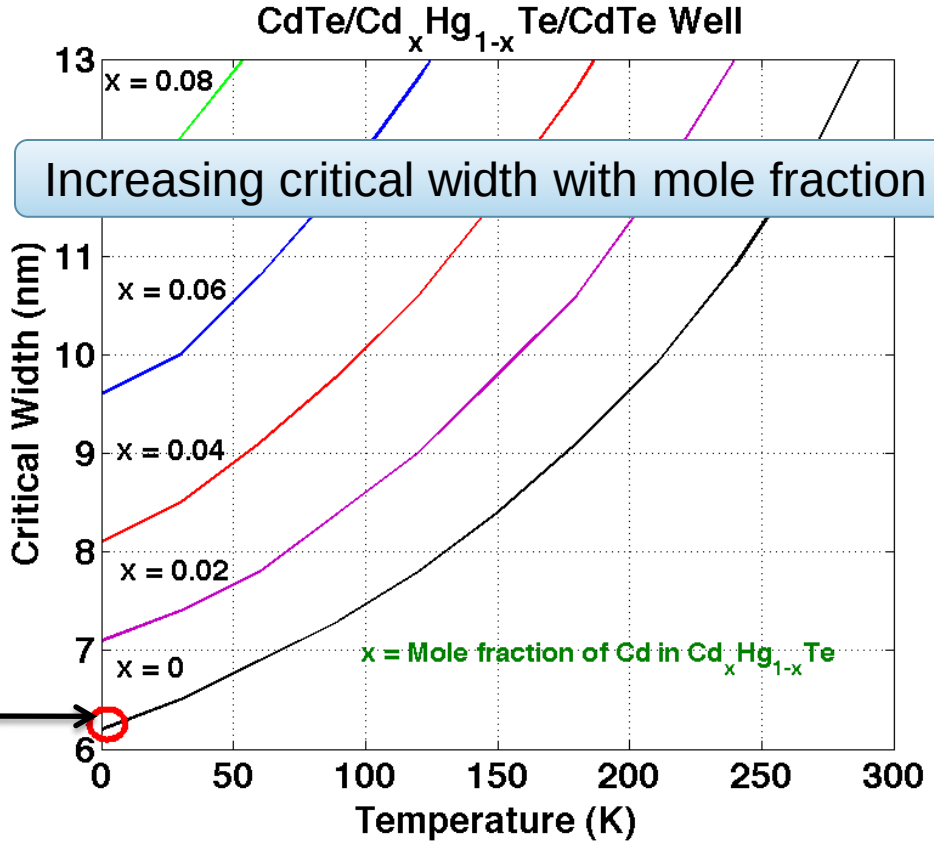
Critical Width as a function of well region



$Cd_xHg_{1-x}Te$ serves as well material



Expt. Value of 6.3 nm

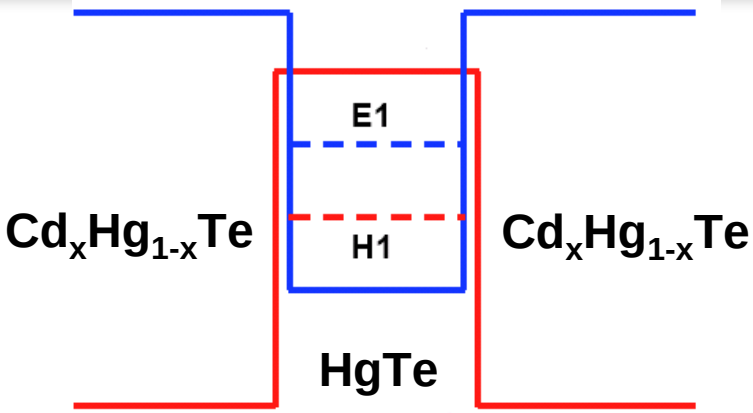


Increasing critical width with mole fraction

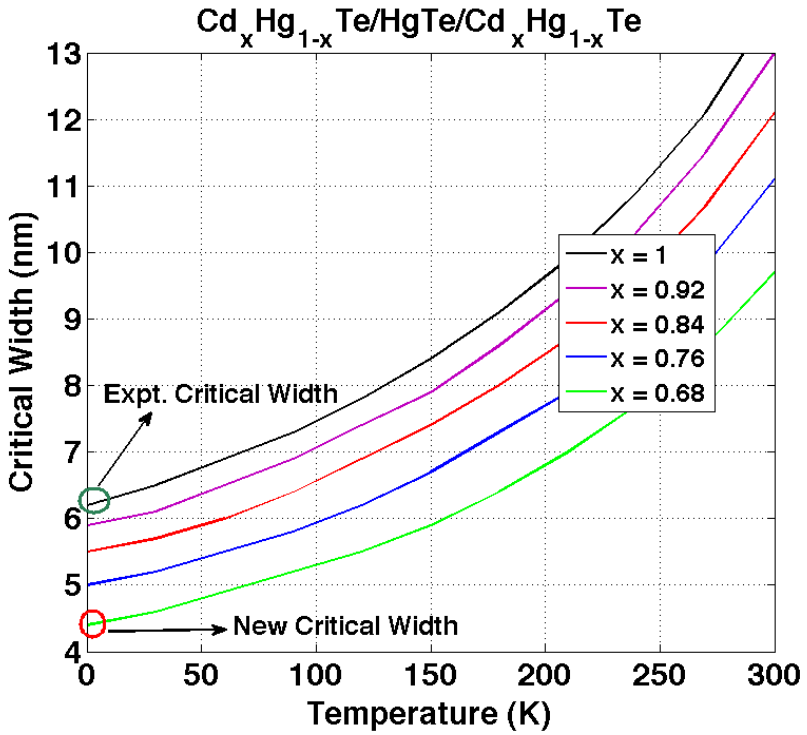
Temperature dependent band gap modulates the critical width

Critical width dependent on temperature and mole fraction

How to reduce the critical width with barrier material

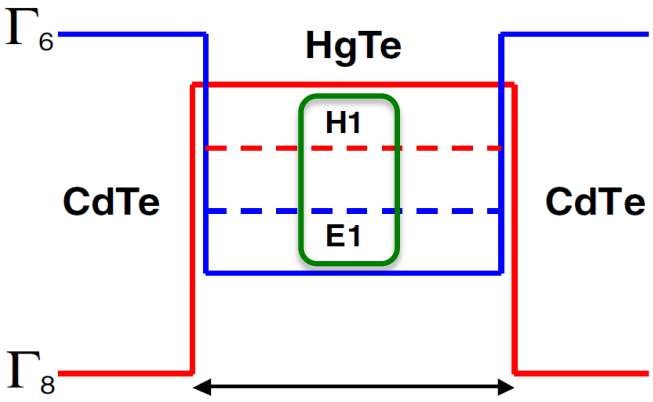


Barrier	Critical Width (nm)	Reduction
CdHgTe	6.3	Standard
$Cd_{0.92}Hg_{0.08}Te$	5.8	7.94 %
$Cd_{0.84}Hg_{0.16}Te$	5.4	14.29 %
$Cd_{0.76}Hg_{0.24}Te$	5.0	20.63 %
$Cd_{0.68}Hg_{0.32}Te$	4.4	28.57 %

