Table of Contents

Bi_2Se_3 topological insulator

Version: 2016.2

Downloads & Links

- PDF version
- Tutorial Synopsis
- Bi2Se3_bulk_configuration.py
- Bi2Se3_bulk.py
- Bi2Se3_slab.py
- dos.py
- bloch_states.py
- spinVector.py
- fermi_surface.py
- TopologicalInvariant3D.py
- Basic QuantumATK Tutorial
- ATK Reference Manual
- Basic QuantumATK Performance Guide

Topological insulators are electronic materials that have a bulk band gap like an ordinary insulator, but still support conducting states on their surface. It can be shown that these states are topologically protected due to a non-trivial topological index of the material and cannot be removed by any distortions. The 2D energy–momentum relation of these surface states has a “Dirac cone” structure similar to that of graphene. Topological insulators therefore constitute a new class of quantum matter governed by exotic physics that may some day be exploited in electronic devices. Refs. [1] and [2] provide recent reviews of this highly active field of research.

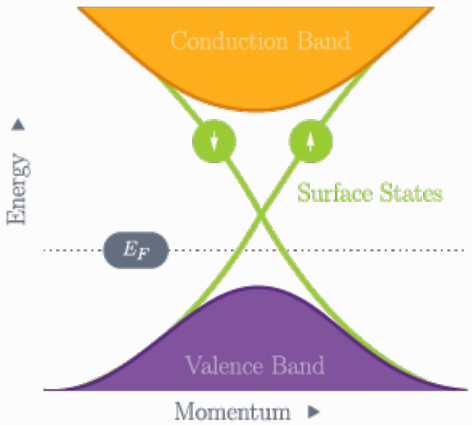


Fig. 49 The valence and conduction bands of a topological insulator are separated by a non-zero band gap, but bands due to surface states cross the band gap and lead to electronic conduction at the surface

of the material.¶

In this tutorial you will learn how to use ATK-DFT to study the Bi_2Se_3 compound, which is a 3D strong topological insulator. Nonequilibrium Green's function DFT calculations were recently reported for a Bi_2Se_3 thin film connected to leads in a two-terminal device setup [3]. However, this tutorial focuses on bulk calculations and properties of the surface states. In particular, you will:

- Use the QuantumATK Crystal Builder to construct the Bi_2Se_3 crystal structure.
- Investigate the bulk Bi_2Se_3 band structure with and without the SOC.
- Construct a Bi_2Se_3 slab configuration and compute the SOC band structure, which exhibits the surface states mentioned above.
- Compute the density of states (DOS) around the Fermi energy, which nicely illustrates the Dirac cone inside the bulk band gap.
- Investigate the surface state penetration depth into the material.
- Plot the spin-resolved Fermi surface of surface states, and investigate how the in-plane spin orientation varies on the Fermi surface.
- Calculate the topological invariants for Bi_2Se_3.

Note

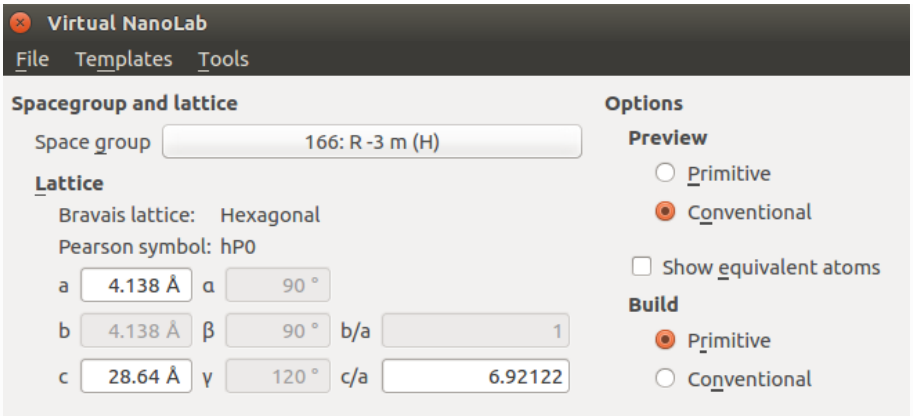
It is essential to include the spin-orbit coupling (SOC) to correctly describe the electronic structure of a topological insulator.

Build the Bi_2Se_3 crystal

Open the QuantumATK Builder and click Add ▸ From Plugin ▸ Crystal Builder. As described in [4], the Bi_2Se_3 crystal is rhombohedral and belongs to space group $\mathrm{R\bar{3}\,m}$. It has lattice constants a=4.138 Å and c=28.64 Å, and internal coordinates μ=0.399 for Bi sites and ν=0.206 for Se sites. The basic Bi_2Se_3 unit cell, called a quintuple layer (QL), contains 5 atoms: One Se atom at coordinate (0, 0, 0), Bi atoms at internal coordinates $(\pm\mu, \pm\mu, \pm\mu)$, and Se atoms at $(\pm\nu, \pm\nu, \pm\nu)$.

Lattice

In the Crystal Builder, choose the *Trigonal* space group number 166 with *Hexagonal* setting, and enter the lattice parameters:

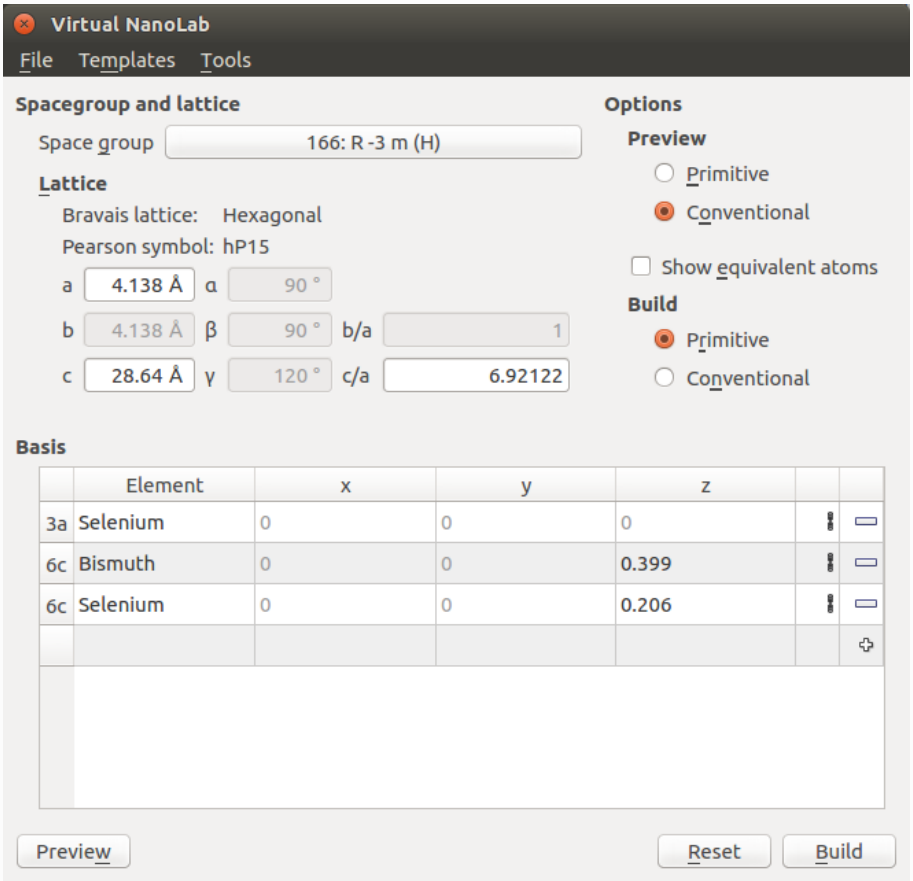


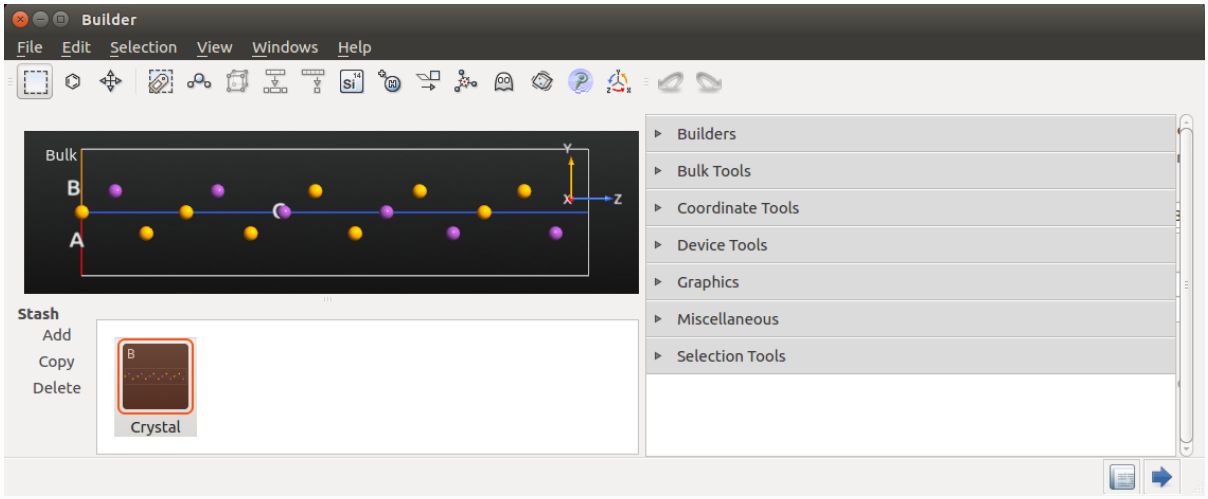
Basis

Then specify the atomic basis with which to decorate the lattice, i.e. enter the internal coordinates of the unique sites of the Bi_2Se_3 crystal and the elements that should be at those sites:

1. Click the ✥ icon and select site *3a: (0,0,0)*, and change the element from hydrogen to selenium.
2. Use the same procedure twice for specifying the remaining sites, but choose *6c: (0,0,z)* for the site type, and enter the internal coordinates z=0.399 for bismuth and z=0.206 for selenium.

