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Coupling QuantumATK with Synopsys tools

Version: 2016.3

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In this tutorial you will learn how to extract band structure data from a first-principles (DFT) calculation in a file format that can be directly imported in **Synopsys** tools for **TCAD simulations**. We will use a simple silicon crystal as the example, but the methodology is general and can in principle be applied to any semiconductor material, subjected to for instance strain, or even a nanowire or 2D thin film.

This tutorial is aimed both at experienced users and those with more limited experience, who are trying this functionality for the first time. In order to keep the tutorial short and succinct, we will not explain so much, but just present the steps you need to follow. It is however a good idea to go through the [Basic QuantumATK Tutorial](#) to learn the basics of QuantumATK (ATK) and its graphical user interface QuantumATK (QuantumATK).

SYNOPSYS[®]
Silicon to Software[™]

If you are familiar with **QuantumATK**, you may skip the following section - just start **QuantumATK** (in any project) and proceed to the next section to install the **addon** needed for this tutorial.

Preparations

You of course first need to download and install the software (there is both a Linux and Windows version).



Start **QuantumATK**, typically by double-clicking the desktop icon. If this is the first time you try **QuantumATK** and you don't have a license, the software will automatically attempt to download a demo license over the internet - naturally you need to be online for this to work. For alternative methods to obtain a license, see the [license](#) to apply for an extended trial license.

Spend just a few minutes to familiarize yourself with the program.

First, a project selection dialog will appear. If this is your first encounter with **QuantumATK**, it is recommended to first open the *Example Project*, to have some data to play around with.

- In the left panel you see a list of files in the project. By checking the little box next to a file name, the

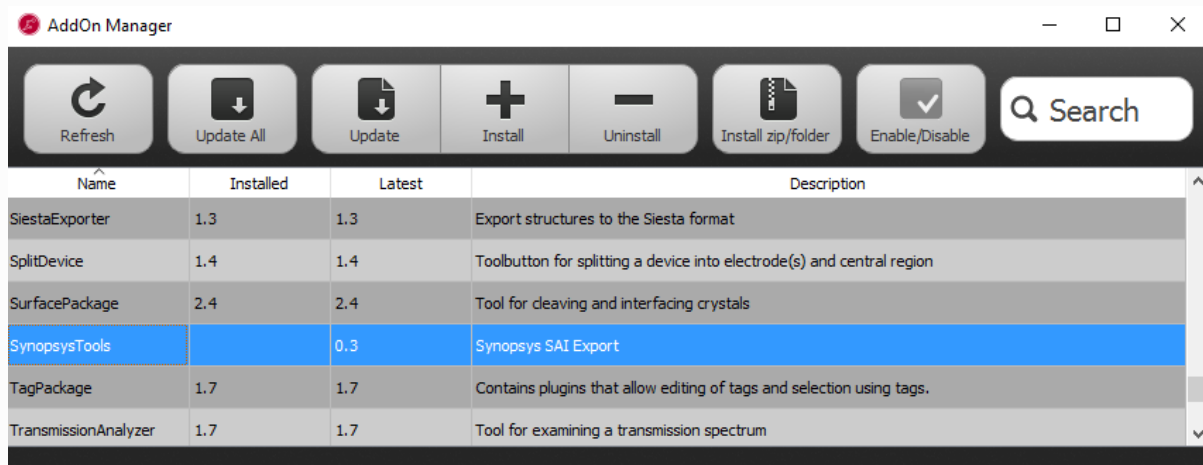
contents of the file will be displayed on the **LabFloor**, the middle panel, provided that the file type is understood by QuantumATK (additional file types can be supported via plugins).

- By selecting an object icon on the **LabFloor**, a set of tools on the right-hand toolbar panel will become active, indicating possible ways you can interact with this object by clicking the corresponding panel button. For instance, a band structure can be opened in the Bandstructure Analyzer.
- Some objects - in particular atomic configurations - can also be dragged with the mouse to e.g. the  **Viewer** to show them in 3D, or the  **Builder** for manipulations of the geometry.

Installing the addon

To export band structures to the **Synopsys SAI** format, you need to install the **SynopsysTools** addon in QuantumATK.

Open the **AddOn Manager** from the **Help** menu. Scroll down to “SynopsysTools” (or type “syn” in the search box) - as you will see, this addon is not installed, but is available on the server (the version number may vary).



Select the SynopsysTools package and click **Install** (alternatively, just click **Update all**) to download and install it.

