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»

Band structure of a SiC
crystal

Band structure of a SiC crystal

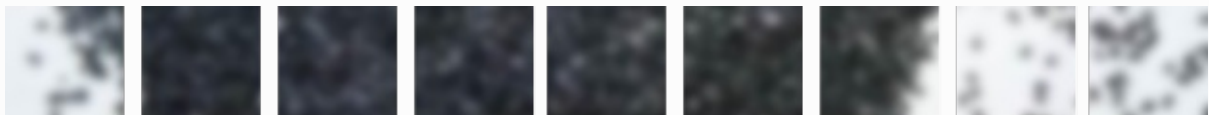
Downloads & Links



PDF

ATK Reference Manual

You will here learn how to use VNL and ATK for calculating the band structure and other properties of a SiC crystal. We shall not discuss the science of such a calculation much; the purpose of the tutorial is to show how to operate VNL, specifically how to set up simple calculations and visualize the results.



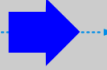
Workflow



WE FOLLOW THE PLAN BELOW:



Build
structure.



Setup
script.



Run
calculations.



Analyze/View
calculations.



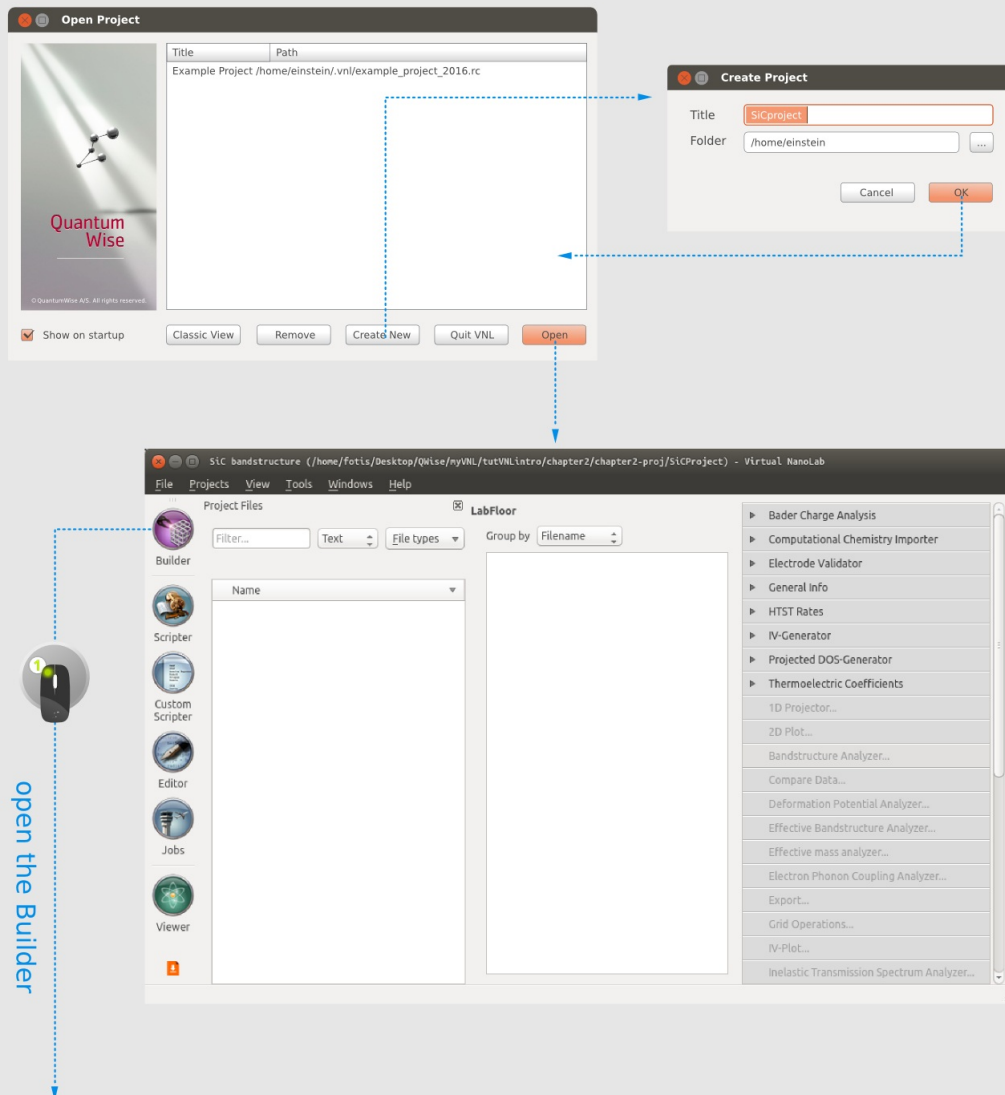
Remember! Any time you can check LabFloor to see your files.