The Crystal Builder window should now look like illustrated below. Click *Build* to build the bulk configuration – it will then appear in the Builder Stash.



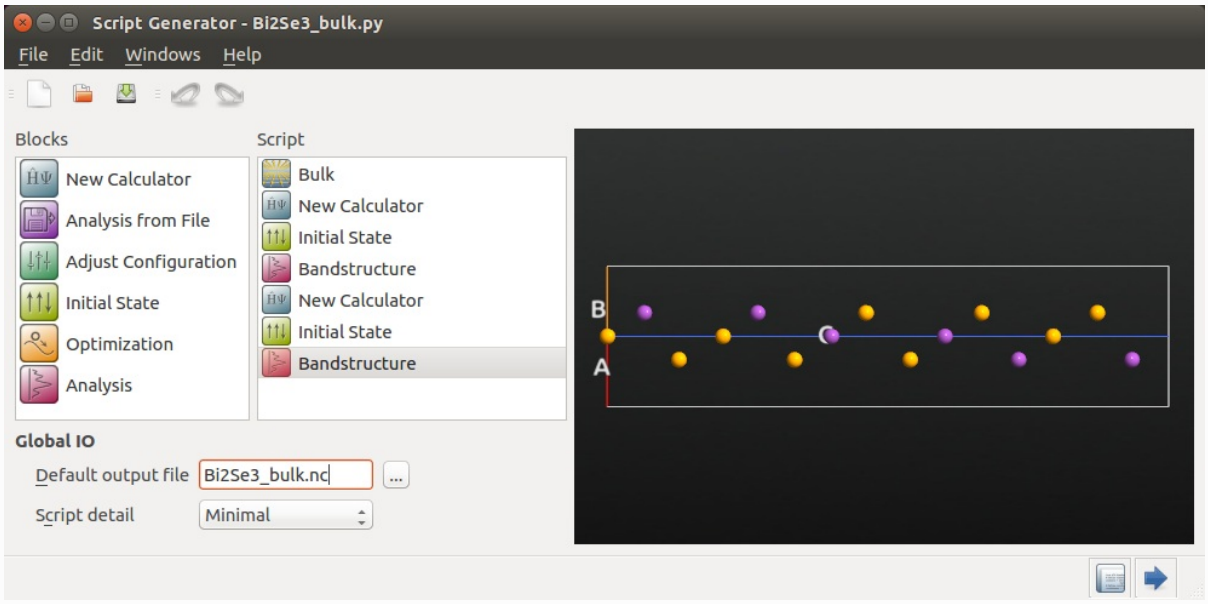


You have now built the Bi_2Se_3 bulk configuration with 3 QLs and 15 atoms in total. Continue to the next section to start doing some DFT calculations for this material. If needed, you can also download the bulk configuration here: Bi2Se3_bulk_configuration.py

Bi_2Se_3 bulk band structure

Send the bulk configuration to the Script Generator, and set up a Python script that uses ATK-DFT to calculate the band structure with and without the spin-orbit coupling. The script should first calculate the self-consistent GGA state and perform band structure analysis, and then use that state as an initial guess for the self-consistent SOGGA state, again followed by band structure analysis.

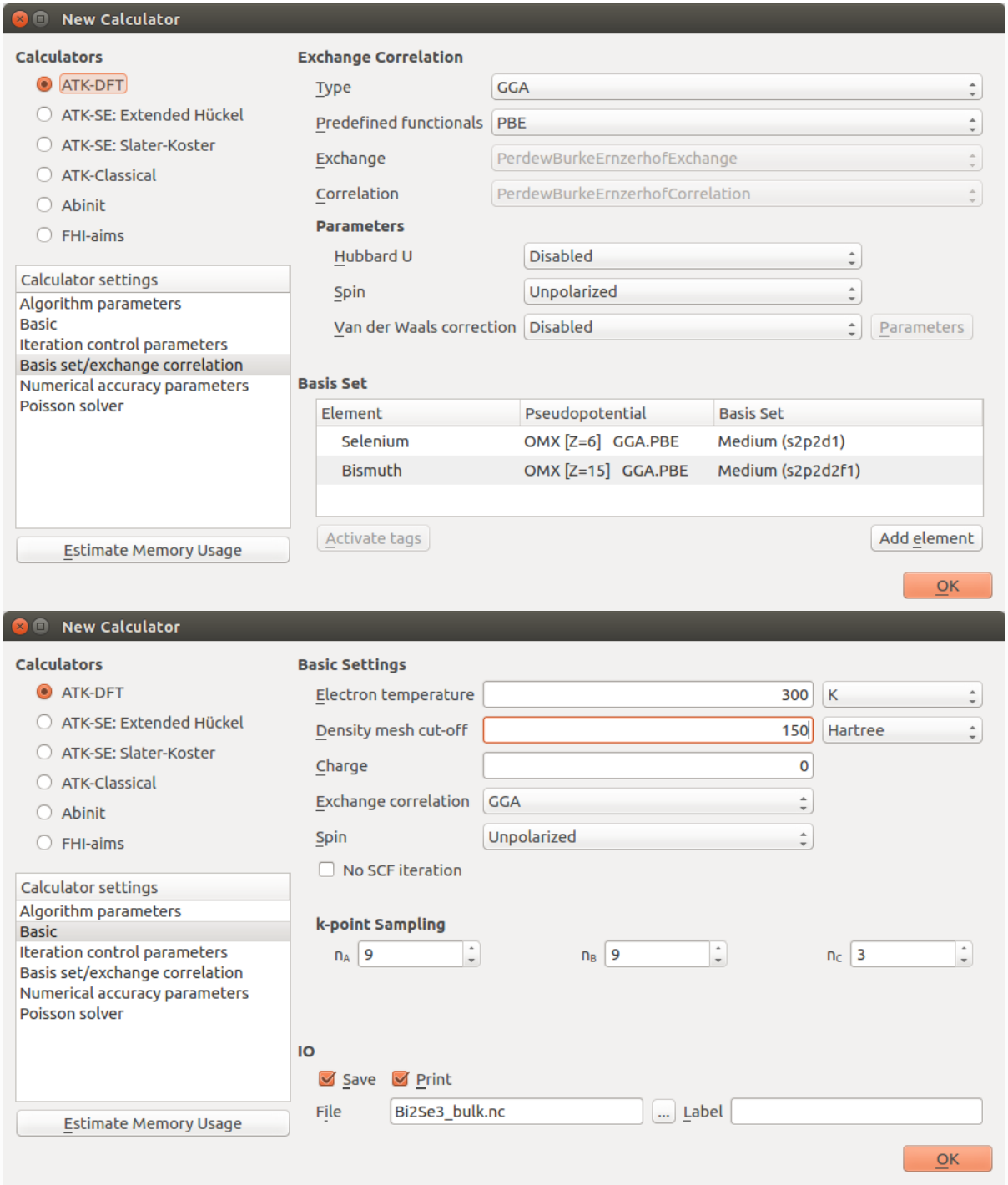
The Script Generator now contains the bulk configuration. Add the New Calculator, Analysis ▸ Bandstructure, and Initial State blocks, as illustrated below. Also change the default output file to `Bi2Se3_bulk.nc`.



GGA calculation

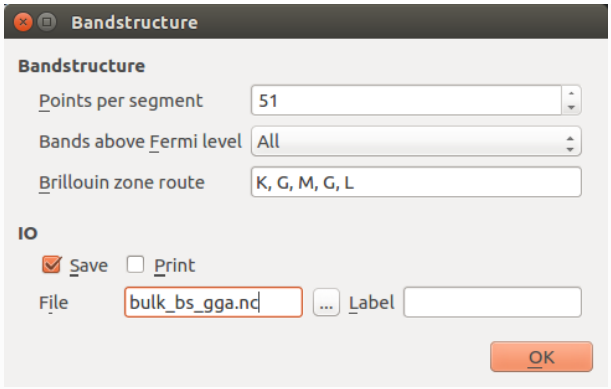
Open the first New Calculator block to edit it:

- Make sure to choose the ATK-DFT calculator.
- In the *Basis set/exchange correlation* settings, choose *GGA* and change the pseudopotentials to the *OMX* family with *Medium* basis sets for both Se and Bi.
- In the *Basic settings* tab, increase the density mesh cut-off to 150 Hartree, and set up a 9x9x3 k-point grid. Click *OK* to save the settings.



