

Table of Contents

Table of Contents	1
Photocurrent in a silicon p-n junction	2
Device ground state	2
Silicon p-n junction	2
NEGF calculation	3
Photocurrent	3
References	5

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Photocurrent in a silicon p-n junction

Version: 0-2018.06

Downloads & Links

- [PDF version](#)
- [silicon_pn_junction.py](#)
- [photocurrent.py](#)

In this tutorial, you will learn how to calculate the photocurrent through a device under illumination. We consider a 7.6 nm sized silicon p-n junction, and showcase the Photocurrent Analyzer introduced with the QuantumATK 0-2018.06 release.

The photocurrent is calculated by adding the electron-photon interaction to the device Hamiltonian, using first-order perturbation theory, as described in [1] and in the ATK Manual: [Photocurrent](#).

Device ground state

At first you will perform the self-consistent device calculation. Then, using the ground-state device Hamiltonian, you will calculate and analyze the photocurrent.

You should use the script [silicon_pn_junction.py](#) to run the ground-state calculation – both the doped device configuration and the appropriate NEGF calculator are defined in the script. Results are saved in `silicon_pn_junction.hdf5`. Simply download the script and run it using the Job manager or from a terminal. Once the calculation is done, you can see the file `silicon_pn_junction.hdf5` on the LabFloor. The calculation takes *ca.* 20 mins with 4 MPI processes.

Brief instructions for building the device configuration and setting up the NEGF calculation are also given below.

Silicon p-n junction

The 7.6 nm silicon device should consist of 28 Si layers (76.0284 Å) and 10.8612 Å left and right electrodes. The *p* and *n* doping levels should be both $2 \cdot 10^{20}$ e/cm³ for this quite short Si device in order to get a reasonable electronic structure with fairly flat band edges near the electrodes and a small gap from the VBM and CBM to the Fermi level.

If you need more information on how to build a junction, please see the tutorial [Silicon p-n junction](#).

Doping

Add doping to the currently selected atoms, by pressing **Add**. Delete doping by selecting a row in the table and pressing **Remove**.

The tag used for the doping can be seen/changed in the first column. The doping type (n/p) can be changed in the second column. The doping value and its desired unit can be changed in the third and fourth columns.

Tag	Doping Type	Value	Unit
doping_0	p-type	2e+20	e/cm ³ (left electrode)
doping_1	n-type	2e+20	e/cm ³ (left electrode)

Add Remove

NEGF calculation

The supplied script [silicon_pn_junction.py](#) uses a NEGF calculator with the settings given below.

- Basis set: *PseudoDojo* and *Low*.
- Exchange-correlation: *GGA-1/2* and *PBE*.
- k-point sampling: 4 \AA density in the A and B directions.
- Density mesh cutoff: 30 Ha .
- Default output file: `silicon_pn_junction.hdf5`.

Run the script using the **Job manager** (click the button to start the calculation).

Photocurrent

You are now ready to calculate the photocurrent. Open the **Script Generator** and add a **Analysis from File**.

- Select the file `silicon_pn_junction.hdf5`.
- Make sure the *DeviceConfiguration* object is ticked.

Next, in order to calculate the photocurrent, add the **Analysis** ▶ **Photocurrent** block. Set the photon energy range to 0 – 5 eV with 31 points, and set the k-point sampling to 9 x 9. Keep all other parameters at default values. You can also download the script [photocurrent.py](#). Send the script to the **Job manager**, save it as `photocurrent.py`, and click on the button to run the calculation.