Build SiC crystal

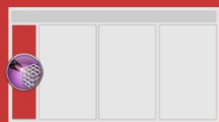
Start VNL and create a new project with the title you prefer, e.g. *SiCproject*. Then open the project.



START VNL, CREATE A PROJECT AND OPEN IT:



Use the **Database** plugin to quickly build the SiC bulk configuration.



Create a SiC crystal in Builder: **Stash** → **Add** → **From Database**

Database - Crystal Cupboard

| Name | Formula | Lattice | Tags |
|------------|---------|---------------------------|-------------------------|
| SiC | SiC | Face Centered Cubic (fcc) | Spinelites (zincblende) |
| Moissanite | SiC | Hexagonal | Wurtzites |

Description

SiC

Chemical formula: Si C

Lattice

- Face Centered Cubic (fcc)
- a = 4.348 Angstrom

Symmetry information

- Space group: 216
- Crystal system: cubic
- Pearson: cF4
- Hermann-Mauguin: F-43m
- Schoenflies: T_d^2

Configuration

TIPS

- Rotate:** [Mouse icon]
- Pan:** [Mouse icon]
- Zoom:** [Mouse icon]
- Zoom:** Ctrl + [Mouse icon]

Builder

Stash

Add

Copy

Delete

Send to Scripter

Tip

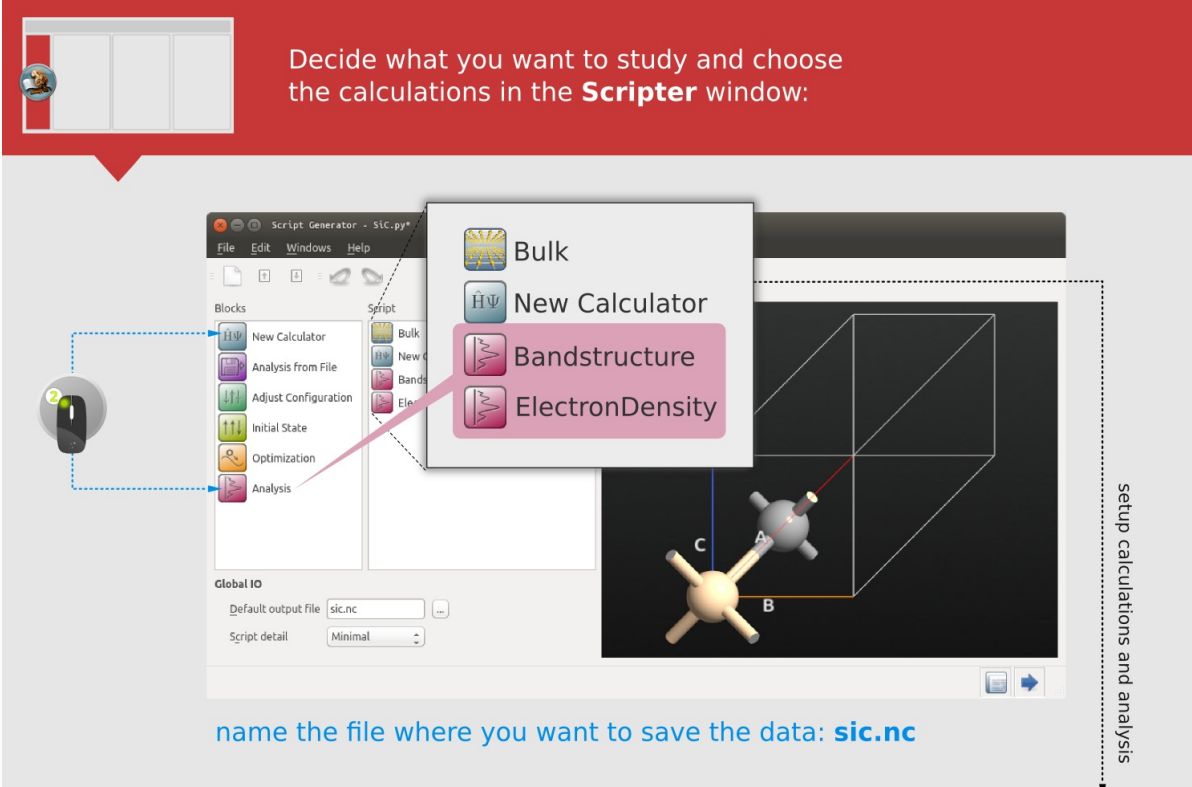
Several VNL tools contain a 3D preview of the currently active configuration. Use the right mouse button to **rotate** the 3D view, use the scroll wheel to **zoom** (or hold down Ctrl and right mouse button and move the mouse), and press the scroll wheel and move the mouse to **pan** the camera (or hold down Shift and the right mouse button and move the mouse).