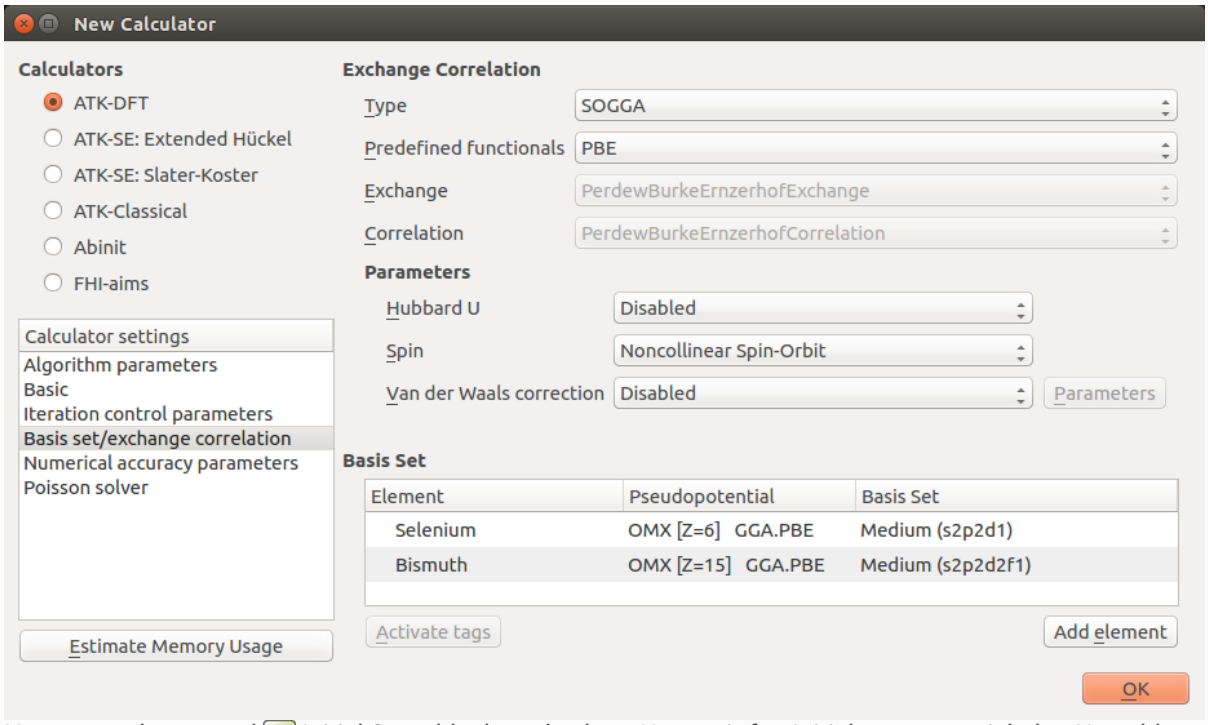
Then open the first Bandstructure block and edit it:

- Increase *points per segment* to 51 to get a nicely resolved band structure.
- Change the Brillouin zone route to *K, G, M, G, L*.
- Change the IO file to `bulk_bs_gga.nc`.

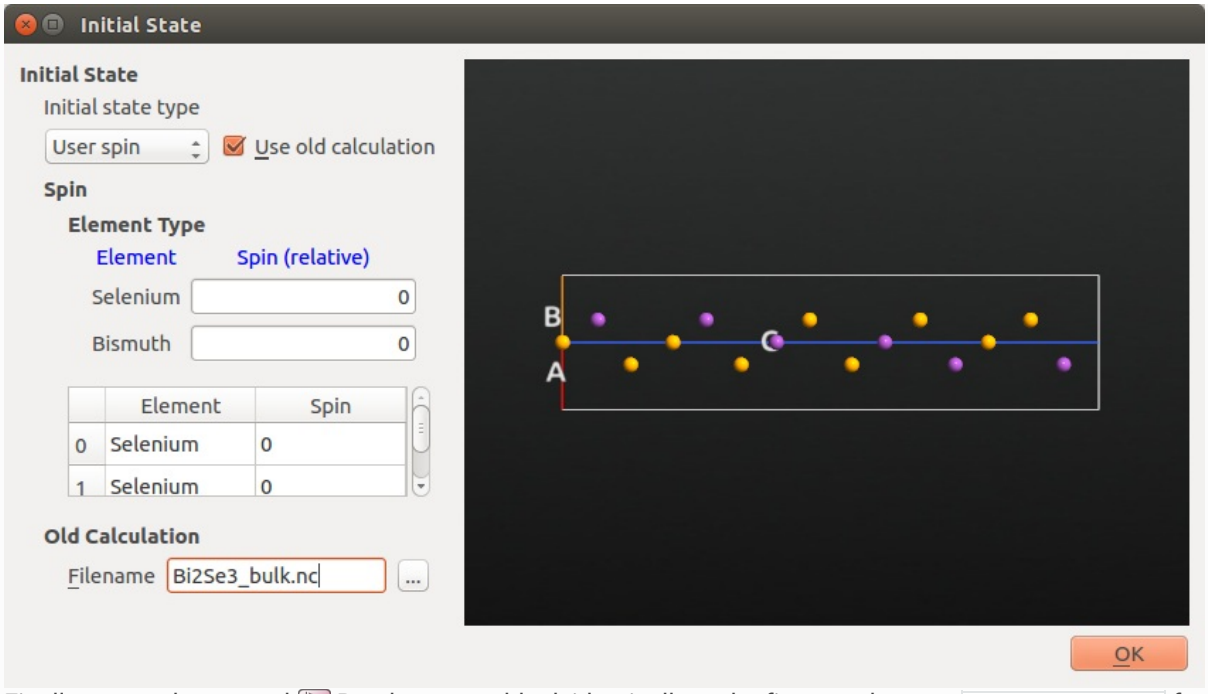


SOGGA calculation

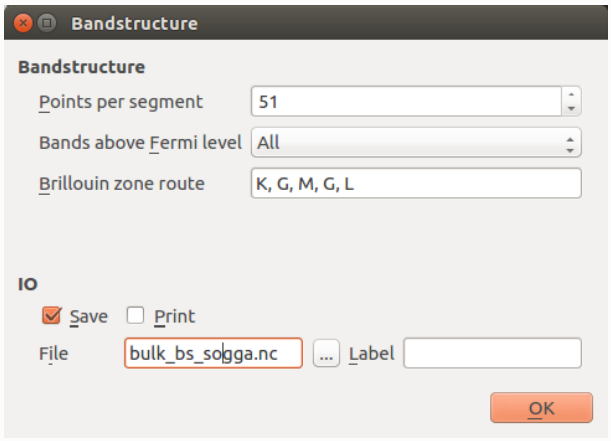
Open the second New Calculator block, and edit it such that the settings are identical to those in the first calculator, but set the *Spin* parameter to *Noncollinear Spin-Orbit* in order to do a SOGGA calculation. Remember to also set the pseudopotentials, density cut-off, and k-points.



Next, open the second Initial State block, and select *User spin* for *Initial state type*, tick the *Use old calculation* option, and enter the file name `Bi2Se3_bulk.nc` from which the GGA state should be read.



Finally, set up the second Bandstructure block identically to the first one, but use `bulk_bs_sogga.nc` for the IO file.



Results

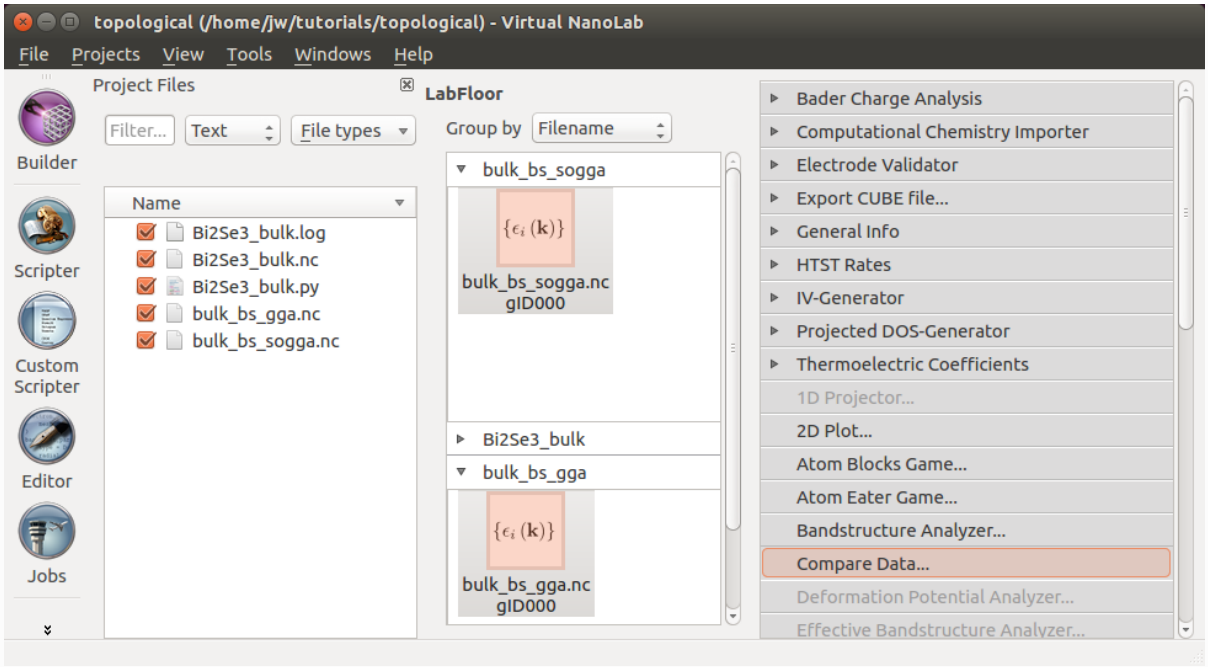
The Python script is now ready. Save it as `Bi2Se3_bulk.py`. If needed, you can also download it here: Bi2Se3_bulk.py

