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Silicon p-n junction

Downloads & Links

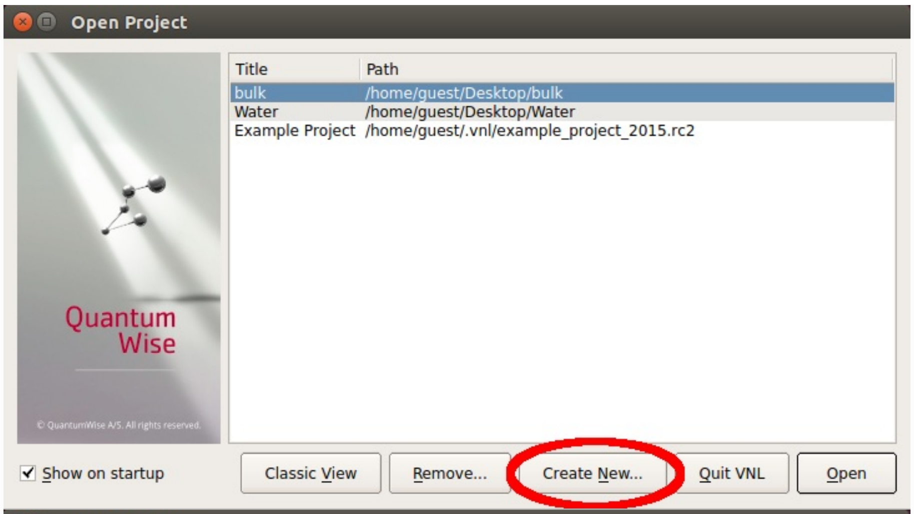
- PDF
- ATK Reference Manual
- MGGA_bulk.py
- bandstructure_fit.py
- ddos_edp.py
- IV_compare.py

In this tutorial you will:

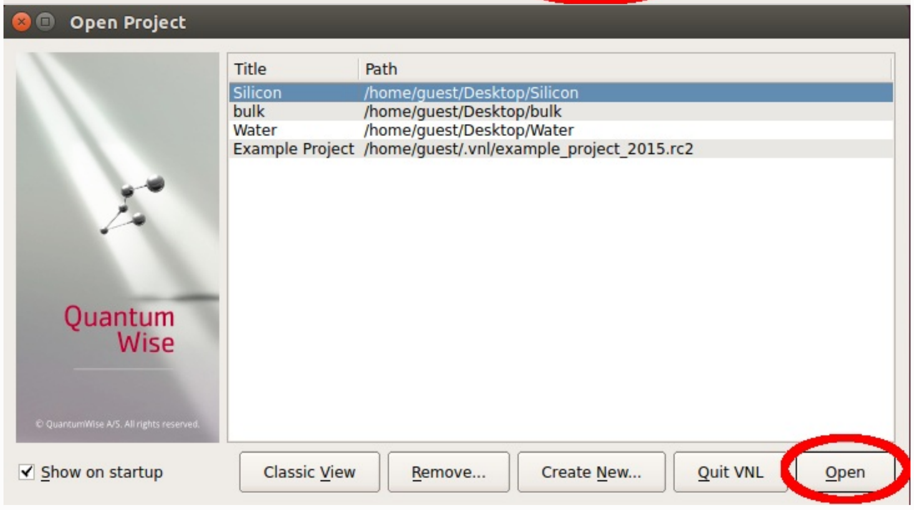
- Learn how to build a p-n junction device.
- Learn how to study the current-voltage characteristic of such a device.
- Compare two different methods: **ATK-SE** and **ATK-DFT**.
- Analyze the electronic structure of the p-n junction by studying and plotting the device density of states at zero bias and at reverse and forward bias.

Silicon bulk: Slater-Koster vs DFT-MGGA

1. Open **QuantumATK** and create a new project by clicking on **Create New**. Give the project a *Title* (here: *"Silicon"*), select a folder for the project, click **OK** and then **Open** to start the project.

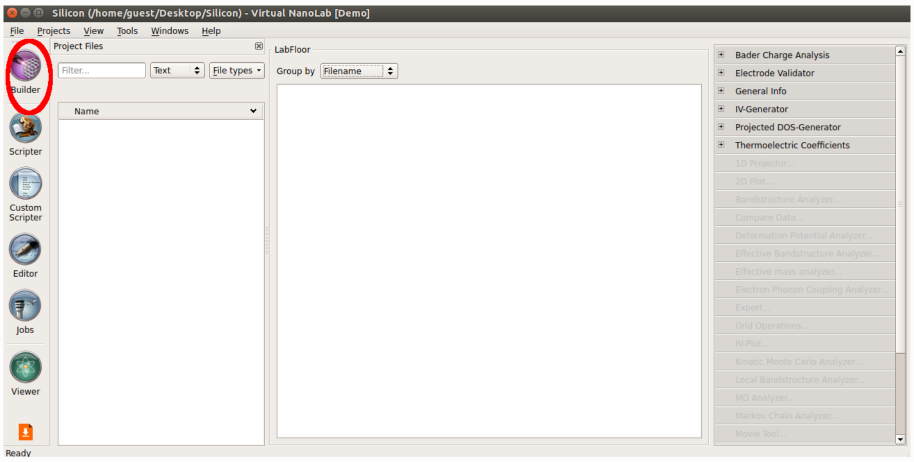


Title	Path
bulk	/home/guest/Desktop/bulk
Water	/home/guest/Desktop/Water
Example Project	/home/guest/.vnl/example_project_2015.rc2

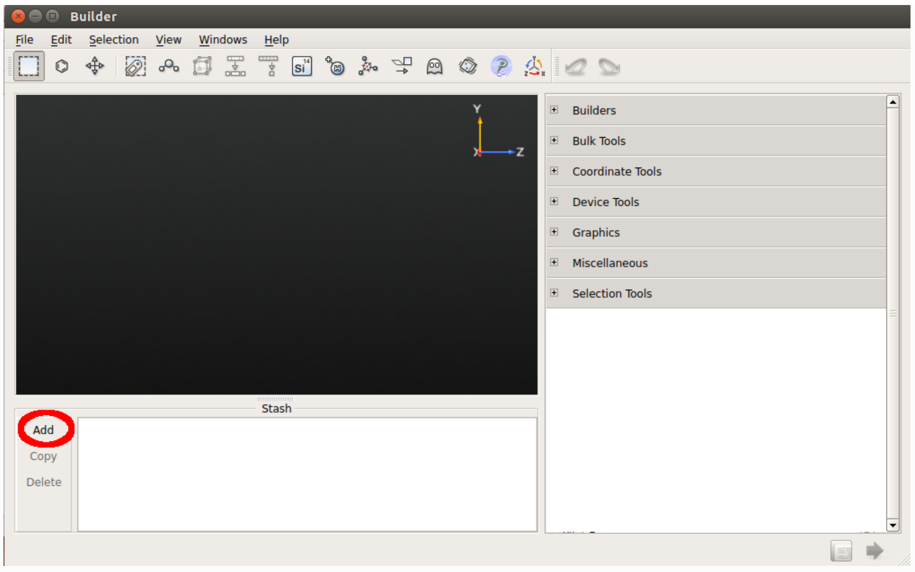


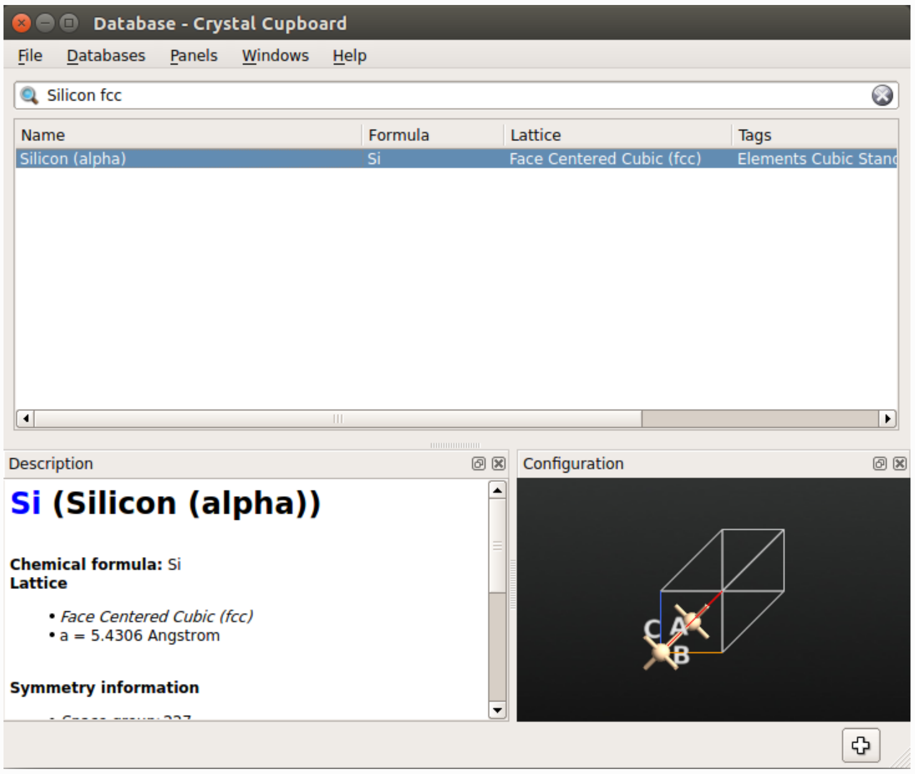
Title	Path
Silicon	/home/guest/Desktop/Silicon
bulk	/home/guest/Desktop/bulk
Water	/home/guest/Desktop/Water
Example Project	/home/guest/.vnl/example_project_2015.rc2

2. In the **QuantumATK** main window, click on the icon to open the **Builder**.



3. In the **Builder**, go to the **Stash**, click Add ‣ From Database and from the menu navigate to Databases ‣ Crystals and search for *"silicon"* in the search window. Then, select *"Silicon (alpha)"* and click the icon, or double-click its line in the list, to send it to the **Stash**.




Database - Crystal Cupboard
File Databases Panels Windows Help
Silicon fcc
Description
Configuration

Name	Formula	Lattice	Tags
Silicon (alpha)	Si	Face Centered Cubic (fcc)	Elements Cubic Stand

Si (Silicon (alpha))

Chemical formula: Si
Lattice

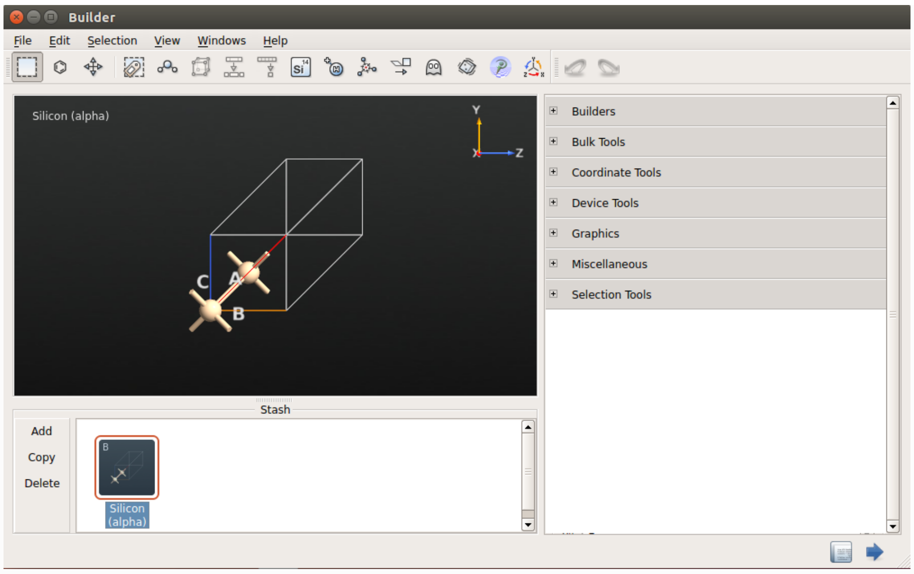
- *Face Centered Cubic (fcc)*
- a = 5.4306 Angstrom

Symmetry information

Slater-Koster calculation

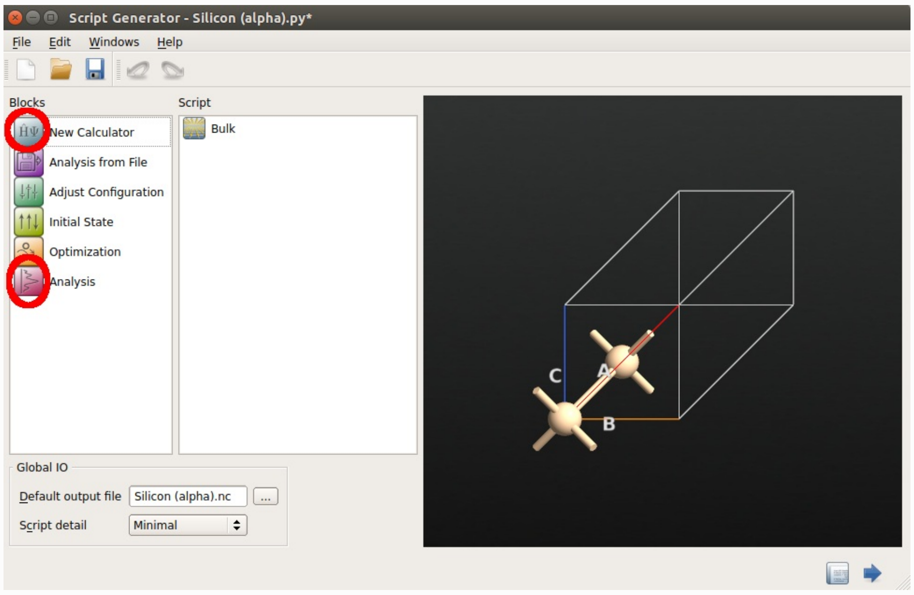
You will now set up an **ATK** semiempirical (**ATK-SE**) calculation using the Slater-Koster model Hamiltonian.

