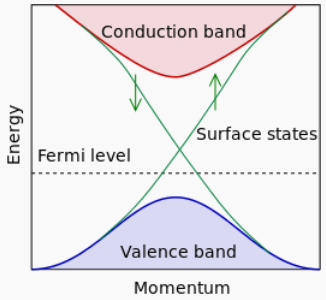
TUTORIAL SYNOPSIS

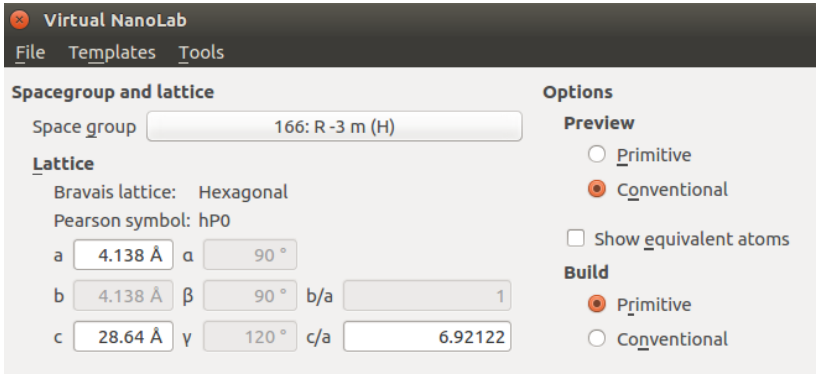
Bi_2Se_3 Topological Insulator

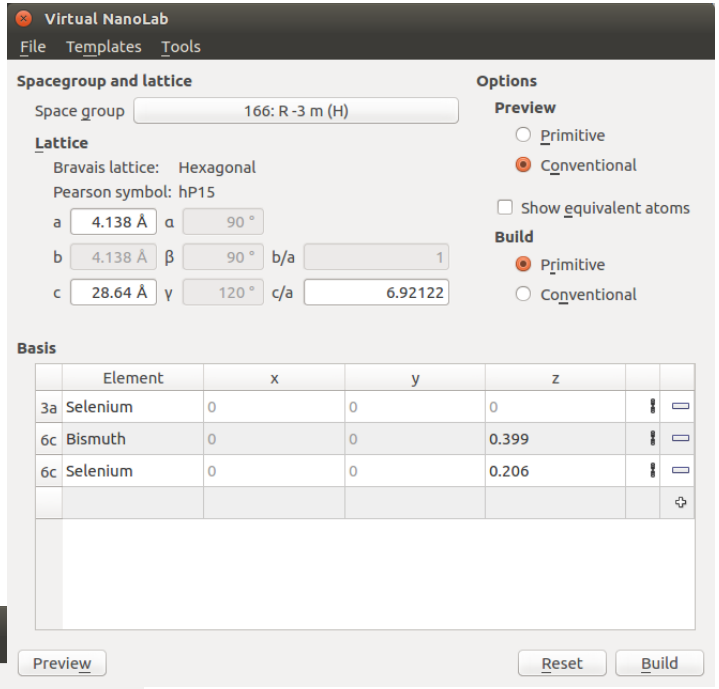
Quantum Wise
When every atom matters

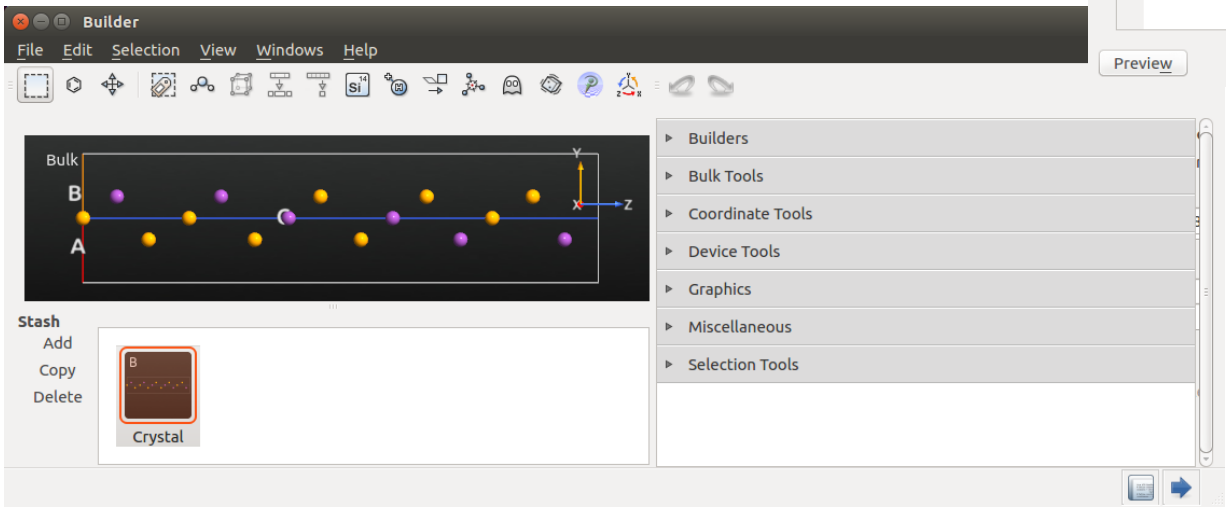


- Use Crystal Builder to create Bi_2Se_3 bulk configuration.
- GGA and SOGGA band structures.
- Use Surface (Cleave) tool to create Bi_2Se_3(0001) slab.
- SOGGA band structure: Surface states emerge and form a Dirac cone.
- SOGGA DOS: Dirac cone finger print.
- Bloch states on the Dirac cone: Penetration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