Execute it using the Job Manager or in a Terminal. The job will take a while, but the wall time can be brought down to around 40 minutes if executed in parallel with 2 MPI processes on 2 CPUs. Note that this requires in total about 15 GB of available memory!

Tip

The tutorial Basic QuantumATK Performance Guide offers tips on QuantumATK performance, including how to deal with memory issues.

Once the calculation has finished, the QuantumATK **LabFloor** contains three sets of data: *Bi2Se3_bulk*, *bulk_bs_gga*, and *bulk_bs_sogga*. The last two contain the GGA and SOGGA band structures. Highlight both band structure objects, and use the **Compare Data** plugin to plot both of them.



The plot is shown below. Including spin-orbit coupling in the calculations (SOGGA) has a significant impact on the band structure, and widens the direct band gap at the Γ-point However, we do not see any bands crossing the Fermi level (the smallest SOGGA band gap is 0.3 eV), so the Bi_2Se_3 bulk material is an insulator.

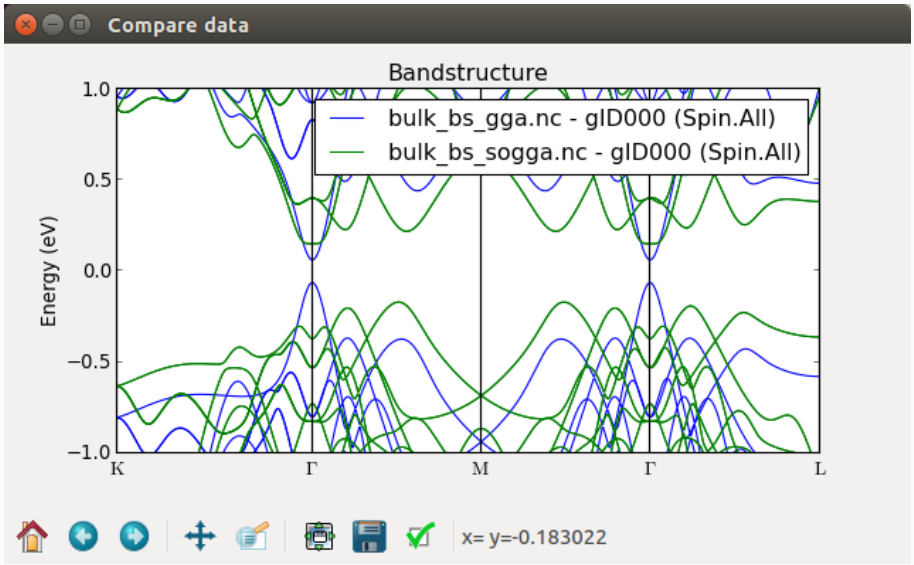


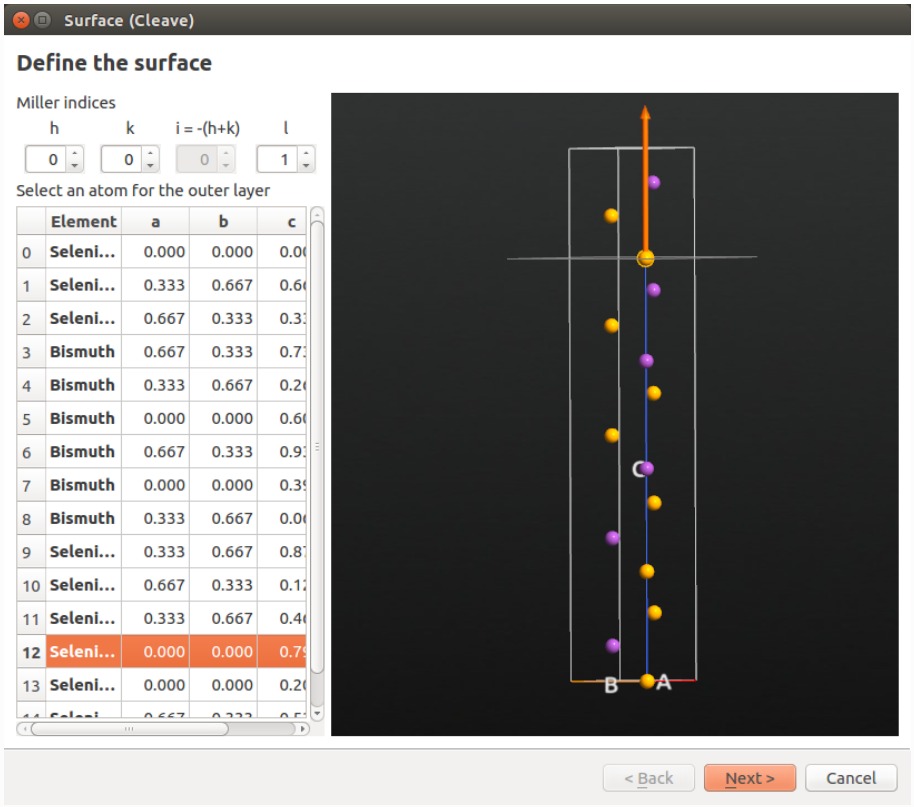
Fig. 50 Comparison of the GGA (blue) and SOGGA (green) band structures of bulk Bi_2Se_3.¶

Bi2Se3 surface: Spin-orbit band structure

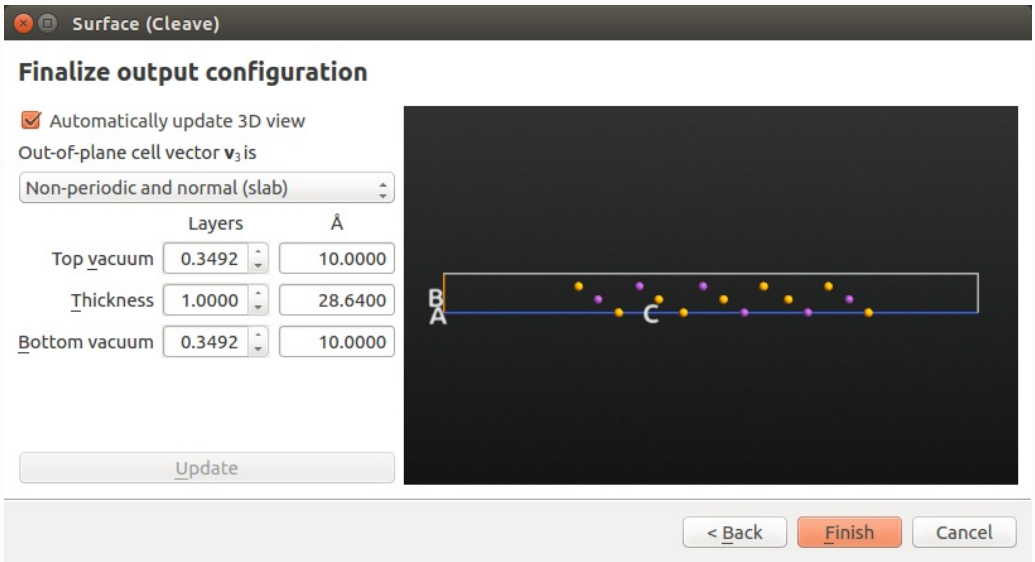
You will now create a Bi_2Se_3 slab configuration, and compute the SOGGA band structure, which will exhibit the topologically protected surface states crossing the band gap around the Γ-point.

