First-principles calculations of electronic structures in topological insulators

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• Summary
Introduction
Topological insulators are electronic materials that have a bulk band gap like an ordinary insulator, but have protected conducting states on their edge (2D) or surface (3D).

[ARPES data of Bi$_2$Se$_3$]

(Ref. Phys. Rev. B 81, 041405 (2010))
Hohenberg-Kohn theorem:
The ground-state energy of an interacting electron gas is a universal functional of the one-particle electron density.

Kohn-Sham scheme:
Anomalous properties of Bi & Bi$_{1-x}$Sb$_x$

- Matrix elements and selection rules for the two-band model of Bi.

- Investigation of the gapless state in Bi-Sb alloys.

- Transport properties of Bi-rich Bi-Sb alloys.

We will commence our investigation by reviewing the two-band model, following closely the methods of COHEN and BLOUNT. The resulting equations are essentially identical to those of the Dirac theory, and many of the methods employed there are useful in the present problem. In particular, the electron energy-momentum relation has the relativistic form:

$$E^2 = \left(\frac{E_G}{2}\right)^2 + E_G \left(\frac{\vec{p} \cdot \vec{\alpha} \cdot \vec{p}}{2}\right)$$

(1)

where $\vec{\alpha}$ is the reciprocal effective mass tensor. Electrons at the Fermi level are quite “relativistic” since, as we have seen, $E_F$ is considerably larger than $E_G/2$. This fact accounts for the rapid variation of electron effective mass with energy.
Recognition of $Bi_{1-x}Sb_x$ as a topological insulator

- Topological insulators with inversion symmetry.
  → Recognition that $Bi_{1-x}Sb_x$ is a topological insulator.

Schematic representation of band energy evolution of $Bi_{1-x}Sb_x$ as a function of $x$. 
Surface states of $\text{Bi}_{0.9}\text{Sb}_{0.1}$

Review on

$Bi_2Se_3$, $Sb_2Te_3$, $Bi_2Te_3$
Bi$_2$Se$_3$, Sb$_2$Te$_3$ and Bi$_2$Te$_3$ share the same rhombohedral crystal structure ($D_{3d}^5$).

- Layered structure with five atomic layers as a basic unit cell, named a quintuple layer (QL).
- Each quintuple layer consists of five atoms with two equivalent Se atoms (denoted as Se 2), two equivalent Bi atoms and a third Se atom (denoted as Se 1).
Topological insulator: $\text{Bi}_2\text{Se}_3$

Band structure of bulk $\text{Bi}_2\text{Se}_3$

without spin-orbit coupling

with spin-orbit coupling

Topological insulator: $Bi_2Se_3$, $Sb_2Te_3$, $Bi_2Te_3$

2D Dirac cones on (111) surfaces

Topological insulator: $\text{Bi}_2\text{Se}_3$

Surface band structure of $\text{Bi}_2\text{Se}_3$


surface Green's functions of semi-infinite system

Fermi velocity: $5.0 \times 10^5$ m/s


LAPW (WIEN2k) calculation of a slab of 12 quintuple layers
Topological insulator: $\text{Bi}_2\text{Se}_3$

Angle-resolved photoemission spectroscopy (ARPES)


Topological vs. simply insulators in $Sb_2Te_3 - Sb_2Se_3$ alloy

- $Sb_2Te_3$ is a topological insulator, while $Sb_2Se_3$ is not.

- The gap energy of bulk $Sb_2(\text{Te}_{1-x}\text{Se}_x)_3$ at the $\Gamma$ point as a function of Se concentration $x$. (TI = topological insulator, SI = simple insulator).
- TI-SI transition occurs at $x = 0.9$.

Our results on

$Bi_2Se_3$, $Sb_2Te_3$, $Bi_2Te_3$
Calculation method

- First-principles density functional calculations
  - Atomic structure of a surface is modeled with a slab in a supercell.
  - Electronic wavefunctions are expanded with pseudo-atomic orbitals.
  - \textit{Ab-initio} nonlocal norm-conserving pseudopotential
  - Generalized gradient approximation (GGA) for electron-electron interaction: Perdew-Burke-Ernzerhof exchange-correlation potential.
  - Spin-orbit coupling (SOC) was implemented in the SIESTA code.

(by Hyungjun Lee)
Real materials = nucleus + all electrons

*Ab initio* pseudopotential method:
Materials = ions + valence electrons
• Spin-orbit interaction term

\[
\sum_{l,m} |Y_l^m\rangle \langle V_l^{SO} \vec{L} \cdot \vec{S} | Y_l^m\rangle = \sum_{l,m} \left[ |\Phi_J^M\rangle \langle V_l^{SO} \vec{L} \cdot \vec{S} | \Phi_J^M\rangle + |\Phi_{J'}^{M'}\rangle \langle V_l^{SO} \vec{L} \cdot \vec{S} | \Phi_{J'}^{M'}\rangle \right] \\
= \sum_{l,m} \left[ \frac{1}{2} l \langle \Phi_J^M | \langle \Phi_J^M | - \frac{1}{2} (l + 1) \langle \Phi_{J'}^{M'} | \langle \Phi_{J'}^{M'} | \right]
\]

