Topological Surface States
Topological Insulators, Superconductors & Beyond

Argonne workshop on Non-Conventional Insulators
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M. Z. Hasan
Dept. of Physics, Princeton Univ.
Overview of this talk

Z2 TI Brief Overview (Expts)
Surface States as a Novel 2DEG
Topo-Phase-Transition

Interaction effects?
Superconductivity, Ferromagnetism
Topo-Phase-Transition & Weyl Fermion?

TI beyond Kane-Mele Z2 theory? TCI phases?
Physics/Experiments Team
David Hsieh, Dong Qian, Andrew Wray, Yuqi Xia, SuYang Xu, MZH

MBE samples: N. Samarth (PennState), Chen et.al., (Purdue)
Bulk Crystals & Chemistry: S. Jia, Y. Hor, R.J. Cava (PU-Chem)
Interface/Heterostructures: S. Oh

LDA/First-Principles: H. Lin, A. Bansil (NEU)
Topological Insulator
\{\nu_0\} (Chern Parity invariants) \(Z_2\) Kane-Mele & many others

Quantum Hall Effect
\(\nu\) (Chern Number): \(Z\) (TKNN)

3D Topological Insulators

Protected Surface States: New 2DEG

2D Topological Insulators

2e^2/h

Edge States (1D) by TRS

Magnetic field —

e^2/h

Chiral Edge States (1D)
Topological Insulator
$\{ \nu \}$ (Chern Parity invariants) $\mathbb{Z}_2$ (Kane-Mele & many others ‘05-’09)

3D Topological Insulators

Bulk-Insulating 3D TI
(>90% surface transport)

Protected Surface States : New 2DEG

Proof of topological nature of Topological surface states

2D Topological Insulators

3D expts are neither derivatives nor extensions of 2D TI expts!
(also they are less than few months apart by the submission dates)

Charge transport Measurement of edge states of quantum spin Hall


Konig et. Science (2007)[Subm. 2007, June]
Experimental Challenge:

experimental “measure” of topological invariants?
(no quantization of charge or spin transport)

cannot be done via transport in Z2 topological insulators
(transport is still interesting and becoming possible)

Experimentally IMAGE boundary/edge/surface states
Experimentally Probe BULK--BOUNDARY CORRESPONDENCE
Experimental prove “topological order”

Spectroscopy is capable of probing
BULK--BOUNDARY correspondence,
Determine the topological nature of boundary/surface states &
experimentally prove “topological order”
QHE phases

\[ \sigma_{xy} = n e^2/h \]

Transport

Spin-sensitive Momentum-resolved Edge vs. Bulk

Topological quantum number

Topo Insulators

\[ \nu_o = \Theta/\pi \]

\[ \Theta = \pi \text{ (odd)} \]

\[ \Theta = 2\pi \text{ (even)} \]

No quantized transport via:

\[ \{ \nu_i \} \]

Topological quantum number

How to experimentally “measure” the topological quantum numbers (\( \nu_i \))?

4 TQNs \( \rightarrow 16 \) distinct insulators

\[ \{ \nu_0, \nu_1, \nu_2, \nu_3 \} \]

Topological “Order Parameters”
Photoelectric Scattering Process

\[ K_x = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}} \sin \vartheta \cos \varphi} \]
\[ K_y = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}} \sin \vartheta \sin \varphi} \]
\[ K_z = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}} \cos \vartheta} \]

- By measuring electron intensity as a function of \( E_{\text{kin}} \), \( \vartheta \) and \( \varphi \), a momentum resolved energy spectrum is obtained.
How to isolate intrinsic Bulk (3D) vs. Surface (2D) states?

Band-structure of Bi(Sn)Sb semiconductors

Fu-Kane PRB’07 Prediction: Bi-Sb $Z_2$ non-trivial since Sb is non-trivial but Bi is trivial

Hsieh et.al., NATURE 08, KITP Proc. (2007)
Protected Fermi surface on the surface on an insulator
(first Topological Insulator (3D): Thermoelectric Bi(Sn)Sb alloy semiconductors)

\( Z_2 \) non-triviality (theory) does not predict the actual Fermi surface

Hsieh et al., Nature 08
Spin Texture on the SS Fermi surface

- Bi$_{0.91}$Sb$_{0.09}$
- $k_x$ and $k_y$ in $\text{Å}^{-1}$
- $E_B$ in eV
- Polarization $P_x$, $P_y$, $P_z$
Can we make a large-gap version of TI ..

