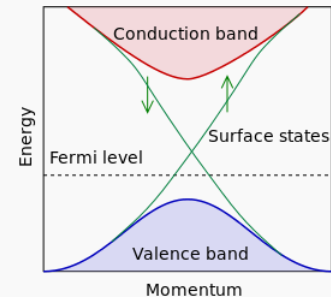


TUTORIAL SYNOPSIS

Bi_2Se_3 Topological Insulator

- ❖ Use Crystal Builder to create Bi_2Se_3 bulk configuration.
- ❖ GGA and SOGGA band structures.
- ❖ Use Surface (Cleave) tool to create $\text{Bi}_2\text{Se}_3(0001)$ slab.
- ❖ SOGGA band structure: Surface states emerge and form a Dirac cone.
- ❖ SOGGA DOS: Dirac cone finger print.
- ❖ Bloch states on the Dirac cone: Penetration depths of surface states located on the top and bottom surfaces.
- ❖ Fermi surface and spin directions.



Use Crystal Builder to set up bulk configuration



Virtual NanoLab

File Templates Tools

Spacegroup and lattice

Space_group 166: R -3 m (H)

Lattice

Bravais lattice: Hexagonal
Pearson symbol: hP0

a 4.138 Å α 90 °
b 4.138 Å β 90 ° b/a 1
c 28.64 Å γ 120 ° c/a 6.92122

Options

☐ Primitive
☒ Conventional

☐ Show equivalent atoms

Build

☒ Primitive
☐ Conventional

Virtual NanoLab

File Templates Tools

Spacegroup and lattice

Space_group 166: R -3 m (H)

Lattice

Bravais lattice: Hexagonal
Pearson symbol: hP15

a 4.138 Å α 90 °
b 4.138 Å β 90 ° b/a 1
c 28.64 Å γ 120 ° c/a 6.92122

Options

Preview

☐ Primitive
☒ Conventional

☐ Show equivalent atoms

Build

☒ Primitive
☐ Conventional

Basis

	Element	x	y	z	
3a	Selenium	0	0	0	
6c	Bismuth	0	0	0.399	
6c	Selenium	0	0	0.206	

Preview Reset Build

Builder

File Edit Selection View Windows Help

Stash

Add
Copy
Delete

Crystal

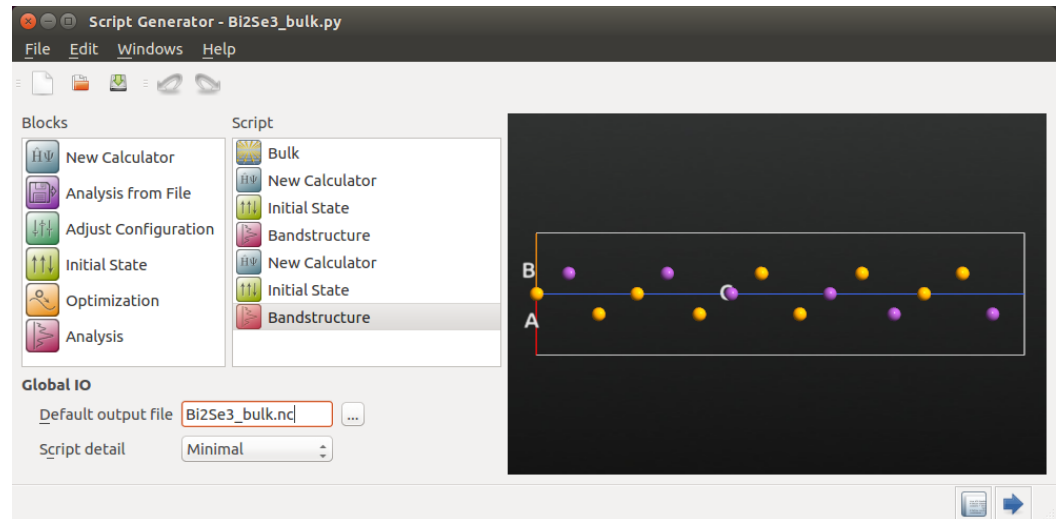
Builders

- Bulk Tools
- Coordinate Tools
- Device Tools
- Graphics
- Miscellaneous
- Selection Tools