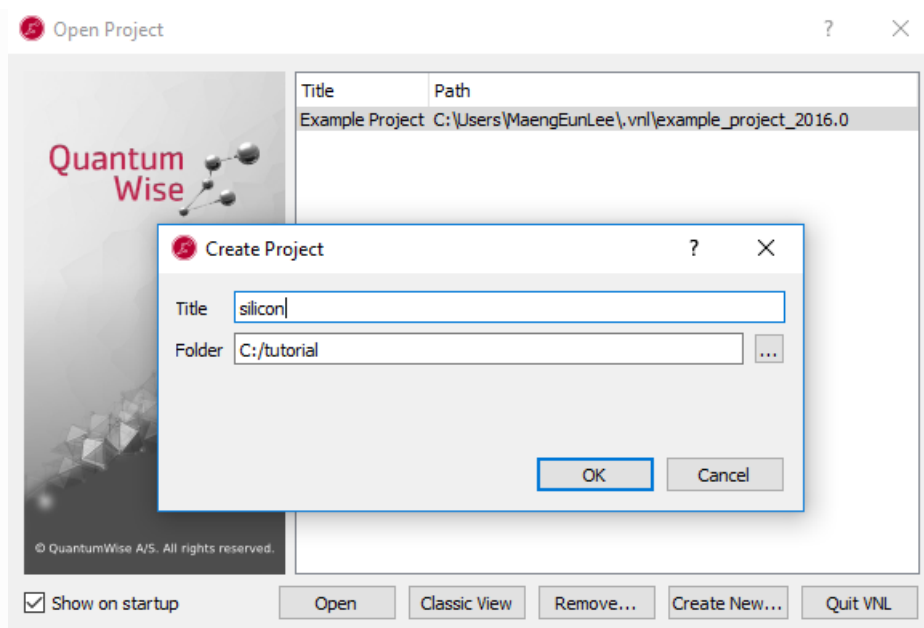
Note

You now need to restart QuantumATK for the plugin to become active.


New project

When QuantumATK starts *again*, make a new project for this tutorial.


1. Create a new project by clicking **Create new** in the dialog shown on startup.
2. Choose a suitable directory (that does not contain any non-Latin characters in the path).
3. Then click **Open** to start the main interface.