Use Crystal Builder to set up bulk configuration



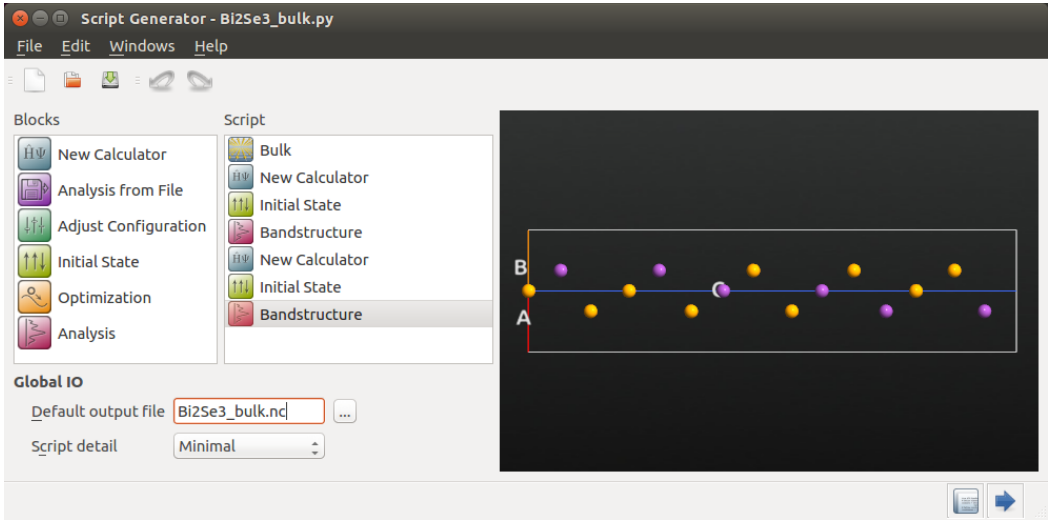




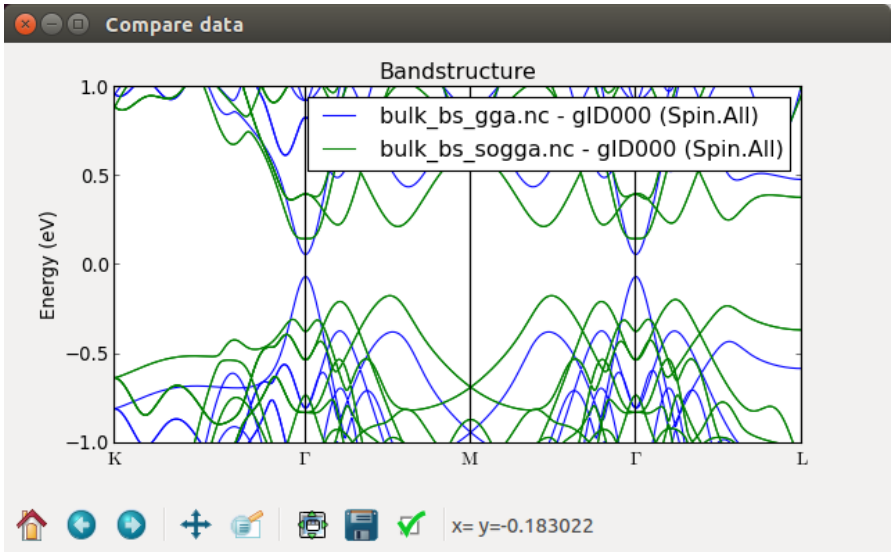
GGA and SOGGA band structures

ATK-DFT

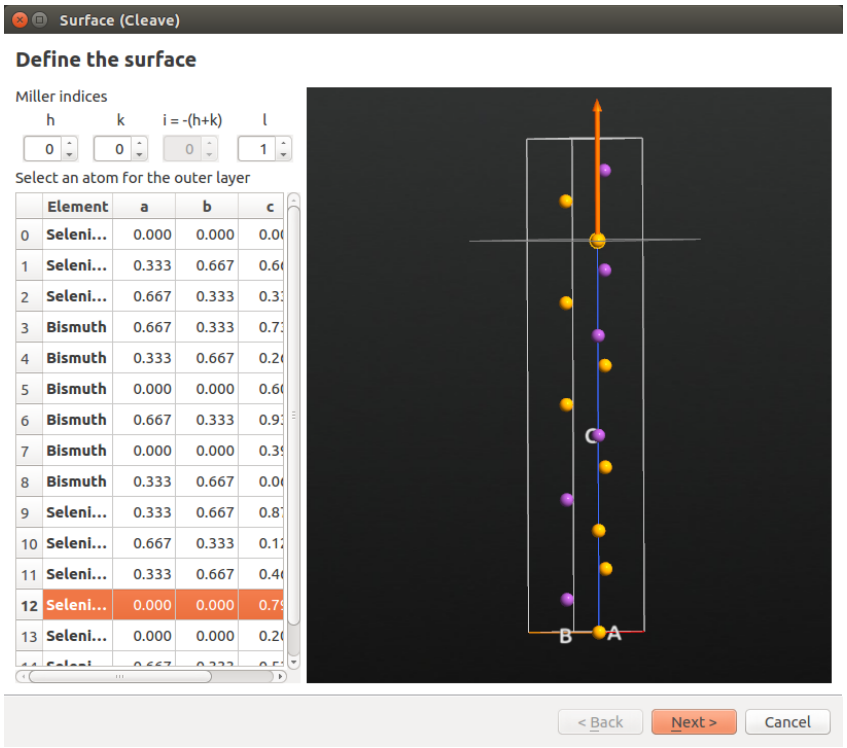
- 9x9x9 k-points
- OMX 150 Hartree
- GGA.PBE and SOGGA.PBE
- Use GGA state as initial guess for the SOGGA state