1. Send the bulk configuration from the **Builder** to the **Script Generator** using the button.

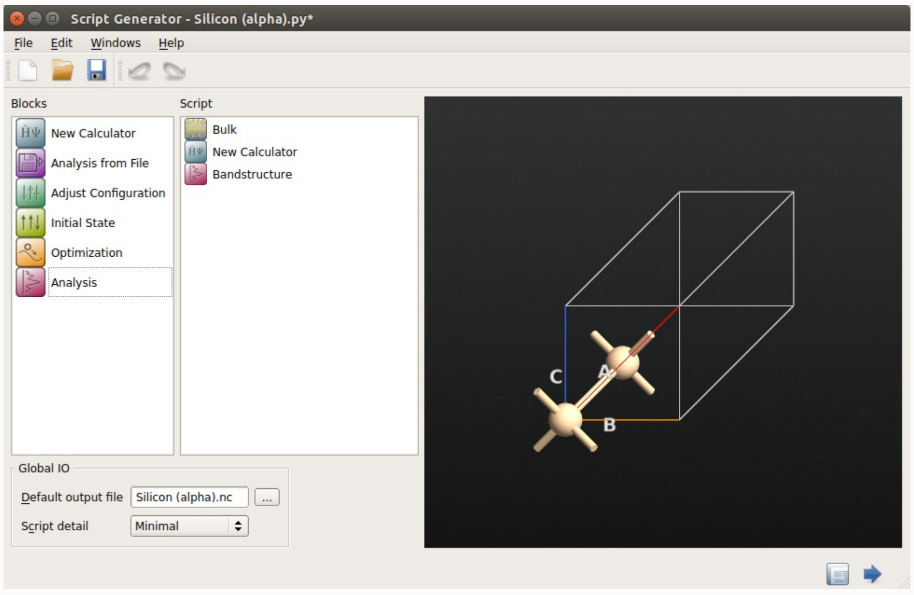


2. Add the following blocks to the *Script* by double-clicking the correspoding icons in the *Blocks* panel:

- New Calculator.
- Analysis ▸ Bandstructure.



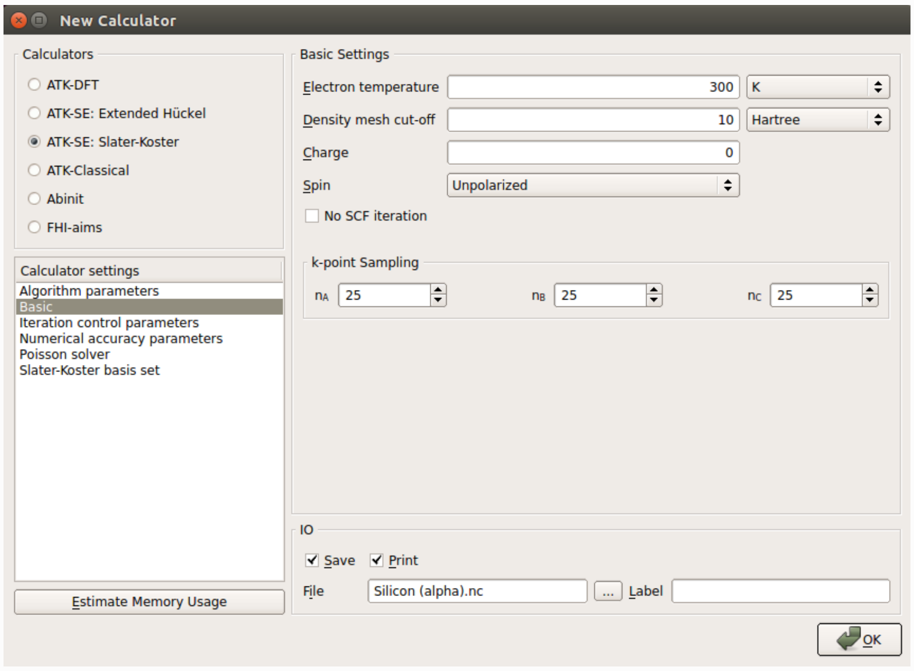
Global IO
Default output file: Silicon (alpha).nc
Script detail: Minimal



Global IO
Default output file: Silicon (alpha).nc
Script detail: Minimal

3. Open the **New Calculator** by double-clicking it.

   - Select the *ATK-SE Slater-Koster* calculator.
   - Use a 25x25x25 k-point sampling.
   - Uncheck the *"No SCF iteration"* box.
   - Select the *"Bassani.Si"* basis set.



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
- Numerical accuracy parameters
- Poisson solver
- Slater-Koster basis set

Estimate Memory Usage

Basic Settings

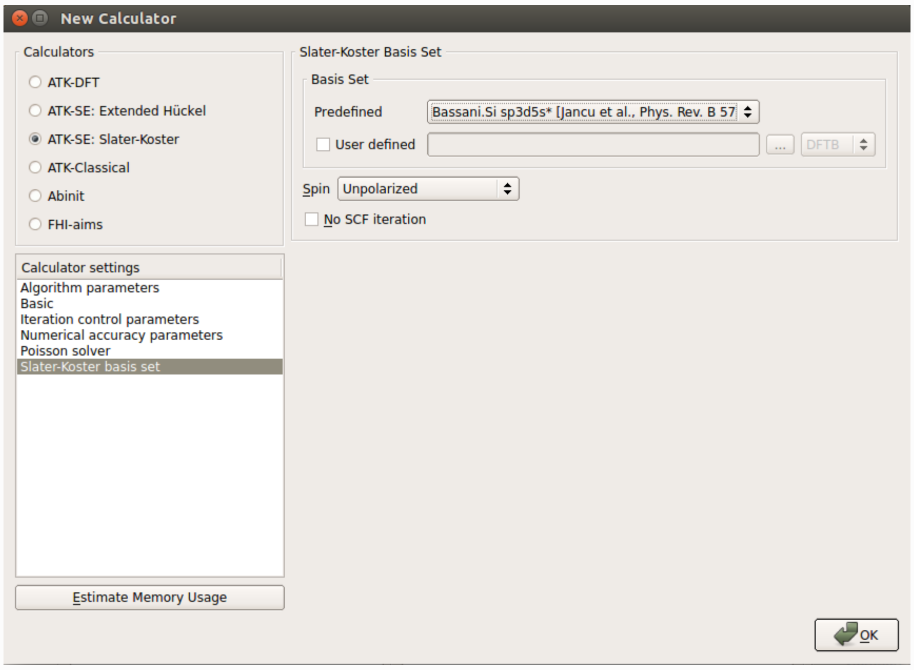
Electron temperature	300	K
Density mesh cut-off	10	Hartree
Charge	0	
Spin	Unpolarized	

☐ No SCF iteration

k-point Sampling: nA 25, nB 25, nC 25

IO: ✓ Save ✓ Print
File: Silicon (alpha).nc ... Label

OK



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
- Numerical accuracy parameters
- Poisson solver
- Slater-Koster basis set

Estimate Memory Usage

Slater-Koster Basis Set

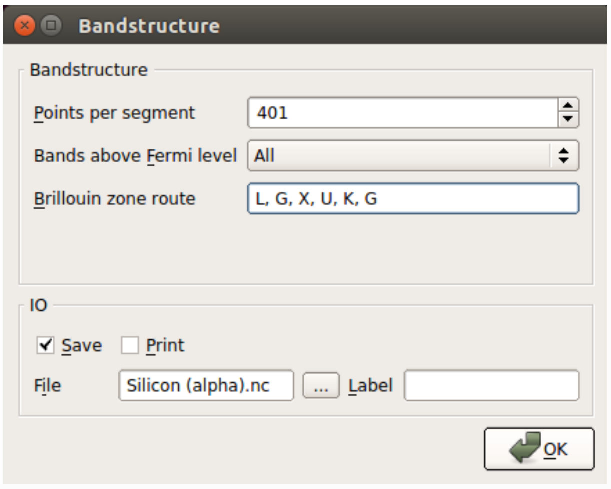
Basis Set
Predefined: Bassani.Si sp3d5s* [Jancu et al., Phys. Rev. B 57
☐ User defined ... DFTB

Spin: Unpolarized

☐ No SCF iteration

OK

4. In **Bandstructure**, select the "L, G, X, U, K, G" Brillouin zone route and 401 points per segment.

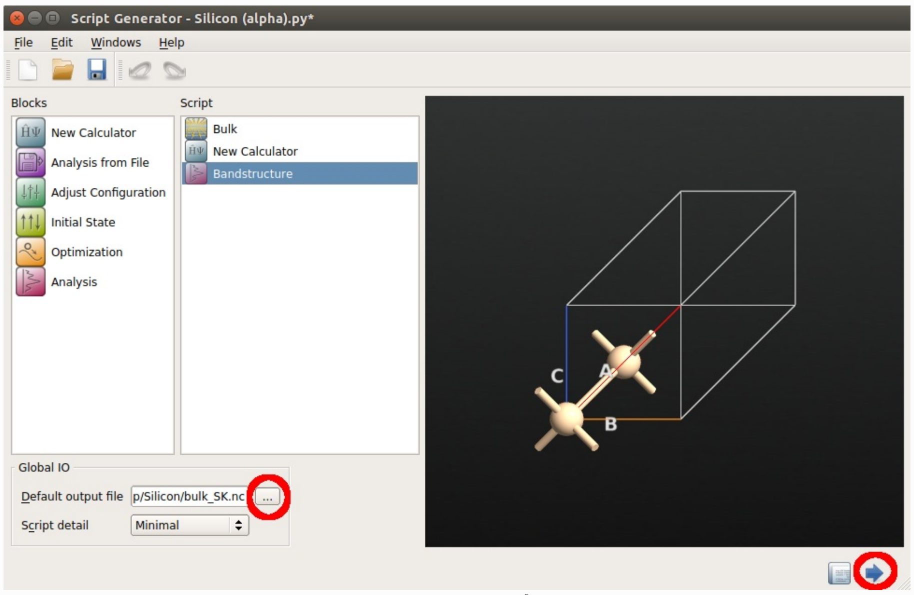


Bandstructure

Points per segment: 401
Bands above Fermi level: All
Brillouin zone route: L, G, X, U, K, G

IO
☑ Save ☐ Print
File: Silicon (alpha).nc
Label:

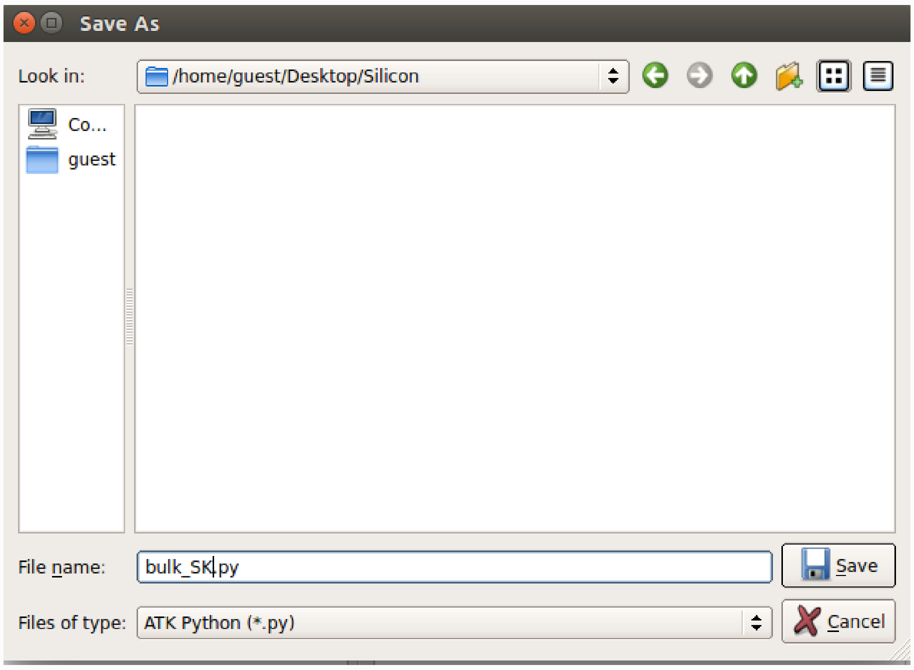
5. Back in the **Script Generator**, set the output filename to `bulk_SK.hdf5`, and send the script to the **Job Manager** using the button.