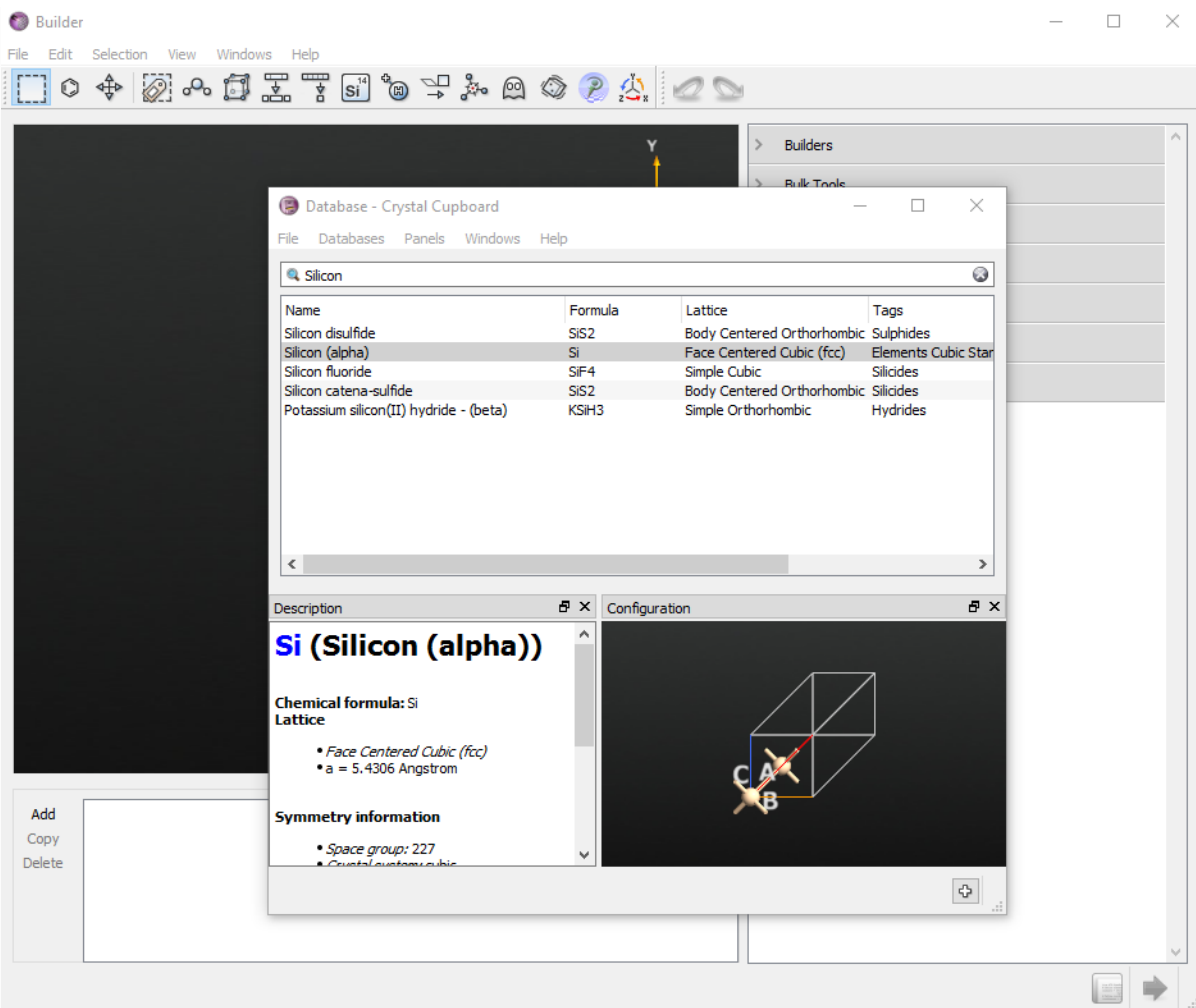
Silicon crystal

Click the  **Builder** to open the atomic geometry builder.

Note

The  **Builder** contains a lot of advanced tools for constructing and manipulating atomic-scale structures, but for this tutorial you will just use a predefined crystal from a database.

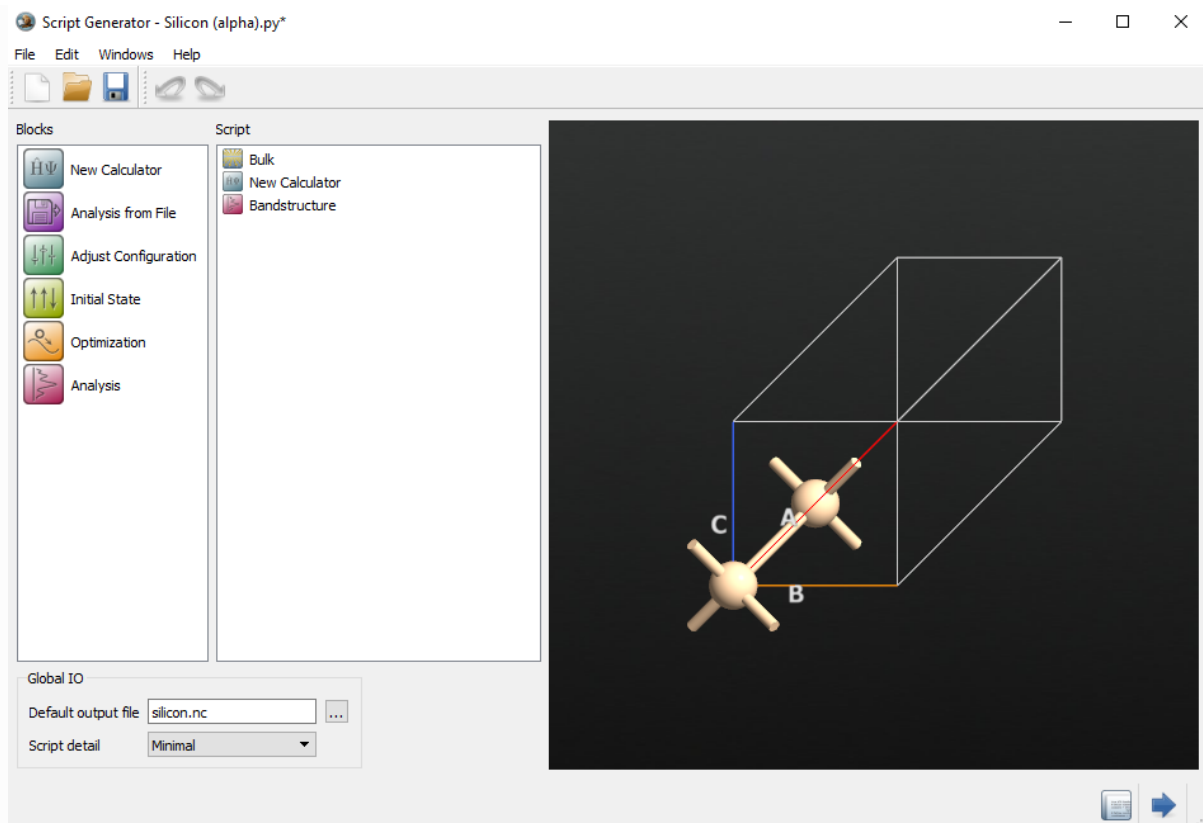
1. Click the button **Add** to the left of the Stash area and choose **From Database...** from the popup menu.
2. Locate the "Silicon (alpha)" structure - for instance by using the search filter - and select it.
3. Click the  plus button to add the silicon crystal to the **Stash**. The database window will automatically close.
4. Now click the  icon in the lower right-hand corner of the Builder, and choose **Script Generator** from the popup menu. This will transfer the geometry to the tool used for setting up the calculation model.




