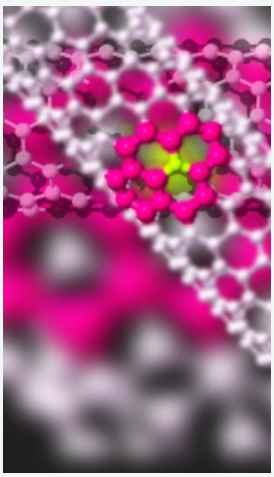
Table of Contents

Stone–Wales Defects in Nanotubes

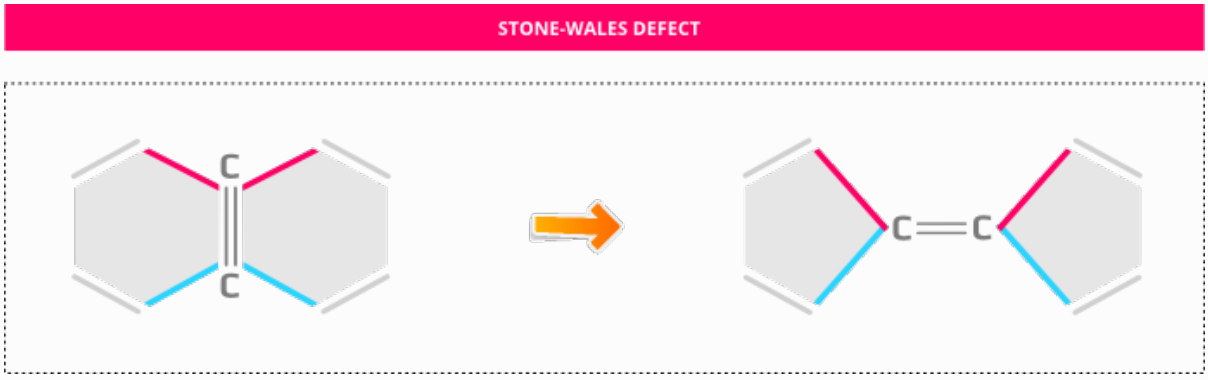
Category: QuantumATK tasks and workflow

Links & Tags:
Prerequicities: TubeWrapper addon
Downloads: PDF version stone_wales_cnt.py

In this tutorial you will learn how to create a Stones–Wales defect in a (9,0) nanotube, and calculate the influence of the defect on the transmission spectrum. The central trick is to first create the defect in a graphene sheet, which makes it easy to define the proper bond rotation of the defect, and then roll the structure into a nanotube.



A Stone–Wales defect changes the connectivity of two π-bonded carbon atoms by rotating them 90° with respect to the midpoint of their bond, as illustrated below:



It is a crystallographic defect that occurs in e.g. nanotubes and graphene, and can have a strong influence on the electronic, chemical, and mechanical properties. It is named after Anthony Stone and David Wales of Cambridge University, who described it in a 1986 paper on fullerenes [SW86], but a similar defect was described much earlier by Peter Thrower in a paper on defects in graphite [Thr69].