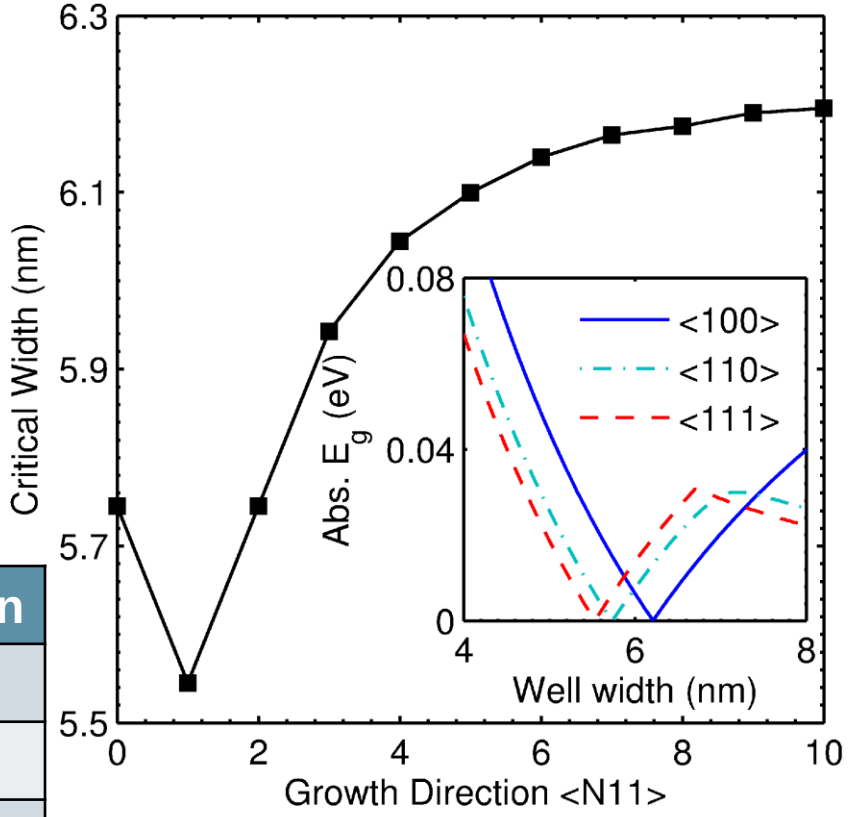


Critical width is reducible up to 4.4 nm with proper barrier material

Reduction of critical width with effective mass



Eff. mass can be changed with crystal growth direction



Coupling can be tuned through variable eff. hole and electron masses

Growth Axis	Critical Width	Reduction
<100>	6.3 nm	Standard
<110>	5.72 nm	9.2 %
<111>	5.52 nm	14.13 %

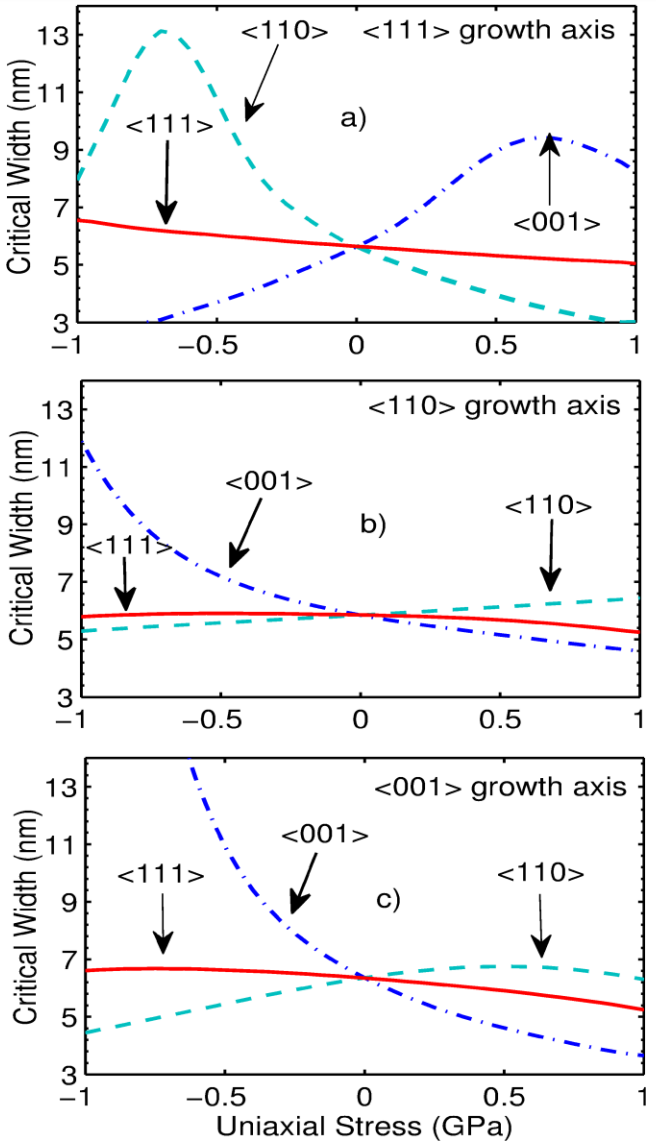
<111> growth axis provides least critical width

Critical width with appl. of strain under diff. growth axis

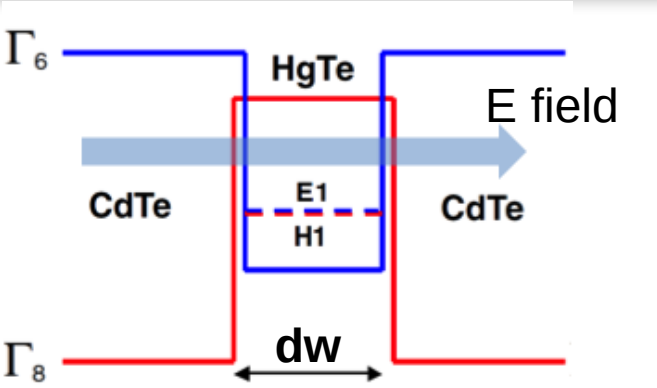
	Tensile Uniaxial Stress		
Growth Axis	<001>	<110>	<111>
<001>	L	H	I
<110>	L	H	I
<111>	H	L	I