DFT model setup

In the  Scripter change the following:

1. double-click  **New calculator** in the "Blocks" panel;
2. double-click  **Analysis** and choose **Bandstructure** from the popup menu;
3. simplify the name of the default output file to `silicon.hdf5`. This is where all results of the calculation will be stored.



Double-click the  **New calculator** block that was inserted in the Script panel. In this tutorial, you will only change the k-point sampling and exchange-correlation.

- Set the k-point sampling as the 2 Å density or the number of k-points to 5 in all three directions (A, B, C)
- Choose the MGGA exchange correlation

Click OK to close the window.

New Calculator ? X

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

Estimate Memory Usage

Basic Settings

Electron temperature K

Density mesh cut-off Hartree

Charge

Exchange correlation MGGA

Spin Unpolarized

k-point Sampling

Grid type Monkhorst-Pack grid Preset densities

Periodic k_x k_y k_z

Density (Å) Sync

Sampling

Number of symmetry reduced k-points: 63 Shift to Γ Show

CheckPoint

File Location ...

Interval (hours)

IO

Save Print

File ... Label

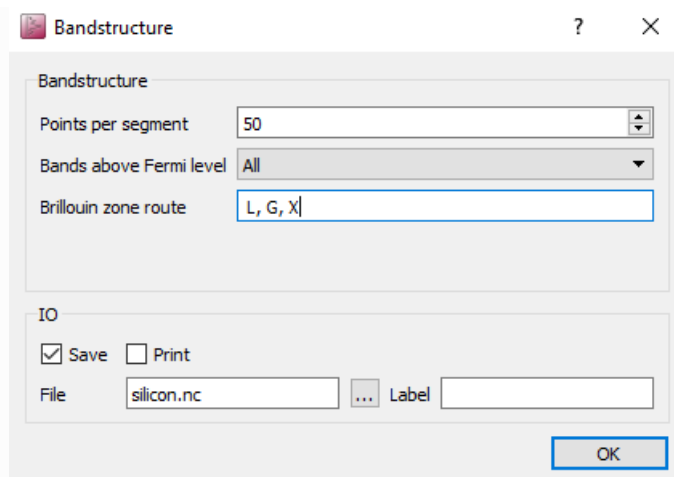
OK



Note

Parameters like the k-point sampling and a few other ones should always be systematically checked for convergence, to obtain accurate results.

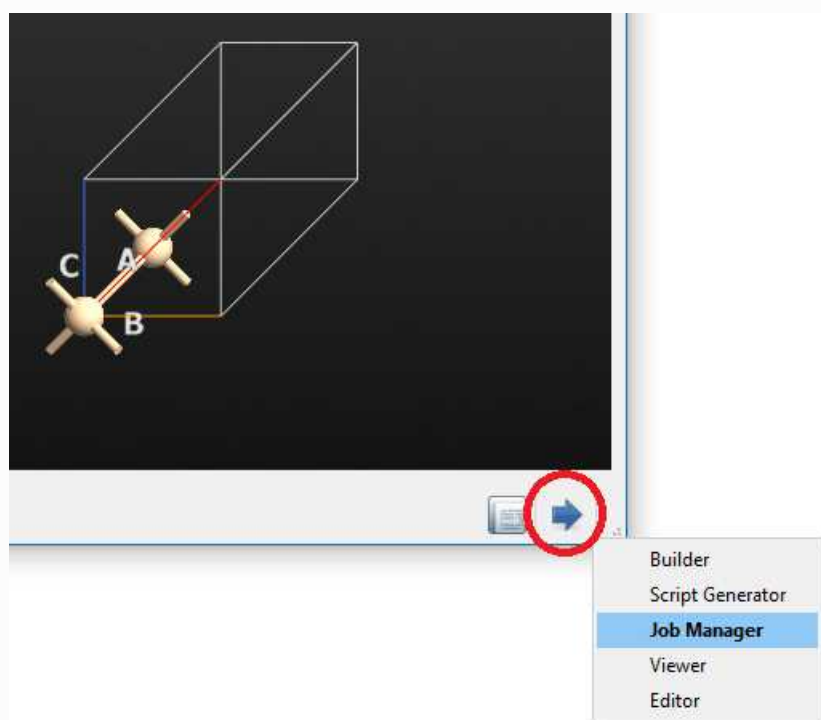
Next, double-click the **Bandstructure** block and set the route in the Brillouin zone to L,G,X, and the number of points to 50, to get a detailed picture of the most important part of the band structure.

