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MoS_2 Nanotubes

Note

Links: DFTB , dftb_atkse, View on YouTube
Prerequisities: TubeWrapper, Twister, CNTBuilder plugins
Downloads: PDF version

Building a carbon nanotube in QuantumATK is rather trivial, since there is a dedicated plugin for it. That tool is also able to create B-N tubes, as well as multiwall structures. But what if you want something more complicated?

A logical approach seems to be to first make a hexagonal sheet, just like graphene, and then wrap it into the shape of a tube. Indeed, such a **TubeWrapper addon** has been developed, and in this tutorial you will learn how to use it to build MoS_2 and other transition metal sulfide TS_2 nanotubes (T = W, Nb, Re), see Refs. [KZH11] and [STT+00].

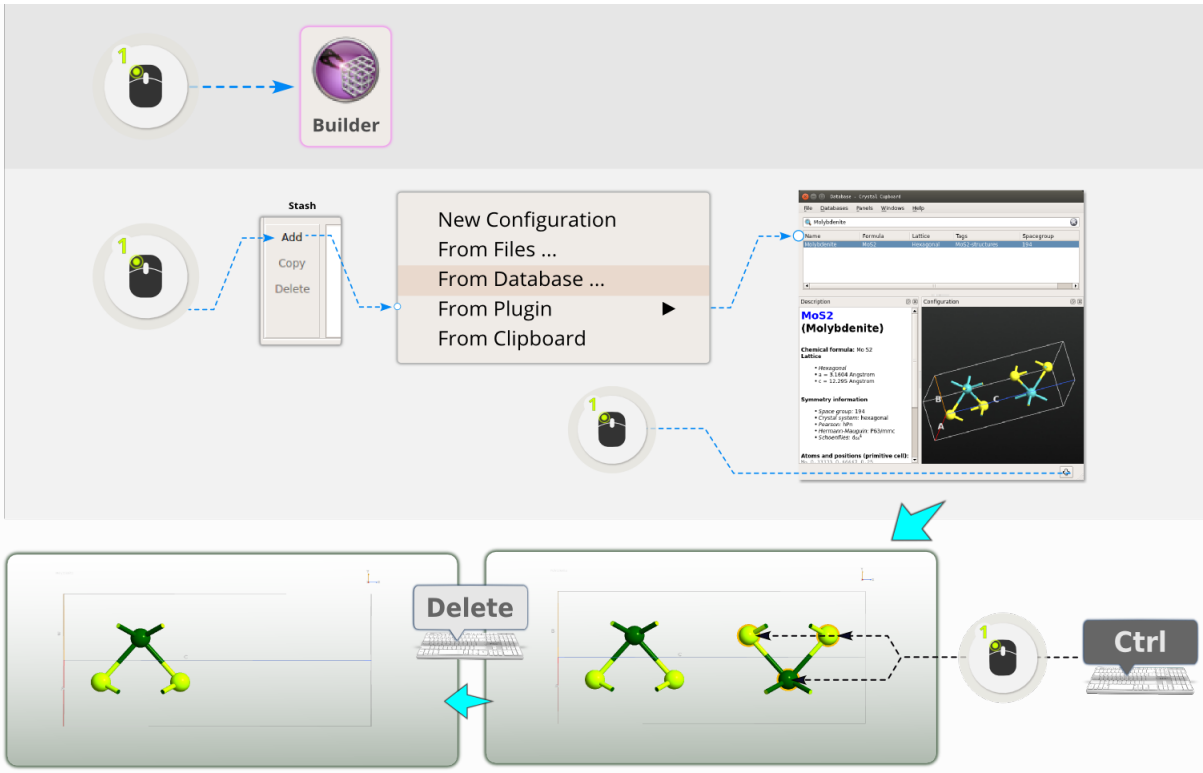
Attention