Script Generator - Silicon (alpha).py*

Global IO
Default output file: p/Silicon/bulk_SK.nc
Script detail: Minimal

6. Save the script in the window that shows up and use the ▶ botton to run the job.



Save As

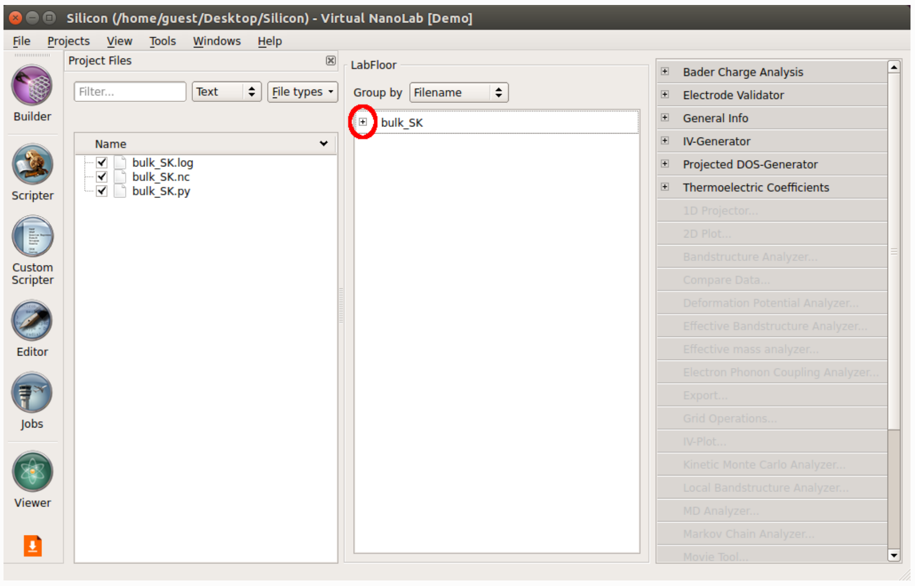
Look in: /home/guest/Desktop/Silicon
File name: bulk_SK.py
Files of type: ATK Python (*.py)

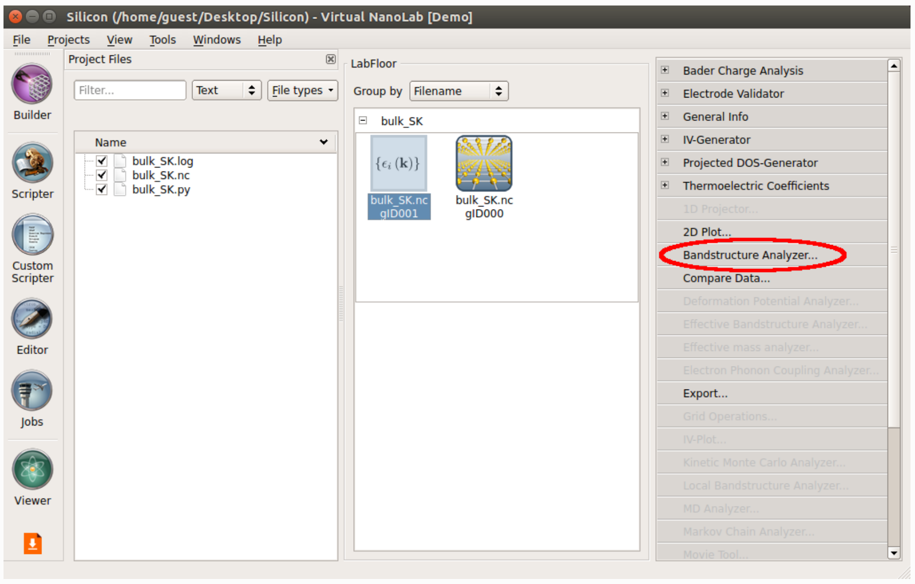
7. Once the calculation is done (it will only take a few seconds) you can find in the **LabFloor** your

Bandstructure object, which is saved in `bulk_SK.hdf5`:

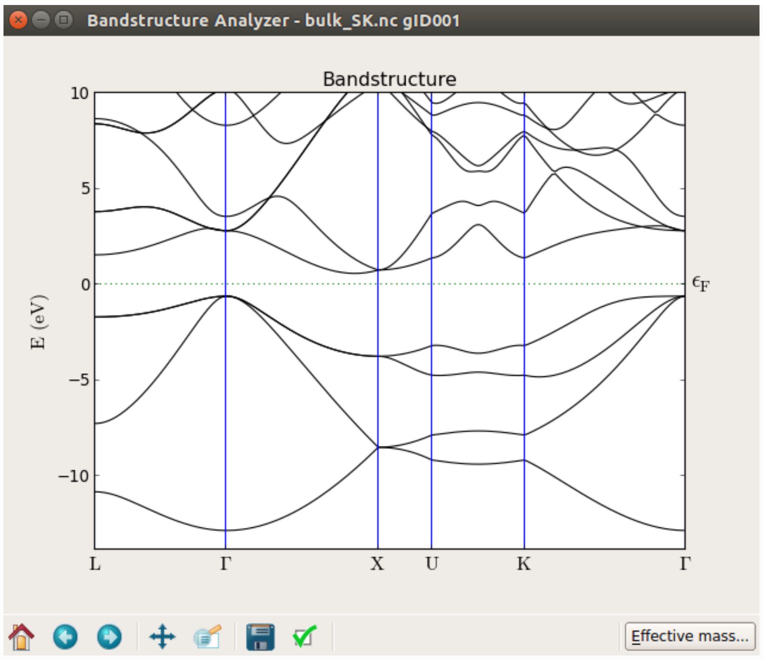
$\boxed{\{\epsilon_i(\mathbf{k})\}}$

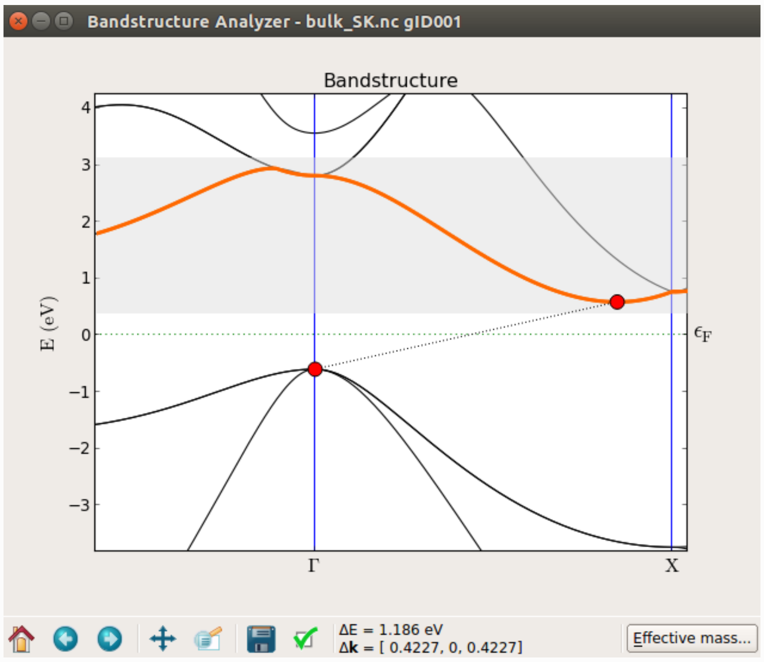
Highlight the object and use the **Bandstructure Analyzer** plugin to plot the bandstructure.





8. You can zoom into a region close to the band edges and precisely measure the calculated indirect band gap, 1.186 eV.





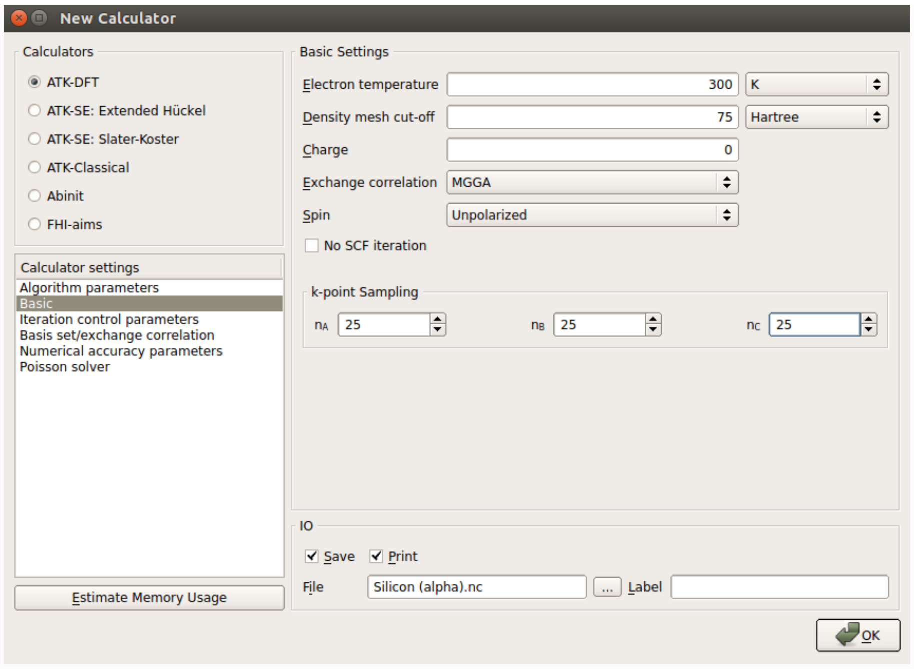
ΔE = 1.186 eV
Δk = [0.4227, 0, 0.4227]

DFT-MGGA calculation

The TB09-MGGA approximation [1] available in **ATK-DFT** is fully explained in the tutorial Meta-GGA and 2D confined InAs. In order to compare the Slater-Koster results with results from the TB09-MGGA method, you will fit a parameter (c) such the TB09-MGGA band gap of silicon matches that calculated with Slater-Koster. Throughout this tutorial you will use this fitted c parameter for the TB09-MGGA calculations.

1. From the **Builder**, send the *Silicon bulk configuration* to the **Script Generator** and add a **New Calculator** to the script. Then edit the calculator parameters:

   - Select *ATK-DFT* and the *MGGA* exchange-correlation functional.
   - Use a 25x25x5 k-point sampling.
   - Select the *SingleZetaPolarized* basis set in order to speed up calculations.


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
- Poisson solver

Estimate Memory Usage

Basic Settings

Electron temperature	300	K
Density mesh cut-off	75	Hartree
Charge	0	
Exchange correlation	MGGA	
Spin	Unpolarized	

☐ No SCF iteration

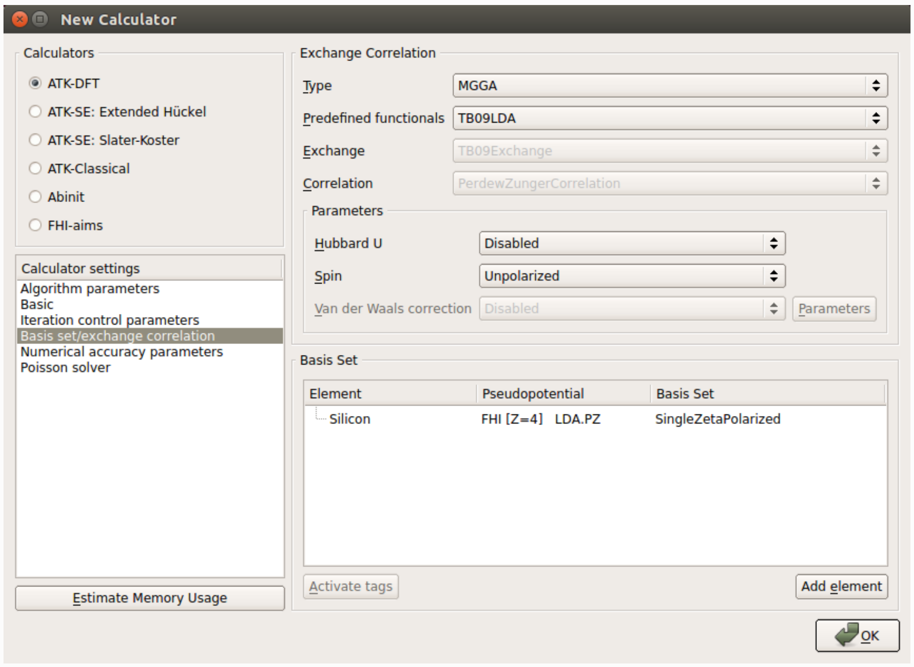
k-point Sampling: nA 25, nB 25, nC 25

IO

☑ Save ☑ Print

File: Silicon (alpha).nc ... Label:

OK


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
- Poisson solver

Estimate Memory Usage

Exchange Correlation

Type	MGGA
Predefined functionals	TB09LDA
Exchange	TB09Exchange
Correlation	PerdewZungerCorrelation

Parameters

Hubbard U	Disabled
Spin	Unpolarized
Van der Waals correction	Disabled

Parameters

Basis Set

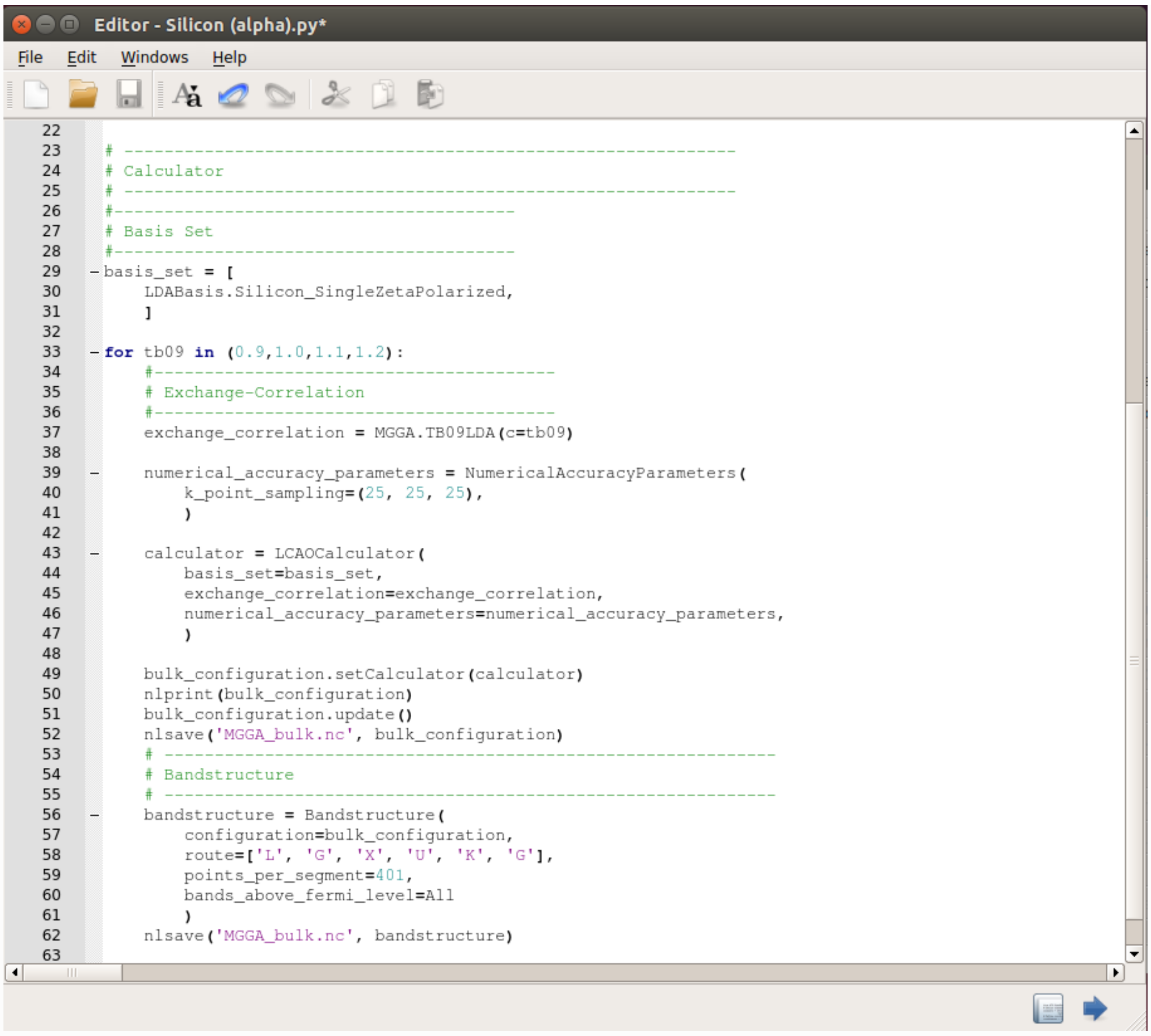
Element	Pseudopotential	Basis Set
Silicon	FHI [Z=4] LDA.PZ	SingleZetaPolarized