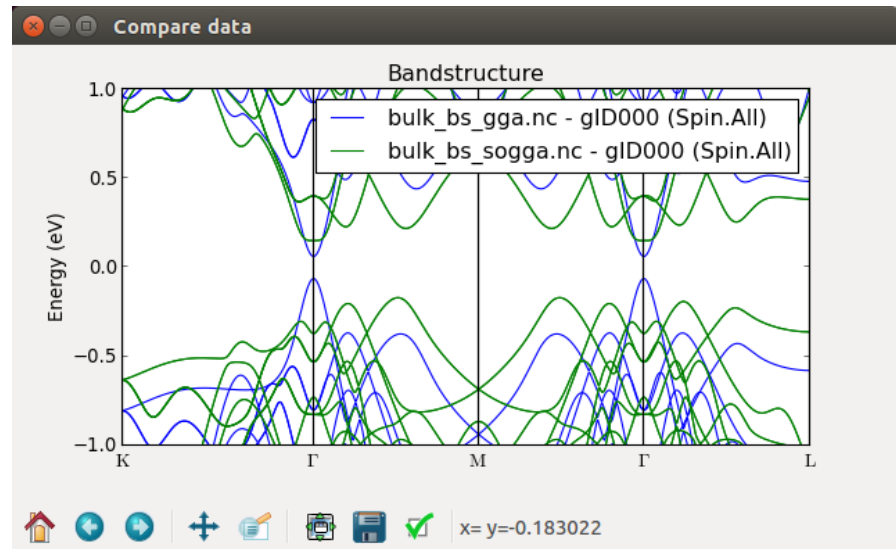


ATK-DFT

- ❖ 9x9x9 k-points
- ❖ OMX 150 Hartree
- ❖ GGA.PBE and SOGGA.PBE
- ❖ Use GGA state as initial guess for the SOGGA state



Bulk Bi_2Se_3 is an insulator



Use Surface (Cleave) to create $\text{Bi}_2\text{Se}_3(0001)$ slab



Surface (Cleave)

Define the surface

Miller indices
 h k $i = -(h+k)$ l

Select an atom for the outer layer

	Element	a	b	c
0	Seleni...	0.000	0.000	0.000
1	Seleni...	0.333	0.667	0.667
2	Seleni...	0.667	0.333	0.333
3	Bismuth	0.667	0.333	0.778
4	Bismuth	0.333	0.667	0.222
5	Bismuth	0.000	0.000	0.667
6	Bismuth	0.667	0.333	0.999
7	Bismuth	0.000	0.000	0.333
8	Bismuth	0.333	0.667	0.000
9	Seleni...	0.333	0.667	0.889
10	Seleni...	0.667	0.333	0.111
11	Seleni...	0.333	0.667	0.444
12	Seleni...	0.000	0.000	0.778
13	Seleni...	0.000	0.000	0.222

< Back Next > Cancel

Surface (Cleave)

Finalize output configuration

☒ Automatically update 3D view
 Out-of-plane cell vector v_3 is
 Non-periodic and normal (slab)

	Layers	Å
Top vacuum	0.3492	10.0000
Thickness	1.0000	28.6400
Bottom vacuum	0.3492	10.0000

Update

< Back Finish Cancel

Lattice Parameters

Choose the lattice type from the dropdown menu.
 Lattice type: Hexagonal

Keep fractional coordinates constant when changing the lattice

Lattice Parameters

Adjust the lattice parameters of the selected lattice type. Only parameters relevant for the lattice type can be changed. Lattice parameters can be exported to the clipboard by right-clicking.

a (Å)	4.138	α	90
b (Å)	4.138	β	90
c (Å)	48.64	γ	120
		b/a	1
		c/a	11.7545

Primitive Vectors

Manipulate the Primitive Vectors directly. This is only possible if UnitCell was chosen from the dropdown menu.

