Evolution of topological surface states of thin HgTe-films with film thickness

Bachelor thesis

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Hello, my name is Tamara Szecsey and I will now give you a talk about my bachelor thesis topic, the evolution of topological surface states of thin HgTe-films with film thickness.

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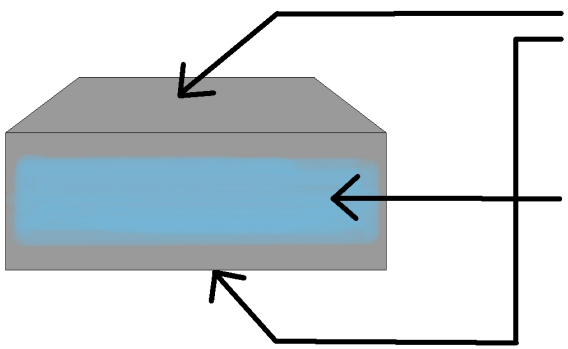
Introduction

HgTe is a II-VI semiconductor and a topological insulator (TI).[1]



TIs are interesting because:

- spin-momentum locking
- protected surface states

Calculations were performed using density functional theory (DFT) through FHI-aims.

Main goal: Evolution of surface states in different slab thicknesses.

[1] F. Virot et al. "Engineering Topological Surface States: HgS, HgSe, and HgTe". In: *Phys. Rev. Letters* 111.146803 (2013).

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Introduction

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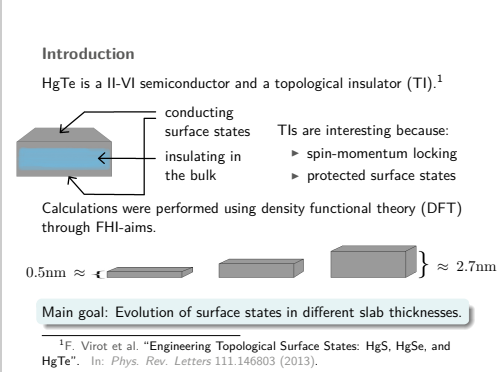

HgTe belongs to the class of mercury-based II-VI(6) semiconductors which appear in zinc-blende structure. It is additionally found to be a topological insulator.
A topological insulator is a material which is insulating in its interior, also called the bulk of a material, and that develops conducting states at the surface.
They are very attractive for potential applications because the spin and the momentum of the electrons at the conducting surfaces are locked. This means, the spin is always perpendicular to the direction of motion of those electrons. The spin-momentum locking make sure that the surfaces are protected if time-reversal symmetry preserved. In other words the surface states remain even for non-magnetic impurities.
The calculations I performed were ab-initio calculations and therefore I used the density functional theory with the exchange-correlation function method PBE, which is short for Perdew-Burke-Ernzerhof through FHI-aims.
HgTe was examined in thin films from approximately 0.5 nm to 2.7 nm, which are 4 to 17 layers of atoms. Surfaces can only be examined in one direction at once. Because otherwise it would went beyond the scope of a bachelor thesis, we chose just direction of observance, namely the (001) direction.

The main goal this thesis pursued was examining the evolution of topological surface states for different slab thicknesses. Therefore I will now explain the theory behind the realization of this examination.

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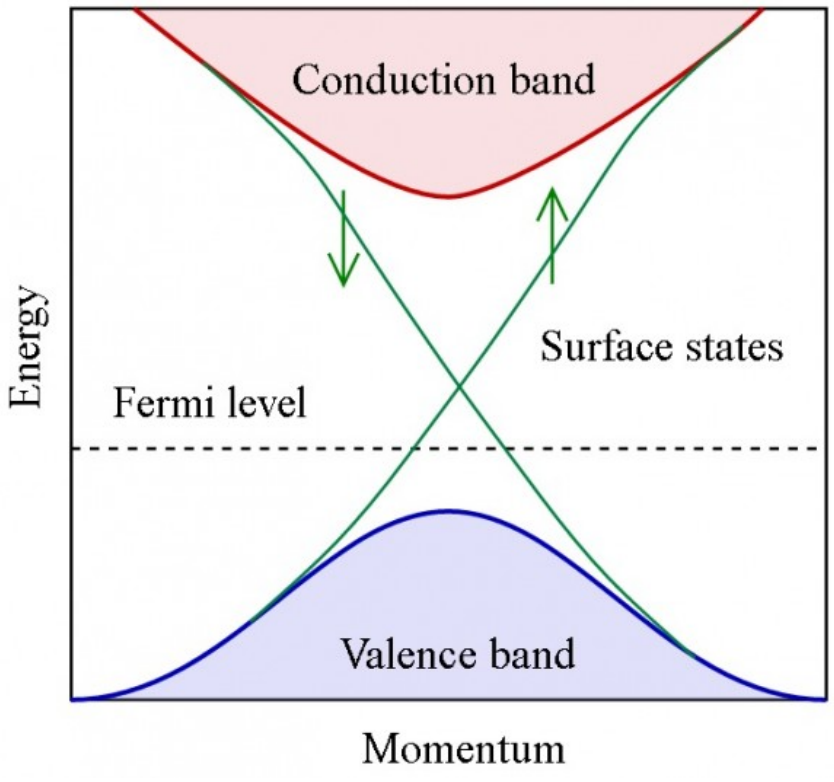
Theory: Topological insulator

2005 Kane and Mele found another class of material:
the topological insulator (TI).
spin-orbit coupling $\rightarrow$ band inversion $\rightarrow$ Dirac cone



2D TI:

have quantum spin edge states found in graphene and HgTe quantum wells.