Activate tags Add element

OK

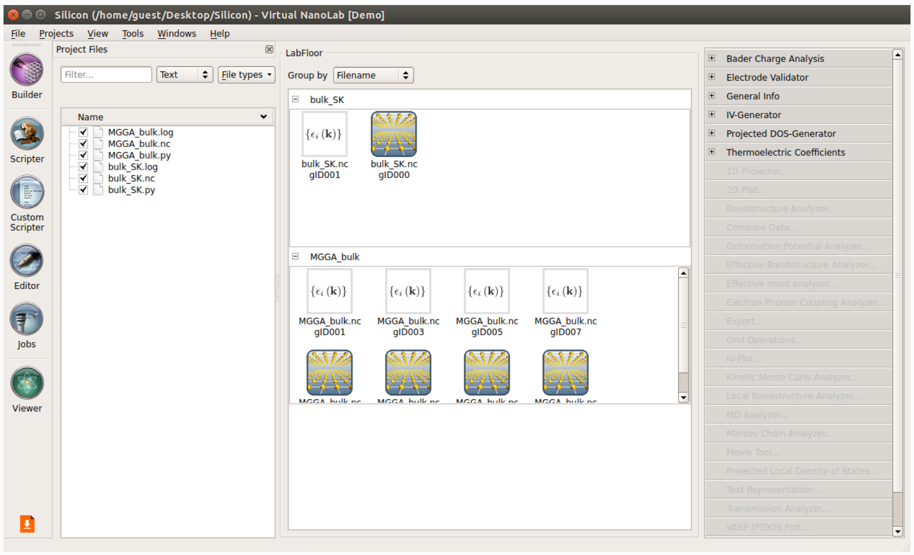
2. Add also a **Bandstructure** analysis object and set it up as you did for the Slater-Koster calculation.
3. Back in the **Script Generator**, set the output filename to `MGGA_bulk.hdf5`.
4. In order to fit the c parameter to the Slater-Koster band gap you will need to run a few calculations for different c parameters and make a linear interpolation. Here, you will run four TB09-MGGA calculations for c = 0.9, 1.0, 1.1 and 1.2. A little manual editing of the script is needed:

   - Send the script to the **Editor** using the button, and modify the exchange-correlation section as shown in the image below. Also, add a loop over the c values to run the four calculations with a single Python script (you can download a copy of the script here: MGGA_bulk.py):



```
# ----------------------------------------------------------------
# Calculator
# ----------------------------------------------------------------
#----------------------------------------
# Basis Set
#----------------------------------------
basis_set = [
    LDABasis.Silicon_SingleZetaPolarized,
    ]

for tb09 in (0.9,1.0,1.1,1.2):
    #----------------------------------------
    # Exchange-Correlation
    #----------------------------------------
    exchange_correlation = MGGA.TB09LDA(c=tb09)

    numerical_accuracy_parameters = NumericalAccuracyParameters(
        k_point_sampling=(25, 25, 25),
        )

    calculator = LCAOCalculator(
        basis_set=basis_set,
        exchange_correlation=exchange_correlation,
        numerical_accuracy_parameters=numerical_accuracy_parameters,
        )

    bulk_configuration.setCalculator(calculator)
    nlprint(bulk_configuration)
    bulk_configuration.update()
    nlsave('MGGA_bulk.nc', bulk_configuration)
    # ----------------------------------------------------------------
    # Bandstructure
    # ----------------------------------------------------------------
    bandstructure = Bandstructure(
        configuration=bulk_configuration,
        route=['L', 'G', 'X', 'U', 'K', 'G'],
        points_per_segment=401,
        bands_above_fermi_level=All
        )
    nlsave('MGGA_bulk.nc', bandstructure)
```

5. Send the script to the **Job Manager** and run the job.
6. On the **LabFloor** you will now have four different **Bandstructure** objects included in the *“MGGA_bulk.hdf5”.*

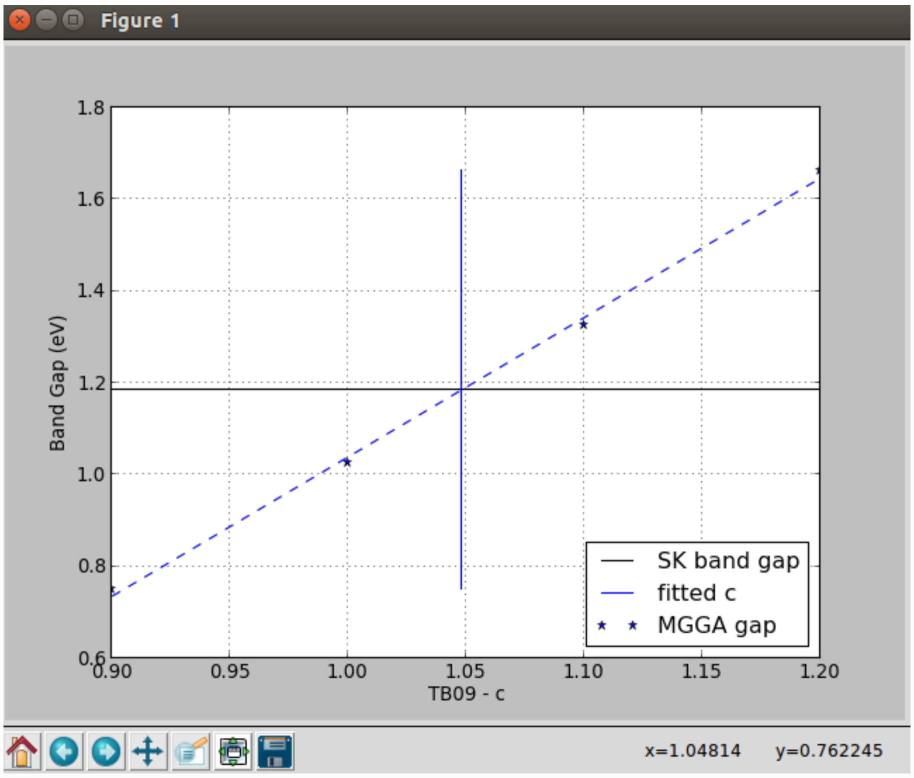


```
☑ MGGA_bulk.log
☑ MGGA_bulk.nc
☑ MGGA_bulk.py
☑ bulk_SK.log
☑ bulk_SK.nc
☑ bulk_SK.py
```

bulk_SK
- bulk_SK.nc gID001
- bulk_SK.nc gID000

MGGA_bulk
- MGGA_bulk.nc gID001
- MGGA_bulk.nc gID003
- MGGA_bulk.nc gID005
- MGGA_bulk.nc gID007

7. You will use the following script to fit the c-parameter: bandstructure_fit.py. Save it in the project directory.
8. Execute the fitting script using the **Job Manager**. The plot shown below should pop up.



It is clear that the TB09 c-parameter has a significant influence on the calculated band gap, and that the dependence is quite linear. The fitted value of c is 1.048.

Note

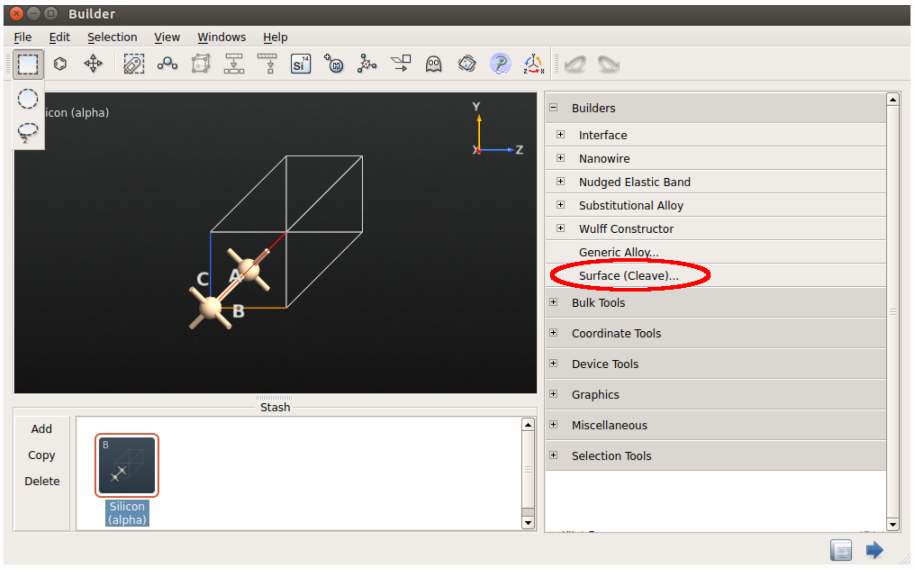
If you take a closer look at the script bandstructure_fit.py, You will see that band gaps are calculated from a **Bandstructure** object like this:

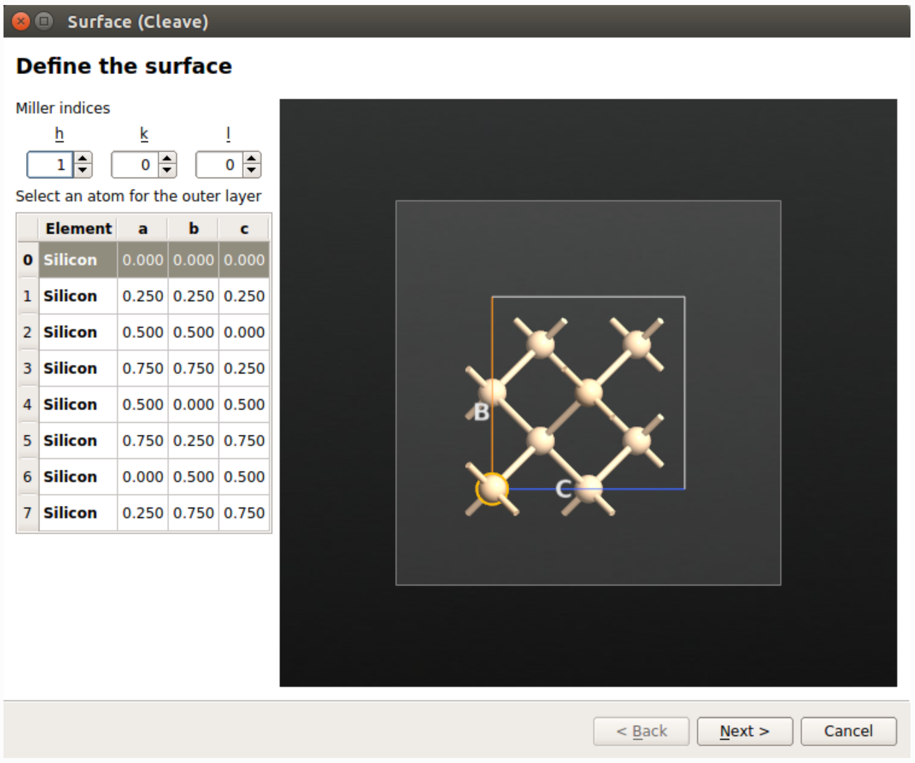
```
bandstructure = nlread("file.hdf5", Bandstructure)[0]
gap_direct   = bandstructure.directBandGap().inUnitsOf(eV)
gap_indirect = bandstructure.indirectBandGap().inUnitsOf(eV)
print "direct gap:   %.2f eV" % gap_direct
print "indirect gap: %.2f eV" % gap_indirect
```

Silicon device

You will now set up the silicon device.

1. Open the **Builder**, highlight *"Silicon (alpha)"* in the **Stash**, and start creating a Si(100) surface:
   - Navigate to Builders ‣ Surface (Cleave).
   - In the **Surface (Cleave)** window, choose the [1,0,0] Miller indices and click *"Next"*.