Topology in Bi-Sb [Hsieh et.al., 08]

Bi-Sb → Pure Sb

Single Dirac cone Bi-Sb (2007)

Bi$_2$Se$_3$

Bi$_2$Sb → Single Dirac cone Bi-Sb (2007)

Bi$_2$Se$_3$ class as TIs:
Xia et.al., *NATURE PHYS* 09, arXiv (2008)
Hsieh et.al. *NATURE* 09
Zhang et.al. *NATURE PHYS* 09

Single Dirac cone in (Bi-Sb alloy)
→ Single Dirac cone ONLY in Bi$_2$Se$_3$ class
Chirality change through the Dirac node

Left handed

Spin-ARPES

Fermi level in Gap

Topological Order

Nature (2009)
Helical Dirac fermions

One to One Spin-Linear-Momentum Locking

Hsieh et al., SCIENCE 09, NATURE 09
Helical spin texture directly implies absence of backscattering

(a) 

(b) 

(c) 

(d)
STM (Roushan et.al.)  
Spin-ARPES (Hsieh et.al.)

Spin-Independent

Spin-Dependent

Roushan et.al., NATURE 09 & Others
Can we make a large-gap version of TI ..

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Single Dirac cone in (Bi-Sb alloy)
→ Single Dirac cone ONLY in Bi$_2$Se$_3$ class
Manipulation & control of TI surface states (Fermi level in gap): (Nature09, Science09)

Electrical Gating is also possible
Mirror Chern number

Hsieh et al., Science 09
Graphene

Excellent Material Properties

Bulk band structure:
Dirac Fermion is a BULK state

\[ \sigma_{xy} = \frac{2e^2}{h} \]
(q-Hall effect)

Topo Insulator

Chirality Inversion

\[ H_{\text{surface}} = -i\hbar v_F \vec{\sigma} \cdot \vec{\nabla} \]

Protected Surface States: New 2DEG

Dirac Fermion is a boundary effect while the BULK is insulating!

\[ \sigma_{xy} = \frac{e^2}{2h} = \frac{1}{4} \]
Ga(Al)As or Hg(Cd)Te limited to low-T (mK)

**Bi$_2$Se$_3$ : Topological Order at Room Temperature**

QH-like topological effect at 300K, No magnetic field

Protected **Surface States** (New 2DEG)

![Diagram depicting Bi$_2$Se$_3$ band structure and topological insulator properties](diagram)

**Fig. 12.** (Color online) Helical fermions: Spin-momentum

Weak electron-phonon coupling at 300K
Band inversion and Topological Phase Transition

Non-inverted

Inverted

S.Y. Xu et al., SCIENCE '11
Evolution of Out-of-plane Spin-Texture

3D Vectorial Spin Textures

Calculation: MZH, Lin et.al. (2009)
Hsieh et.al., NATURE ‘09, SuYang Xu et.al., SCIENCE ‘11
Topo-insulators in nature

2D Topological Insulators: Ga(Al)As, Hg(Cd)Te

Quantum Hall state (Breaks T-invariance)  \( \text{IQH} \)
Cryogenic, Large Magnetic field, high-purity crystals

Quantum spin Hall state (Preserves T-invariance) \( \rightarrow 2 \text{ IQH} \)
Cryogenic, No Magnetic field, high-purity crystals,

3D Topological Insulators: Bi-Sb, Bi\(_2\)Se\(_3\), Bi\(_2\)Te\(_2\)Se

Topological insulator (Preserves T-invariance)
Room Temperature operation, No magnetic field, Dirty crystals?

Protected Surface States: New 2DEG

AFM/FM/Magnetism in doped topo insulator: Topo-Order & Broken-Symmetry
Superconductivity in doped topo insulator: Topo-Order & Broken-Symmetry
Can we make a large-gap version of TI..

**Single Dirac cone Bi-Sb (2007)**

Bi-Sb → Pure Sb

**Bi$_2$Se$_3$**

Topology in Bi-Sb [Hsieh et.al., 08]

**Bi$_2$Se$_3$ class as TIs**: 
Xia et.al., *NATURE PHYS* 09, arXiv (2008)
Hsieh et.al. *NATURE* 09
Zhang et.al. *NATURE PHYS* 09

Single Dirac cone in (Bi-Sb alloy) → Single Dirac cone ONLY in Bi$_2$Se$_3$ class
Experiments on Topological Insulators (3D)

Surface Magnetic Impurity Coulomb perturbation etc.