Setup ATK calculation

You are now ready to setup an ATK Python script that calculates the electronic ground state of the SiC crystal followed by analysis of the band structure and electron density. This is what the **Script Generator** is used for ("Scripter" for short).

Transfer the SiC crystal from the Builder to the Scripter by clicking the **Send to** icon ➡ in the lower-right corner of the Builder window, and select "Script Generator" from the pop-up menu. The Scripter appears and the Builder window is automatically minimized.

The script already contains the SiC bulk configuration. Add the **Calculator** block and two **Analysis** blocks.



Decide what you want to study and choose the calculations in the **Scripter** window:

name the file where you want to save the data: **sic.nc**

setup calculations and analysis

New Calculator block

The calculator computes the ground state of the SiC crystal. It contains a wide range of settings, all of which have sensible default values. However, you will most often need to change at least a few of them in order to make the calculation match your scientific goals.

Double-click the **New Calculator** block to edit it:

New Calculator

Calculators

- ☒ ATK-DFT
- ☐ ATK-SE: Extended Hückel
- ☐ ATK-SE: Slater-Koster
- ☐ ATK-Classical
- ☐ Abinit
- ☐ FHI-aims

Calculator settings

Algorithm parameters

Basic

Iteration control parameters

Basis set/exchange correlation

Numerical accuracy parameters

Parallel parameters

Poisson solver

Basic Settings

Electron temperature: 300 K

Density mesh cut-off: 75 Hartree

Charge: 0

Exchange correlation: MGGA

Spin: Unpolarized

☐ No SCF iteration

k-point Sampling

n_x : 5 n_y : 5 n_z : 5

IO

☒ Save ☒ Print

File: sic.nc Label:

Estimate Memory Usage

OK

choose Meta-GGA to get accurate semiconductor band gaps

set all k-points sampling to 5

save and exit

Analysis blocks

The **Bandstructure** and **ElectronDensity** blocks perform post-SCF analysis. Double-click the Bandstructure block to increase the Brillouin zone sampling:

Bandstructure

Bandstructure

Points per segment: 100

Bands above Fermi level: All

Brillouin zone route: G, X, W, L, G, K, X, U, W, K, L

IO

☒ Save ☐ Print

File: sic.nc Label:

OK

set to 100 to obtain smoother curves

save and exit

Saving the script

The ATK script is now done, and it is good practice to immediately save it. Use the **File** menu in the **Script Generator**, or the keyboard shortcut Ctrl+Shift+S.



Run calculations


You need to run the ATK Python script in order to execute the calculations. This can be done from a

terminal:

```
atkpython example.py > example.log
```

A very convenient alternative is to use the  **Job Manager** to run the script directly from inside VNL:

- Click the  in the lower-right corner of the **Script Generator**, and select “Job Manager” from the menu.
- The “Save As” dialog appears, prompting you to make sure the script is saved, followed by the Job Manager window and the “Select Machine” dialog.
- Choose a “Local” machine type, and click OK. The ATK Python script is added to the job queue of the chosen machine.
- Select your script and click the  button to start executing the calculation.

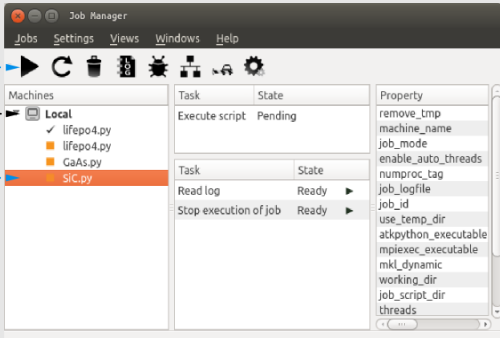


Send your file to **Job Manager** and **Run** it!