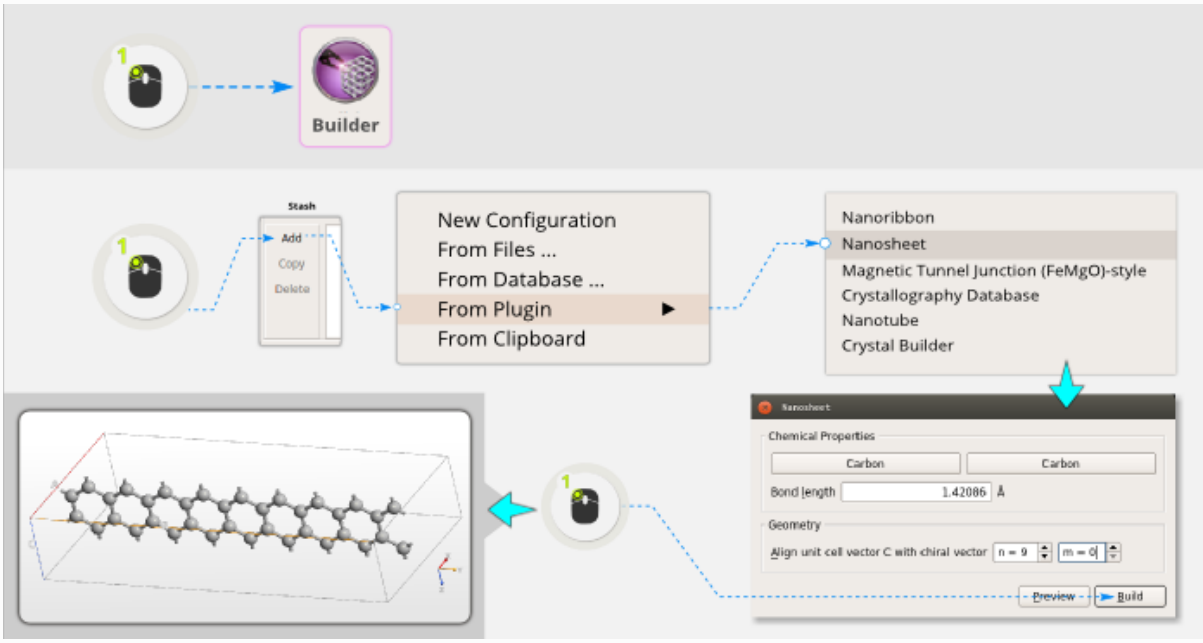
Note

You will create the Stone–Wales defect in graphene and then wrap it into a tube. You will therefore

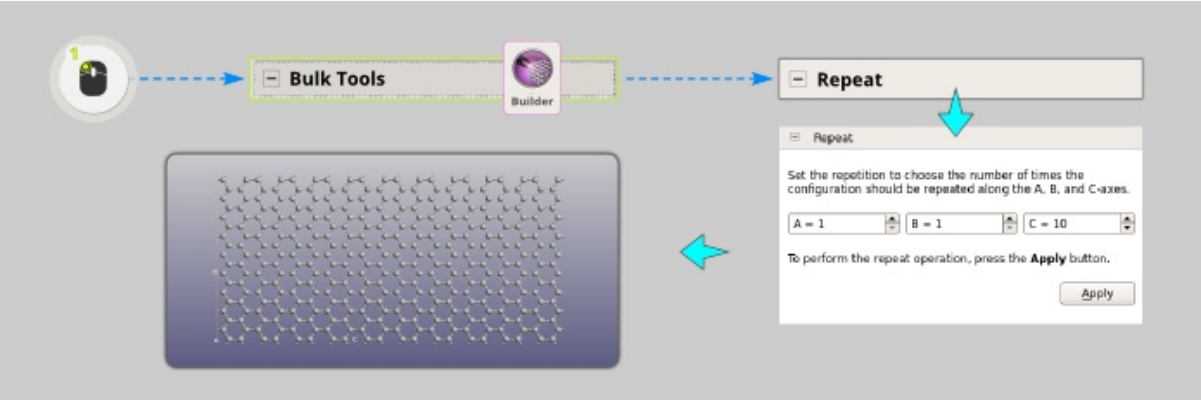
need the **TubeWrapper** addon. Download the TubeWrapper.zip file and install the addon following the instructions in the How to create AddOns for QuantumATK page.