Define the surface

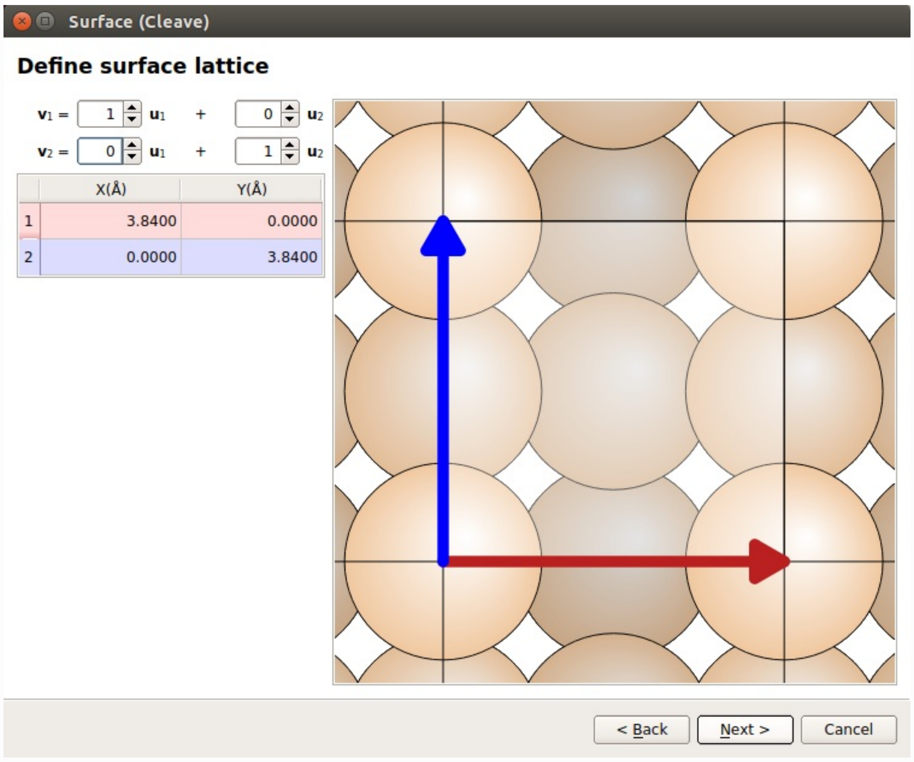
Miller indices

h	k	l
1	0	0

Select an atom for the outer layer

	Element	a	b	c
0	Silicon	0.000	0.000	0.000
1	Silicon	0.250	0.250	0.250
2	Silicon	0.500	0.500	0.000
3	Silicon	0.750	0.750	0.250
4	Silicon	0.500	0.000	0.500
5	Silicon	0.750	0.250	0.750
6	Silicon	0.000	0.500	0.500
7	Silicon	0.250	0.750	0.750

2. Keep the 1 ×1 surface unit cell and click *"Next"*.


Surface (Cleave)

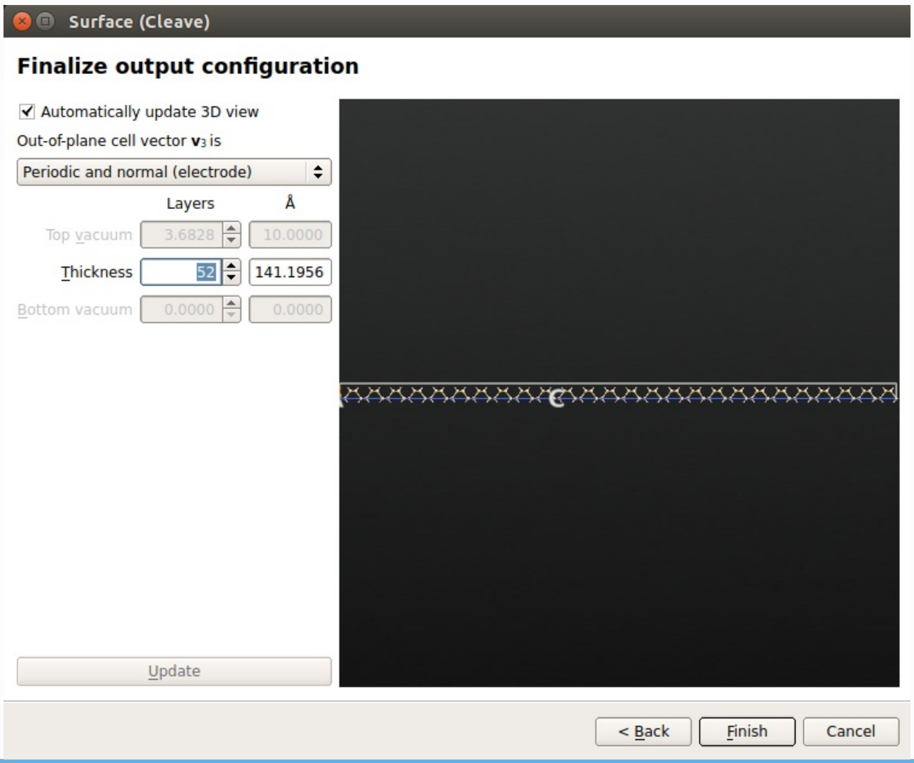
Define surface lattice

v1 = 1 u1 + 0 u2

v2 = 0 u1 + 1 u2

	X(Å)	Y(Å)
1	3.8400	0.0000
2	0.0000	3.8400

3. Select a thickness of 52 layers and click *“Finish”*.


Surface (Cleave)

Finalize output configuration

☑ Automatically update 3D view

Out-of-plane cell vector v3 is

Periodic and normal (electrode)

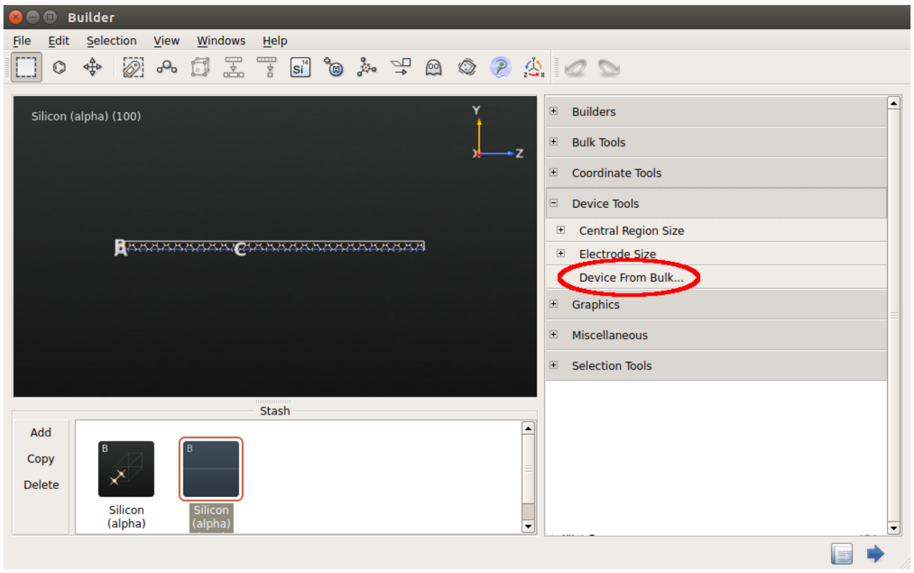
	Layers	Å
Top vacuum	3.6828	10.0000
Thickness	52	141.1956
Bottom vacuum	0.0000	0.0000

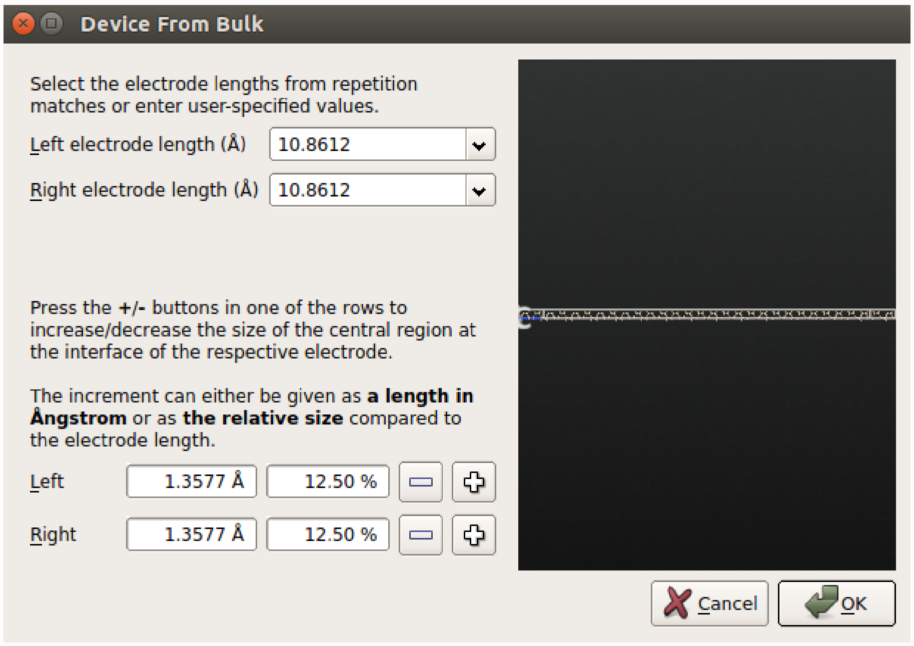
Note

The 52 layers will constitute the central region of your device. You need such a relatively long device (~14 nm) because of the long screening length in the silicon semiconductor, as explained in the NiSi2−Si interface tutorial. Still, as you will see later, this device is not long enough to have perfectly converged results. However, you will use the 52 layers device throughout this tutorial to be able to perform the TB09-MGGA calculations faster.

4. Your Si(100) configuration is now constructed, and you will use it to construct a device with the

transport direction along (100). Navigate to Device Tools ‣ Device From Bulk, keep the default parameters, and simply click *"OK"*.





Select the electrode lengths from repetition matches or enter user-specified values.

Left electrode length (Å) 10.8612

Right electrode length (Å) 10.8612

Press the **+/-** buttons in one of the rows to increase/decrease the size of the central region at the interface of the respective electrode.

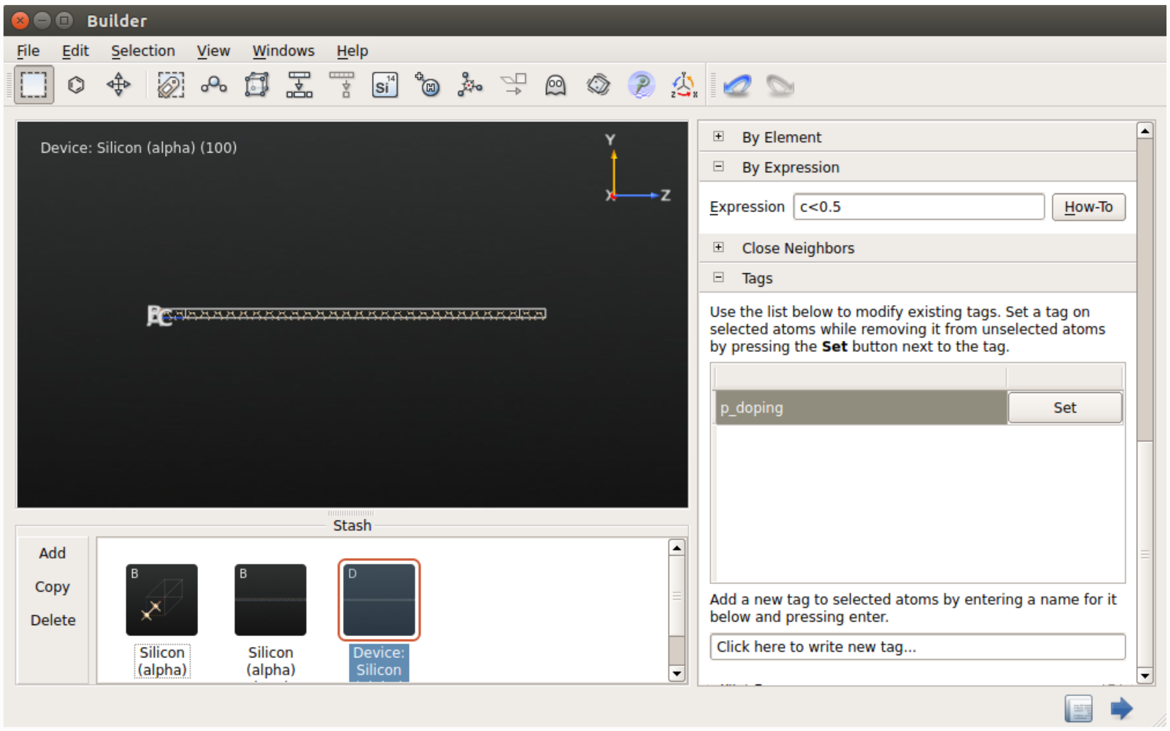
The increment can either be given as **a length in Ångstrom** or as **the relative size** compared to the electrode length.

Left 1.3577 Å 12.50 %

Right 1.3577 Å 12.50 %

5. It will prove convenient to assign tags to atoms in the regions that should be doped p-type and n-type, respectively.

   - Highlight the device configuration in the Stash and go to Selection Tools ‣ By Expression.
   - Type in *c < 0.5* and press *Enter* to select all atoms in the left hand side of the device.
   - Use Selection Tools ‣ Tags to assign the tag *"p_doping"* to the selected atoms.
   - Follow the same procedure to select atoms with *c > 0.5* and assign the tag *"n_doping"* to those atoms.



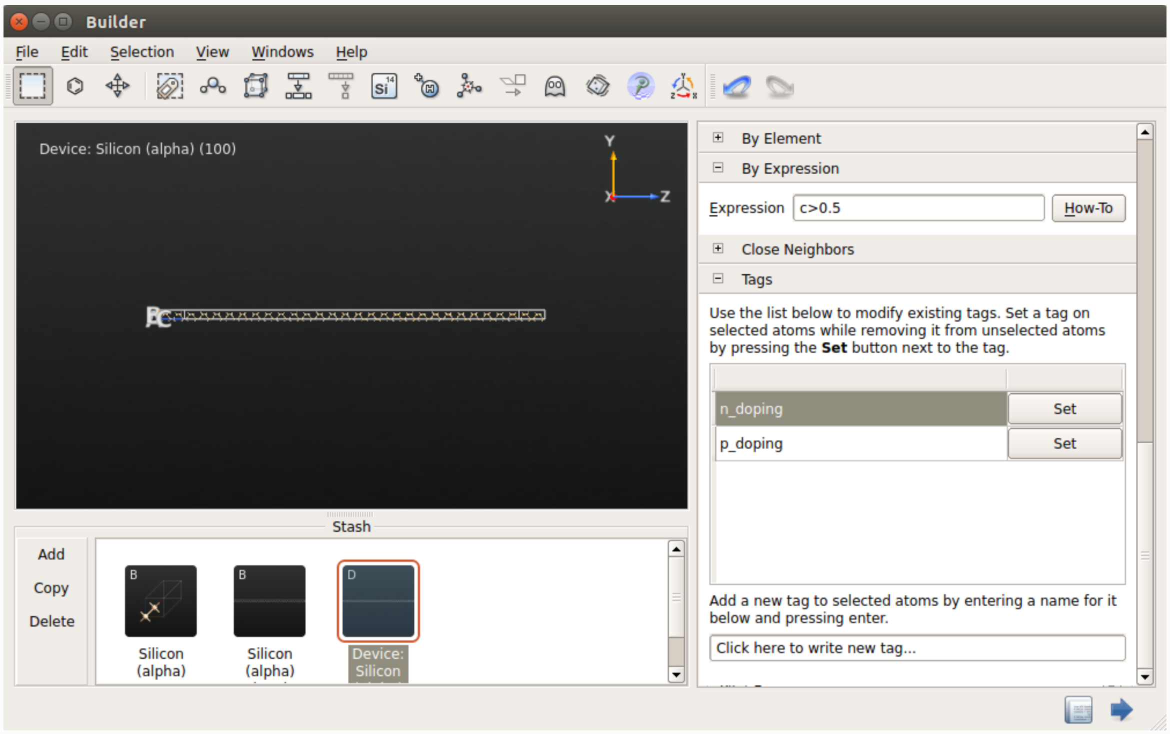
Expression c<0.5

Use the list below to modify existing tags. Set a tag on selected atoms while removing it from unselected atoms by pressing the **Set** button next to the tag.

p_doping	Set

Add a new tag to selected atoms by entering a name for it below and pressing enter.

