Use Crystal Builder to create $\text{Bi}_2\text{Se}_3$ 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
**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$_2$Se$_3$ is an insulator*
Use Surface (Cleave) to create $\text{Bi}_2\text{Se}_3(0001)$ slab

Define the surface

- **Miller indices**
  - $h$ = 0
  - $k$ = 0
  - $l$ = 1

- **Select an atom for the outer layer**
  - Element: Selenite
  - Atom positions:
    - 0: $a = 0.000$, $b = 0.000$, $c = 0.000$
    - 1: $a = 0.333$, $b = 0.667$, $c = 0.667$
    - 2: $a = 0.667$, $b = 0.333$, $c = 0.333$
    - 3: $a = 0.333$, $b = 0.333$, $c = 0.7$
    - 4: $a = 0.333$, $b = 0.667$, $c = 0.2$
    - 5: $a = 0.667$, $b = 0.000$, $c = 0.000$
    - 6: $a = 0.667$, $b = 0.333$, $c = 0.9$
    - 7: $a = 0.333$, $b = 0.000$, $c = 0.3$
    - 8: $a = 0.333$, $b = 0.333$, $c = 0.6$
    - 9: $a = 0.333$, $b = 0.667$, $c = 0.8$
    - 10: $a = 0.667$, $b = 0.667$, $c = 0.1$
    - 11: $a = 0.667$, $b = 0.333$, $c = 0.4$
    - 12: $a = 0.333$, $b = 0.000$, $c = 0.7$
    - 13: $a = 0.333$, $b = 0.667$, $c = 0.2$

Finalize output configuration

- **Automatically update 3D view**
- **Out-of-plane cell vector $\mathbf{v}_z$**
  - Type: Non-periodic and normal (slab)
  - Layers: 10 Å
  - Top vacuum: 0.3492 Å, 10.0000 Å
  - Thickness: 1.0000 Å, 28.6400 Å
  - Bottom vacuum: 0.3492 Å, 10.0000 Å

Lattice Parameters

- **Lattice type**: Hexagonal
- **Keep coordinates** constant when changing the lattice
- **Primitive Vectors**
  - $x$: 2.069, $y$: -3.58361, $z$: 0
  - $A$: 2.069, $B$: -3.58361, $C$: 0
  - 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
**BlochState analysis**

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

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**Figure Description**

- A graph showing band structure with labels for bands and angles.
- Band structure is indicated with different lines and markers.
- Directions and angles are labeled accordingly.

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**Additional Information**

- **Bi$_2$Se$_3$ Topological Insulator**
- **QuantumWise**
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