• By using KB projector

\[
|\Phi_J^M\rangle \langle V_l^{SO} | \Phi_J^M\rangle = \sum_\xi \langle V_l^{SO} \overline{R}_J \xi | \Phi_J^M\rangle \frac{1}{c_{J\xi}} \langle \overline{V}_l^{SO} \overline{R}_{J'\xi} | \Phi_J^M\rangle \\
\text{where } c_{J\xi} = \langle \overline{R}_J \xi | \overline{V}_l^{SO} | \overline{R}_{J'\xi}\rangle
\]

\[
|\Phi_{J'}^{M'}\rangle \langle V_l^{SO} | \Phi_{J'}^{M'}\rangle = \sum_\xi \langle V_l^{SO} \overline{R}_{J'\xi} | \Phi_{J'}^{M'}\rangle \frac{1}{c_{J'\xi}} \langle \overline{V}_l^{SO} \overline{R}_J \xi | \Phi_{J'}^{M'}\rangle \\
\text{where } c_{J'\xi} = \langle \overline{R}_{J'\xi} | \overline{V}_l^{SO} | \overline{R}_J \xi\rangle
\]
We obtained the band structures of Bi$_2$Se$_3$, Sb$_2$Te$_3$ and Bi$_2$Te$_3$ with and without spin-orbit coupling (SOC).

With SOC turned on, the band structure is changed around the Γ point.

Our results agree with reported results.
- We obtained the bulk band structures with and without spin-orbit coupling (SOC).
- Our result agrees with reported result.
• We obtained the band structure of Bi$_2$Se$_3$, Sb$_2$Te$_3$ and Bi$_2$Te$_3$ slab with 10-QLs.

Our results are in agreement with reported results.

reported results [Nature Phys. 5, 438 (2009)]
In our surface band structure for $\text{Bi}_2\text{Se}_3$, bulk conduction band minimum is $\sim 0.35 \text{ eV}$ higher than the Dirac point.

Angle-resolved photoemission spectroscopy (ARPES)


Energy contour near Dirac point

- Cubic warping term is strongest in Bi$_2$Te$_3$. 

```plaintext
Bi$_2$Se$_3$

Sb$_2$Te$_3$

Bi$_2$Te$_3$
```
Spin vectors from surface-state wavefunctions

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• S = 0.5 for fully spin-polarized states
- The real space distribution of a surface state wave function is analyzed.

- The distribution of wave function is very localized to the surface region, with a typical spread of about 2QL (about 2 nm in thickness).
Review on other topological insulators
Thallium-based III-V-VI$_2$ ternary chalcogenides

- Theoretical prediction of topological insulators in thallium-based III-V-VI$_2$ ternary chalcogenides, B. Yan et al., EPL 90, 37002 (2010)

- TIBiQ$_2$, TISbQ$_2$ (Q=Te, Se, S)
Ge-Sb-Te (GST) compounds

- Prediction of topological insulating behavior in crystalline Ge-Sb-Te.
  J. Kim et al., PRB 82, 201312 (2010)

\[ \text{Ge}_2\text{Sb}_2\text{Te}_5 \text{ Petrov sequence} \]

\[ \text{Ge}_2\text{Sb}_2\text{Te}_5 \text{ KH sequence} \]
Ternary Heusler compounds


zinc-blende

Heusler (C1_b), XYZ

Orange: X
Blue: Y
Yellow: Z
Ternary Heusler compounds

Ternary Heusler compounds

Our results on side surface of $\text{Bi}_2\text{Se}_3$
Side surface of $\text{Bi}_2\text{Se}_3$

Atomic structure of the $\text{Bi}_2\text{Se}_3$ (221) surface.

(a) Side view with perspective. QLs are slanted by 58 degrees.

(b) Top view of the topmost atomic layer, with surface unit vectors denoted by $a_1$ and $a_2$.

Using the experimental bulk structure, the length of $a_1$ is 4.14 Å, the $y$-component of $a_2$ is 11.26 Å long.

Side surface of Bi$_2$Se$_3$

Band dispersions

Wave function in real space

Anisotropic 2D Dirac fermions on the side surface of $\text{Bi}_2\text{Se}_3$

Low-energy effective Hamiltonian

$$H = \hbar(-v_x \sigma_y k_x + v_y \sigma_x k_y)$$

Ray optics of Dirac fermions in topological insulators

- Refraction at (111)/(221) interface

\[ T = \frac{\cos(\phi - \theta') + \cos(\phi + \theta')}{1 + \cos(\phi + \theta')} \]

Ray optics of Dirac fermions in topological insulators

- Fabry-Perot interferometer

\[
R = \frac{\sin^2(q_y D)(\sin \phi - \sin \theta')^2}{\cos^2 \phi \cos^2 \theta' + \sin^2(q_y D)(\sin \phi - \sin \theta')^2}
\]

Summary

• Conventional band theory with spin-orbit coupling is suited for topological insulators. Bulk and surface electronic structures of Bi$_2$Se$_3$ and other topological insulators are reviewed briefly.

• Our calculations of bulk and surface electronic structures of Bi$_2$Se$_3$, Sb$_2$Te$_3$, and Bi$_2$Te$_3$ agree well with previous published works.

• Our results on the side surface of Bi$_2$Se$_3$ show low-velocity anisotropic Dirac fermions, which opens a new perspective of topological insulators for "surface ray optics".