Constructing the surface

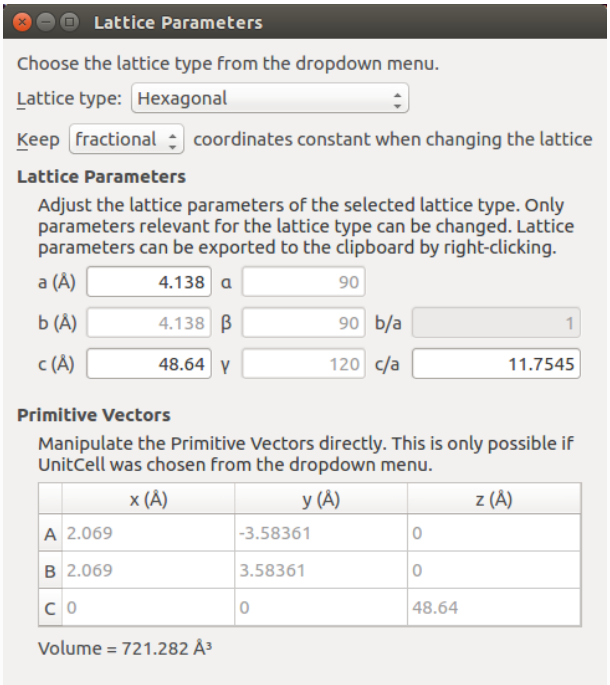
Back in the **Builder**, highlight the Bi_2Se_3 bulk configuration (named Crystal), and open the Builders ▸ Surface (Cleave) plugin. Choose Miller indices (0001), and select selenium atom #12 as the top atom in the slab. Then click *Next*.



Leave settings at defaults in the “Define surface lattice” options window. In the “Finalize output configuration” options, choose a *Non-periodic and normal (slab)* out-of-plane cell vector, and enter 10 Å for both top and bottom vacuum. Then click *Finish*.



The slab configuration, named Crystal (0001), has now appeared in the Stash. As a final touch, highlight the item and use the Bulk Tools ▸ Lattice Parameters plugin to convert the lattice type to *Hexagonal* while keeping the fractional coordinates constant:

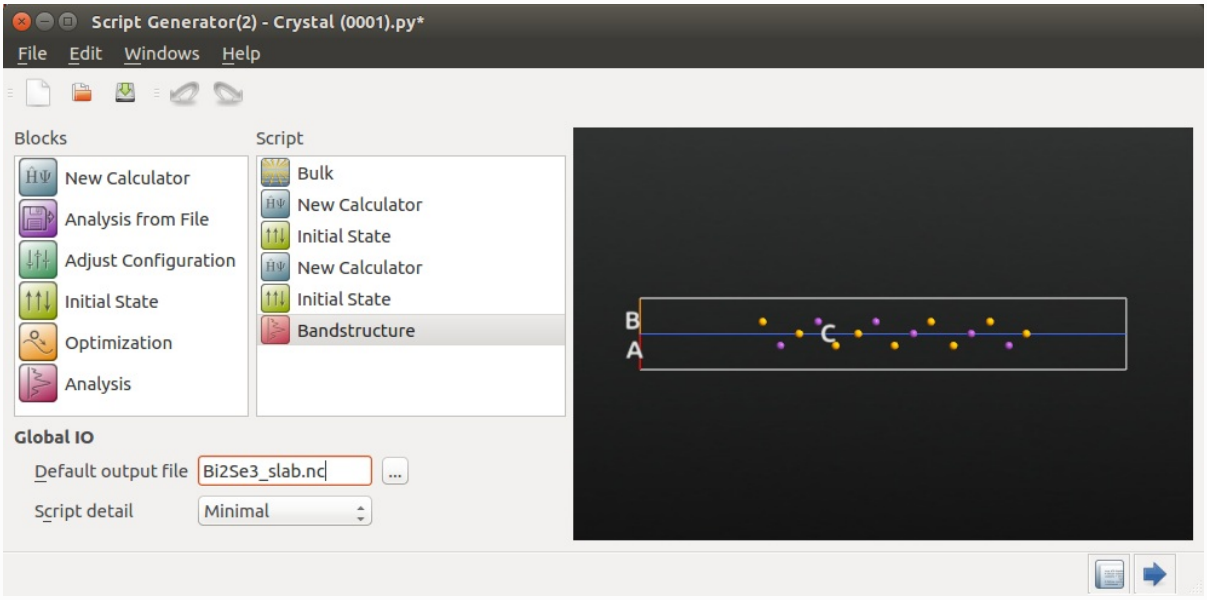


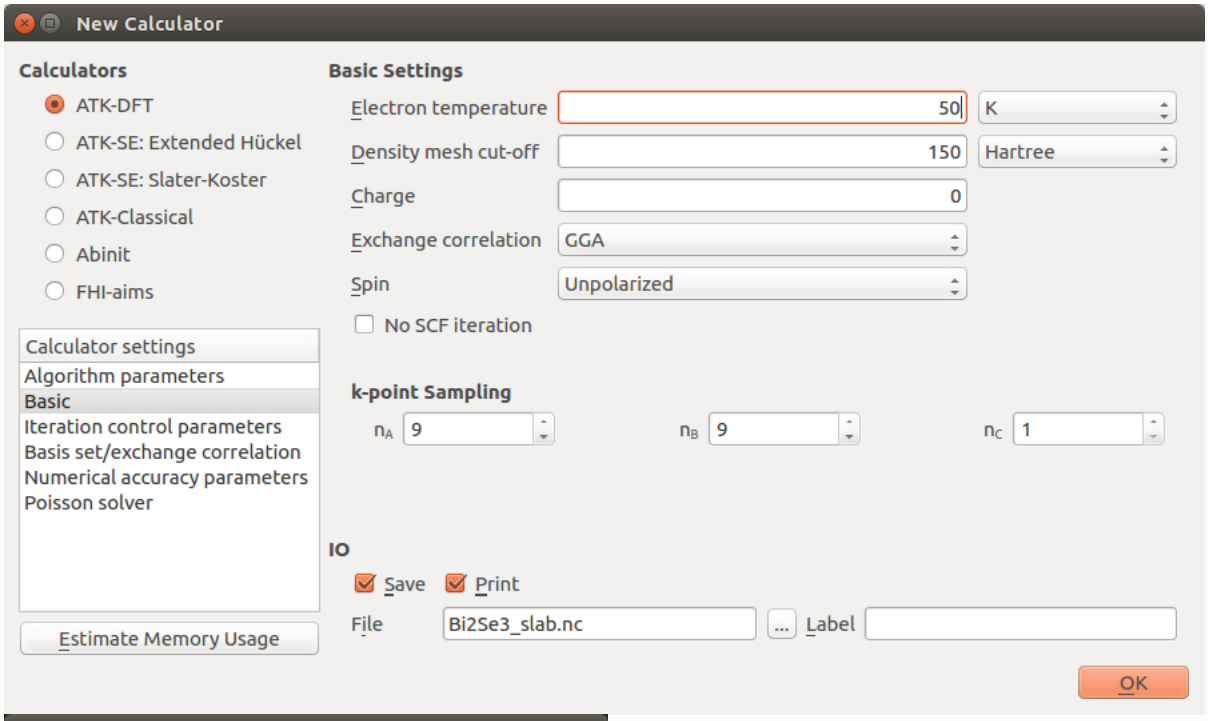
DFT-SOGGA calculations

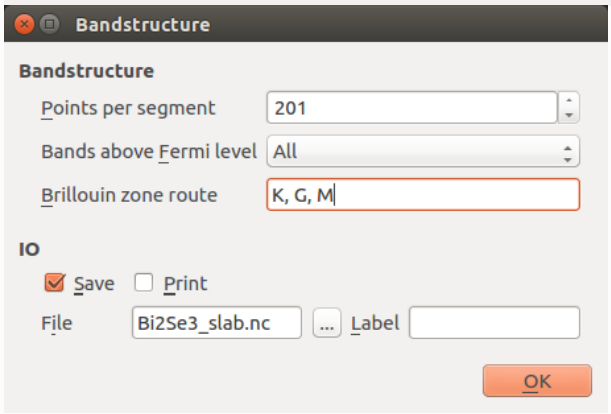
You can now send the slab configuration to the **Script Generator**, and set up the SOGGA band structure calculation similarly to what you did above for the bulk, but with slight changes:

- You will not need the GGA band structure analysis.
- Use `Bi2Se3_slab.nc` as default output file.
- Use a 9x9x1 k-point grid (the slab is not periodic along the C-direction).
- Decrease the electron temperature from 300 to 50 K. This will improve the DFT description of electron occupations close to the Fermi level.
- Use 201 points per segment for the SOGGA band structure analysis, and the *K*–*G*–*M* Brillouin zone route.

Alternatively, you can simply skip the above and go directly to the next section to use a pre-made Python script with a few additional features.







Convenient Python script

Click here: Bi2Se3_slab.py to download a Python script that was made using the procedure outlined above, but also has a few extra features:

- The “MemoryUsage” functionality is used to estimate the memory required for the GGA and SOGGA calculations immediately before they are executed.
- The SOGGA calculator is constructed as a copy of the GGA calculator, and is then modified accordingly.
- A special density mixing algorithm is used for the non-collinear calculation.

Run the calculation using the Job Manager or in a Terminal. The job will take roughly 30 minutes if executed in 2 parallel MPI processes on 2 CPUs.