Click here to write new tag...



Expression c>0.5

Use the list below to modify existing tags. Set a tag on selected atoms while removing it from unselected atoms by pressing the **Set** button next to the tag.

n_doping	Set
p_doping	Set

Add a new tag to selected atoms by entering a name for it below and pressing enter.

Click here to write new tag...

Slater-Koster IV curve

You will use the Slater-Koster model to calculate the I-V characteristics for the p-n doped silicon junction.

1. Send the device configuration from the **Builder** to the **Script Generator**.
2. Add a **New Calculator** to the script and set the following parameters:

    - Select the *ATK-SE Slater-Koster* calculator.
    - Use a 7x7x100 k-point sampling.
    - Select the *Bassani.Si basis set* and uncheck the *"No SCF iteration"* box.

3. You can now add all the analysis objects needed. Add the following ones:

- ElectronDensity
- DeviceDensityofStates
- ElectrostaticDifferencePotentials
- IVCurve

4. Edit the **DeviceDensityofStates** parameters:

   - Increase considerably the k-point sampling. Use a 21x21 grid.
   - Energy: from -2 to 2 eV with 401 points.

5. Edit the **IVCurve** parameters:

   - *Voltage Bias*: sample from -1 V to 1 V with 21 points.
   - *Energy*: from -1.1 eV to 1.1 eV with 401 points.
   - *k-point sampling*: 21x21.

   Note

   A full explanation of all the parameters is given in the *Doping in QuantumATK: the Ni silicide - :ref:`nisi2-si* and in the ATK Reference Manual.

6. Change the output filename to something like `IV_2e19_SK.hdf5`.

Doping the silicon junction

You need to set up the proper doping to finally have a p-n junction. To this end, send the script to the **Editor** and locate the part of the script that defines the device configuration:

```
device_configuration = DeviceConfiguration(
central_region,
[left_electrode, right_electrode]
)
```

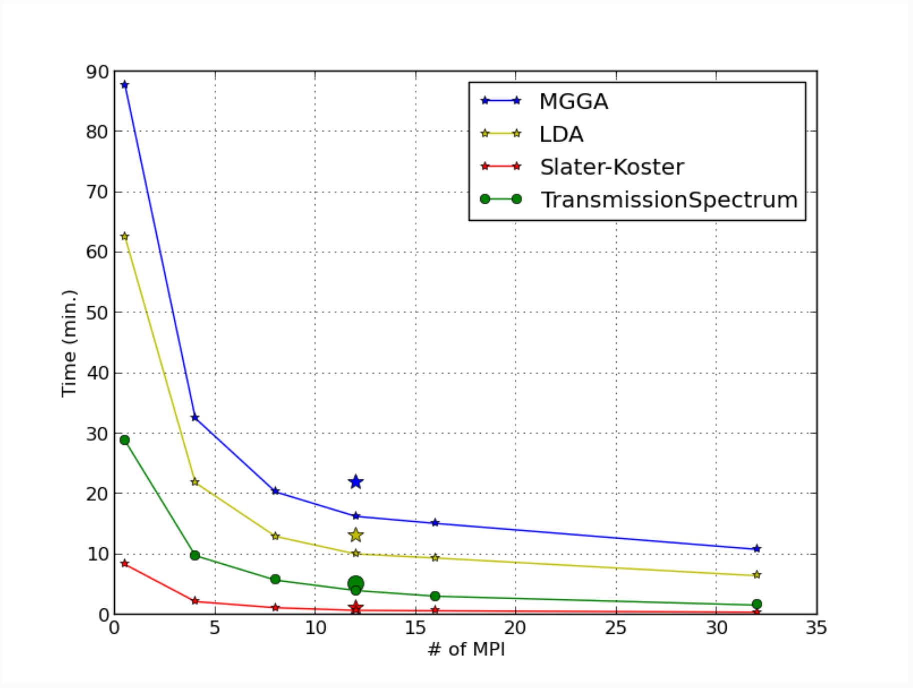
Just before those lines, add the following lines to define a p-n junction with a doping concentration of 2 $\cdot 10^{19}$ cm^{-3}:

```
# -------------------------------------------------------------
# Add Doping
# -------------------------------------------------------------
doping_density = 2e+19
# Calculate the volume  and convert it to cm^-3
# Note: right and left electrodes have the same volume,
volume = right_electrode_lattice.unitCellVolume()
volume = float(volume/(0.01*Meter)**3)
# Calculate charge per atom
doping = doping_density * volume / len(right_electrode_elements)
# Add p- and n-type doping to the central region
external_potential = AtomicCompensationCharge([
     ('p_doping', -1*doping), ('n_doping',doping)
     ])
central_region.setExternalPotential(external_potential)
# Add doping to left and right electrodes
left_electrode.setExternalPotential(
   AtomicCompensationCharge([(Silicon, -1*doping)]))
right_electrode.setExternalPotential(
   AtomicCompensationCharge([(Silicon, doping)]))
```

Running the calculation

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

Depending on the analysis objects included in the script, and on the number og parallel processes executed by the **Job Manager**, the calculation may take a few minutes for the zero bias part and up to few hours to calculate the whole IV curve. The performance of **ATK 2014** for different methods (**ATK-SE** and **ATK-DFT**) and for a transmission spectrum calculation are reported in the figure below.



Note

The calculations are run in parallel on different Intel Xeon e5472 3.0 GHz machines. The single points at 12 MPI are run with QuantumATK 13.8. Overall, QuantumATK 2014 is 25-30% faster compared to QuantumATK 13.8.

Calculation details: zero-bias, 7x7x100 k-point sampling for SCF part and 21x21 for the transmission spectra. All other parameters are set as in this tutorial.

Note that the Slater-Koster SCF calculation is much faster than the post-SCF calculation of the transmission spectrum.

DFT-MGGA IV curve

While the Slater-Koster job is running you can set up the DFT-MGGA calculation. Simply go back to the **Script Generator** and change the **Calculator** block:

- Choose *ATK-DFT*.
- Exchange correlation: *MGGA*.
- *SingleZetaPolarized* basis set.

Remove all analysis objects except the **IVCurve**. Then set up the device doping and run the calculation.

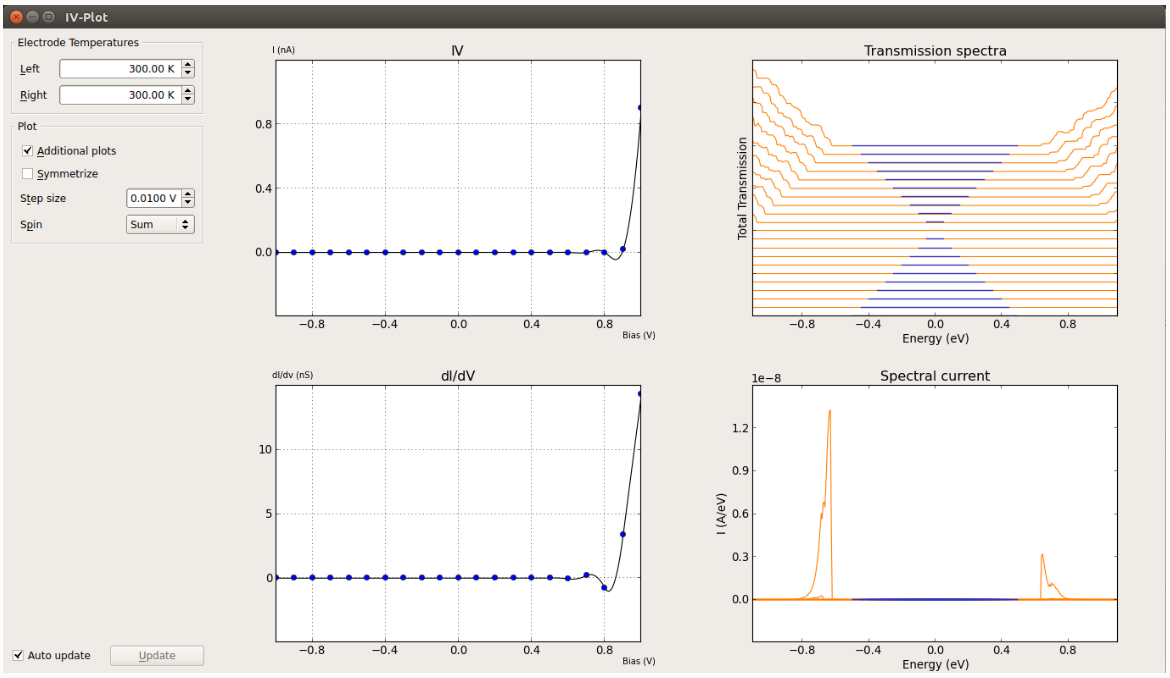
Analyzing the results

IV Curve

Once the two calculations are done and you have the output nc files in the project directory you will see the two **IVCurve** objects loaded in the **LabFloor**:

$I(V)$

1. Select one of the **IVCurve** objects and use the **IV-Plot** plugin to plot the IV curve. If you check the *Additional plots* option, you will also see plots of dI/dV, transmission spectra, and the spectral current.



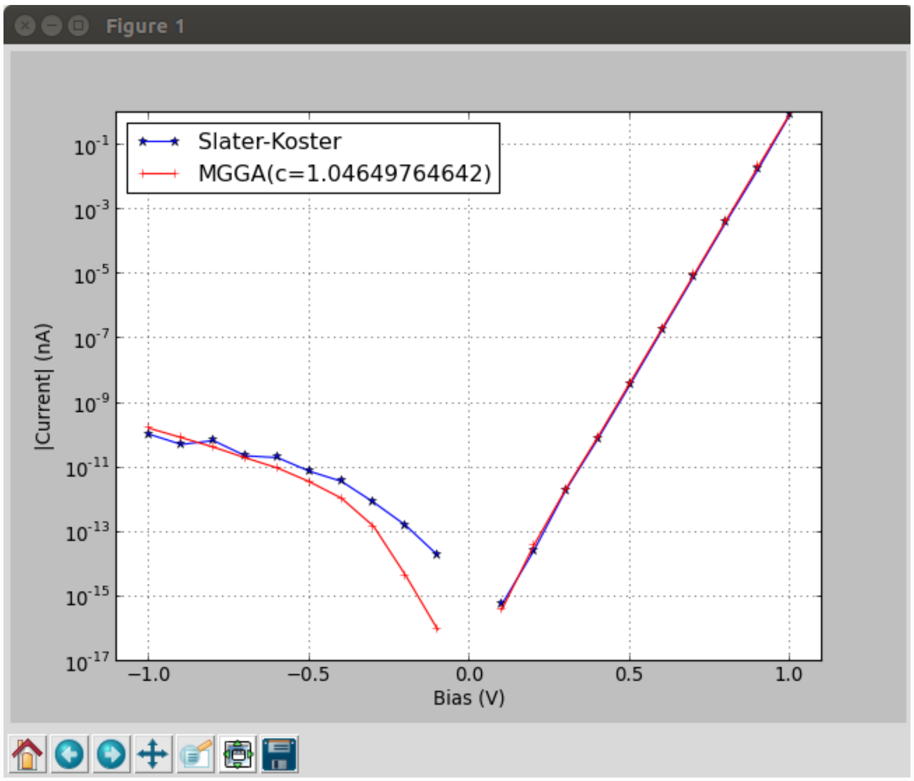
IV-Plot

Electrode Temperatures
Left 300.00 K
Right 300.00 K

Plot
[✓] Additional plots
[ ] Symmetrize
Step size 0.0100 V
Spin Sum

[✓] Auto update
Update

2. In order to compare the **Slater-Koster** and **MGGA** IV curves, and send the script to the **Job Manager** to create the figure below, where you can compare directly the two IV curves. You can also open the script with the **Editor** and modify it to tune the plot to your best convenience.