Creating the defect and wrapping the tube

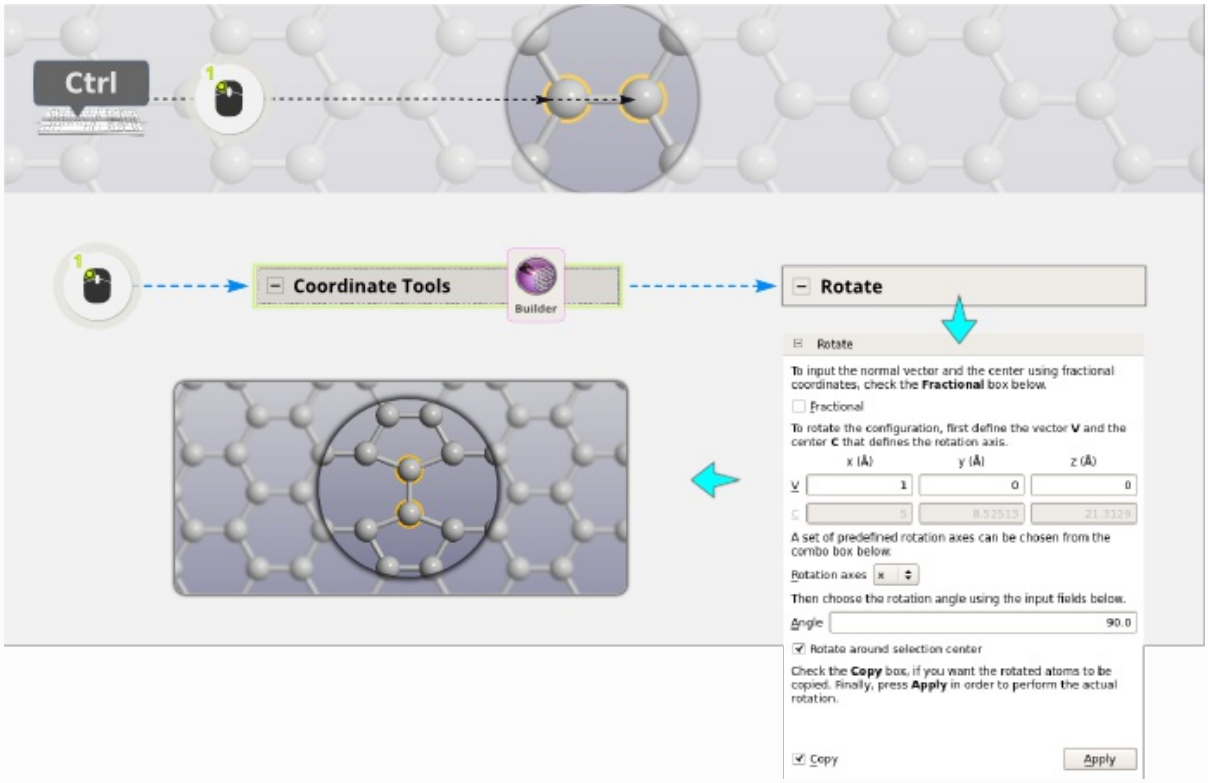
- **Step 1:** First create a graphene sheet by using the Add ▸ Add From Plugin ▸ Nanosheet plugin. Select **n=9** and **m=0** for the chiral indices, and click **Build**.



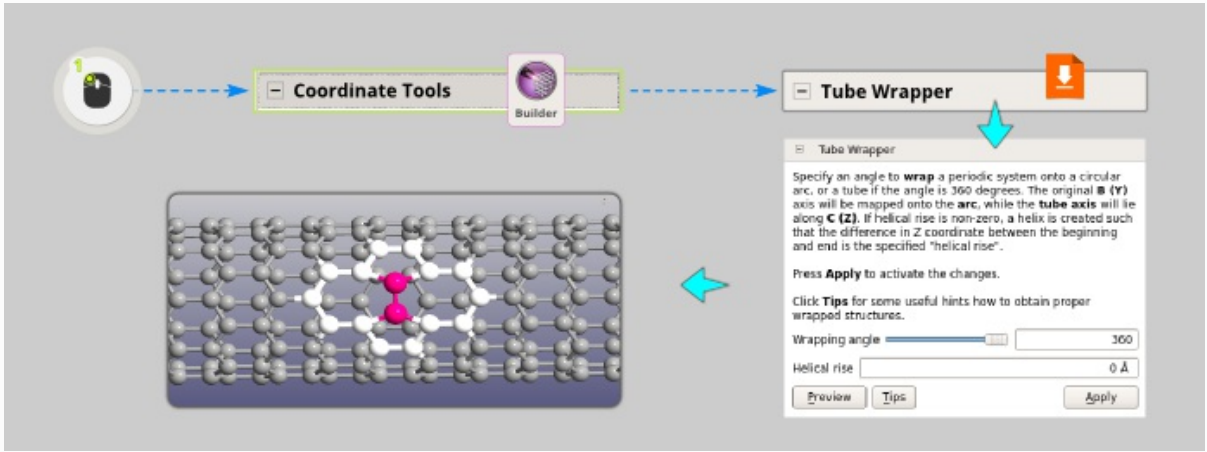
- **Step 2:** The purpose is to study an isolated defect, so it is necessary to make a large structure where a single carbon–carbon bond can be rotated. **Repeat** the configuration 10 times along the C direction using the Bulk Tools ▸ Repeat tool, and press Ctrl+R to reset the view.