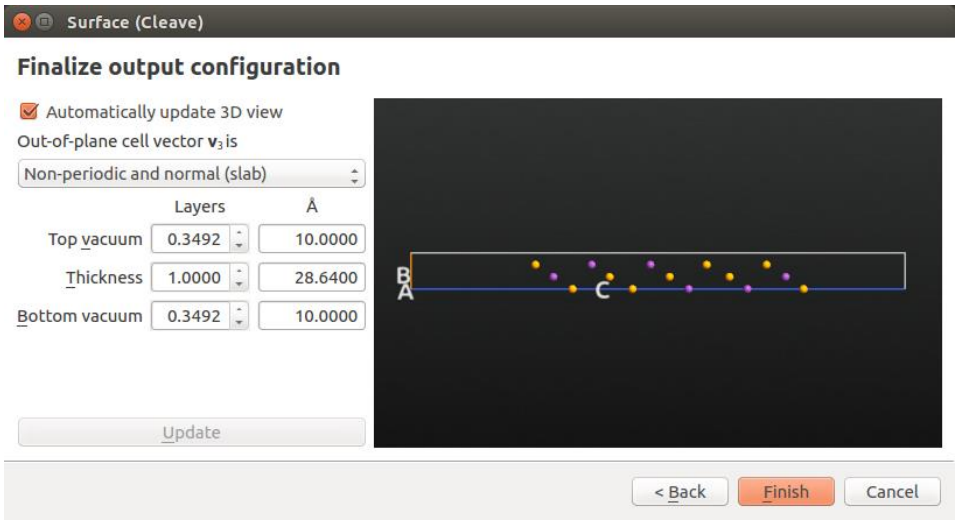


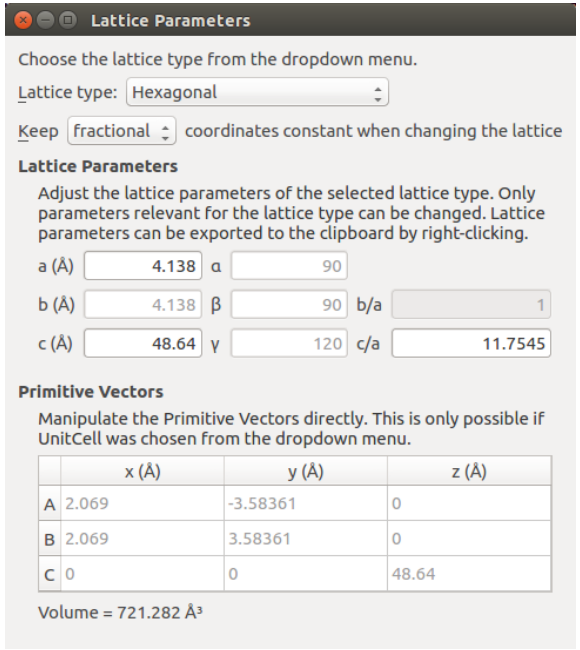
Bulk Bi_2Se_3 is an insulator



Use Surface (Cleave) to create Bi_2Se_3(0001) slab