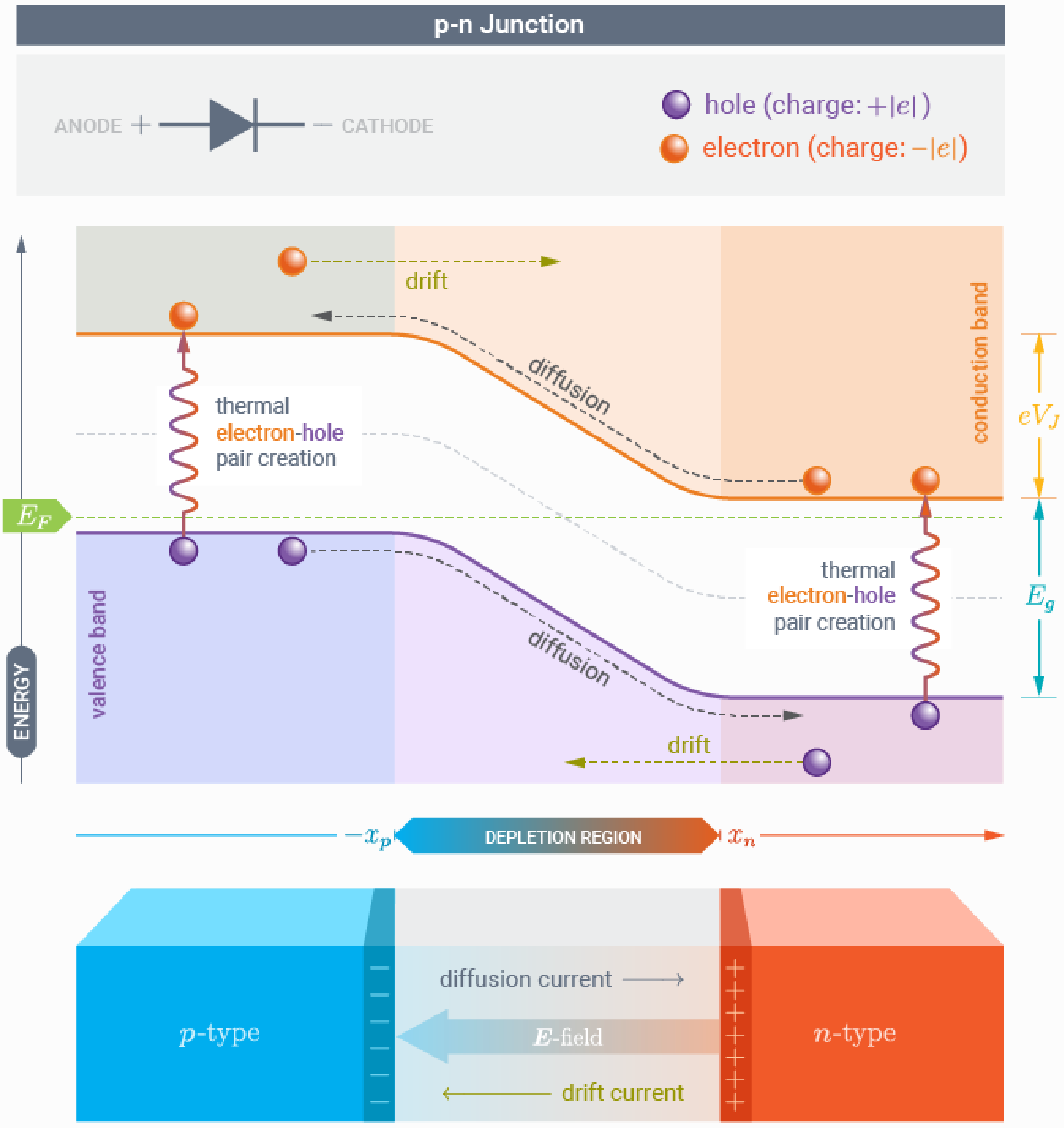


Attention

From the plot above you can see that the results from the semiempirical **Slater-Koster** model and the **DFT-MGGA** method are virtually the same.

Device Density of States

A classical picture of the electronic structure of a p-n junction is the one reported below, where the potential energy is plotted as a function of position along the transport direction of the device.



Using **QuantumATK** and **ATK** it is possible to perform this analysis through the **DeviceDensityOfStates** or the **LocalDensityOfStates** analysis objects.

Attention

Here, you will analyze the **DeviceDensityOfStates** and plot it along the device transport direction using a script.

In order to run the script and make the plots shown below you need an `.hdf5` file containing the analysis objects **DeviceConfiguration**, **DeviceDensityOfStates** and **ElectrostaticDifferencePotential**. You can open the script with the **Editor** and customize the plot according to your wish.

In particular, the ddos_edp.py script will read:

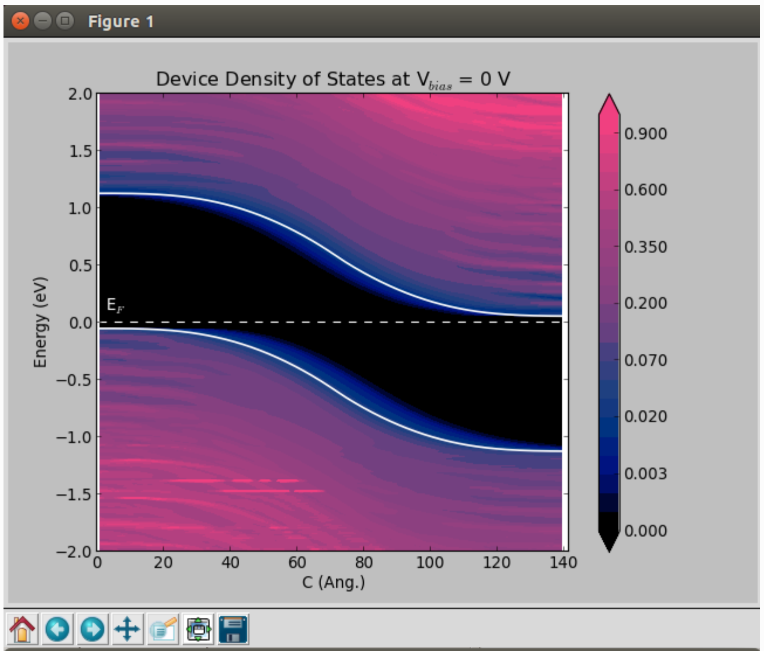
- **DeviceConfiguration**: to determine the spatial resolution along the device by defining a projection list used to plot the DDOS. Also, the electrode voltages are extracted from this object.
- **DeviceDensityOfStates**: besides reading and plotting the projected density of states, this object is also used to exctract the band edges at the left electrode. These informations are printed and used to align the electrostatic difference potential plots.

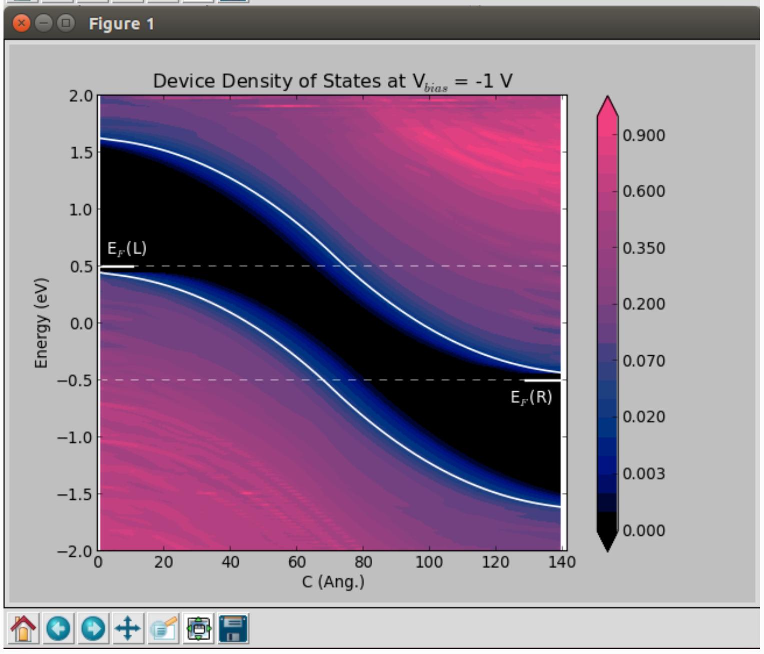
- **ElectrostaticDifferencePotential**: to plot the average electrostatic difference potential across the device.

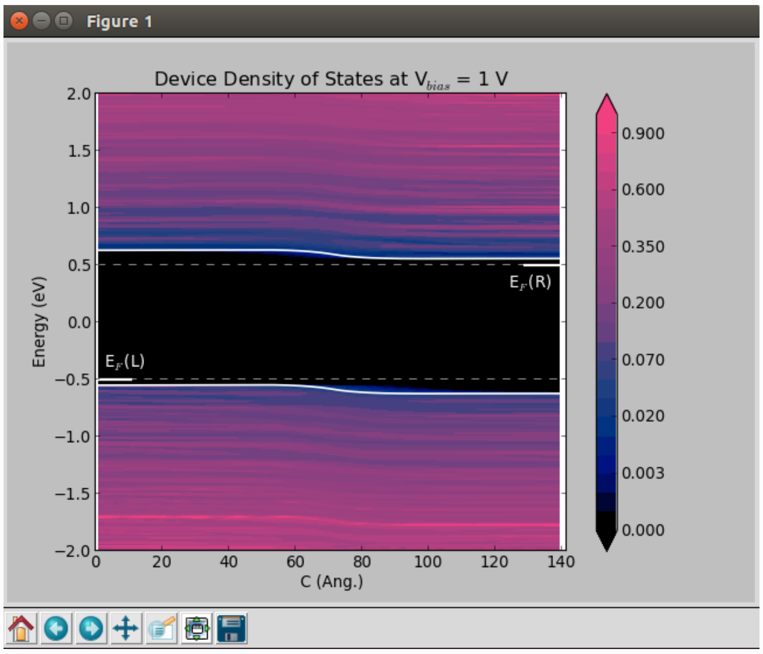
In order to get the **DeviceDensityOfStates** plot without an applied bias, run the script from a terminal:

```
atkpython ddos_edp.py IV_2e19_SK.hdf5
```

where `IV_2e19_SK.hdf5` contains the analysis objects described above. You can also create plots for finite bias. See the section Finite-bias calculations. Results are illustrated below.



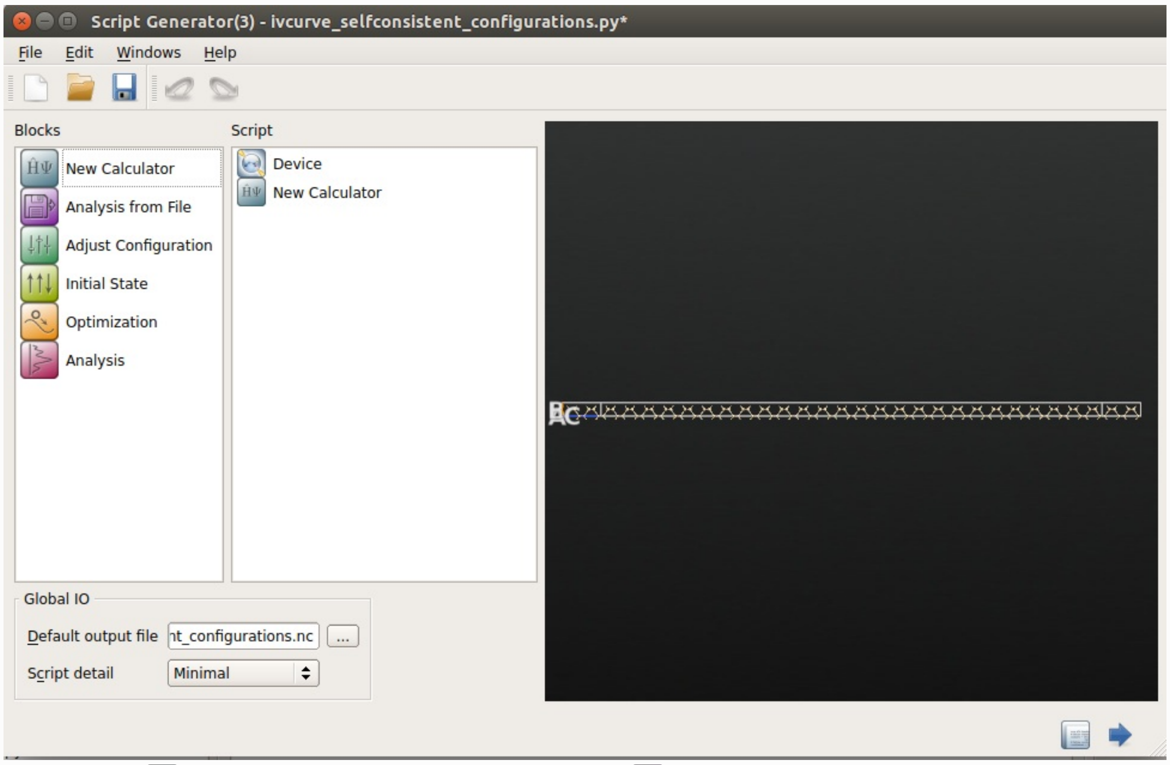




Finite-bias calculations

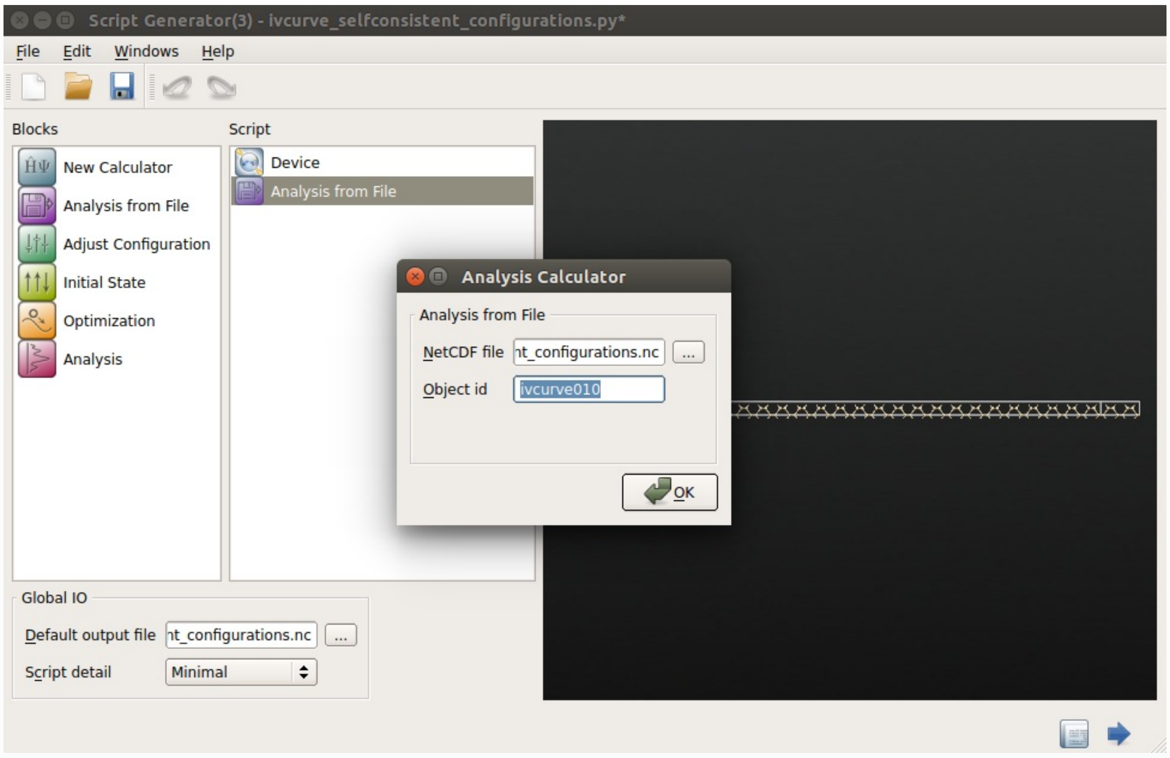
In order to create the finite-bias plots (V_{bias} = -1 and 1 V), do as follows:

1. Go to the **Labfloor** and from the `ivcurve_selftconsistent_configuration.hdf5` file select the device configuration obtained at V_{bias} = -1 V, and drag and drop it onto the **Scripter**. The following window will show up.