- **Step 3:** Next, **create the defect**: Select two atoms in the middle of the structure, and open the Coordinate Tools ▸ Rotate tool. Select the rotation axis to be *X* (this is the default) and enter 90 degrees for the rotation angle. It is important that the checkbox *Rotate around selection center* is ticked. Then click **Apply**.



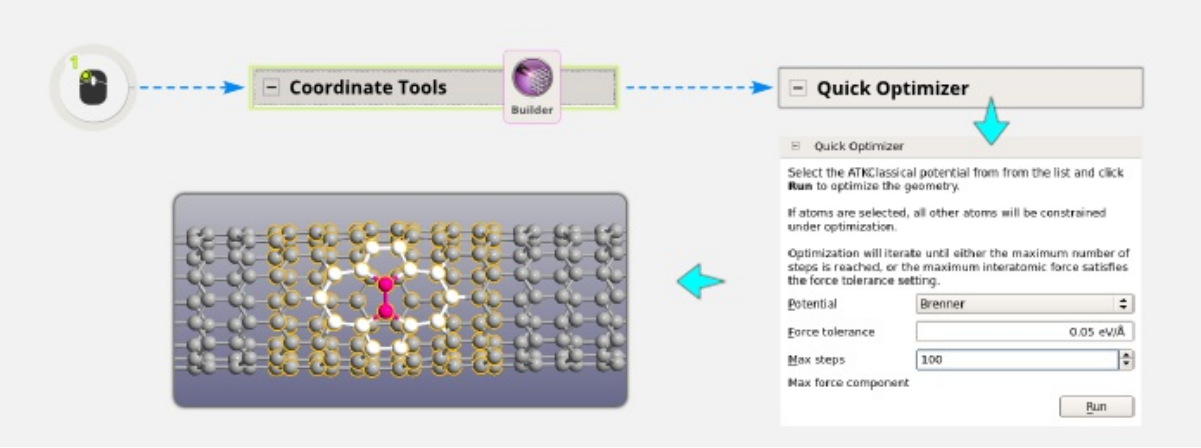
- **Step 4:** You can now **wrap** the graphene sheet into a tube. The sheet is periodic along the B and C directions. The tube axis should be along C, so the graphene sheet should be rolled up along B. Use the Coordinate Tools ▸ Tube Wrapper tool to accomplish this; set the angle to 360 degrees and click **Apply**.