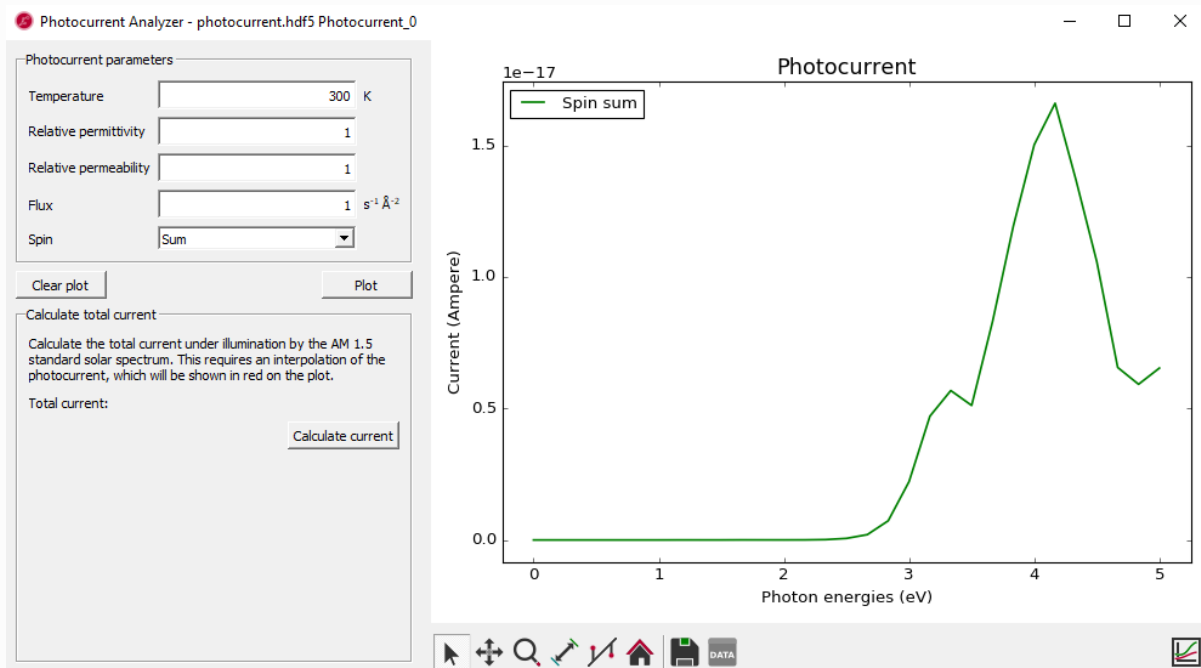
Note

The photocurrent calculation takes *ca.* 3.5 hours with 4 MPI processes, so you may consider running the calculation on a remote computing cluster, if possible.

Once the calculation is done, you can see the file `photocurrent.hdf5` in the **LabFloor**. Note that the calculation can be made faster by decreasing the number of photon energies and increasing the `energy_resolution`, leading to fewer electron energy points.

Select the *Photocurrent_0* object of `photocurrent.hdf5` on the **LabFloor**. Open the **Photocurrent Analyzer** in the right-hand panel.

You can easily plot the current vs. photon energies by clicking Plot. This is shown in the figure below.



You can also calculate the total current based on illumination by the AM1.5 standard solar spectrum obtained from [Solar spectra website](#). Once you click **Calculate current**, the interpolated photocurrent will be indicated by a red line. This interpolated function is multiplied with the flux from the reference spectrum at each photon energy, and the result is then numerically integrated to calculate the total current from the device under the given illumination.