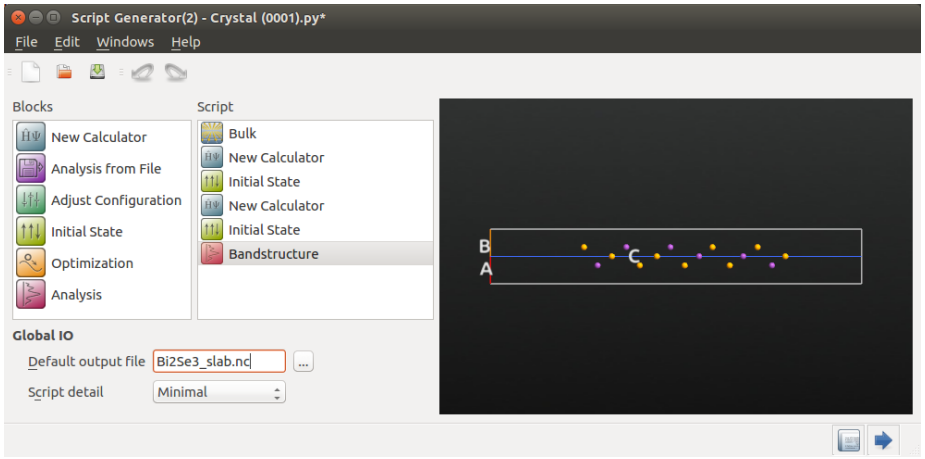


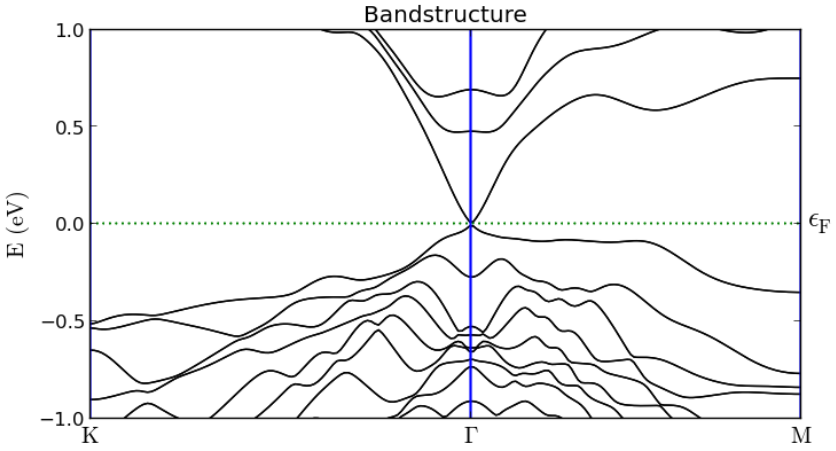


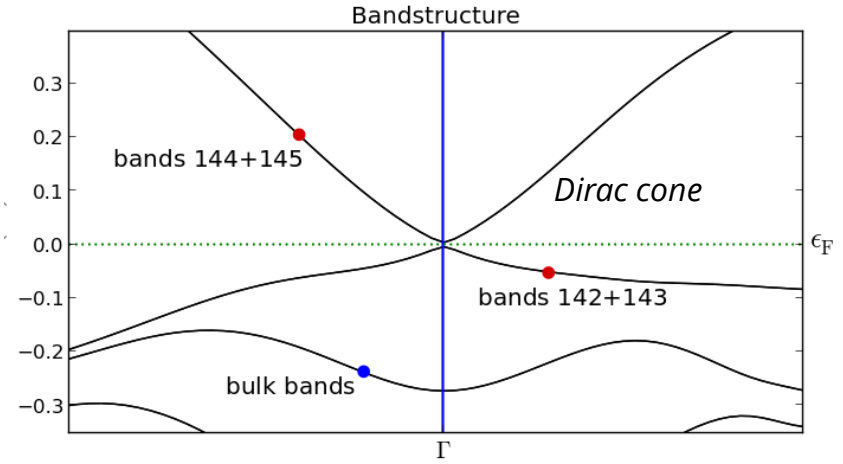
SOGGA band structure: Surface states emerge and form a Dirac cone