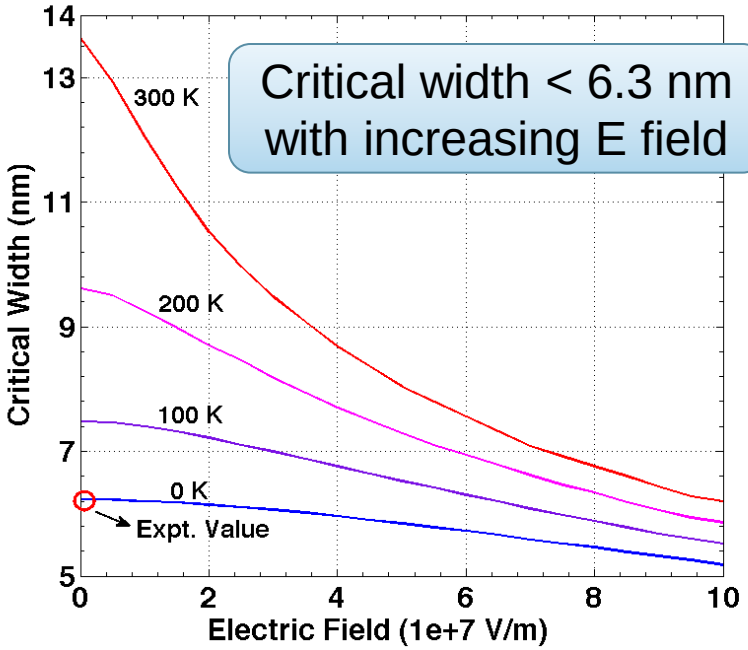
	Comp. Uniaxial Stress		
Growth Axis	<001>	<110>	<111>
<001>	L	H	I
<110>	L	H	I
<111>	H	L	I

L = Least; H = Highest; I = Intermediate

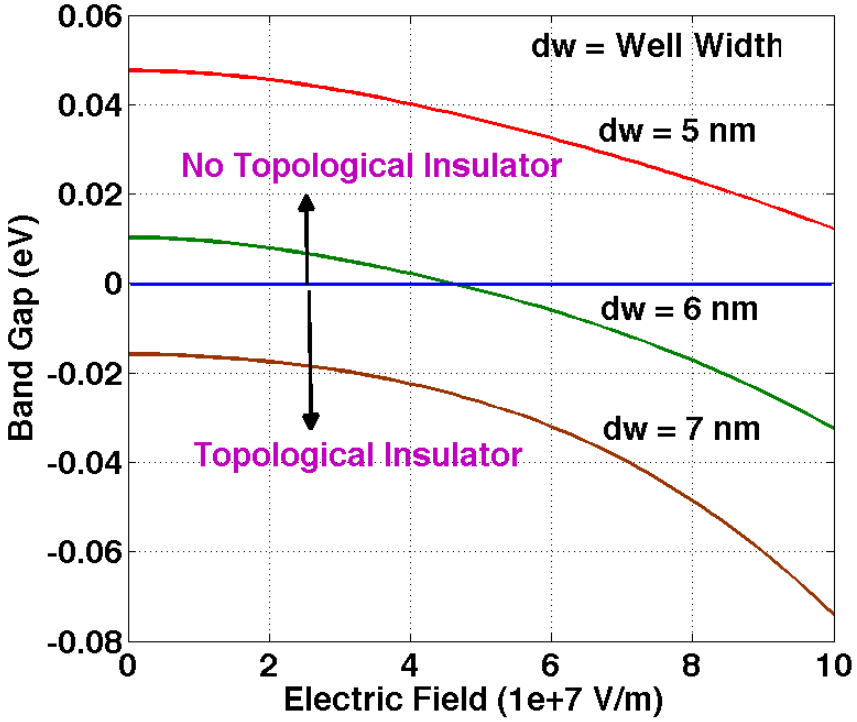


Impact of external electric field





Electric field induced TI



CdTe/HgTe heterostructure acts as a *topological switch* under electric field

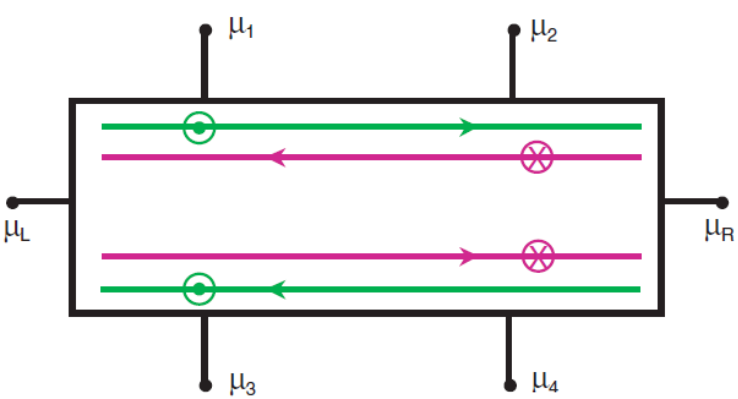
Can such TI-based electronic components incorporated in a fast switching environment?

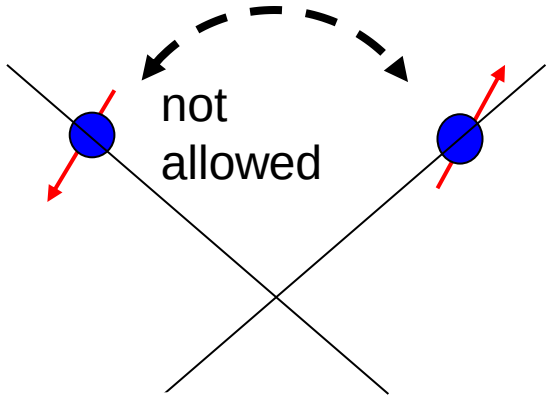
A fast switching environment needs faster transmission

Topological insulators are characterized by *high electron mobility* on the surface

Material	Mobility(cm^2 /V.s)	Method	Reference
Bi_2Te_3 (bulk)	10,200	Hall meas.	Science 329, 821 (2010)
Bi_2Se_3 (bulk)	13,200	SdH	Nano Lett.,12 (3), 1486 (2012)
Bi_2Te_3 (NR)	4,560-5,790	SdH	Nature Nanotech 6,216 (2011)

Silicon electron mobility is **1400 cm^2 /V.s** at room temperature (300 K)



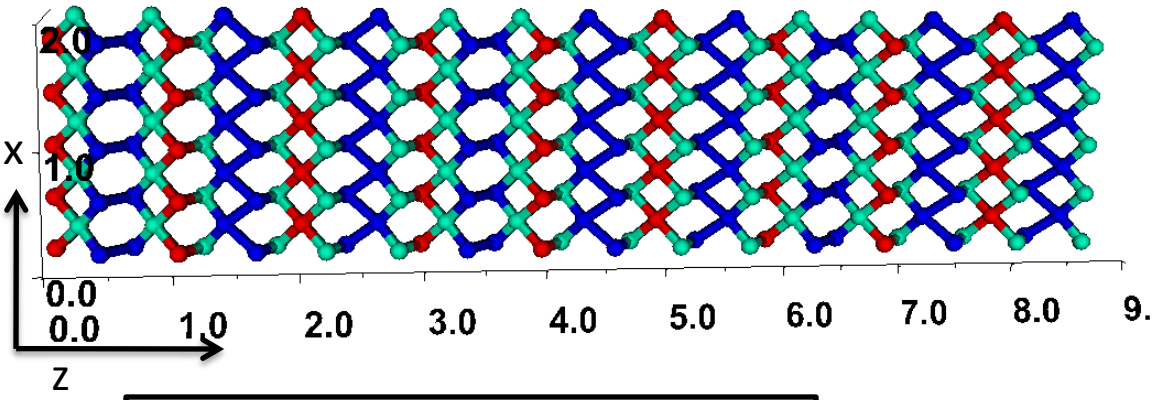


Back Scattering is forbidden

TIs have high mobility: Is a real fast transistor possible ?