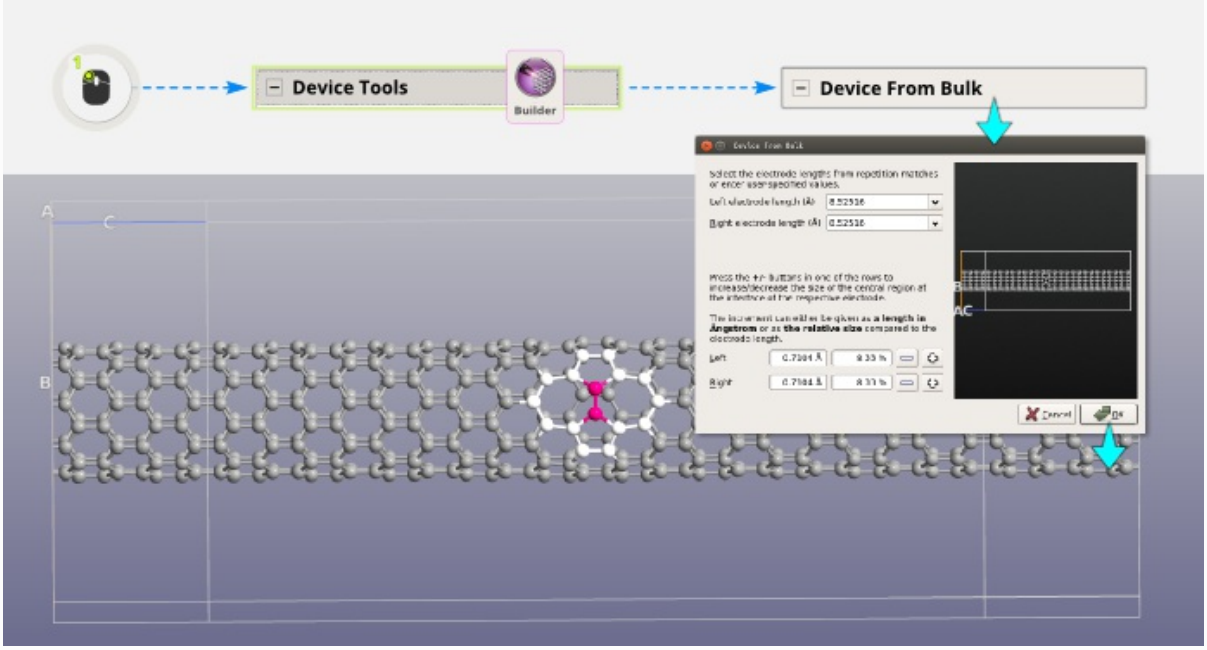
Optimizing the structure

The defect was created by a simple rotation of two carbon atoms, and is most likely not in its equilibrium shape. You should therefore geometry optimize the defect. The **ATK-ForceField** engine with the Brenner potential will provide a great starting point (conveniently available in Coordinate Tools ▸ Quick Optimizer), but for a truly correct structure, you should run a full DFT optimization. In both cases, the ends of the tube should be constrained so they remain perfectly periodic, in order to use it for a device calculation later on.

Anyway, as a first approximation, select the defect atoms (white and pink in the figure below), and atoms immediately around the defect, to locally optimize the defect geometry. Use the **Quick Optimizer** with the Brenner potential (you will need to increase the number of steps to 100).



Then, convert the structure to a **device** using Device Tools ▸ Device From Bulk (just click Create, the default settings are fine).



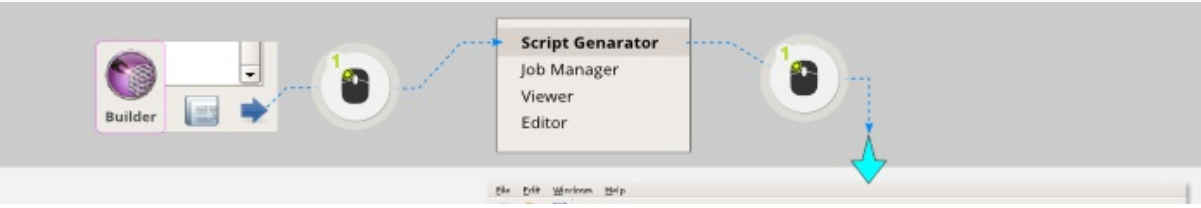
Save the device in a file (say) as **Device_stone.hdf5** in your project directory for other future calculations.