Hint

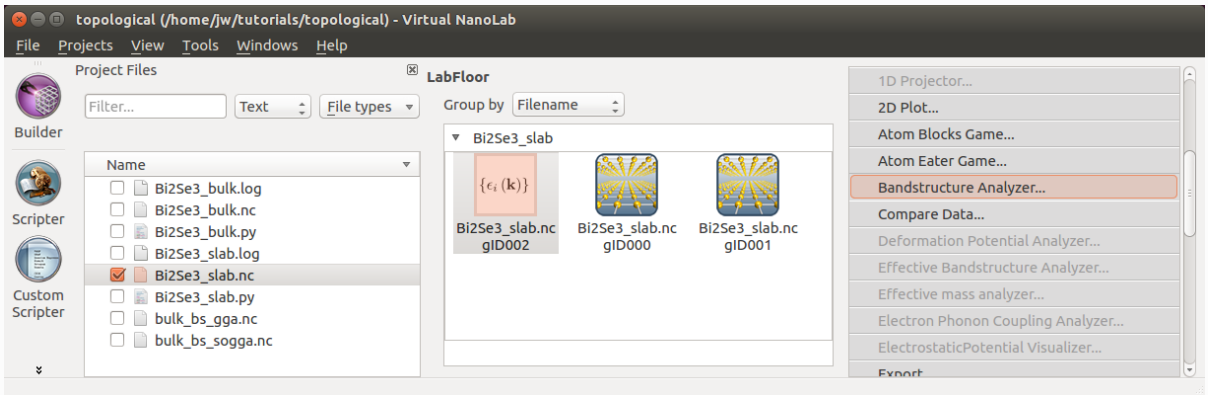
If you look at the log file during the calculation, you will see that the estimated peak memory requirements are 756 MB per MPI process for the GGA calculation, and 3.8 GB per MPI process for the SOGGA calculation. These are estimates, and in practice you should expect the full calculation to require almost 5 GB per MPI process.

```
GGA:
+-----------------------------------------------------------+
| Memory usage estimate                                     |
| --------------------------------------------------------- |
| Base: Sparse matrices                          44 Mbyte   |
| Base: GridTool+Basis set                      100 Mbyte   |
| Base: SCF history                             442 Mbyte   |
| Base: NLEngine                                 70 Mbyte   |
| Base: Grid terms                               39 Mbyte   |
| Sum of the base terms                         696 Mbyte   |
| --------------------------------------------------------- |
| Peak: Diagonalization                          60 Mbyte   |
| Peak: Grid terms                               19 Mbyte   |
| --------------------------------------------------------- |
| Estimated Peak memory requirement             756 Mbyte   |
+-----------------------------------------------------------+

SOGGA:
+-----------------------------------------------------------+
| Memory usage estimate                                     |
| --------------------------------------------------------- |
| Base: Sparse matrices                          272 Mbyte  |
| Base: GridTool+Basis set                       100 Mbyte  |
| Base: SCF history                             2726 Mbyte  |
| Base: NLEngine                                 70 Mbyte   |
| Base: Grid terms                               157 Mbyte  |
| Sum of the base terms                         3326 Mbyte  |
| --------------------------------------------------------- |
| Peak: Diagonalization                          446 Mbyte  |
| Peak: Grid terms                               58 Mbyte   |
| --------------------------------------------------------- |
| Estimated Peak memory requirement             3772 Mbyte  |
+-----------------------------------------------------------+
```

Results

The QuantumATK **LabFloor** should now contain the results of the calculation. Select the band structure object, and use the **Bandstructure Analyzer** to plot it.



The calculated band structure of the Bi_2Se_3 slab is shown below. Bands are now present around the Fermi level at the
Γ-point – these are surface states. There are four such surface states crossing the Fermi level (indicated by red dots); bands 142 and 143 form a single degenerate band immediately below the Fermi energy, while bands 144 and 145 form a degenerate band above E_F. The bulk valence bands are below those surface states (indicated by blue dot). It is clear that the dirac cone is located inside the bulk band gap. There is a tiny gap between the valence and conduction surface bands of size 7 meV. This is a finite size effect from the use of a slab model, which arise from the interaction of the surface bands on opposite sides of the slab. For a larger slab the gap will be reduced.

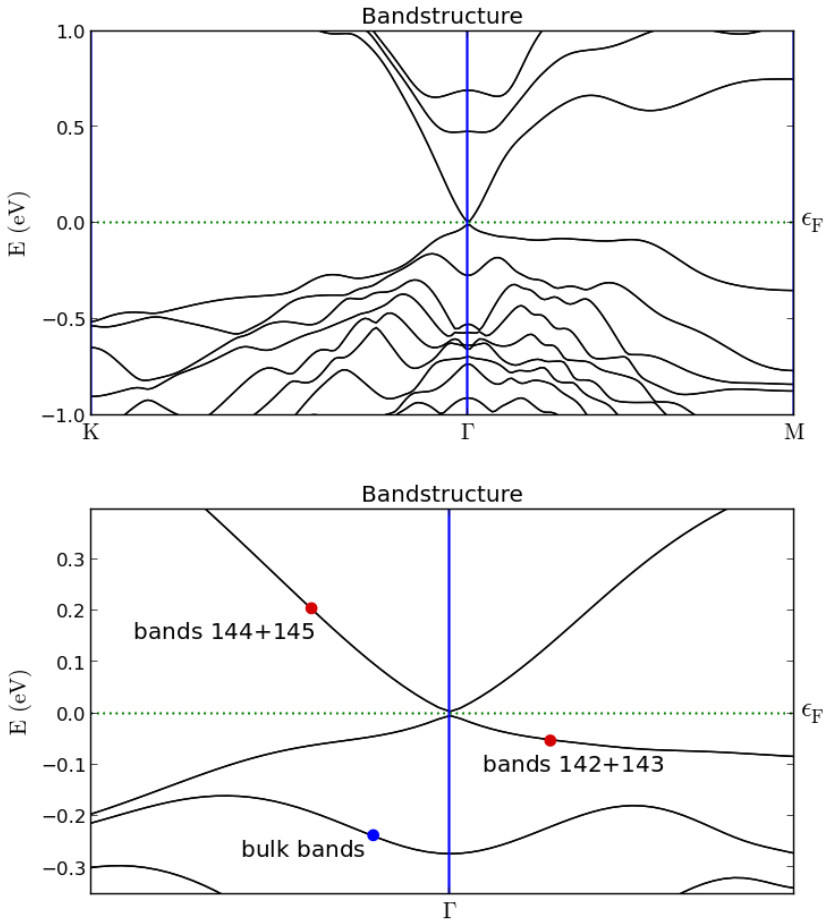
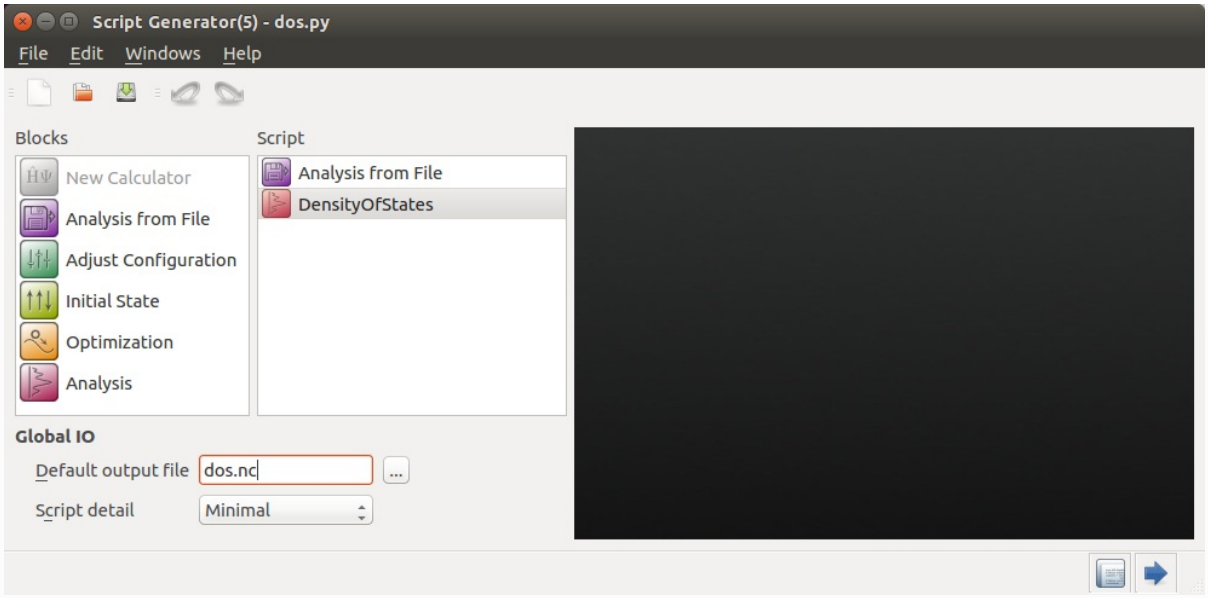


Fig. 51 SOGGA bandstructure of the Bi_2Se_3 slab configuration. The bottom panel is a zoom-in on the topologically protected Dirac cone. Both surface state bands (red dots) are both doubly degenerate and are located above the bulk valence bands (blue dot).¶