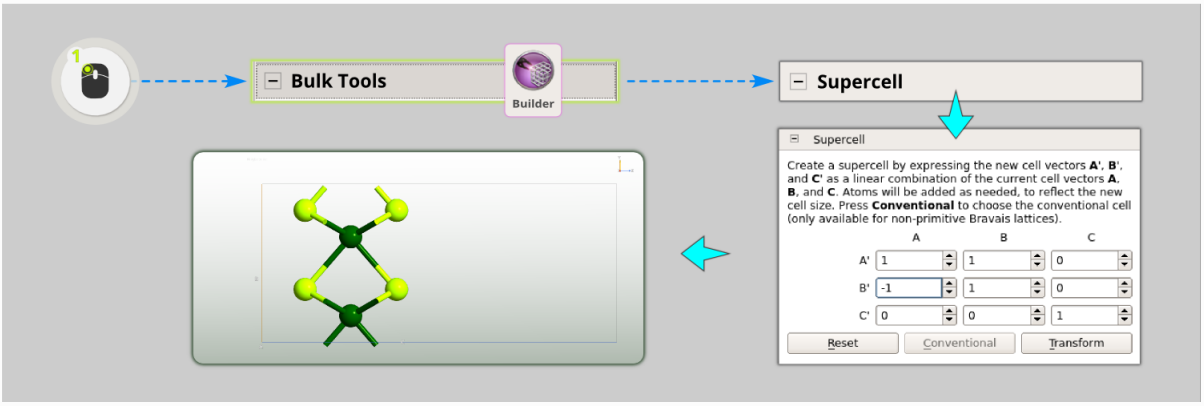
The recipe is simple enough:

1. Create a bulk crystal of MoS_2.
2. Change it into a monolayer.
3. Wrap it using the **TubeWrapper addon**.

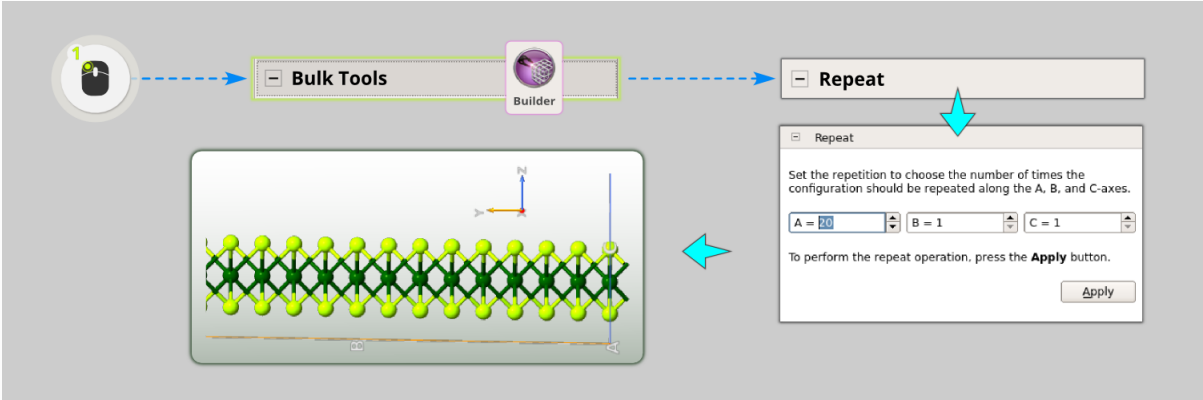
This approach can then easily be adapted for other TS_2 structures.

- **Step 1:** Download the TubeWrapper.zip file and install the addon following the instructions in the How to create AddOns for QuantumATK page.
- **Step 2:** Click Add ▸ Add from Database and locate **molybdenite**. Add it to the Stash (clicking ✚). Use the mouse to select and delete the three atoms to the right in the cell. This leaves a single layer of MoS_2. The cell is hexagonal cell, but to make the tube it is necessary to have an orthorhombic supercell to work with. Therefore, open Bulk Tools ▸ Supercell and use the settings illustrated below.