Two TI attributes are useful:

1. They have metal-like surface states
2. Surface states possess high mobility

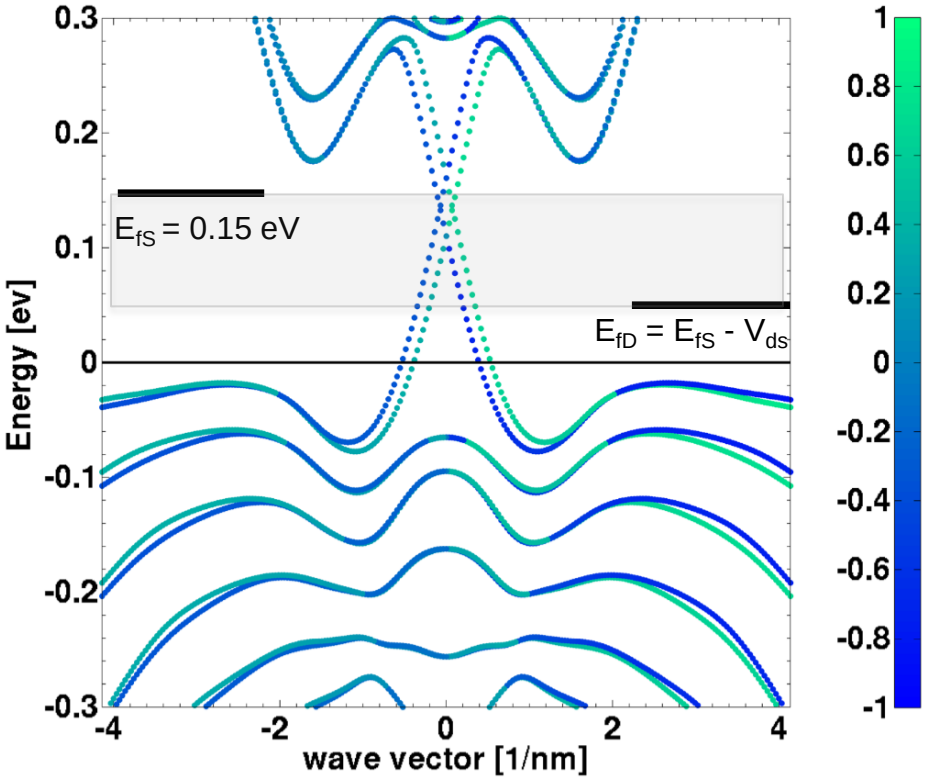


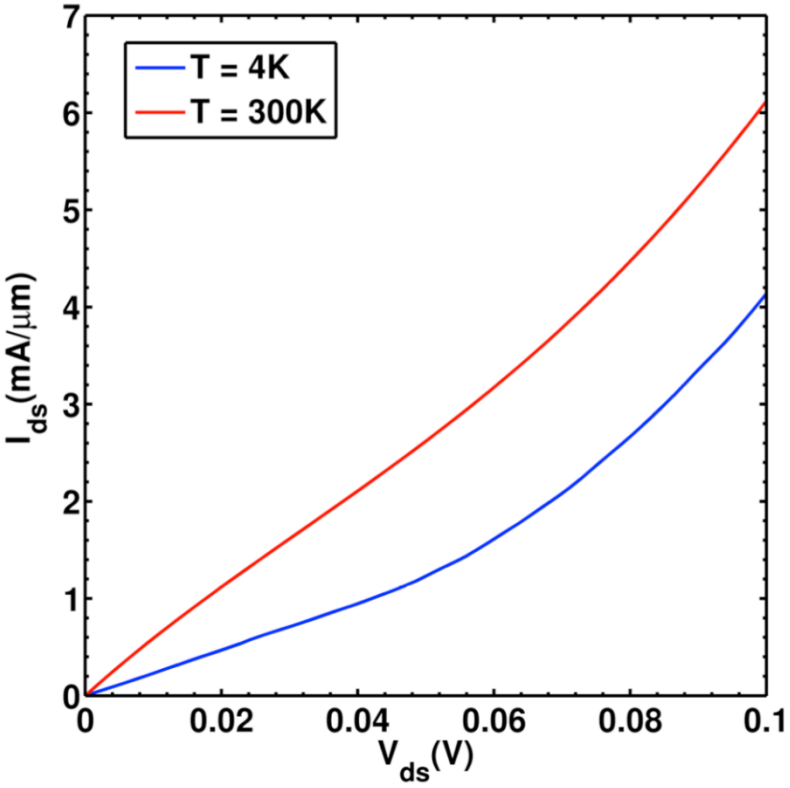
Simulation structure for Bi_2Te_3 ultra-thin-body

- Geometric confinement: 8.942 nm (z-axis)
- Open boundary condition (transport direction): 1.972 nm (x-axis)
- Periodic direction : y axis

- Temperature of operation : 4K / 300K
- Chem. potential of drain = 0 eV relative to band structure
- Chem. potential of source = [voltage] eV relative to band structure
- Flat bands

I_d vs. V_d characteristics of Bi_2Te_3





Nominal externally applied voltage between source and drain results in a sufficiently high current

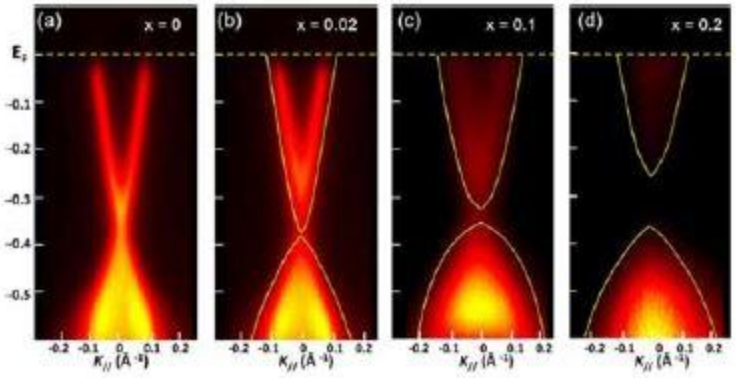
Turning off the TI transistor

The TI transistor has metal-like conduction at surface with high mobility!