	x (Å)	y (Å)	z (Å)
A	2.069	-3.58361	0
B	2.069	3.58361	0
C	0	0	48.64

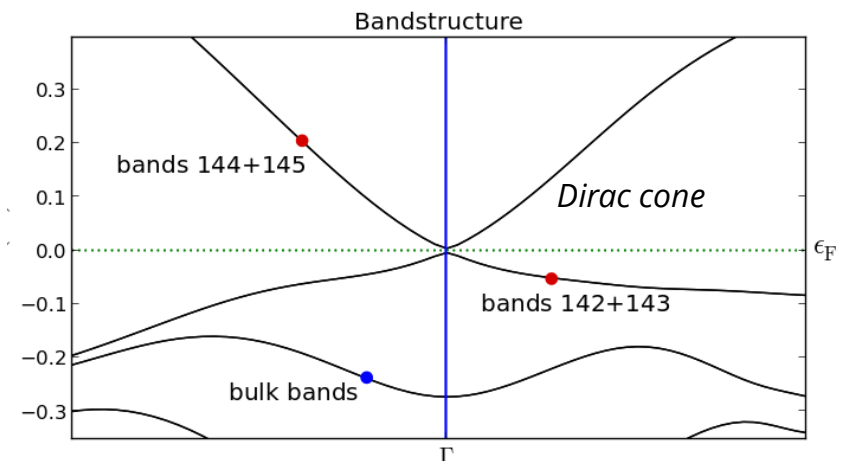
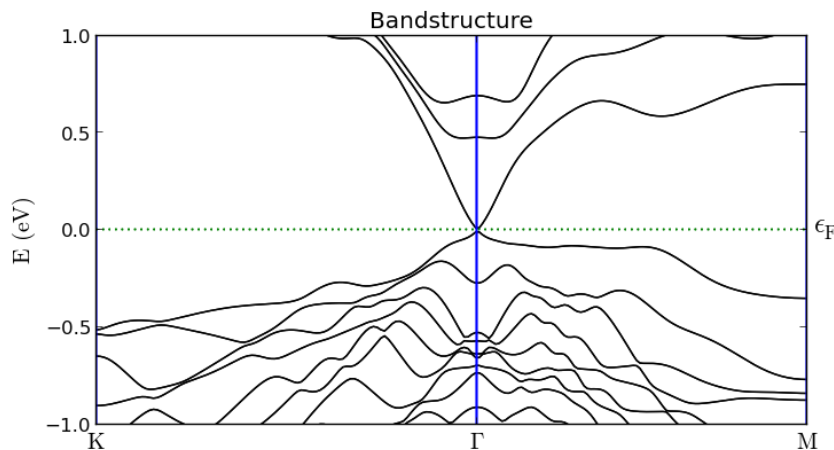
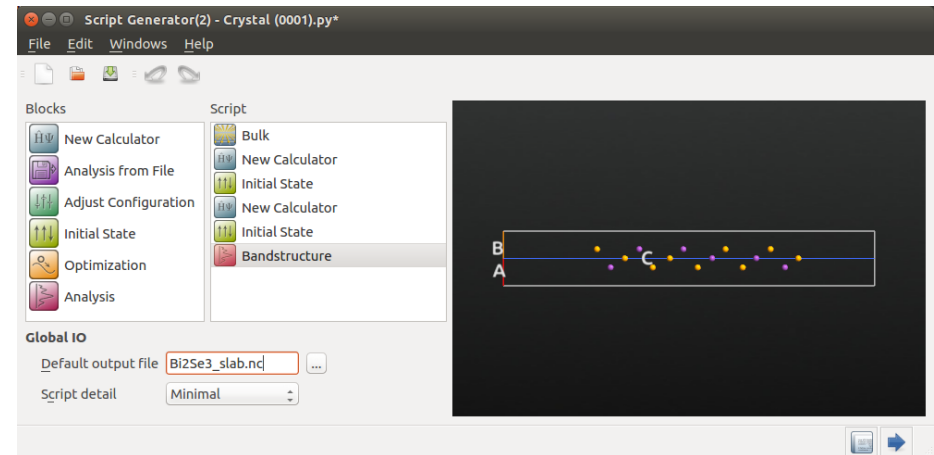
Volume = 721.282 Å³