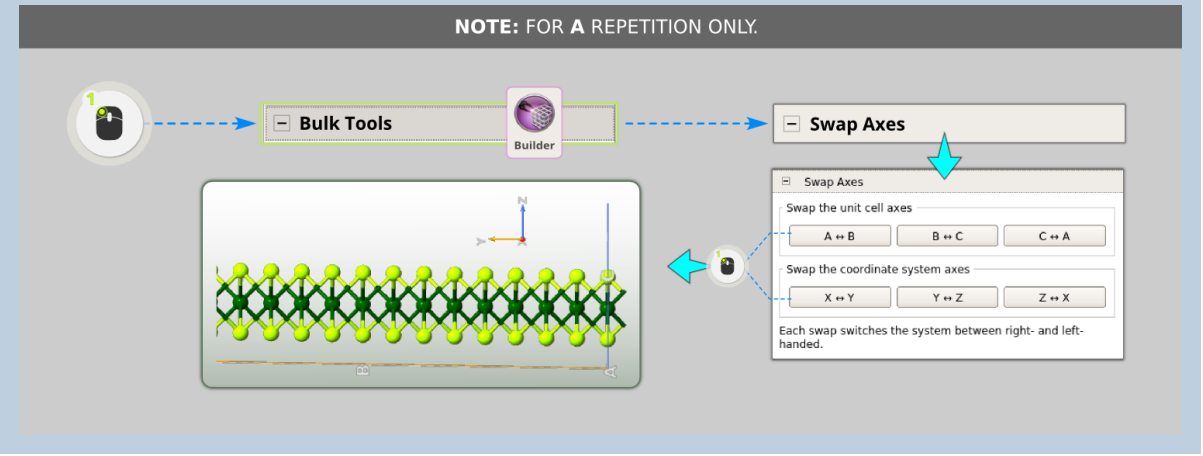
- **Step 3:** Open Bulk Tools ▸ Repeat. You now have two choices: Repeat in **A** or **B** – this will give either armchair (A) or zigzag (B) tubes. Repeat some decent number, like 20 – the new size of the system in the repeated direction will directly determine the circumference of the tube.



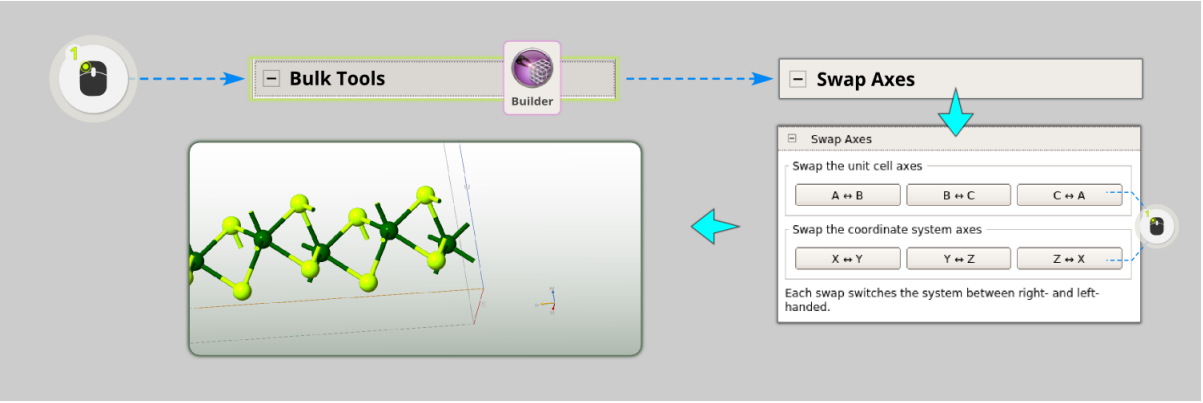
Note

If you repeated in A, use Bulk Tools ▸ Swap Axes and click **A<->B** then **X<->Y** to reorient the system. If