execute script

choose machine
[local in this example]

choose the script
you want to run



Tip

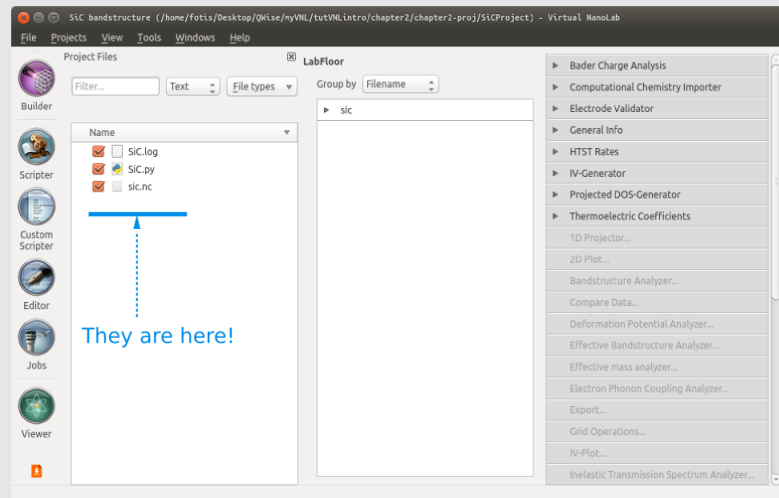
See the tutorials [Local](#) and [Remote](#) for more instructions on using the Job Manager for multi-CPU execution of ATK Python scripts on your local machine and on remote supercomputers.

Calculation output

Any output (data, log, etc.) should appear in the **Project Files** list. New `.nc` files are automatically scanned and their contents displayed on the **LabFloor**.






Main VNL Window: Where are my **Project Files**?



Analyze and visualize results

The calculation has now finished and you are ready to study the results. To this end, return to the VNL main window to select one of the saved **data items** and see the list of applicable **analysis plugins**.

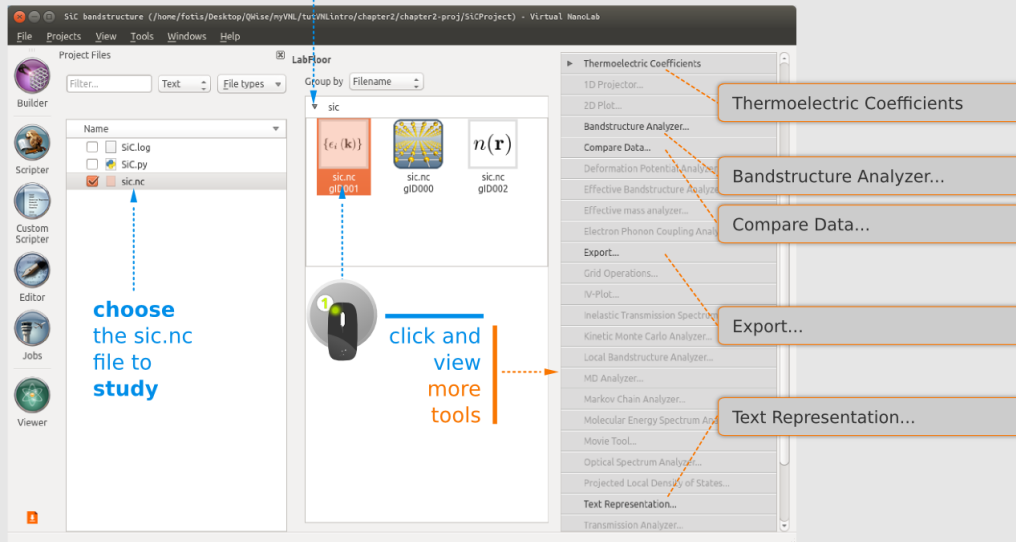
The saved items all have a unique *ID*:

- *gID000* –  BulkConfiguration
- *gID001* –  Bandstructure
- *gID002* –  ElectronDensity



Use the **Analysis** plugins to visualize and analyze your data.