ATK-DFT

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



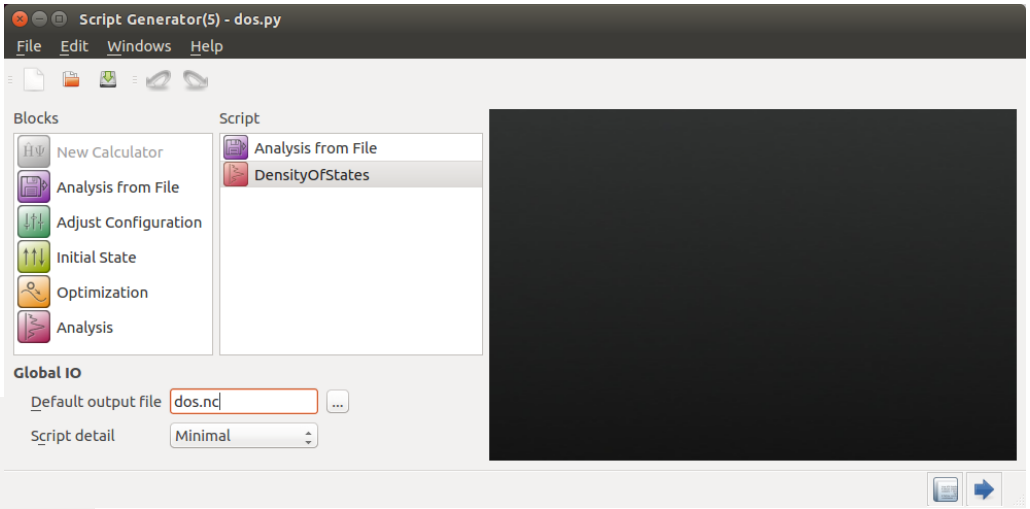


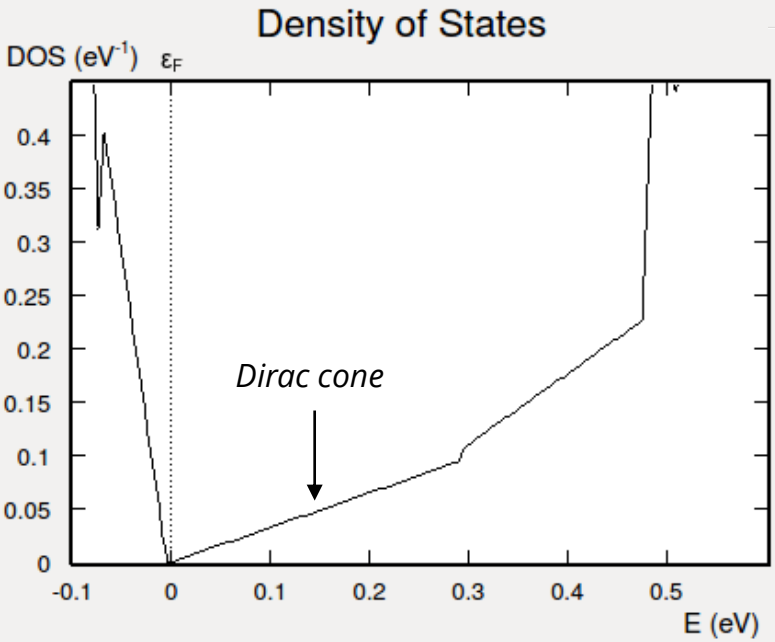


SOGGA DOS: Dirac cone finger print

Analysis from File

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

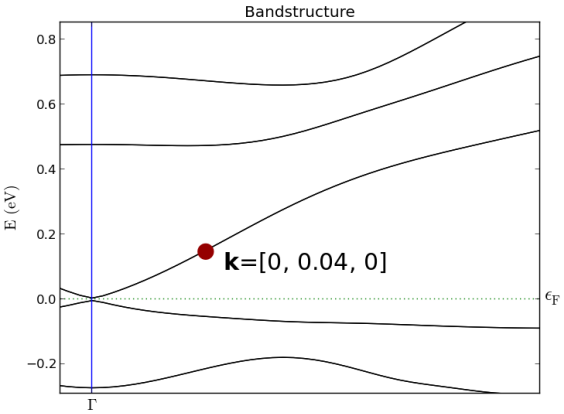


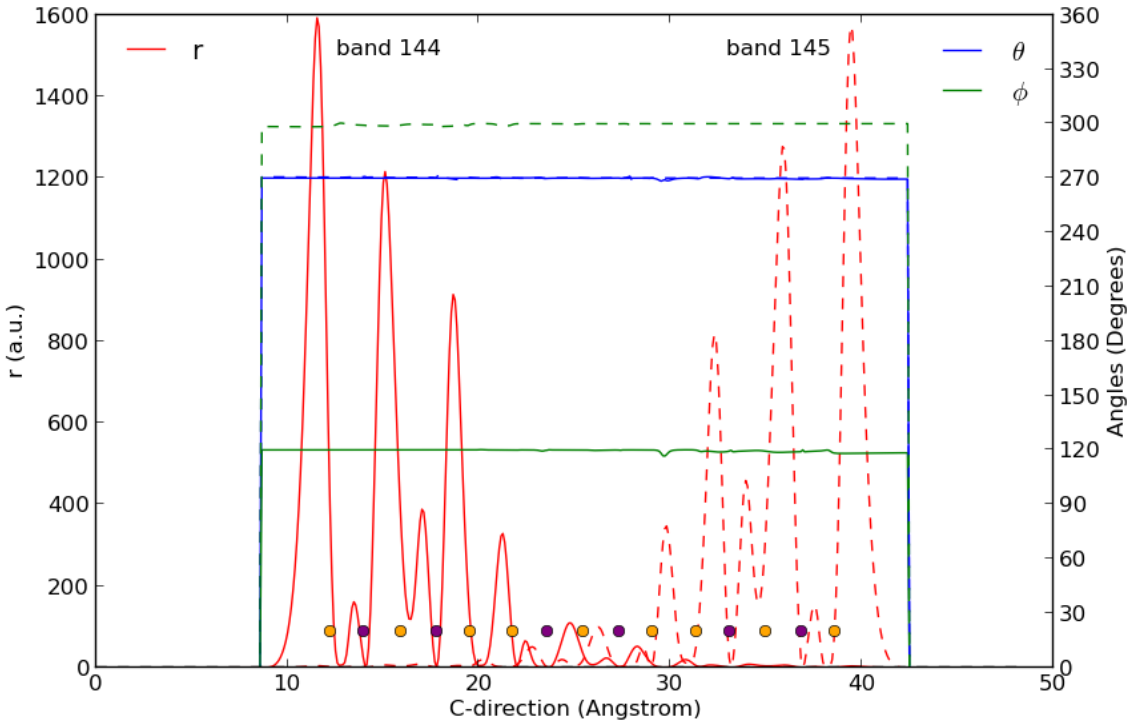


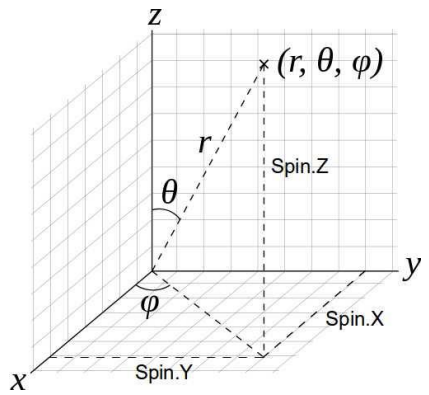
Bloch states on the Dirac cone: Penetration depth of surface states located on the top and bottom surfaces

BlochState analysis

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







Fermi surfaces and spin directions

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