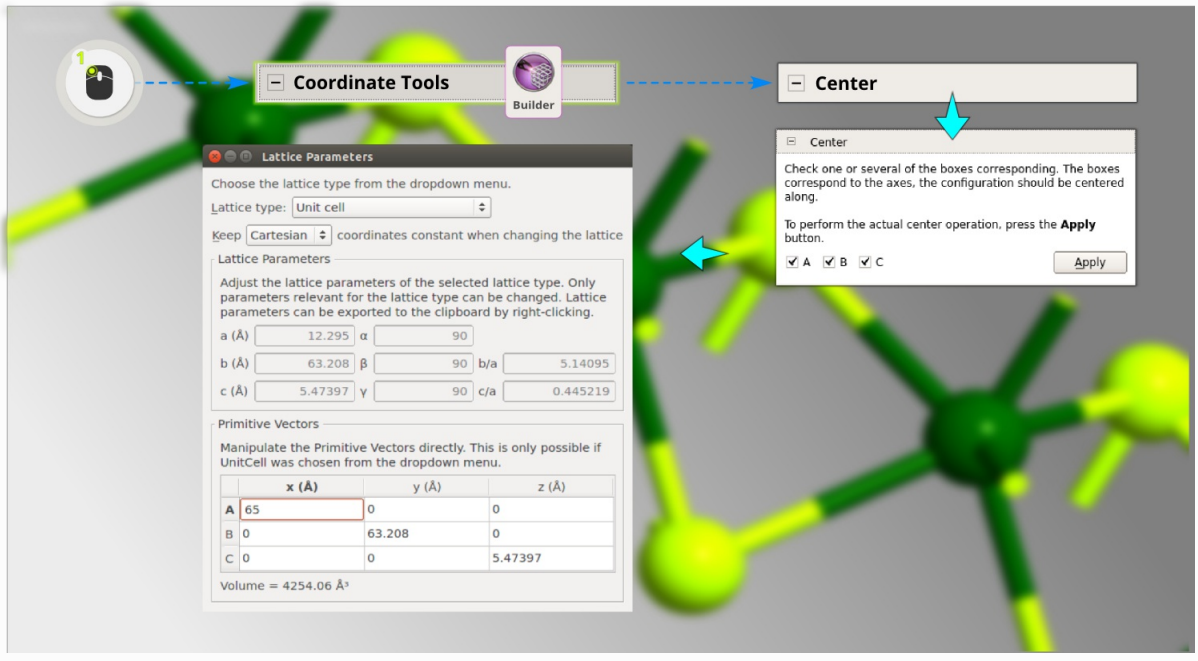
you repeated in B, skip this step.



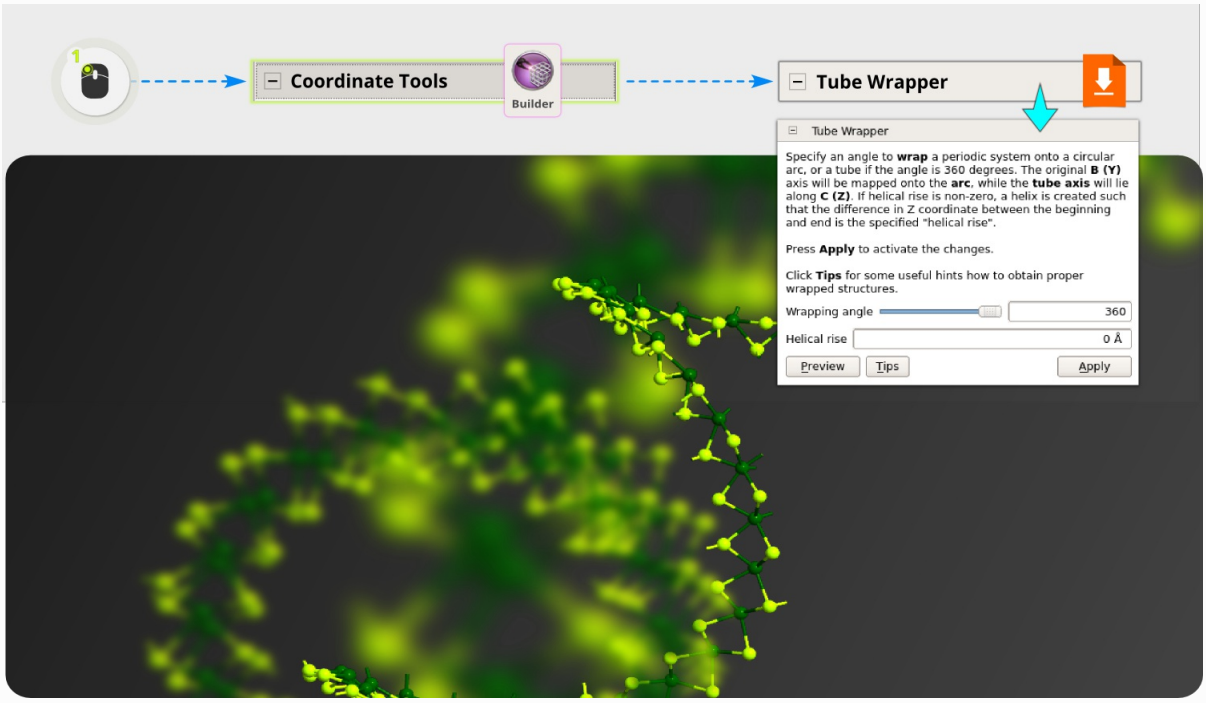
- **Step 4:** Using Bulk Tools ▸ Swap Axes, click **C<->A** then **X<->Z** (do this regardless of whether you repeated in **A** or **B**):