Click OK to close the window.




Click the  icon in the lower right-hand corner of the  **Scripter**, and choose **Job Manager**.


A file dialog will pop up, prompting you to save the input file. Choose a suitable filename, such as `silicon.py` (the file is a python script, so always use the `.py` extension). Make sure the file is saved in the current project directory.



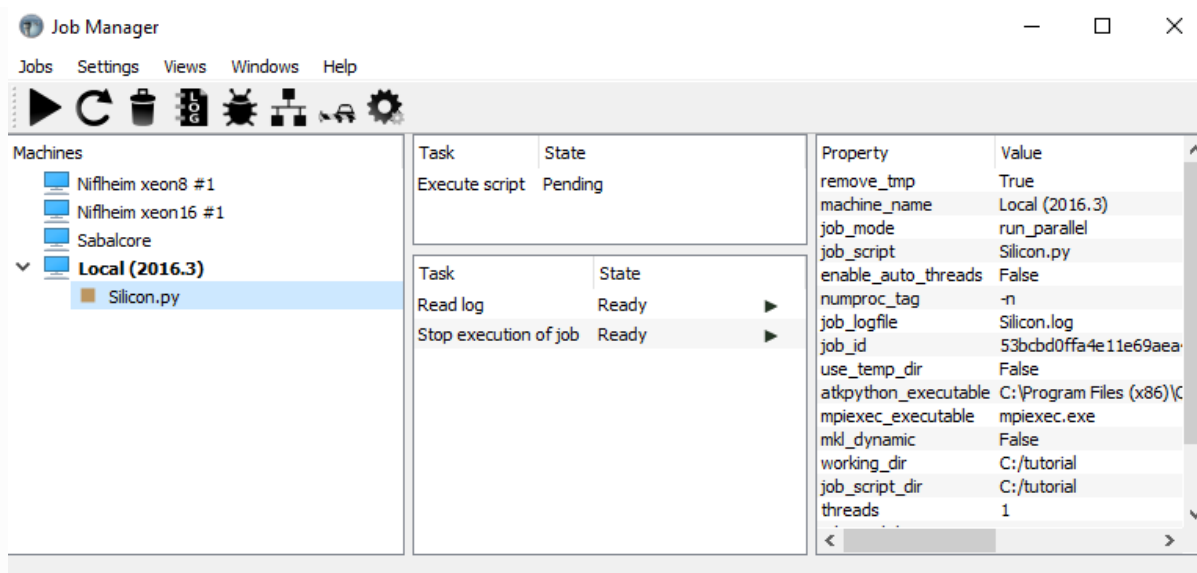
Running the calculation

After you have saved the script, the  **Job Manager** opens up, and asks where you would like to run the script. Choose "Local" to run the calculation on your own machine, and click OK.

Note

A small job like this can be run on any computer, even a simple laptop, but for more complex simulations, the  **Job Manager** offers the possibility to submit jobs to remote clusters and servers.