Bi$_2$X$_3$

STM Landau quantization
Xue et.al., PRL 2010
Analytis et.al, NatPhys ’10
Xiong et.al., arXiv’11

Quantum Hall effect

Bi-Sb

Hsieh et.al., NATURE 08 (sub. 2007)
Hsieh et.al., SCIENCE 09
Roushan et.al., NATURE 09

Topo.Phase Transition

S.-Y. Xu et.al., 2011
Science ’11, arXiv’11

Superconductivity

Xia et.al, 2008 (arXiv’08, KITP 08)
Xia et.al, 2009 (Nature Phys.)
Hsieh et.al., Nature 2009
Chen et.al, Sci ’09, Zhang et. NatP ‘09

Hsieh et.al., NATURE 08 (sub. 2007)
Hsieh et.al., SCIENCE 09
Roushan et.al., NATURE 09
Magnetic vs. Non-magnetic doping (Mn)

Doping dependence of surface Dirac gap

Sample layout:
- a-Se cap
- Mn-doped Bi$_2$Se$_3$ film
- ZnSe buffer (~3 nm)
- GaAs buffer (~3 nm)
- GaAs 111A substrate

Graphs showing binding energy $E_b$ (eV) vs. momentum $k$ (Å$^{-1}$):
- 0% Mn
- 2.5% Mn
Resonant (Circular Pol.) X-ray Scattering + ARPES

S.-Y. Xu et al., Nature Physics (2012)
Mott det ARPES
Route to Weyl Fermions & other cool stuff..

Topo-Ins. near criticality TI $\rightarrow$ NI  
(Xu et.al., Science 2011)

Magnetize it (Ferromagnetic)  
(Xu et.al., Nat. Phys. 2012)
STI/Superconduct interface

2D interface state with energy gap and exotic topological order

Resembles 2D spinless $p_x+ip_y$ superconductor but does not violate time reversal symmetry

**Fu-Kane proposal**

$$H = \psi^\dagger (-iv \vec{\sigma} \cdot \vec{\nabla} - \mu)\psi + \Delta \psi^\dagger \downarrow \psi \uparrow + \Delta^* \psi \downarrow \psi^\dagger$$

Dirac surface states
(no spin degeneracy)

proximity induced superconductivity

Majorana bound state at a vortex:
- bound state solution to BdG equation at exactly zero energy
- $c_0 = c_0^\dagger$ (electron=hole) Majorana fermion = “1/2 a state”

**Also predicted in** $\nu=5/2$ FQHE, $\text{Sr}_2\text{RuO}_4$, cold atoms, etc
Topological Surface States: Superconductivity in doped topological insulators

Wray et.al., Nature Physics (2010)
Surface States at superconducting composition

$\text{Cu}_x\text{Bi}_2\text{Se}_3$ ($T_c \sim 3.8\text{K}$) : Hor et.al., PRL 2010

Wray et.al., Nature Physics (2010)
Topological Superconductor (TSC)?
Kitaev/Ludwig D3 class of TSC (proposed by Fu & Berg 09)

If ODD parity → TSC
[ analog of SF He-3(B) ]

ARPES Expts

Wray et.al., Nature Physics (2010)
Candidate Topological Superconductors ..

**Centrosymmetric**

- $\text{Cu}_x(\text{Bi}_2\text{Se}_3)$ 3.8K
- $\text{Pd}_x(\text{Bi}_2\text{Te}_3)$ 4.0K
- $\text{TlBiTe}_2$ 0.1K

**Non-Centrosymmetric**

- $\text{LaPtBi}$ 0.3K
- $\text{Li}_2\text{Pt}_3\text{B}$ 3.0K
- $\text{CePt}_3\text{Si}$ 0.7K

Order parameter sym must be determined
Path to Topological Devices?

Some of the materials are reported at S.-Y. Xu et.al., arXiv:1007.5111v1

Magnetoelectric interface

Majorana interface
\( \text{Bi}_2\text{Te}_2\text{Se}_{1} \) (more insulating than Si at 4K)

5 Ohm-cm (more insulating than Si at low-T)

S.-Y. Xu et.al., preprint (2012)
Highly Bulk-Insulating Topological Insulators

Surface contribution to transport more than 90%
Surface Mobility $\sim 3000 \text{ cm}^2/\text{Vs}$

Surface conductivity $\rho (\text{mOcm})$
- Bi$_2$Te$_3$ native: 5000
- Bi$_2$Te$_3$ improve1: 2500
- Bi$_2$Te$_3$ improve2: 500
- BTS221 native1: 2500
- BTS221 native2: 500

Surface conductivity $\rho (\text{mOcm})$
- Bi$_2$Te$_3$: 5000
- Bi$_2$Te$_3$: 2500
- Bi$_2$Te$_3$: 500
- BTS221 native1: 2500
- BTS221 native2: 500

$G_{surface} (T \sim 0) = (e^2/\hbar)k_F L = (e^2/h)k_F v_F T$

Surface conductivity $\rho (\text{mOcm})$ vs. temperature (K)
- Bi$_2$Te$_3$ native: 10000
- Bi$_2$Te$_3$ improve1: 5000
- Bi$_2$Te$_3$ improve2: 1000
- BTS221 native1: 10000
- BTS221 native2: 1000