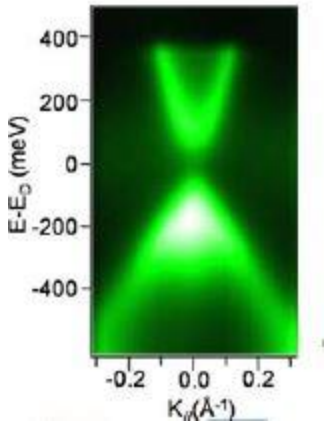
But gapless surface states mean → *No electrical tuning* of Fermi level in a band gap region → No *"turn-off"* possible

A band gap can be induced in a TI in three possible ways

1. Doping with a ferromagnet (FM)
2. Coating with a ferromagnet
3. Superconductor in proximity of a TI



ARPES* measurements of Cr based Bi_2Se_3



Gapped surface states of a TI grown on a FM*

*PSS, RRL 7 (2013)

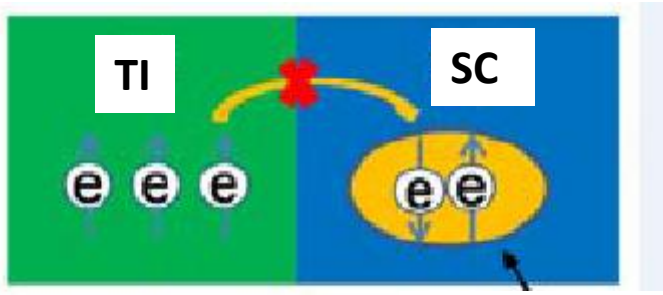
The TI-superconductor heterostructure

→ Band gap created on TI surface

TI grown epitaxially on a SC

SC film on top of a TI film

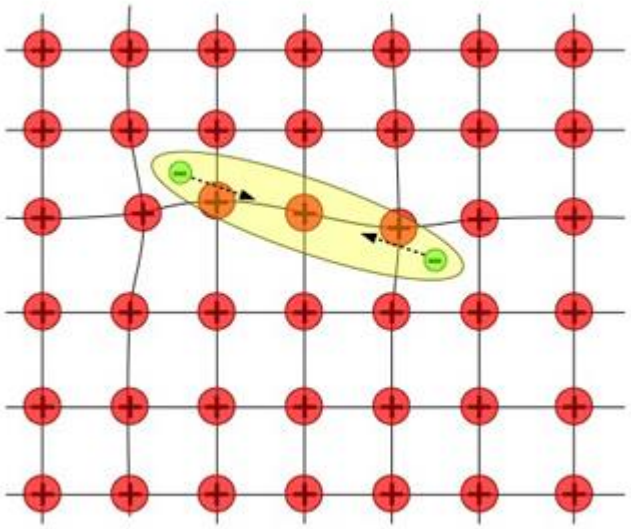
Explanation lies in the proximity effect between a superconductor and the TI's surface state



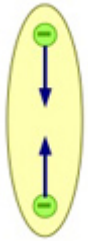
Cooper pair

Cooper pairs: The microscopic origin of superconductivity

- There is no one single theory that describes superconductivity
- Common to all superconductors is the *pairing of electrons* that allows dissipation-less transport
- Several mechanisms (*not yet fully understood*) can give rise to electron-pairing
- The well-accepted (*experimentally verified*) **BCS*** theory explained superconductivity at temperatures close to absolute zero for elements and simple alloys



Cooper pairs within a lattice

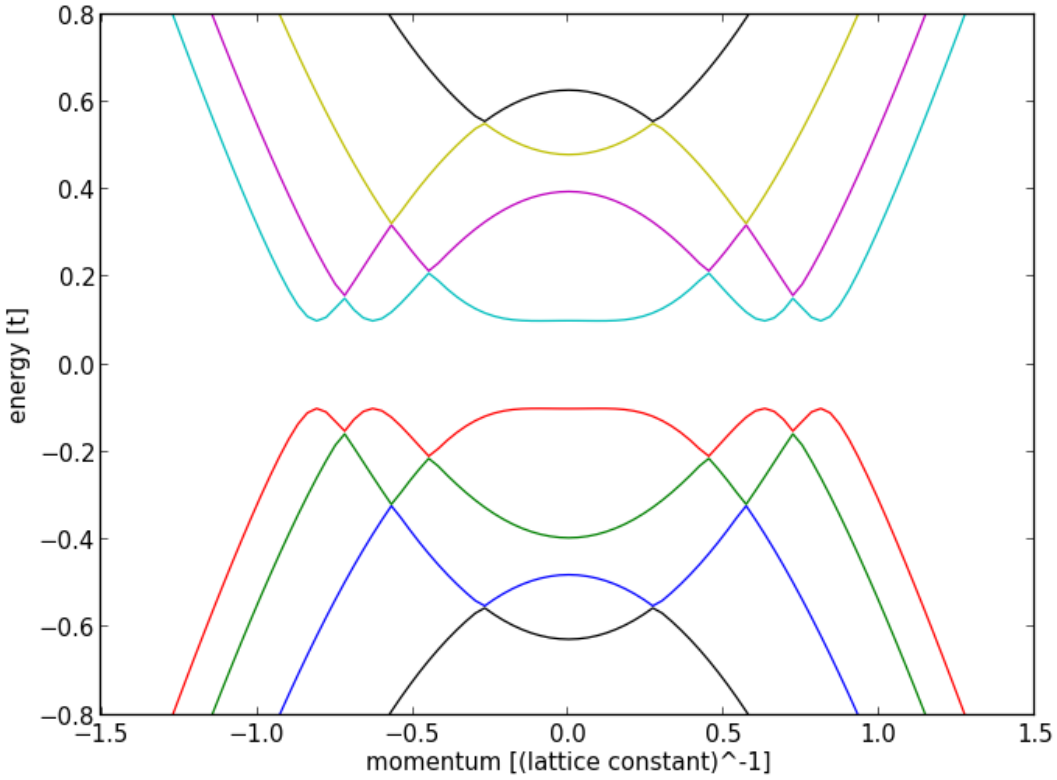


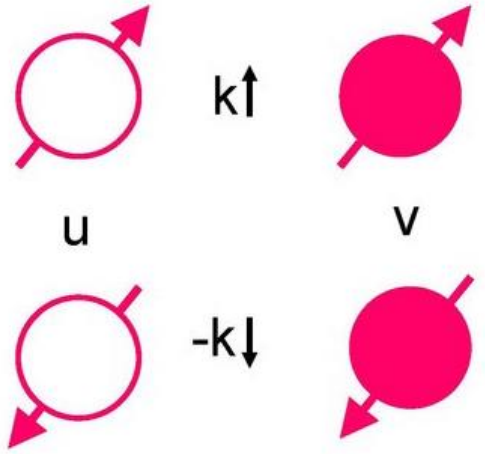
Paired electrons are called Cooper pairs