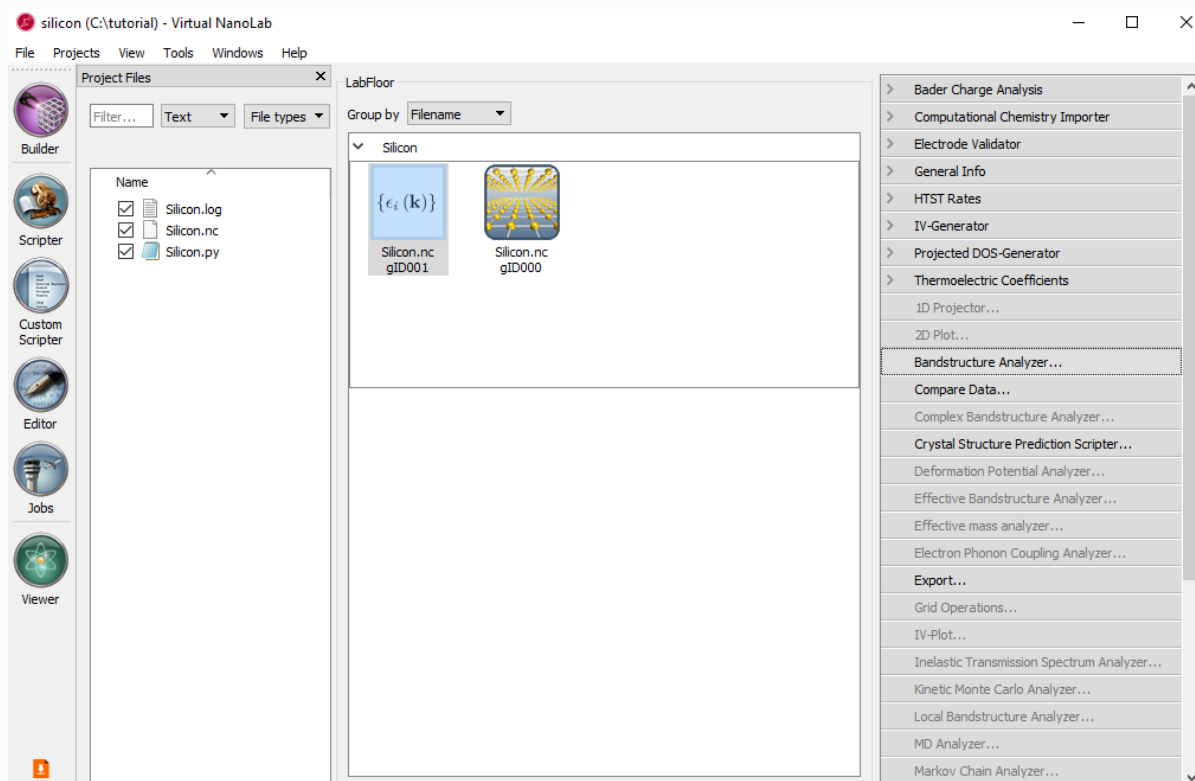
To run the job, click the  start button on the toolbar.



Visualizing the band structure

The job should take less than a minute or so to complete. When it's done, you will note that a new file (`silicon.hdf5`) has appeared in the project (along with a log file for the calculation), and its contents are already visible on the LabFloor in the main QuantumATK window: a band structure and a bulk configuration.

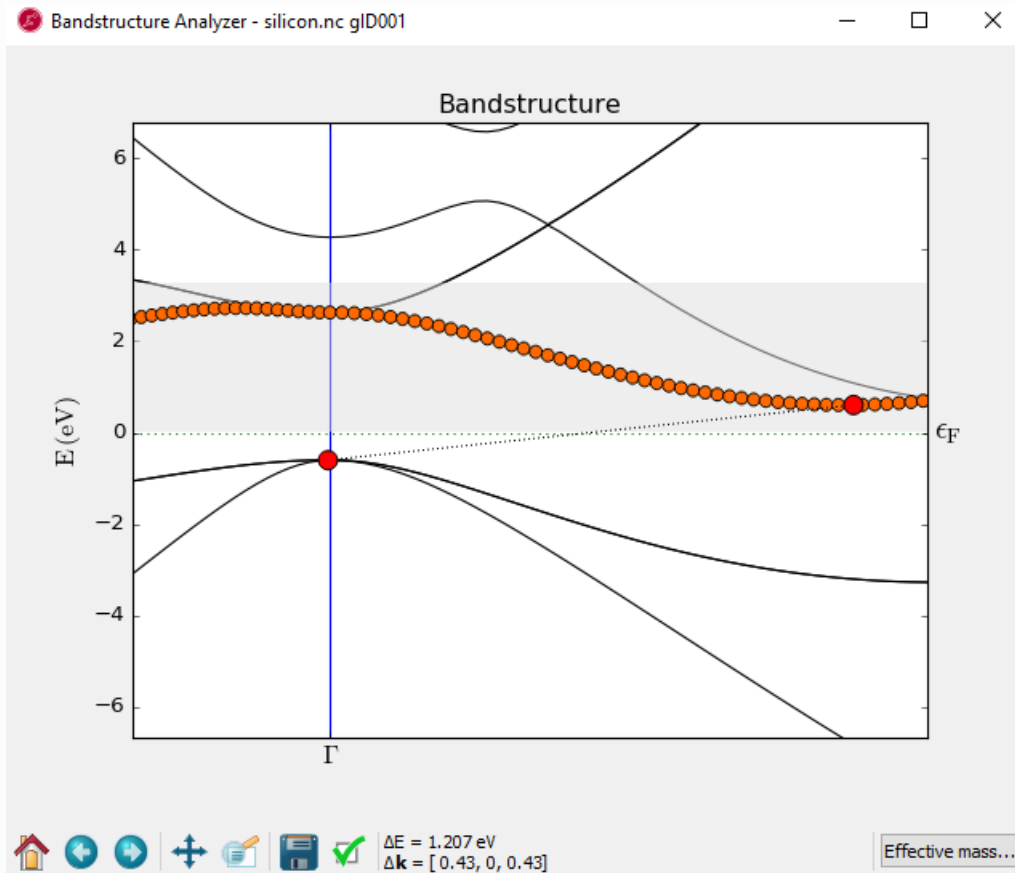
1. Select the *band structure* object;
2. Click **Bandstructure Analyzer** on the right-hand side panel of analysis tools.