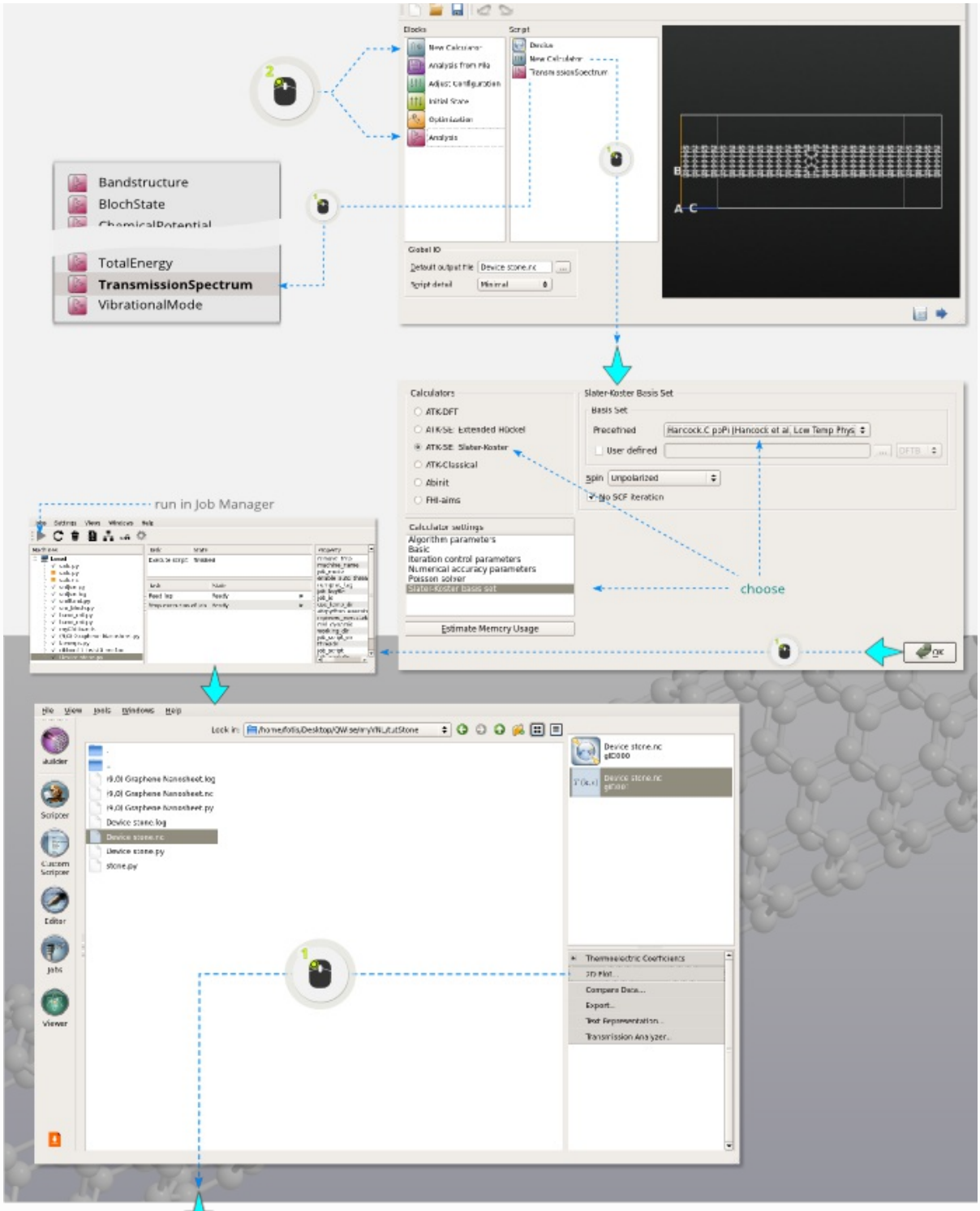
Transmission spectrum

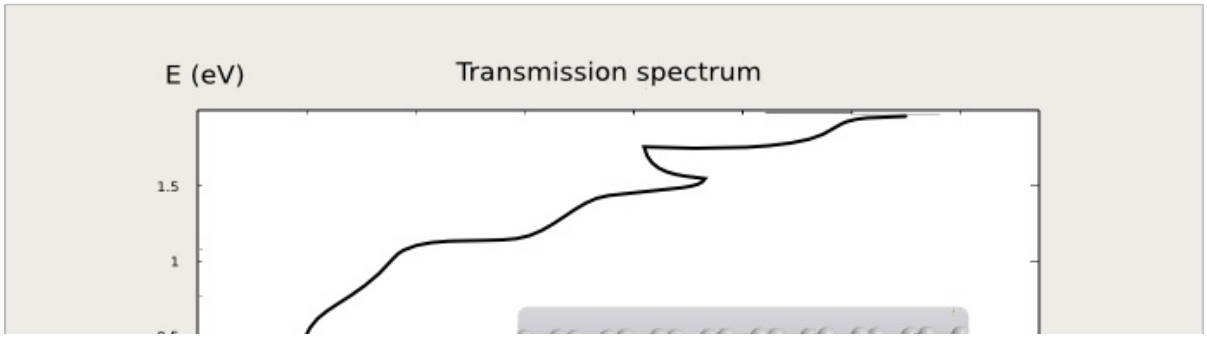
Let's extract the transmission spectrum of the last device structure. This is a rather large device – the central region contains 360 atoms – but with the **ATK-SE** engine you can calculate the electron transmission spectrum in just a few minutes.