expand to see contents

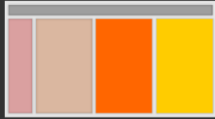


Tip

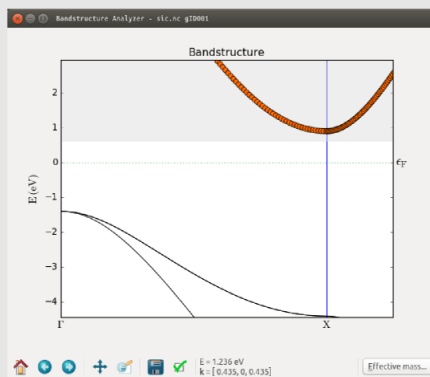
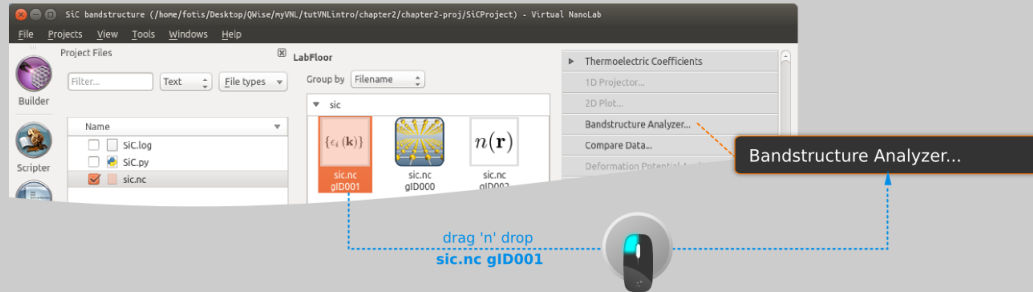
Use the keyboard shortcut **Alt+W** to activate the **Windows** menu, which allows you to easily switch between different VNL windows.

Band structure

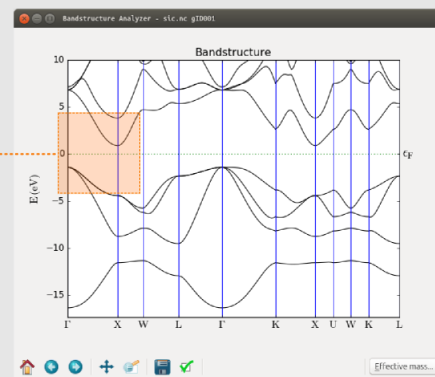
The NetCDF data file is `sic.nc`. Make sure the file is ticked in the Project Files list in order to see its contents on the LabFloor. You may have to expand the LabFloor item. Select the band structure item (*gID001*) and click the **Bandstructure Analyzer** in the right-hand Panel Bar.




Example: Plot the band structure of your system.



zoom-in on Γ X area:
drag mouse forming
a square lasso



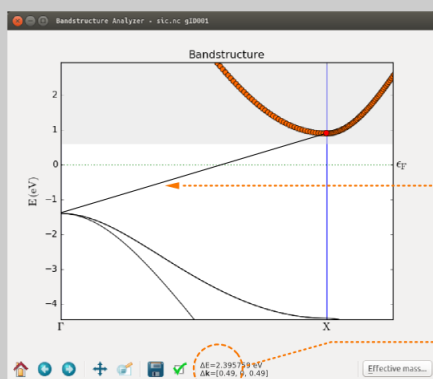
It is easy to measure the indirect **band gap**, which in this case is between the Γ and X points in reciprocal space:

1. Click the  icon to activate the **Zoom to rectangle** function, and zoom into the relevant part of the band structure.
2. Deactivate Zoom, and use the mouse to measure the indirect band gap.

The calculated gap is 2.40 eV, in excellent agreement with the experimental value of 2.36 eV for fcc SiC.



Example: **Measure a band gap.**



How to measure a band gap:
Choosing a point on a band drag
your mouse to another one.

$\Delta E = 2.395759 \text{ eV}$
 $\Delta k = [0.49, 0, 0.49]$

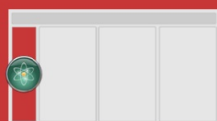
You can see the
- band gap energy and the
- corresponding Δk

YOU CAN CLICK
OR HOVER ON ANY
BAND AND SEE
IMMEDIATELY ITS
PROPERTIES

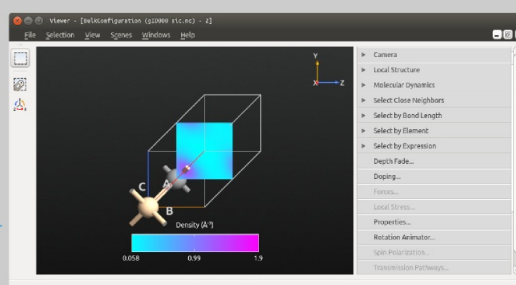
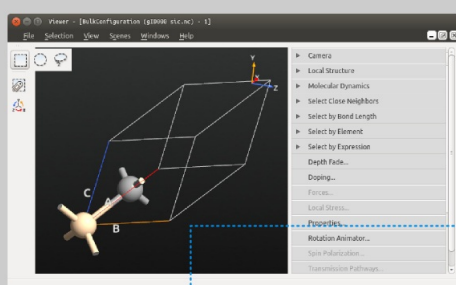
Electron density

The **Viewer** is used to visualize configurations and also data that is represented on 3D grids. You can visualize the SiC unit cell and the self-consistent electron density in a single view:

1. Drop the SiC bulk configuration (*glD000*) on the Viewer.
2. Select on the LabFloor the **ElectronDensity** item, $n(\mathbf{r})$, and just drop it on the SiC visualization.
Choose a cut-plane representation.