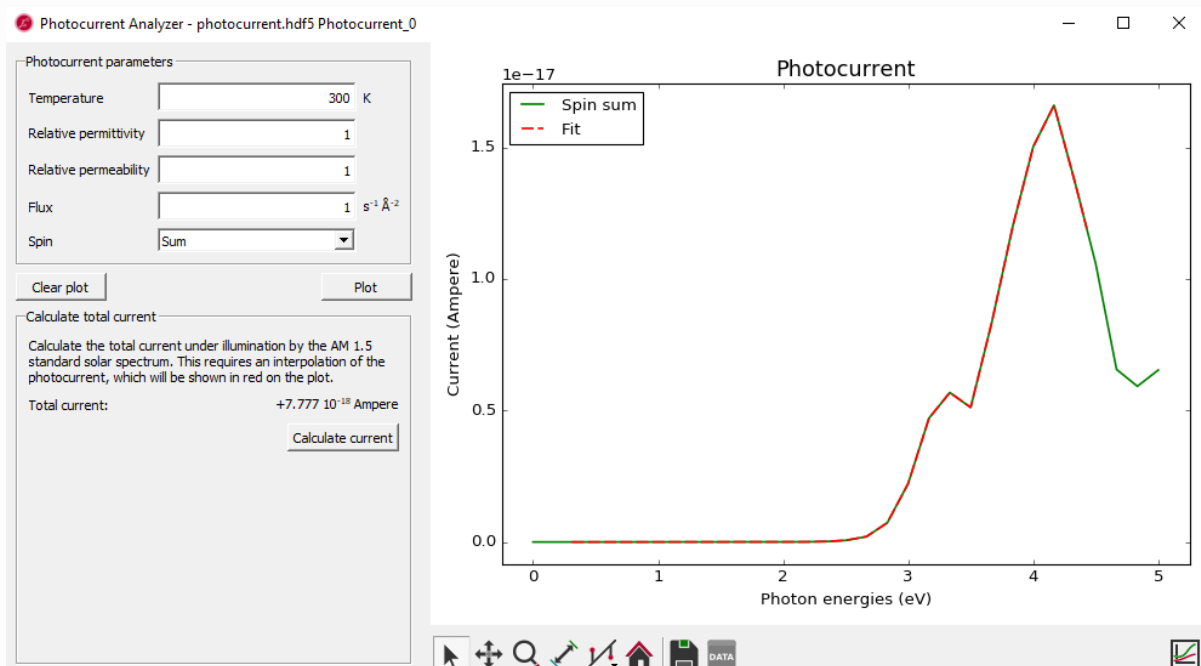
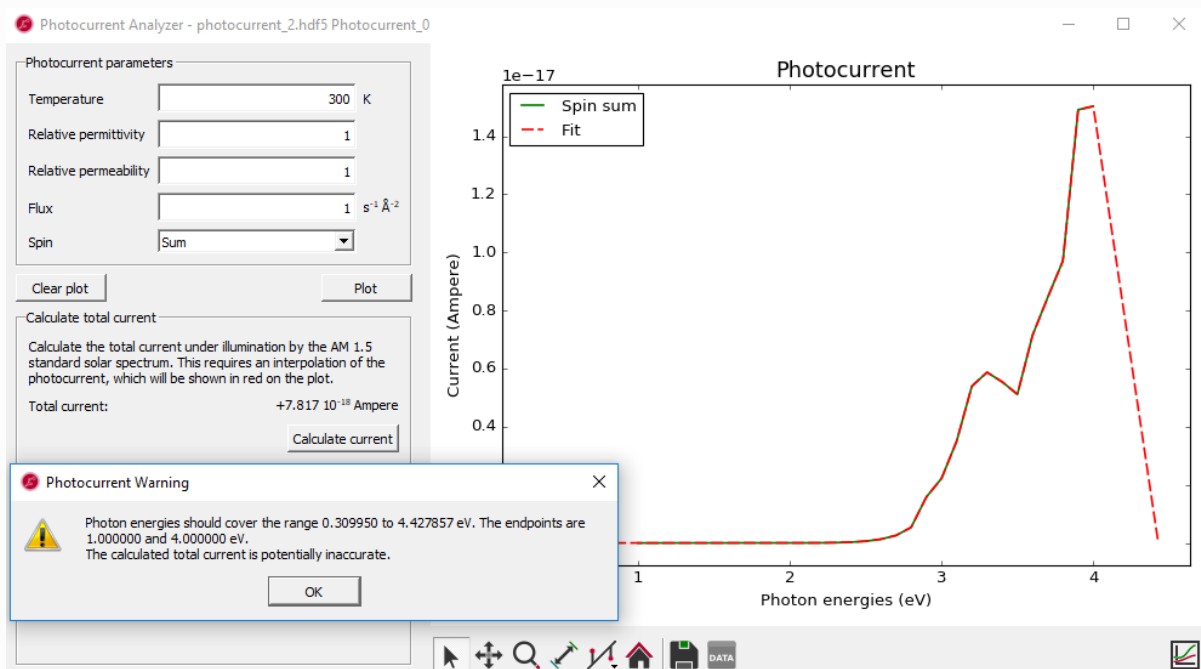


Fig. 1 The total current is calculated as 7.777 $\cdot 10^{-18}$ Ampere under the illumination by the AM 1.5 standard solar spectrum.

If the photon energies used to calculate the photocurrent do not cover the range of photon energies in the AM1.5 spectrum, you will see a warning message. In this case, the interpolation will include data outside the data range, so the calculated total current may therefore be inaccurate. We therefore recommend to calculate the total current only from photocurrents covering the full range of the AM1.5 standard solar spectrum, which is 0.3 eV to 4.43 eV. Photocurrents covering a larger range is not a problem, as data outside the range of the reference spectrum simply do not contribute. The figure below shows an example

of this.



References

- [1] Mattias Palsgaard, Troels Markussen, Tue Gunst, Mads Brandbyge, and Kurt Stokbro. Efficient first-principles calculation of phonon assisted photocurrent in large-scale solar cell devices. *arXiv:1801.03683*, 2018. URL: <http://arxiv.org/abs/1801.03683>.

← Previous

Next →