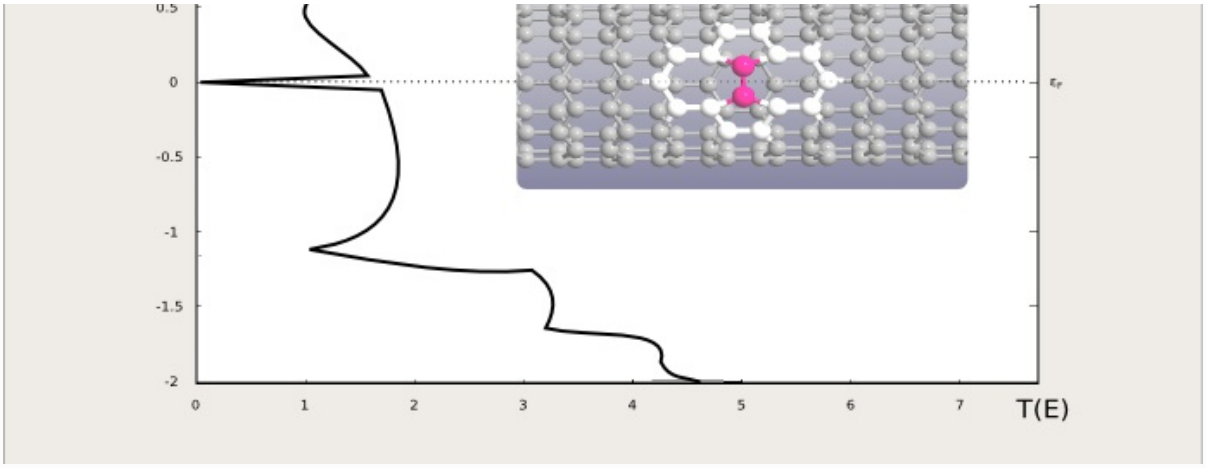
Use the Script Generator to create a Python script including a *Slater–Koster calculator* with the *Hancock.CppPi* basis set and a *TransmissionSpectrum* analysis block. Then run the calculation using the Job Manager, and use the 2D Plot plugin to visualize the calculated transmission spectrum.

The resulting transmission spectrum is also available for download: Device_stone.hdf5.




Bandstructure
BlochState
TotalEnergy
TransmissionSpectrum
VibrationalMode
run in Job Manager
choose
Estimate Memory Usage
OK


E (eV)
Transmission spectrum
1.5
1



The transmission spectrum is shown above. It was computed using the Hancock single-band tight-binding model with up to 3rd nearest neighbor interactions from Ref. [HSU+08]. A perfect (9,0) tube would have a step-like transmission spectrum around the Fermi level, but the defect introduces strong scattering and significantly modifies the electronic transmission. This will most certainly have a noticeable influence on the I-V curve.

Tip

You can easily calculate the corresponding I-V curve: Simply start a new Script Generator session and use **Analysis from File** and the **IVCurve** analysis object to create the script. Plot the results using the **IV-Plot** plugin.

You can also calculate the transmission spectrum and I-V curve for the defect free (9,0) nanotube and compare to the results found above.

References

[HSU+08] Y. Hancock, K. Saloriutta, A. Uppstu, A. Harju, and M. J. Puska. Spin-Dependence in Asymmetric, V-Shaped-Notched Graphene Nanoribbons. *J. Low Temp. Phys.*, 153(5):393–398, 2008. doi:10.1007/s10909-008-9838-y.

[SW86] A.J. Stone and D.J. Wales. Theoretical studies of icosahedral c60 and some related species*Chemical Physics Letters*, 128(5–6):501 – 503, 1986.doi:10.1016/0009-2614(86)80661-3.

[Thr69] P. Thrower. The study of defects in graphite by transmission electron microscopy.*Chemistry and Physics of Carbon*, 5:217–320, 1969.

Previous Next