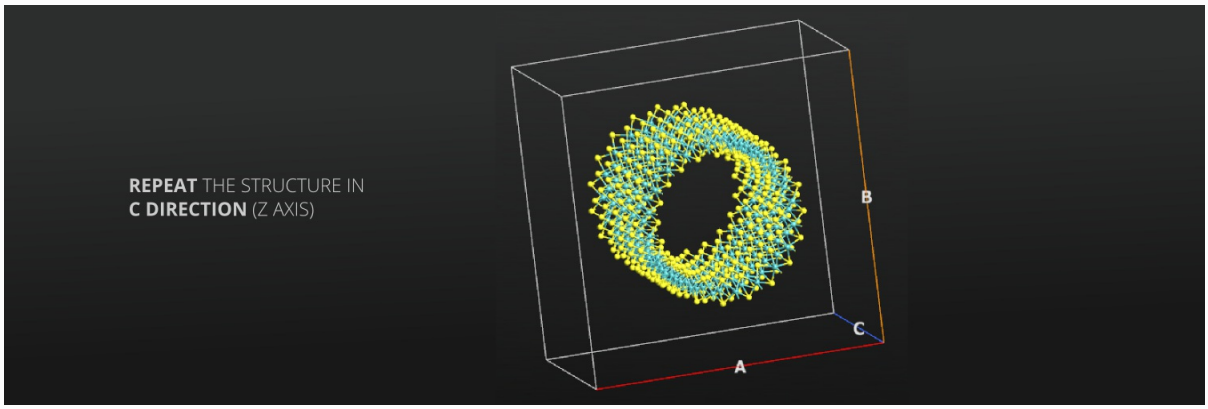
- **Step 5:** Open Bulk Tools ▸ Lattice Parameters and select **Cartesian** coordinates. Then change the first cell vector **A** so that the size of the cell in X is at least as large as in Y. Open Coordinate Tools ▸ Center and center the system.



- **Step 6:** Finally, open the plugin you just installed, Coordinate Tools ▸ Tube Wrapper and wrap the tube. You can use 360 degrees directly to get a fully wrapped tube, or perhaps 180 degrees for some interesting novel work!



- **Step 7:** In the end, it's a good idea to adjust the cell size (it was necessary to keep it large during the building procedure) and then center the system in **A** and **B** and afterwards repeat in z direction:



Tip

What's next?

Now you can perform calculations on MoS_2 nanotubes just as easily as CNTs. The DFTB model used in Ref. [STT+00] is also available in QuantumATK, and you can request the Mo/S parameters from DFTB , and run QuantumATK with those. How to install DFTB parameters is described in another tutorial: dftb_atkse.

You can of course also use the method outlined here to make carbon nanotubes, even though the dedicated plugin Add ▸ Add from Database ▸ Nanotube is much faster to use for a perfect, simple CNT. An interesting example where the Tube Wrapper plugin is anyway useful also for CNTs is for the creation of Stone–Wales defects, which are much easier to define in for a mololayer sheet than for the rolled-up tube. Or, you can make "open" or partially wrapped nanotubes.

References

[KZH11] A. Kuc, N. Zibouche, and T. Heine. Influence of quantum confinement on the electronic structure of the transition metal sulfide ts2. *Phys. Rev. B*, 83:245213, Jun 2011. doi:10.1103/PhysRevB.83.245213.

[STT+00] *(1, 2)* Gotthard Seifert, Humberto Terrones, Mauricio Terrones, Gerd Jungnickel, and Thomas Frauenheim. Structure and electronic properties of mos2 nanotubes. *Phys. Rev. Lett.*, 85:146–149, Jul 2000. doi:10.1103/PhysRevLett.85.146.

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