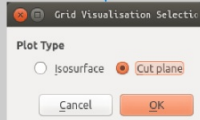
Drag 'n' drop file(s) in **Viewer**



drag 'n' drop
on Viewer window

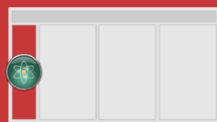


import
cut plane
(for example)



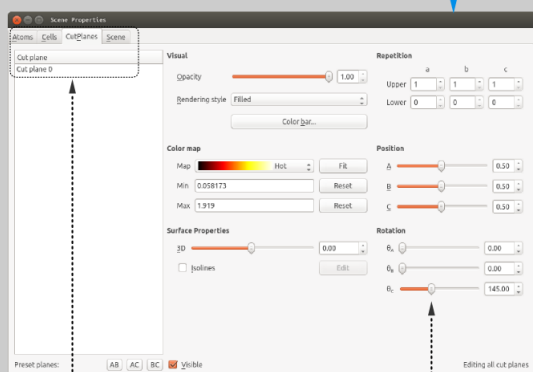
drag 'n' drop from
LabFloor to **Viewer**
or
click the **Viewer** button
at the **PanelBar**

A default visualization style is used. Use the **Properties** tool in the Viewer panel bar to adjust the visualization settings as you prefer.



Adjust visualization **Properties**.

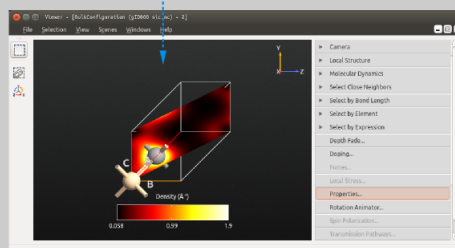
Properties...



tabs to set more properties

Example: Change angle of the cut plane to **145**.