The band structure plot will appear, and you can verify the band gap to be 1.2 eV.

To measure the band gap,

1. Click the **zoom** button, and draw a rectangle with the mouse to zoom in around the Fermi level. Then click the zoom button again, to exit zoom mode.
2. Click a point in the band structure and hold down the mouse button, while moving the mouse to another point, and the difference in energy will be displayed in the toolbar.



Note

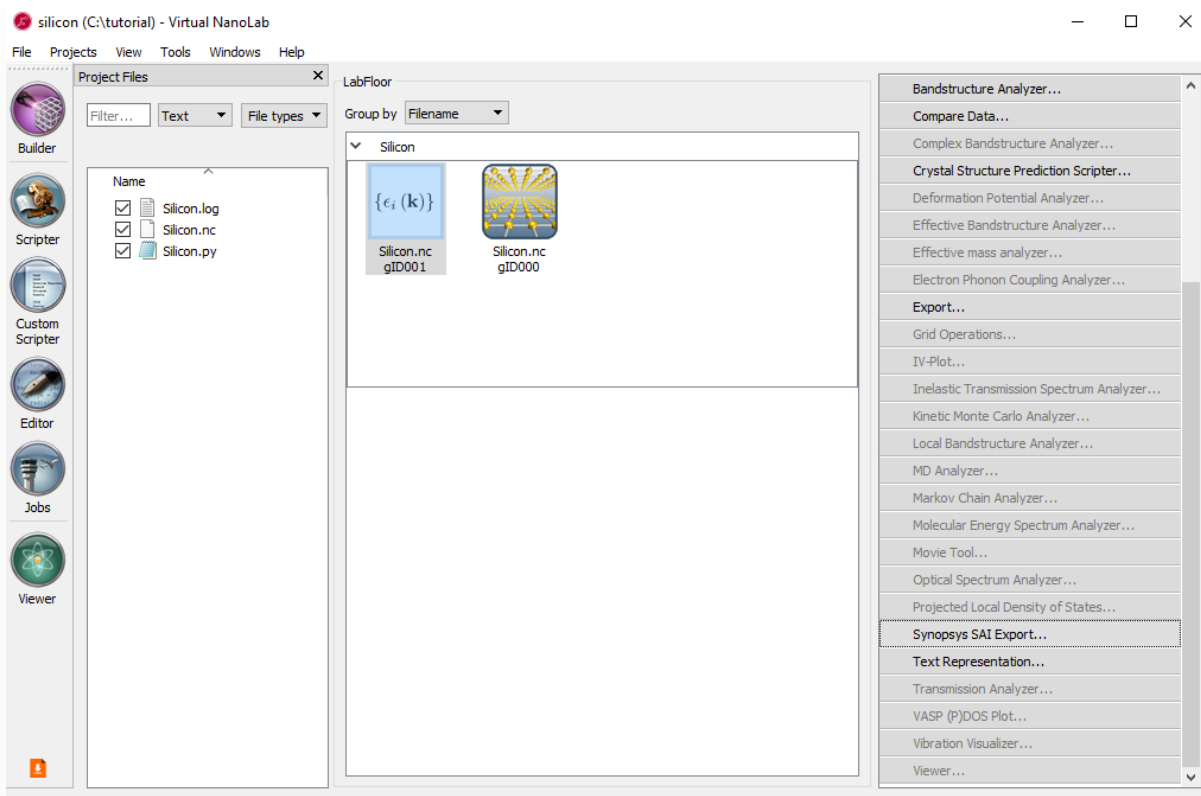
It is well-known that “standard” DFT fails to give good band gaps. In this tutorial you have, however, found that by using the TB09 meta-GGA (MGGA) exchange-correlation functional, the gap comes out close to the experimental value for silicon (and the same is true for many other semiconductors). In fact, the TB09-MGGA functional you used actually contains a tunable parameter which can be used to fit the gap very precisely.