$E_g (\text{eV})$ vs. momentum ($k (A^{-1})$)
- Bi$_2$Te$_3$ native: 0.4
- Bi$_2$Te$_3$: 0.4
- Bi$_2$Te$_3$: 0.4
- BTS221 native1: 0.4
- BTS221 native2: 0.4

100-nm Film equivalents $\sim 10^{10}$ carriers

Very large Gap $\sim 200 \text{ meV}$ (unlike HgTe)

Ong et al., as-grown

even Bulk crystals $> 5 \text{ Ohm-cm}$
Our experiments on Topological Surface States (new type of 2DEG)

1. Robust & Protected to alloying, Non-mag. disorder: Nature 08
   TSS survive various bulk, surface doping, annealing disorders etc.
2. FS encloses odd no. of Dirac points (1/4 Graphene): Nature Phys 09
3. Spin-Linear Momentum Locking (Helical Fermions): Nature 09
   Room temperature topological order demonstration.
4. Berry’s phase $\pi$ around the Dirac cone pocket: Science 09
   Nearly 100% spin polarized, Spins lie mostly in plane
5. Opposite to Anderson Localization (“Anti-localization”): Nature 09
   STM(A.Y.)+Spin-ARPES(Z.H.) → Absence of backscattering
6. Dirac node is destroyed if TRI is broken (Doping effect): Nature 09
   Magnetic impurity on the surface makes it a band insulator
7. New platform for topological quantum phenomena: NatureMat 10
Topo Insulators beyond Kane-Mele $Z_2$ theory?

TR invariance $\leftrightarrow \rightarrow$ SG symmetry (TCI)

Space group symmetry protected topological insulators (Fu PRL’11)

Pb(1-x)Sn(x)Te:
Space group symmetry protected topological insulators

Pb(1-x)Sn(x)Te :
Space group symmetry protected topological insulators

Pb(1-x)Sn(x)Te:
Space group symmetry protected topological insulators
Pb(1-x)Sn(x)Te:
Space group symmetry protected topological insulators
Topo Insulators beyond Z2 theory?


Also see Work by Story and Ando grps (arXiv)
Topo (Band) Insulator $\rightarrow$ **Topo Mott insulator (TMI)**

Emergent physics in TMI

Pesin & Balents 2010

5d-Oxides

Coulomb Interaction

Spin-Orbit coupling
Visions and challenges:  
*Semiconductor+ Emergent Pheno.*

**Topological Condensed Matter Physics (new book on solid-state physics)**

Topological classification of quantum solids including many-body systems
- Magnetoelectric effects, - Quantum Anomalous Hall effect
- Superconducting proximity effects
- Creating and manipulating Majorana fermions
- Observe topological phenomena at room temperature
- Expand the types of topological phases and discover them in real materials.

Example: topo. crystalline insulators, topo. Anderson insulators, new topo. superconductors, Weyl semi-metals, topo. Mott insulators, etc.

Observe, Control and Manipulate these new states of matter
- Reduce the density of bulk carriers to a negligible level
- Induce a robust gap

**Materials Synthesis** quality materials bulk crystals and thin films (long-term)

US is not internationally competitive in materials

**New experimental tools** hybrid spectroscopies+transport, high precision etc.
Conclusions

1. A novel experimental approach to Topological phenomena

2. Topological Insulator A new quantum phase of matter
   has been identified (bulk Topological-Insulator) whose surface
   is a new type of 2DEG (spin-momentum locked $\frac{1}{2}$ Dirac gas)
   protected by time-reversal symmetry.
   Bulk Insulating samples are now realized.

3. Topological Phase Transition Spin-texture and half Dirac gas is
   one-to-one correlated with a topological (quantum) phase transition
   Bulk-boundary correspondence

4. Ferromagnetism in Topological Insulators
   new physics of competing order : Broken symmetry vs. Topo Order

5. Topological Superconductors: some results but a lot more work..

6. Route to Weyl Fermions (Future)

7. TIs protected by SGS (Topo Cryst. Insulators)

Items 1) & 2) : MZH & CL Kane Rev. Mod. Phys. 82, 3045 (2010)
(also reviews by others including Qi&Zhang (2011))
Items 3)-7) are new frontiers (interactions + New Topo Phases!)
Thanks!
Topological Insulator
\{v_o\} (Chern Parity invariants) \(Z_2\) (Kane-Mele & many others ’05-’09)

3D Topological Insulators

Protected Surface States : New 2DEG

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3D expts are neither derivatives nor extensions of 2D TI expts!
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Bulk-Insulating 3D TI
(>90% surface transport)

Proof of topological nature of Topological surface states


Konig et. Science (2007)[Subm. 2007, June]

Charge transport
Measurement of edge states of quantum spin Hall

QSH edge States (1D) by TRS