SOGGA band structure: Surface states emerge and form a Dirac cone



ATK-DFT

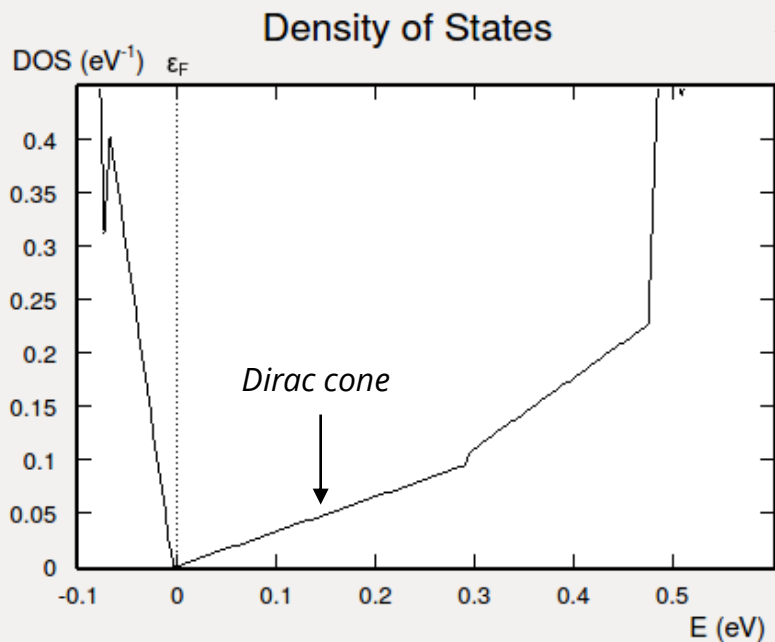
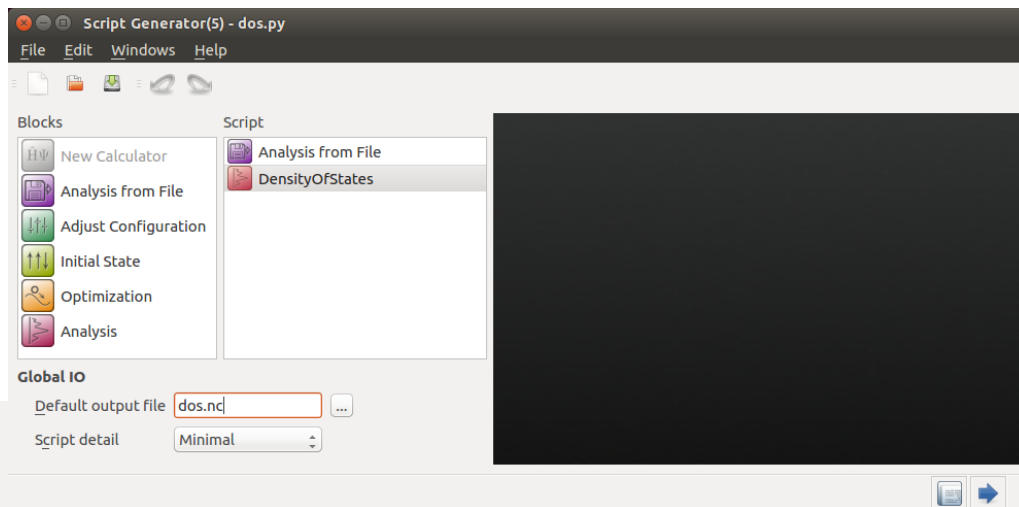
- ❖ 9x9x1 k-points
- ❖ OMX 150 Hartree
- ❖ Electron temperature = 50 K
- ❖ SOGGA restarted from GGA state