*Bardeen, Cooper, Schrieffer
Nobel Prize (Physics) 1972

The BCS ground state

The most distinctive consequence of BCS theory is that an energy gap opens up between the ground state and the lowest excited state



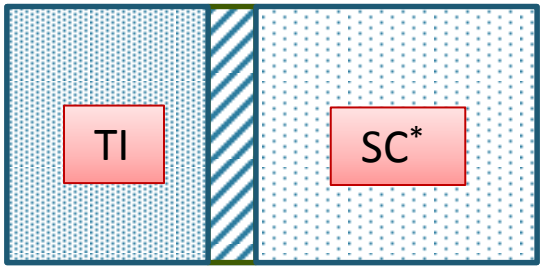


The ground state of the wave function is a superposition of states in which pair $(k\uparrow, -k\downarrow)$ are occupied or unoccupied

Proximity effect of a superconductor

- The Cooper pair ordering of electrons in superconductor is observed in a non-superconductor placed in contact
- Electrons cannot lose their ordering abruptly → Coherence is lost over a distance
- Gapped state of the superconductor is induced in the adjacent contact
- Most extensively studied are metal-superconductor junctions

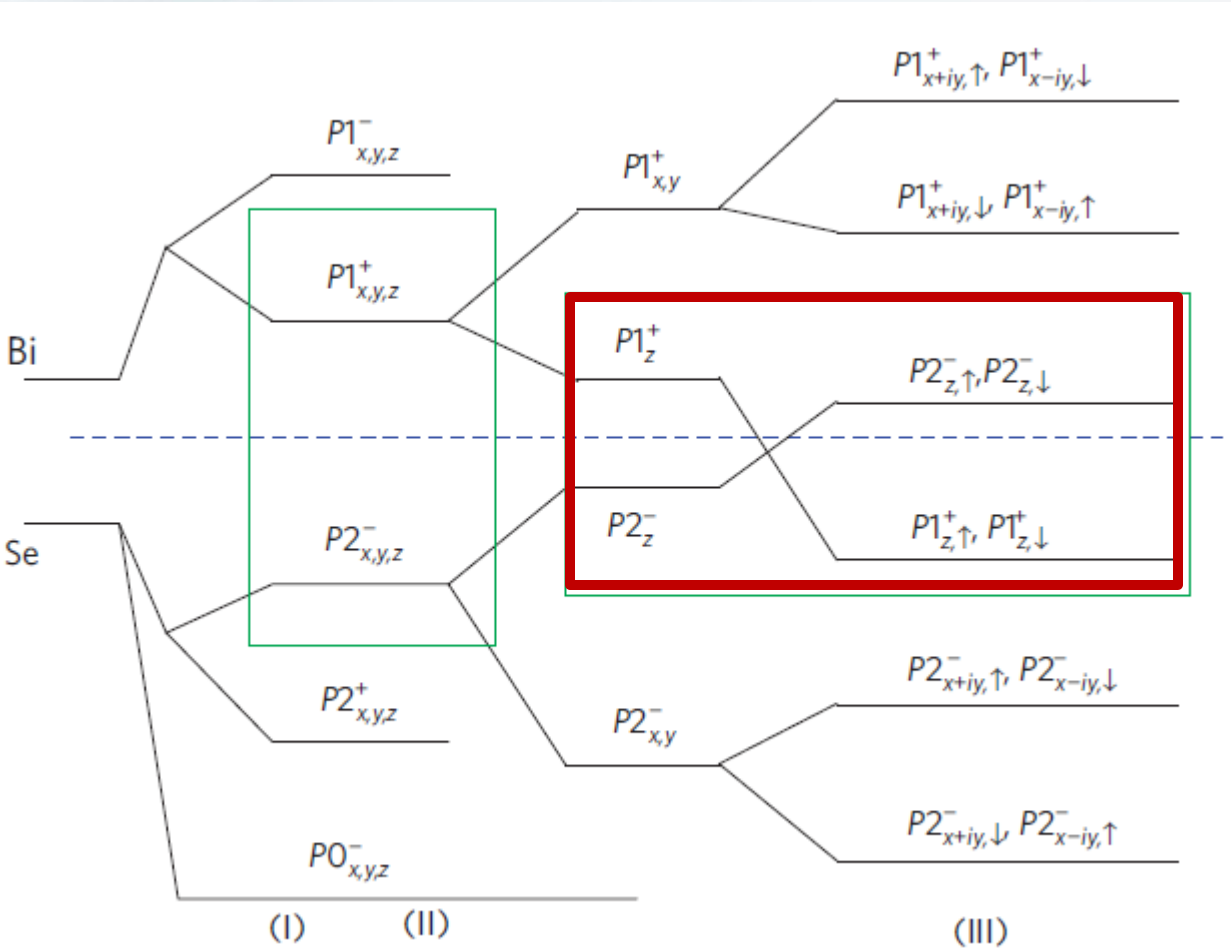
The same proximity effect is visible in a topological insulator-superconductor junction



Hatched region is TI + SC

*s-wave superconductor

Participating orbitals in surface state bands



Stage 1:Bi and Se atoms combine to produce the P1 and P2 orbitals

Stage 2: Crystal field splitting : Low-energy sub-space

Stage 3: Spin-orbit coupling

The four low-lying states at Γ are $P^+_{1z}\uparrow\downarrow$ and $P^-_{2z}\uparrow\downarrow$

Writing the composite TI-superconductor Hamiltonian

The Hamiltonian for a superconductor cannot be solved analytically

An approximation known as the Bogoliubiv de-Gennes is used to solve the Hamiltonian

The general form of the Hamiltonian is

$$H = \begin{pmatrix} h-\mu & \Delta \\ \Delta^* & \mu - ThT^{-1} \end{pmatrix} \longrightarrow$$

Effectively turned in to 8N x 8N sized Hamiltonian

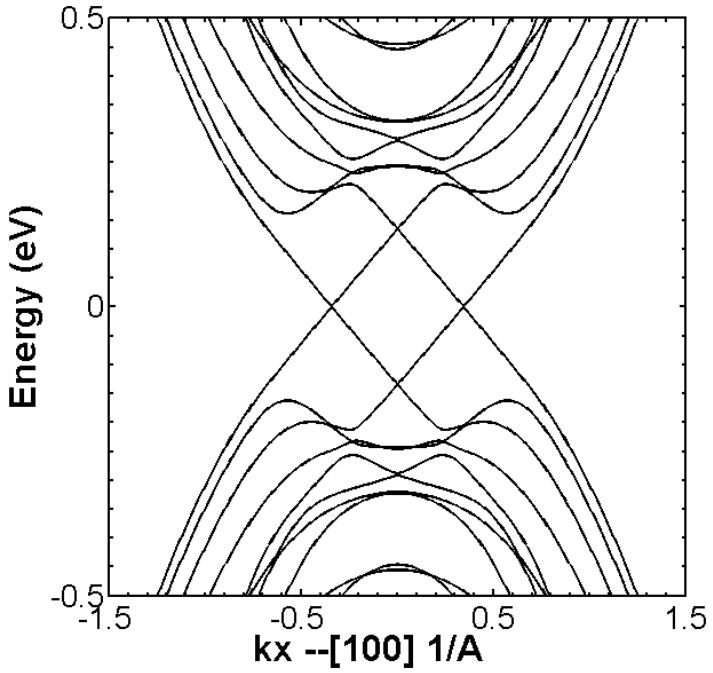
h is the Hamiltonian of the system without superconductivity (4-band model for TI)