3D TI:

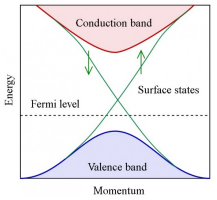
strong and weak ones
HgTe is semi metal but under strain Γ_6 and Γ_8 bands can close up at Fermi level.

└Theory: Topological insulator

Besides from insulators and conductors, Kane and Mele 2005 found another class of material which is the so-called topological insulator.

Theory: Topological insulator

2005 Kane and Mele found another class of material:
the topological insulator (TI).
spin-orbit coupling → band inversion → Dirac cone



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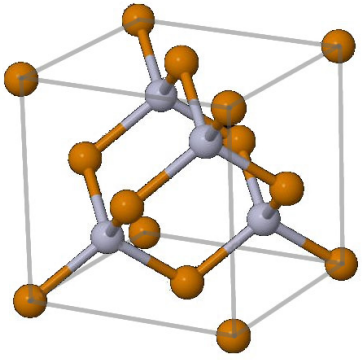
Theory: Crystal and surface description part 1

Translation Vector: $\boldsymbol{R}_i = x_i\boldsymbol{a}_1 + y_i\boldsymbol{a}_2 + z_i\boldsymbol{a}_3$

contains basis for lattice forming a unit cell.
Smallest primitive unit cell is the Wigner Seitz cell.

Bravais lattice

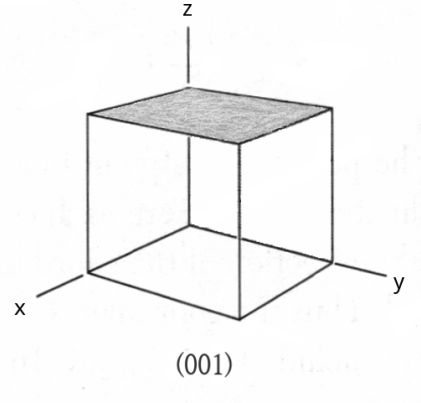
fcc lattice with two atomic basis $\rightarrow$ diamond or zinc-blende structure



	x	y	z
$\boldsymbol{a}_1$	0	$\frac{a}{2}$	$\frac{a}{2}$
$\boldsymbol{a}_2$	$\frac{a}{2}$	0	$\frac{a}{2}$
$\boldsymbol{a}_3$	$\frac{a}{2}$	$\frac{a}{2}$	0
Te	0	0	0
Hg	$\frac{a}{4}$	$\frac{a}{4}$	$\frac{a}{4}$

Miller indices: (hkl)

$$h : k : l = \frac{1}{x} : \frac{1}{y} : \frac{1}{z}$$



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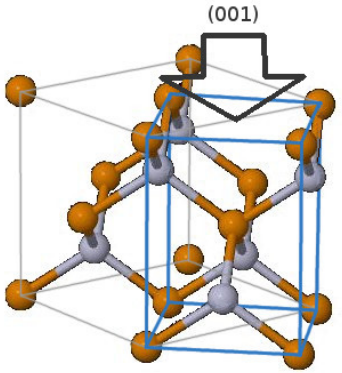
Theory: Crystal and surface description part 2

Basis for (001) direction of zinc-blende structure:



	x	y	z
$\boldsymbol{a}_1$	$\frac{a}{\sqrt{2}}$	0	0
$\boldsymbol{a}_2$	0	$\frac{a}{\sqrt{2}}$	0
$\boldsymbol{a}_3$	0	0	a

	x	y	z
Te	0	0	0
Hg	$\frac{a}{2\sqrt{2}}$	0	$\frac{a}{4}$
Te	$\frac{a}{2\sqrt{2}}$	$\frac{a}{2\sqrt{2}}$	$\frac{a}{2}$
Hg	0	$\frac{a}{2\sqrt{2}}$	$\frac{3a}{4}$