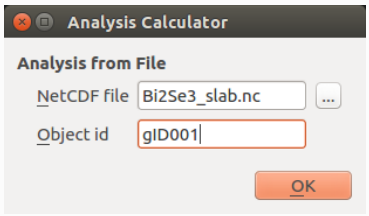
DOS analysis: Dirac cone finger print

As stated in the introduction, the electronic structure of the surface states close to the Fermi level resembles that of a Dirac cone, where the electron momentum depends linearly on the energy. Since the surface states are the only states present inside the bulk energy gap, we should expect the electronic density of states close to E_F to be linear. It is easy to compute and plot the DOS as a post-SCF analysis:

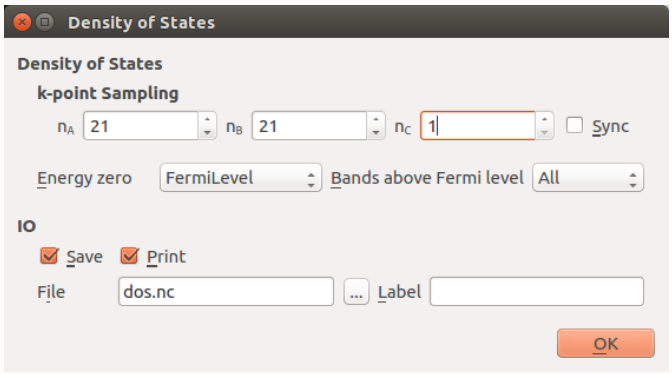
Open the **Script Generator** and add the Analysis from File and Analysis ▸ DensityOfStates blocks. Change the default output file to `dos.nc`.



Open the first block, and point to the `Bi2Se3_slab.nc` file and Object id *gID001*, which is the self-consistent SOGGA state.



Then open the DensityOfStates analysis block, and set up a dense k-point sampling along k_x and k_y, 21x21x1. You will need to uncheck the *sync* option. Remember: It is important in this case to sample the Γ-point, so we use use an odd k-grid.



Save the script as `dos.py` and run it. You can also download it here: dos.py.

Then locate the DOS object on the **LabFloor**, and use the **2D Plot** plugin to visualize it. With a bit of zooming you should be able to see the expected linear dependence of the DOS on energy, as illustrated below. The sharp increase in DOS at E=0.47 eV are due to the lowest bulk conduction bands.

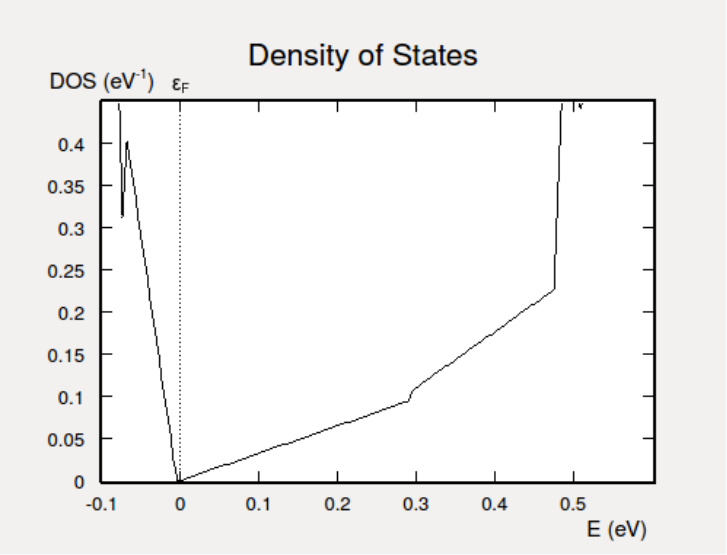


Fig. 52 Electronic DOS for the Bi_2Se_3 slab. Due to the Dirac cone, the DOS depends linearly on the energy in the vicinity of the Fermi level.¶

Penetration depth of surface states

An essential feature of the topologically protected surface states close to the Dirac point is that they are highly localized to the surface region. The penetration depth into the bulk material may be as small as 2–3 nm [4]. Moreover, the degenerate surface states observed in a band structure calculation are in each specific k-point composed of states with opposite spin and localized on opposite sides of the slab.

You will now investigate this by performing a **BlochState analysis** in a specific k-point on the Dirac cone for bands 144 and 145. You will then project both Bloch states onto the C-axis of the Bi_2Se_3 slab unit cell, and plot the magnitude and direction of the non-collinear spin vectors as a function of the C-coordinate.

Calculations

You will need the following two scripts: bloch_states.py and spinVector.py. Download the scripts and execute the first one (`bloch_states.py`) using the Job Manager or in a Terminal. It reads in the SOGGA state from `Bi2Se3_slab.nc`, performs the two BlochState analyses for k-point [0, 0.04, 0], and then computes the length
r and polar angles
θ and
ϕ for both Bloch states and plots them.

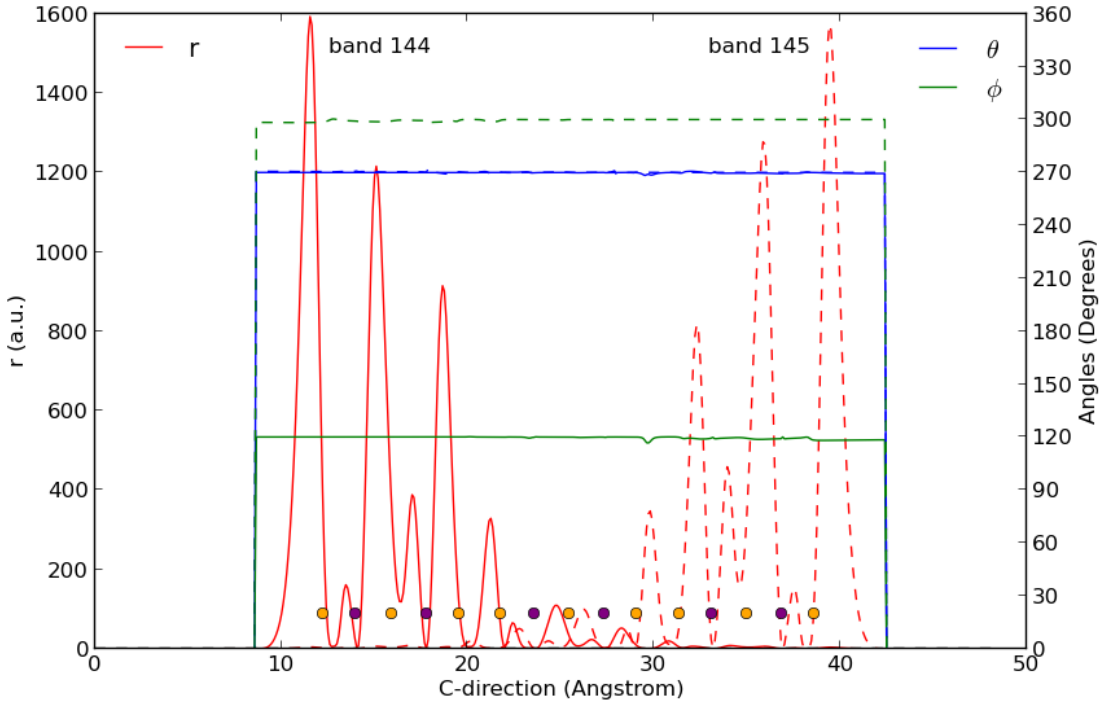


Fig. 53 Surface Bloch states in bands 144 and 145 evaluated in k-point [0, 0.04, 0]. The states are projected onto the C-direction. The states are localized on opposite sides of the slab configuration, and their spin directions are opposite.¶

The resulting figure is shown above. Orange and purple dots at the bottom indicate the position of the Se and Bi atoms, respectively. The two states are clearly localized on opposite sides of the slab (red curves) and have very little overlap in the middle of it. The polar angle ϕ is 270° for both states (blue curves), but the in-plane angle ϕ is 120° for band 144 and rotated by 180° to 300° for band 145 (green curves). The two spin states therefore point in opposite directions!

Fermi surface and spin directions

Finally, it is interesting to study the Fermi surface of the Bi_2Se_3 slab in the vicinity of the Dirac cone. This is easily done by sampling the band structure on a dense k-grid centered at the Γ-point.

Download and execute this pre-made script: fermi_surface.py. It reads in the SOGGA state from `Bi2Se3_slab.nc`, performs band structure analysis in all points on a $k_x \times k_y$=51 $\times$51 grid, and creates a contour plot of the eigen-energies of the surface state in energy band 144.

Note

For users of QuantumATK 2017: Use instead the script fermi_surface_2017.py.