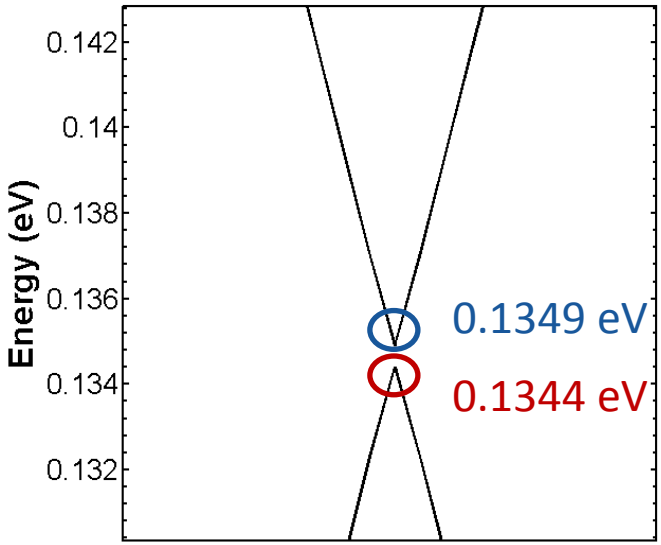
Δ is the order parameter, μ the Fermi-level and T is the time reversal operator

$P_{1z}^{+}\uparrow, -P_{1z}^{+}\downarrow$ are paired by Δ_1 and $P_{2z}^{-}\uparrow, -P_{2z}^{-}\downarrow$ are paired by Δ_2

Superconductivity induced band gap on surface of a 3D TI

A s-wave superconductor and 8 quintuple layer (8.0 nm) thick Bi_2Te_3 heterostructure





A gap of 0.5 meV induced on surface of TI

Band gap induced is of the same order as the superconducting gap

Conclusion

1. General idea of metals, semiconductors, and insulators
2. New material topological insulator (TI) : Dual properties of metal and insulator
3. Robust protected surface states : 2-D and 3-D topological insulators
4. Electronic structure calculation for TIs: *20 band TB and k.p*

1. Internal polarization induced 2D-TIs – Unconventional since it *does not use so-coupling*
2. Design principles for HgTe based 2D-TIs – *Tunability of the critical width*
3. Topological insulator based *switching*

1. I-V characteristics of Bi_2Te_3 UTB – No band gap *prevents turn-off*
2. *Inducing a band gap* on surface of a 3D-TI → TI-Superconductor heterostructure

Electronic structure calculation for broken-gap devices

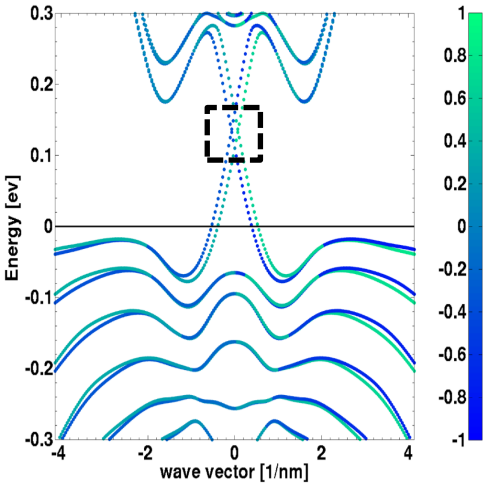
P. Sengupta, T. Kubis, Y. Tan, M. Povolotskyi, and G. Klimeck

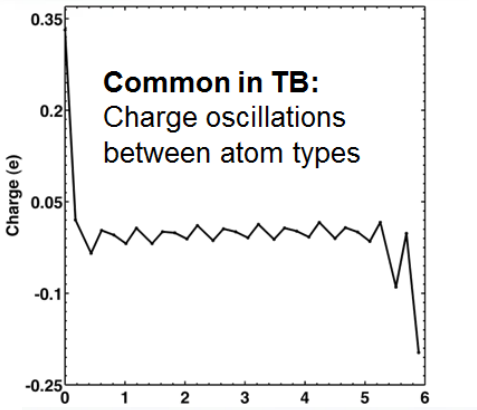
Objective

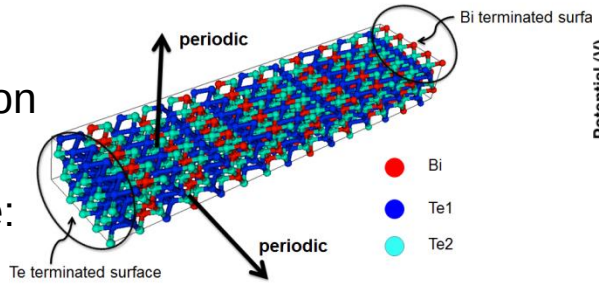
- Accurately model the eigen spectrum of broken-gap devices and topological insulators → Applicable when classical electron hole description fails

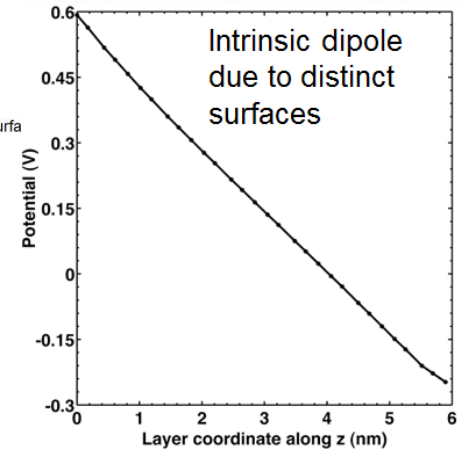
Method

- Consider all states as electronic and assume a positive charge background
- Screening of core shell electrons is neglected (ε = 1)
- Total charge density per atom = - electron density per atom + ionic charge
- To compute positive background charge: Calculate bulk density in TB
- Electron density at each atom = positive ionic charge
- Bulk parameters are transferred to heterostructures
- Self-consistently solve the Schrodinger-Poisson equation with bulk parameters









Result

- Charge self-consistent tight-binding calculation done for a Bi_2Te_3 thin-film
- Energy separation between Dirac cones gets enhanced
- Fermi velocity of Dirac states changes