right click to export image




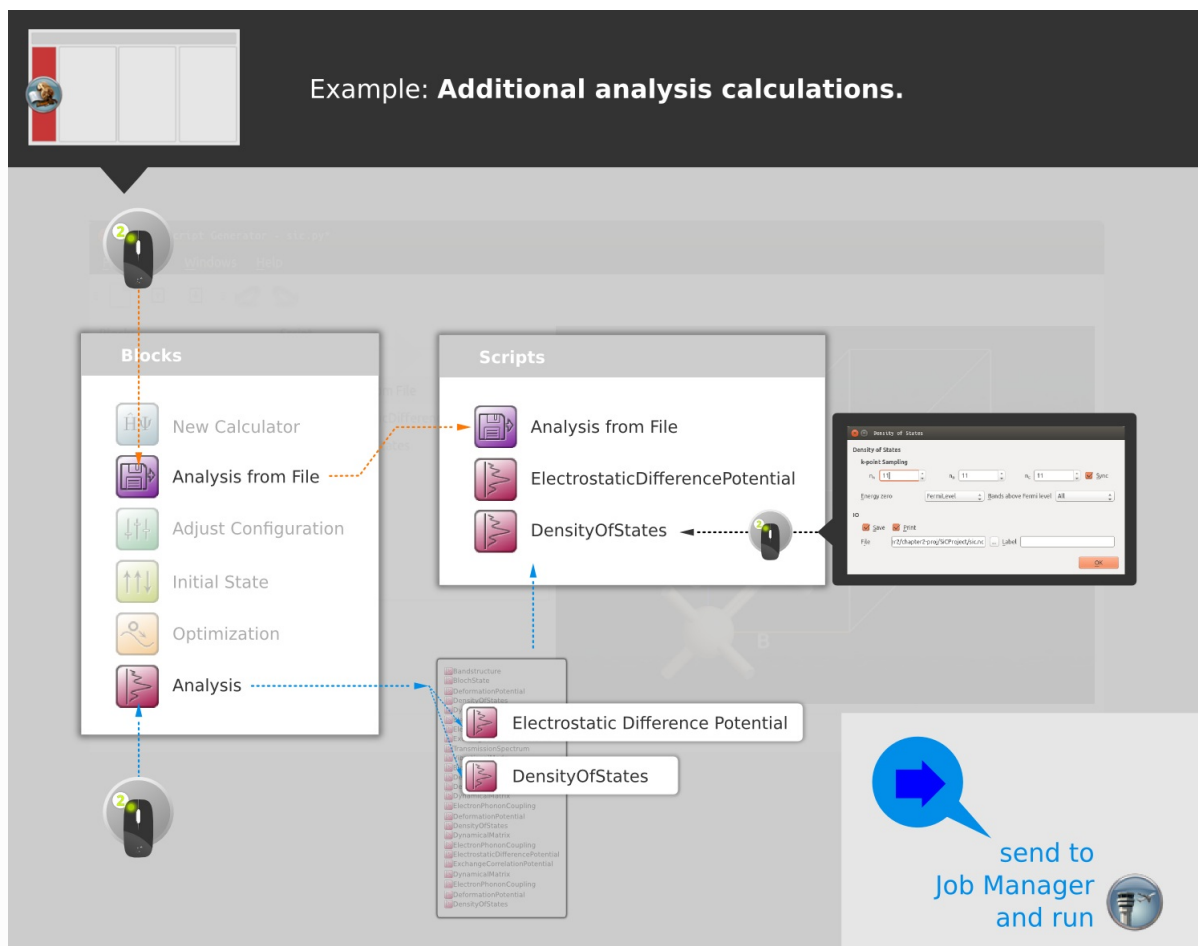
Tip

To export the visualization as an image, use the right mouse button menu **Export image**.

Additional analysis

Suppose you now want to perform some additional analysis of the SiC crystal, e.g. compute the electronic density of states (DOS). This is easily done by creating and running a new ATK Python script that uses the **Analysis from File** functionality.

Simply open the  **Script Generator** and create the script as illustrated below. In the Analysis from File block, load the saved NetCDF file `sic.nc`. The widget should automatically detect and select the BulkConfiguration `gID000`. Lastly, change the default output filename to `sic.nc` and save the script as `analysis.py`.



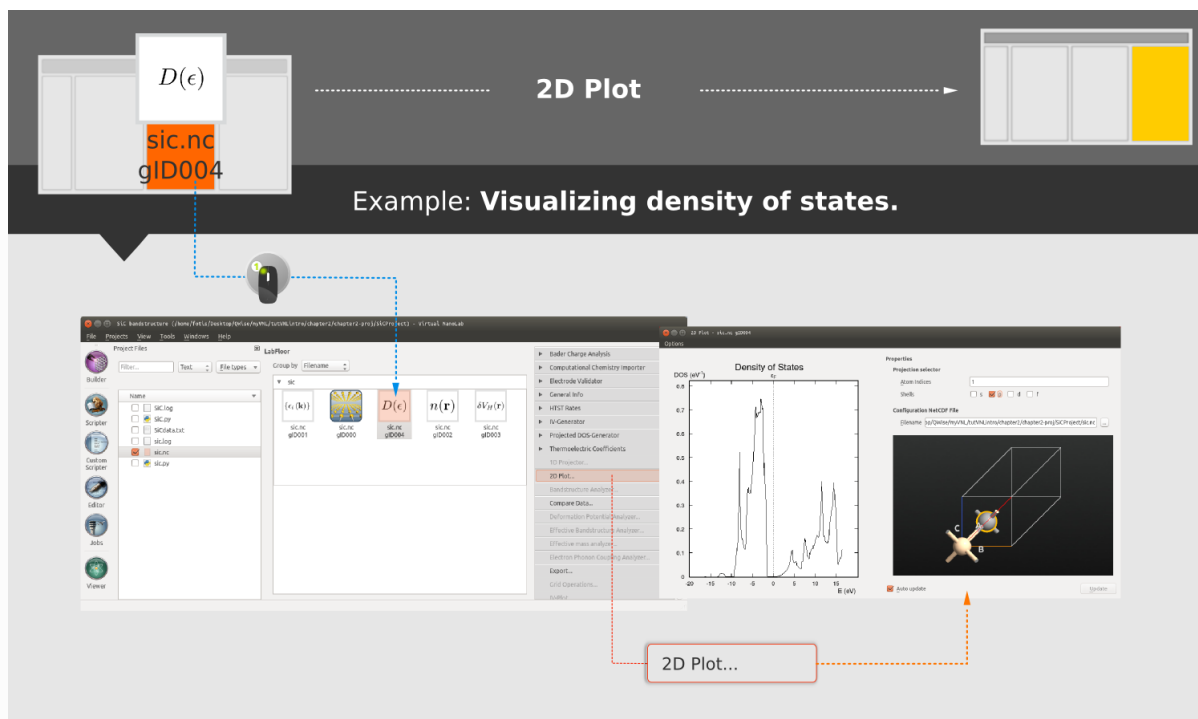
What happens in the ATK Python script you just made is this:

1. The self-consistent electronic structure of the SiC bulk was previously calculated, so here we simply read that state using Analysis from File.
2. Two different post-SCF analyses are then performed; first the electrostatic difference potential is computed, and then the density of states. Both data items are appended to the existing data file `sic.nc`.