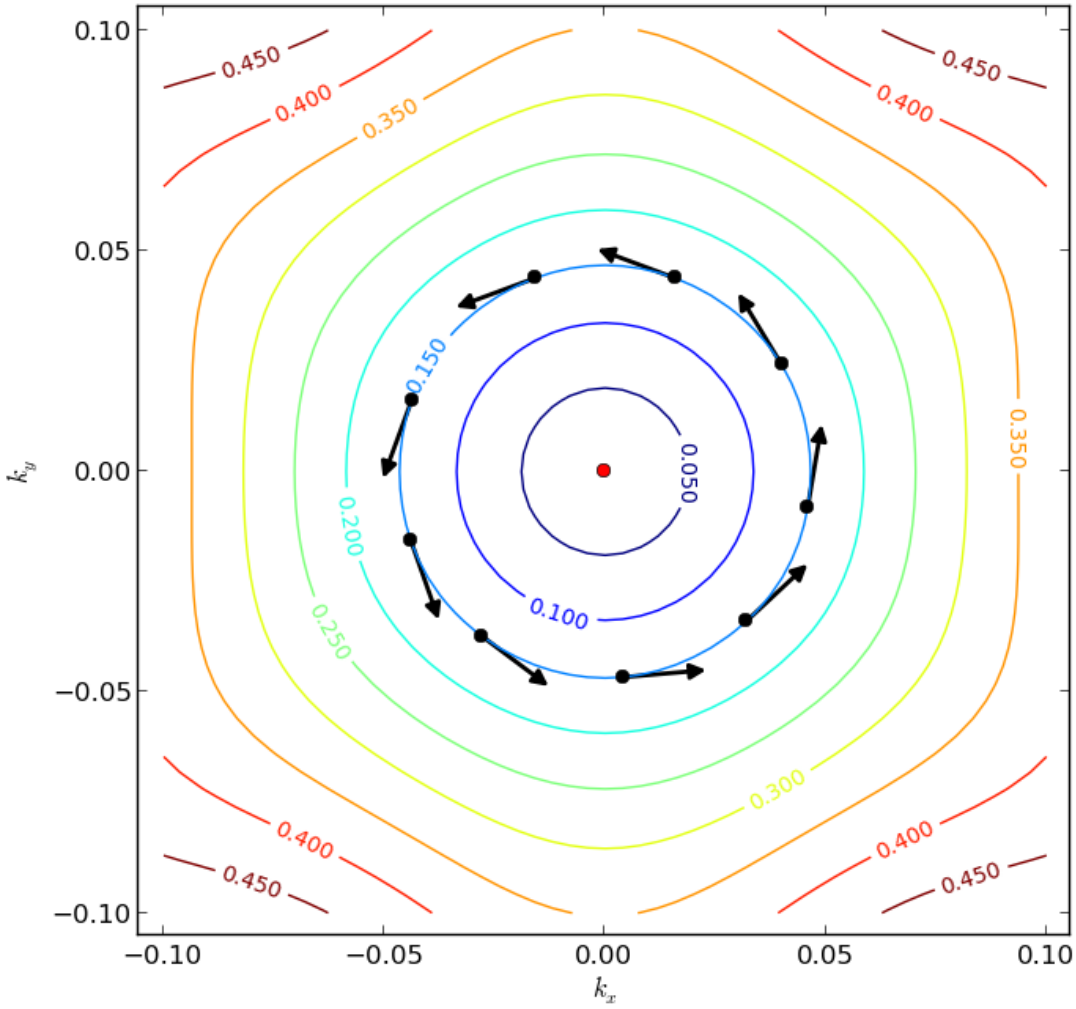


Fig. 54 Fermi surfaces on the Dirac cone centered at the
Γ-point. The arrows indicate how the in-plane spin direction varies as an electron circles around the Dirac point.¶

The resulting plot is illustrated above. As expected for a Dirac cone, the Fermi surface is circular close to the apex (red dot), but in this case it turns more hexagonal in shape for higher energies.

The Python script has also extracted the contour corresponding to E_F=0.15 eV and computed the Bloch state for every 10th (k_x, k_y) point around that contour. In each point, an arrow indicates the in-plane spin orientation (
ϕ). It is clear that the spin rotates by
2π as it circles around the Dirac point.

The reason for this is simple: Time-reversal symmetry requires that states at momenta **k** and -**k** have opposite spin. However, the Dirac cone for surface states originating from a *single* surface is *not* spin degenerate. The spin must therefore rotate with **k** as it goes around the Fermi surface. See Ref. [1] for more details.

Topological Invariants

The properties of a 3-D topological insulator is determined by four topological invariants [5], [6], [7], which describe properties of the band structure at special k-points, i.e. the
Γ-point and the Brillouin zone edges.

The first topological invariant describes the difference in the wavefunction symmetry at the different

special k-points. This invariant distiguishes “strong” topological insulators, and when present, the system will have topologically protected surface bands. The topological invariant is robust towards atomic disorder and any time-invariant perturbation cannot remove the surface bands.

For a system with inversion symmetry the topological invariants can be calculated from the symmetry of the Bloch function at 8 special Brillouin zone points [8],

$$\Gamma_{i=(n_1,n_2,n_3)} = \frac{1}{2}(n_1\mathrm{b}_1 + n_2\mathrm{b}_2 + n_3\mathrm{b}_3),$$

where
b_i are the reciprocal lattice vectors and
$n_i = 0, 1$.

Let
$\psi_{i,n}$ be the nth occupied Bloch function at
Γ_i, then we define the symmetry function

$$\delta_i = \Pi_n \sqrt{\langle \psi_{i,n} | \Theta | \psi_{i,n} \rangle}$$

where
Θ is the inversion operator. Once the symmetry functions are known the strong topological invariant, ν_0, is given by

$$(-1)^{\nu_0} = \Pi_{i=1}^{8} \delta_i.$$

There are three weak invariants,
ν_1,
ν_2, and
ν_3, given by products of four
δ_i's, for which
Γ_i reside in the same plane:

$$(-1)^{\nu_k} = \Pi_{n_k=1, n_{j\neq k}=0,1} \delta_{i=(n_1,n_2,n_3)}.$$

The weak invariants are not robust towards atomic disorder, and do not guarantee the existence of metallic surface bands.

Python script for the calculating the topological invariants

Download the script TopologicalInvariant3D.py, which implements the equations given above for calculating the topological invariants. The script will only work for systems with inversion symmetry. An example of usage is given with the python script below.

```
from TopologicalInvariant3D import topologicalInvariant3D

bulk_configuration = nlread('Bi2Se3_bulk.nc', BulkConfiguration)[-1]

print '-----------------------------------'
print 'Topological Invariants = ', topologicalInvariant3D(bulk_configuration)
print '-----------------------------------'
```

which when run will produce the output

```
-----------------------------------
Topological Invariants =  [1 0 0 0]
-----------------------------------
```

We see that Bi_2Se_3 is a strong 3D topological insulator, because
$\nu_0 = 1$, while the three weak invariants are all 0.

You can now easily screen a range of 3D materials with inversion symmetry for their topological indices to figure out if they are strong or weak topological insulators.

Note

For users of QuantumATK 2017 and later: The script TopologicalInvariant3D.py will **not** work with QuantumATK 2017 and later versions. Download instead the script TopologicalInvariant3DATK2017.py and use it like this:

```
from TopologicalInvariant3DATK2017 import topologicalInvariant3D

bulk_configuration = nlread('Bi2Se3_bulk.nc', BulkConfiguration)[-1]

print '-----------------------------------'
print 'Topological Invariants = ', topologicalInvariant3D(bulk_configuration)
print '-----------------------------------'
```

References

[1] (1,2)
M. Z. Hasan and C. L. Kane. Colloquium: topological insulators. *Rev. Mod. Phys.*, 82:3045–3067, Nov 2010. doi:10.1103/RevModPhys.82.3045.

[2]
Xiao-Liang Qi and Shou-Cheng Zhang. Topological insulators and superconductors. *Rev. Mod. Phys.*, 83:1057–1110, Oct 2011. doi:10.1103/RevModPhys.83.1057.

[3]
Po-Hao Chang, Troels Markussen, Søren Smidstrup, Kurt Stokbro, and Branislav K. Nikolić. Nonequilibrium spin texture within a thin layer below the surface of current- carrying topological insulator bi2se3: a first-principles quantum transport study. *Phys. Rev. B*, 92:201406, 2015. doi:10.1103/PhysRevB.92.201406.

[4] (1,2)
Wei Zhang, Rui Yu, Hai-Jun Zhang, Xi Dai, and Zhong Fang. First-principles studies of the three-dimensional strong topological insulators Bi2Te3, Bi2Se3 and Sb2Te3. *New Journal of Physics*, 12(6):065013, 2010. doi:10.1088/1367-2630/12/6/065013.

[5]
Liang Fu, Charles L Kane, and Eugene J Mele. Topological insulators in three dimensions. *Physical Review Letters*, 98(10):106803, 2007. doi:10.1103/PhysRevLett.98.106803.

[6]
Joel E Moore and Leon Balents. Topological invariants of time-reversal-invariant band structures. *Physical Review B*, 75(12):121306, 2007. doi:10.1103/PhysRevB.75.121306.

[7]
Rahul Roy. Topological phases and the quantum spin hall effect in three dimensions. *Physical Review B*, 79(19):195322, 2009. doi:10.1103/PhysRevB.79.195322.

[8]
Liang Fu and Charles L Kane. Topological insulators with inversion symmetry. *Physical Review B*, 76(4):045302, 2007. doi:10.1103/PhysRevB.76.045302.

Previous Next

© Copyright 2023 Synopsys, Inc. All Rights Reserved.