3D-TI based nanowires

P. Sengupta, T. Kubis, Y. Tan, M. Povolotskyi, and G. Klimeck

Objective

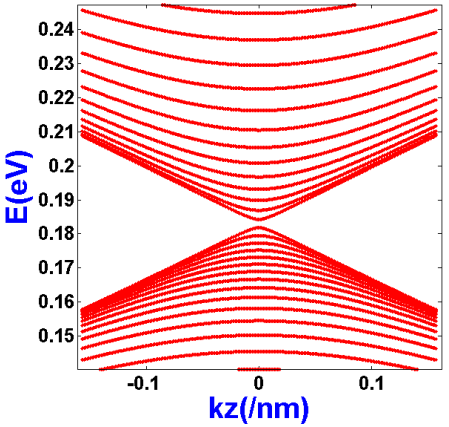
- Gain understanding of surface states (SS) on cylindrical topological insulator (TI) nanowires
- Influence of B-field on SS dispersion
- Study A-B oscillations on TI nanowires

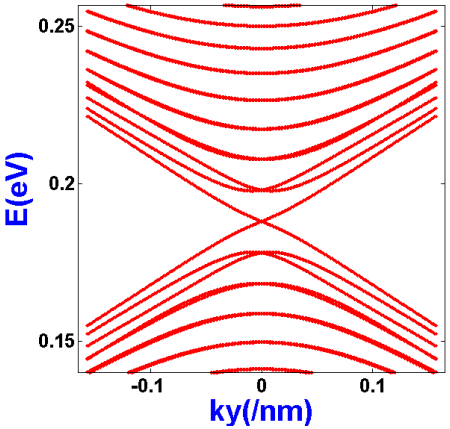
Method

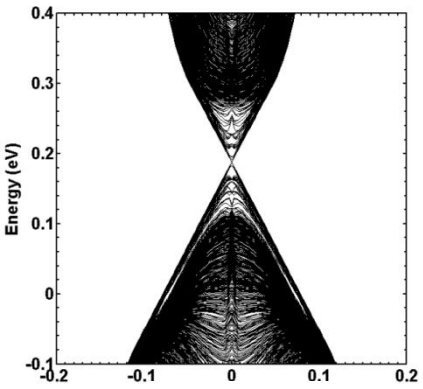
- 20-band tight binding and 4-band k.p Hamiltonian
- B-field implemented with the Peierls phase and Peierls substitution for TB and k.p respectively

Results

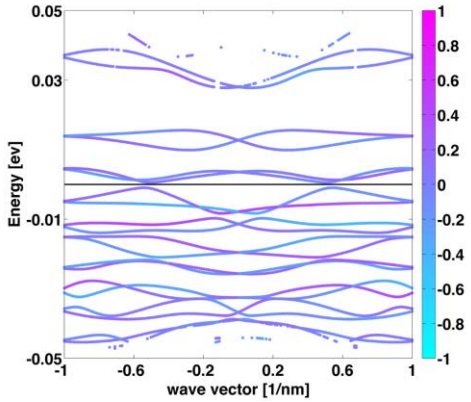
- Diameter of TI nanowires must be more than 30 nm to observe SS
- Wires grown along z-axis do not have TI states
- Wires grown along z-axis show band-gap closing under half magnetic flux quantum







Band-gap closing under half-magnetic flux quantum



Small diameter nanowires lead to surface volume hybridization
→ No TI states found

Numerical study of surface states of 3D-TI materials

P. Sengupta, T. Kubis, Y. Tan, M. Povolotskyi, and G. Klimeck

Objective

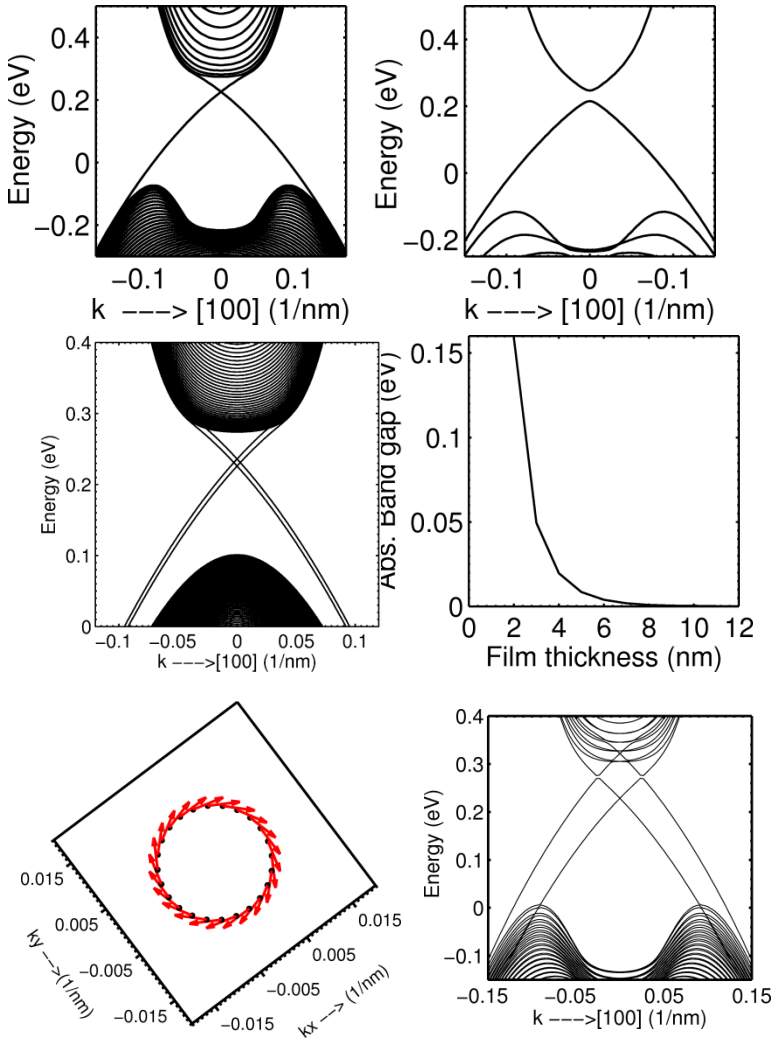
- Determine optimal conditions for existence of surface states (SS) on a 3D-TI
- Control the spin polarization of SS by placing two 3D-Tis together

Method

- 4-band k.p Hamiltonian for Bi_2Se_3 and Bi_2Te_3
- Bias added to Hamiltonian to mimic asymmetric surface terminations
- Spin-polarizer device parameters analyzed using 2D-Dirac equation

Results

- Physical and chemical attributes of TI thin-film impact the SS dispersion
- Low film thickness and asymmetric growth conditions form displaced Dirac-hyperbolas
- Spin-polarized components have unequal strength in asymmetric film



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