Analysis from File

- ❖ 21x21x1 k-point grid
- ❖ Important to include the Gamma point

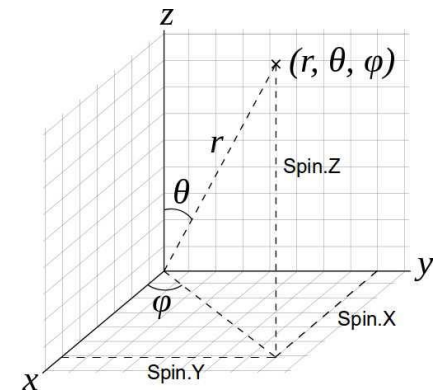
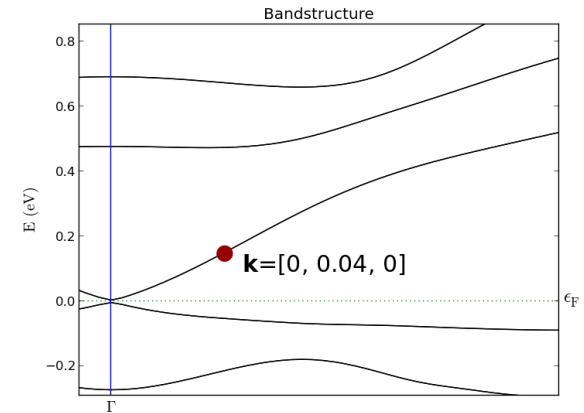
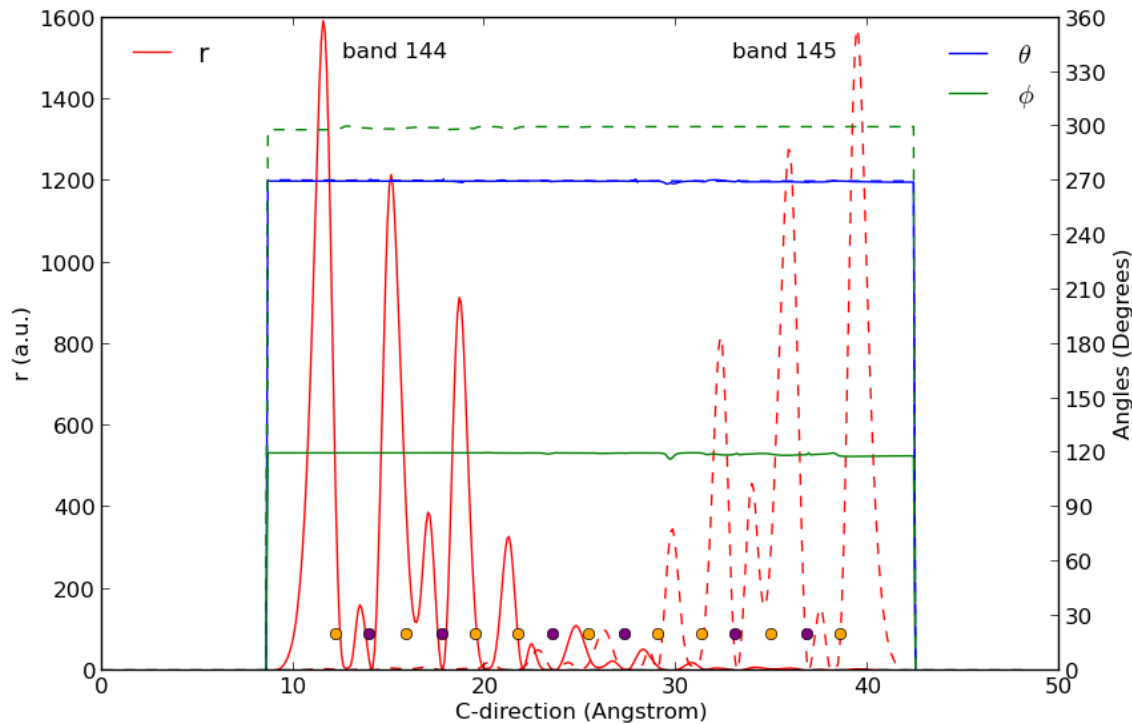


Bloch states on the Dirac cone: Penetration depth of surface states located on the top and bottom surfaces



BlochState analysis

- ❖ Script provided
- ❖ Surface Bloch states projected onto the C-direction





Bandstructure and BlochState analyses

- ❖ Script provided for Bandstructure analysis on a dense k-grid in the vicinity of the Dirac point
- ❖ Plots the Fermi surfaces for a single surface state as a contour plot
- ❖ Also extracts and plots the spin directions on the $E_F=0.15$ eV contour