Exporting the band structure to SAI format

The ultimate goal of this tutorial is to export the band structure in a format that can be imported in Synopsys tools. To do this, ensure that the band structure object is still selected, then locate the **Synopsys SAI Export...** button on the right-hand side toolbar.

Click it - then provide a filename and click Save. You have now exported an `.sai` file which can be imported in Synopsys tools, for further use in TCAD simulations.

It is also possible to select multiple band structure objects on the **LabFloor** and export them all with a single click on the **Synopsys SAI Export...** button. In this case, the filename of the `.sai` file will be automatically determined by the lab floor item title.



Note

Specifically, each SAI file will be saved in the same directory as the HDF5 file containing the corresponding band structure, with the extension switched from “nc” to “sai” and with the unique object ID (seen in the label for each lab floor item - it is gID001 for the band structure created in this tutorial) appended to the filename to handle the case where there are several band structures in the same HDF5 file.

Batch processing and command line usage

A major advantage of QuantumATK is that in addition to the graphical user interface, you can also perform tasks via Python scripting.

First of all, to convert a single bandstructure, saved in an HDF5 file, to the SAI format, you just need 3 lines of Python code (assuming the addon has been installed, of course):

```
from Add0ns.SynopsysTools.saiExporter import saiExporter
import sys
saiExporter(sys.argv[1], sys.argv[2])
```

Download this script [atd_input_qw.py](#) and save it in the folder containing the HDF5 file. Then run, as also described in the Synopsys *Ab-Initio to Device User Guide*:

```
atkpython atd_input_qw.py $NC_FILE $SAI
```

where `$NC_FILE` denotes the HDF5 (.hdf5) output file containing the BandStructure object, and `$SAI` denotes the desired output `.sai` file.

However, the scripting interface also makes it possible to do batch processing. For instance, assume you have a set of HDF5 files in a particular directory, and each one contains only one band structure. Then,

open the  Editor in QuantumATK and insert the following code:

```
from Add0ns.SynopsysTools.saiExporter import saiExporter
import glob, sys
for nc_file in glob.glob("*.hdf5"):
    bs = nread(nc_file, Bandstructure)[0]
    sai_file = nc_file.replace(".hdf5", ".sai")
    print(nc_file, ">", sai_file)
    saiExporter(bs, sai_file)
```

Save the script in the same folder where the HDF5 files are (for instance with a name like `many_to_sai.py`), and run it from the command line (in the directory where the files are) as

atkpython many_to_sai.py

This will produce `silicon.sai` from `silicon.hdf5`, and so on. Of course, if you want to select only a subset of HDF5 files, you just need to modify `glob.glob` (`"*.hdf5"`) to reflect your desired selection.

If you have HDF5 files with several band structures, use a modified script:

```
from Add0ns.SynopsysTools.saiExporter import saiExporter
import glob, sys
for nc_file in glob.glob("*.hdf5"):
    all_bs = nread(nc_file, Bandstructure)
    for i, bs in enumerate(all_bs):
        sai_file = nc_file.replace(".hdf5", "%i.sai" % i)
        print(nc_file, i, ">", sai_file)
        saiExporter(bs, sai_file)
```

This will make one SAI file for each band structure, and the files will be named after the HDF5 file (just like before) but with `_1`, `_2`, *etc* added.

As an alternative to specifying the HDF5 files inside the script, replace the line

```
for nc_file in glob.glob("*.hdf5"):
```

with

```
for nc_file in sys.argv[1]:
```

and run it as

atkpython many_to_sai_2.py silicon*.hdf5

The possibilities to customize tasks like this with scripts in QuantumATK are endless.