Default output file: nt_configurations.nc
Script detail: Minimal

2. Remove the **New Calculator** object and add instead **Analysis from File**.
3. In **Analysis from File**, set the *HDF5* file and the *Object id* of the device configuration object.



Analysis from File

NetCDF file: nt_configurations.nc

Object id: ivcurve010

Default output file: nt_configurations.nc

Script detail: Minimal

4. Then, add the **Electrondensity**, **DeviceDensityOfStates** and **ElectrostaticDifferencePotential** analysis objects and set the parameters as described above.
5. Change the output file to `Analysis_ivcurve_10.hdf5`.
6. Before running the job, send the script to the **Editor**, and add the following line to get the *device_configuration* file within the `Analysis_ivcurve_10.hdf5` output file.

```
# ----------------------------------------------------------------
# Analysis from File
# ----------------------------------------------------------------
device_configuration = nlread('ivcurve_selfconsistent_configurations.hdf5', object_id='ivcurve010')
```

7. After this part and just before **ElectronDensity**, add the following line:

```
nlsave('ivcurve_selfconsistent_configurations.hdf5', device_configuration)
```

8. Lastly, save the script and run the job. Once the job have finished, run the script ddos_edp.py in order to get the *Device Density of States* plot. Run the script as follows:

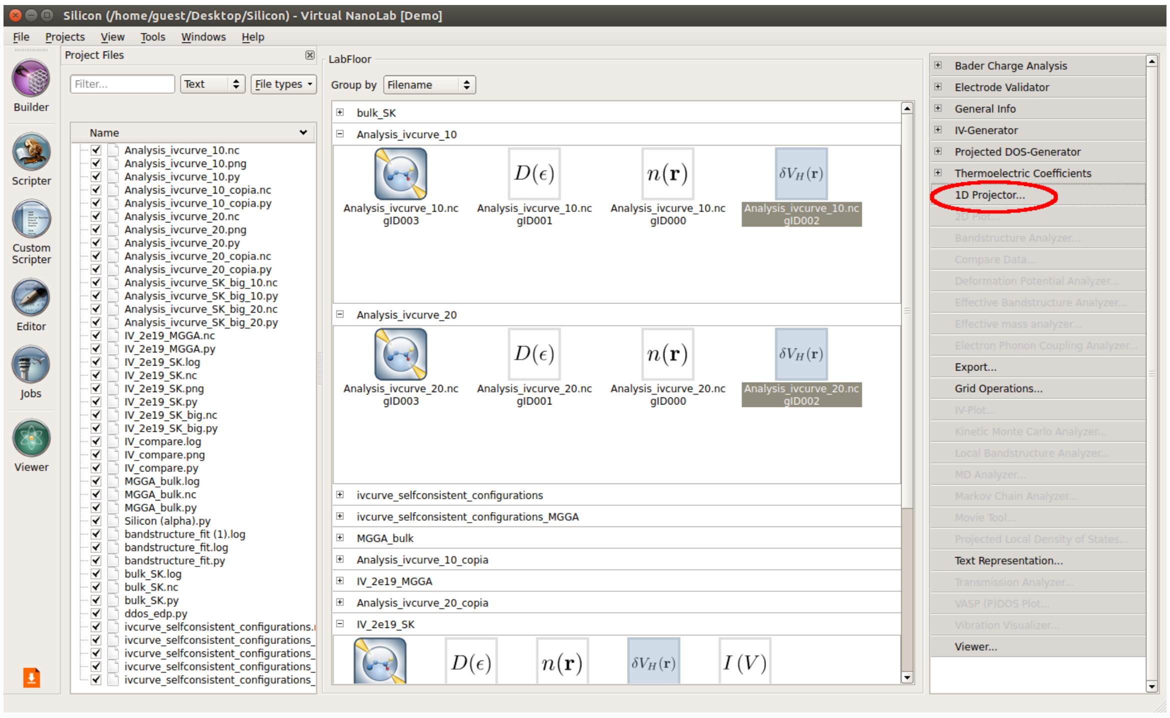
```
atkpython ddos_edp.py Analysis_ivcurve_10.hdf5
```

You can plot the *Device Density of States* plot following the same procedure for the `ivcurve_selftconsistent_configuration.hdf5ivcurve020` file.

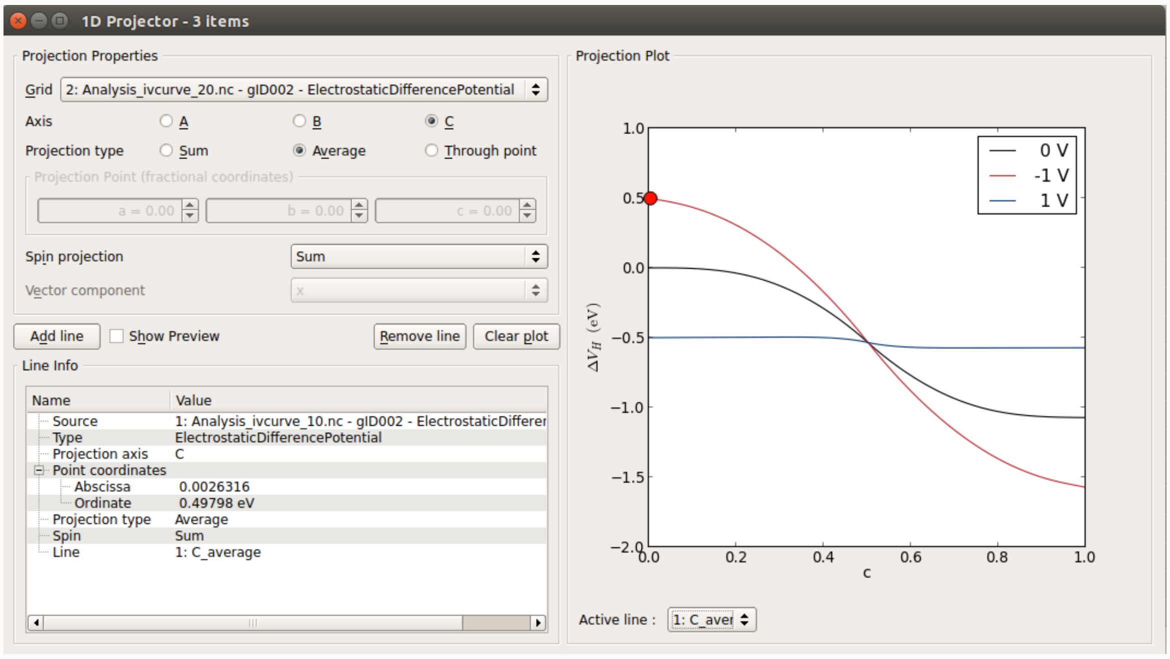
Electrostatic potential

$$\delta V_{\mathbf{E}}(\mathbf{r})$$

1. In the **Labfloor**, select the **ElectrostaticDifferencePotential** objects obtained for V_{bias} = 0, -1, 1,


Silicon (/home/guest/Desktop/Silicon) - Virtual NanoLab [Demo]
File Projects View Tools Windows Help
Builder
Scripter
Custom Scripter
Editor
Jobs
Viewer
Project Files
Filter...
Text
File types
Name
Analysis_ivcurve_10.nc
Analysis_ivcurve_10.png
Analysis_ivcurve_10.py
Analysis_ivcurve_10_copia.nc
Analysis_ivcurve_10_copia.py
Analysis_ivcurve_20.nc
Analysis_ivcurve_20.png
Analysis_ivcurve_20.py
Analysis_ivcurve_20_copia.nc
Analysis_ivcurve_20_copia.py
Analysis_ivcurve_SK_big_10.nc
Analysis_ivcurve_SK_big_10.py
Analysis_ivcurve_SK_big_20.nc
Analysis_ivcurve_SK_big_20.py
IV_2e19_MGGA.nc
IV_2e19_MGGA.py
IV_2e19_SK.log
IV_2e19_SK.nc
IV_2e19_SK.png
IV_2e19_SK.py
IV_2e19_SK_big.nc
IV_2e19_SK_big.py
IV_compare.log
IV_compare.png
IV_compare.py
MGGA_bulk.log
MGGA_bulk.nc
MGGA_bulk.py
Silicon (alpha).py
bandstructure_fit (1).log
bandstructure_fit.log
bandstructure_fit.py
bulk_SK.log
bulk_SK.nc
bulk_SK.py
ddos_edp.py
ivcurve_selfconsistent_configurations.
ivcurve_selfconsistent_configurations_
ivcurve_selfconsistent_configurations_
ivcurve_selfconsistent_configurations_
ivcurve_selfconsistent_configurations_
LabFloor
Group by Filename
bulk_SK
Analysis_ivcurve_10
Analysis_ivcurve_10.nc gID003
$D(\epsilon)$ Analysis_ivcurve_10.nc gID001
$n(\mathbf{r})$ Analysis_ivcurve_10.nc gID000
$\delta V_H(\mathbf{r})$ Analysis_ivcurve_10.nc gID002
Analysis_ivcurve_20
Analysis_ivcurve_20.nc gID003
$D(\epsilon)$ Analysis_ivcurve_20.nc gID001
$n(\mathbf{r})$ Analysis_ivcurve_20.nc gID000
$\delta V_H(\mathbf{r})$ Analysis_ivcurve_20.nc gID002
ivcurve_selfconsistent_configurations
ivcurve_selfconsistent_configurations_MGGA
MGGA_bulk
Analysis_ivcurve_10_copia
IV_2e19_MGGA
Analysis_ivcurve_20_copia
IV_2e19_SK
$D(\epsilon)$ $n(\mathbf{r})$ $\delta V_H(\mathbf{r})$ $I(V)$
Bader Charge Analysis
Electrode Validator
General Info
IV-Generator
Projected DOS-Generator
Thermoelectric Coefficients
1D Projector...
Bandstructure Analyzer...
Compare Data...
Deformation Potential Analyzer...
Effective Bandstructure Analyzer...
Effective mass analyzer...
Electron Phonon Coupling Analyzer...
Export...
Grid Operations...
IV-Plot...
Kinetic Monte Carlo Analyzer...
Local Bandstructure Analyzer...
MD Analyzer...
Markov Chain Analyzer...
Movie Tool...
Projected Local Density of States...
Text Representation...
Transmission Analyzer...
VASP (P)DOS Plot...
Vibration Visualizer...
Viewer...

2. Use the **1D Projector** plugin to plot the data.



Grid: 2: Analysis_ivcurve_20.nc - gID002 - ElectrostaticDifferencePotential

Axis: A B [✓ C]

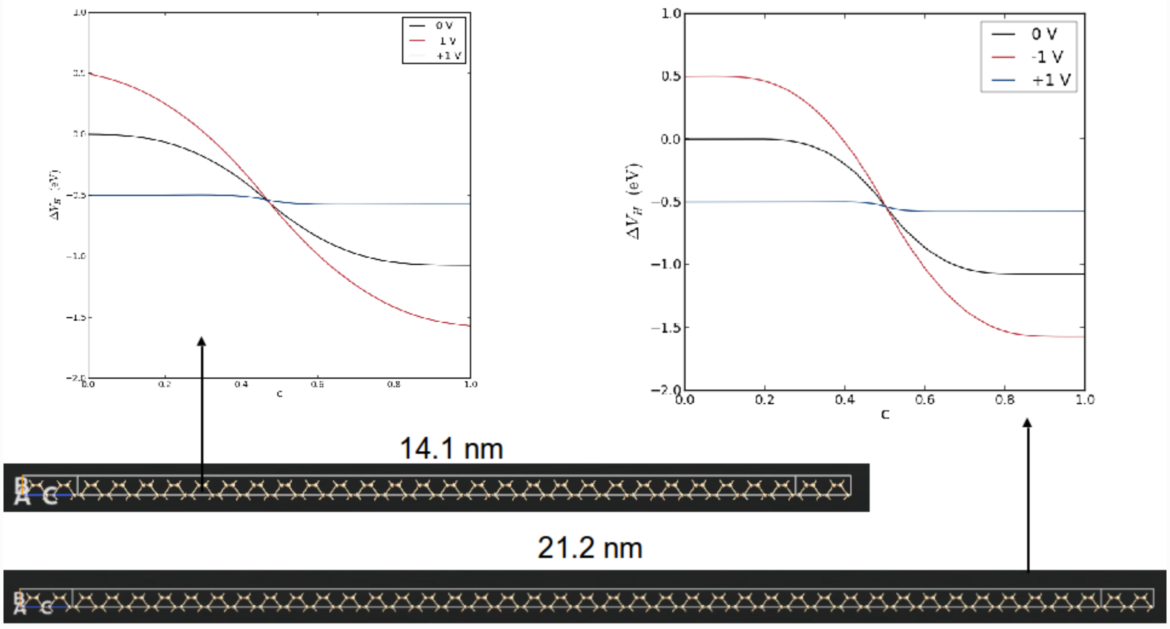
Projection type: Sum [✓ Average] Through point

Spin projection: Sum

Line Info

Name	Value
Source	1: Analysis_ivcurve_10.nc - gID002 - ElectrostaticDifferer
Type	ElectrostaticDifferencePotential
Projection axis	C
Point coordinates	
Abscissa	0.0026316
Ordinate	0.49798 eV
Projection type	Average
Spin	Sum
Line	1: C_average

You can see that the results are not perfectly converged wrt. the length of the device, because the gradient of the electrostatic potential is not zero at the ends of the device central region. The figure below compares the **ElectrostaticDifferencePotential** of the device used in this tutorial with results for a longer one.



References

[1]
F. Tran and P. Blaha. Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential. *Phys. Rev. Lett.*, 102:226401, 2009. doi:10.1103/PhysRevLett.102.226401.

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