Send the script to the **Job Manager** and run the calculations.

Plotting the density of states

The SiC density of states is now easily plotted; select the DOS object on the LabFloor, `D(ϵ)`, and click the **2D Plot** plugin in the right-hand Panel Bar. You should now see a plot of the computed DOS vs. electron energy eigenvalue (referenced to the Fermi level). Use the mouse to zoom in on the plot if needed.

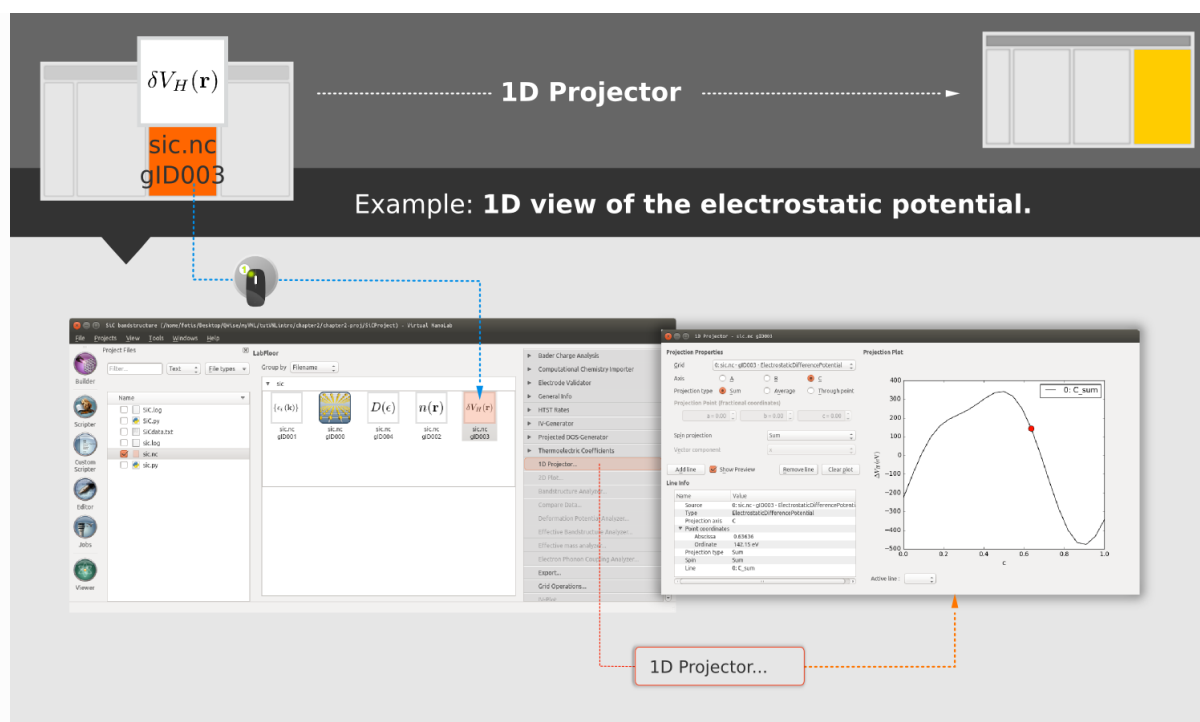


You can also plot the projected DOS using the **Projection selector**: Select the carbon atom (index 1) and tick only the p-shell in order to see the PDOS corresponding to the p-orbital of the C atom.

1D projection of the electrostatic potential

The electrostatic difference potential (EDP) is represented on a 3D grid, and you could visualize it as an isosurface or a cut plane in the 3D Viewer. However, VNL also offers a very convenient tool for creating 1D projections of 3-dimensional grid data – the **1D Projector**:

- Select the EDP data item on the LabFloor, $\delta V_{el}(\mathbf{r})$, and click the 1D Projector plugin.
- Choose “C” as the projection axis and “Sum” as the projection type.
- Then click *Add line* to produce the plot.



Note

The plot above shows the summed EDP along the C-axis of the SiC bulk configuration, i.e. summed in the AB plane for each value of C. You can also choose to average the grid values instead of summing them. Use the “Through point” projection type to avoid summing or averaging the grid values altogether.

Please proceed to the next chapter:

Example 2: Transport in a graphene nanoribbon with a distortion.

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Next