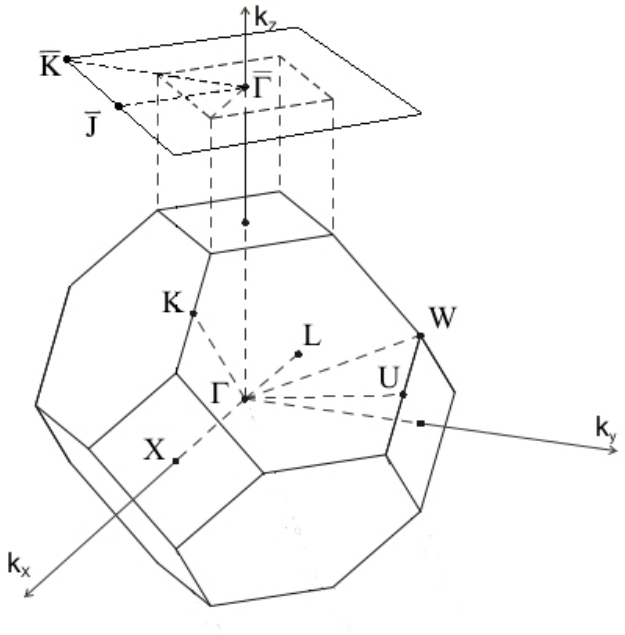
Reciprocal lattice: $e^{i\boldsymbol{K}\boldsymbol{R}} = 1$

$\boldsymbol{K}$ is reciprocal translation vector.

First Brillouin zone (BZ) is Wigner Seitz cell for reciprocal space.

Super symmetrical points:

$$\overline{\Gamma} = 0; \quad \overline{\mathrm{J}} = \frac{1}{2}\boldsymbol{b}_1; \quad \overline{\mathrm{K}} = \frac{1}{2}\boldsymbol{b}_1 + \frac{1}{2}\boldsymbol{b}_2$$



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Theory: Surface modeling

Termination

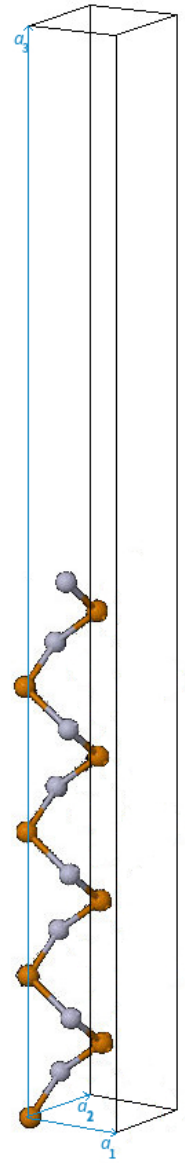
Two surfaces with symmetric Hg-Hg, Te-Te terminations or antisymmetric Te-Hg terminations.
Add hydrogen atoms in order to saturate dangling bonds.

Number of layers

Atoms with same z component are in the same layer.
Odd for symmetric, even for antisymmetric termination.
I studied 3 different thicknesses for each termination.

Supercell approach

Infinite repetition only possible in all directions.
In order to avoid interactions between slabs in k_z direction: add vacuum space.



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Theory: Density functional theory (DFT)

First Hohenberg-Kohn Theorem:

$\rho(\boldsymbol{r})$ can be uniquely converted into the $V_{\text{ext}}(\boldsymbol{r})$

Second Hohenberg-Kohn Theorem:

Ground state energy can be expressed in a density functional:

$$E^{\text{HK}}[\rho(\boldsymbol{r}); v_{\text{ext}}(\boldsymbol{r})] = T_0[\rho] + V_{\text{H}}[\rho] + \int v_{\text{ext}}(\boldsymbol{r})\rho(\boldsymbol{r})\mathrm{d}\boldsymbol{r} + E_{\text{xc}}[\rho]$$

Kohn-Sham equation

Minimizing $E^{\text{HK}} \rightarrow$ Kohn-Sham eigenfunctions $\boldsymbol{p}hi_i(\boldsymbol{r})$:

$$E_0[\rho_0] = E_{\text{nucl}} + E_{\text{kin}} + E_{\text{H}} + E_{\text{xc}}$$

Perdew-Burke-Ernzerhof (PBE) functional

$$E_{\text{xc}}^{\text{PBE}} = \int \mathrm{d}^3 r \rho(\boldsymbol{r})\, \epsilon_{\text{xc}}^{\text{PBE}}(r_s(\boldsymbol{r}), s(\boldsymbol{r}), \zeta(\boldsymbol{r}))$$

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Theory: Spin-orbit coupling

Dirac equation: $$\left(c\boldsymbol{\alpha}\cdot\boldsymbol{p}+c^2(\beta-1)+V\right)\Psi=\epsilon\Psi$$

Separate Ψ into two spinors: $$\Psi=\begin{pmatrix}\Psi_L\\ \Psi_S\end{pmatrix}$$

Substitute and dissolve:

$$\left(\boldsymbol{p}\frac{c^2}{2c^2+\epsilon-V}\boldsymbol{p}+i\boldsymbol{p}\frac{c^2}{2c^2+\epsilon-V}\times\boldsymbol{p}\cdot\boldsymbol{\sigma}+V\right)\Psi_L=\epsilon\Psi_L$$

First part with V is relativistic Schrödinger equation.
Expanding in $\frac{\epsilon-V}{2c^2}$ in zeroth order gives non-relativistic Schrödinger equation.
Expanding just second part in first order gives:

$$V_{SOC}=\frac{i}{4c^2}\boldsymbol{p}V\times\boldsymbol{p}\cdot\boldsymbol{\sigma}$$

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Conclusion

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