

## Table of Contents

Table of Contents	1
Building a molecular junction	2
Benzene to DTB: Building the molecule	2
Cleaving gold into two surfaces	4
Combining the molecule and the surfaces	8
Converting the central region to a device configuration	11
References	11

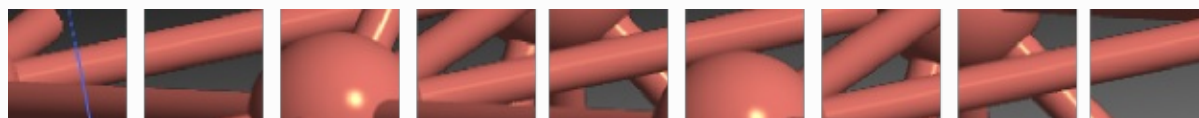


## Building a molecular junction

### Downloads & Links

- [PDF version](#)
- [molecular\\_junction.py](#)

In this tutorial you will learn how to use the Builder in QuantumATK to construct one of the most famous molecular junctions - a dithiole-benzene, DTB (sometimes also known as benzene-dithiole, BDT) embedded between two gold (111) surfaces.



### Note

The work flow described below will walk you through a rather broad overview of the various tools in the Builder. The individual operations are not specific for this surface and this molecule, but can be applied to any other molecule or similar structure. This is the idea of the Builder - by applying a specific sequence of generic operations, you can easily build even highly specialized structures.

The recipe is quite simple and includes the following simple steps:

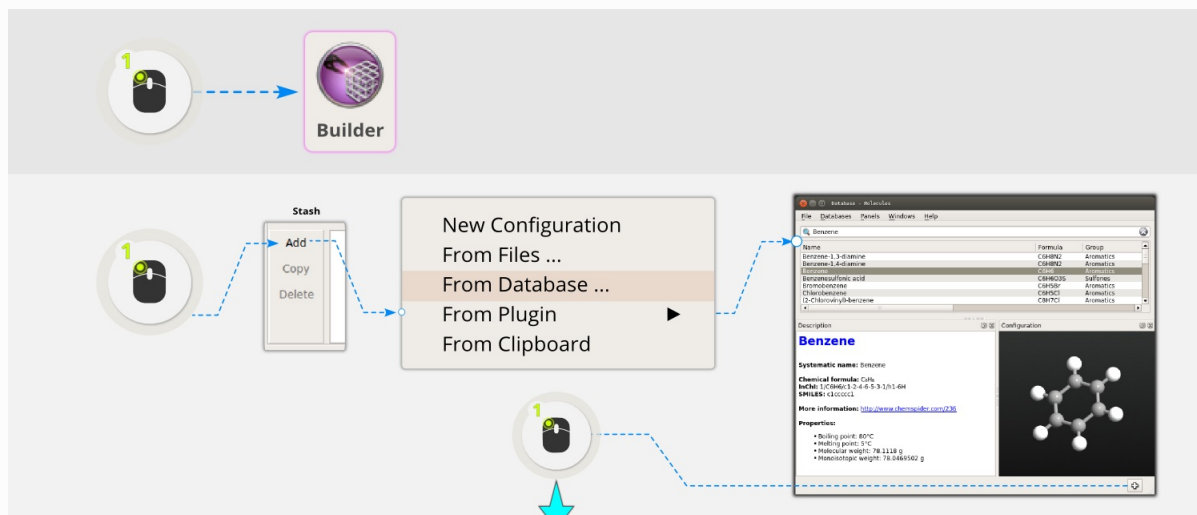
- Construct the molecule. (Sometimes trivial, if you have it ready in the Database or as an external file; in our case we will modify benzene to make DTB.)*
- Construct the surfaces, by cleaving the bulk crystal and creating a copy, to make two electrodes.*
- Place the molecule on the surface of the left electrode, and connect the right electrode to the molecule.*
- Finalize the device geometry.*


The instructions below may appear a bit complicated, since each step contains many operations, but with a bit of training the whole process can be carried out in under 5 minutes. Also remember - if you make a mistake anywhere along the line, use Undo (Ctrl+Z)!

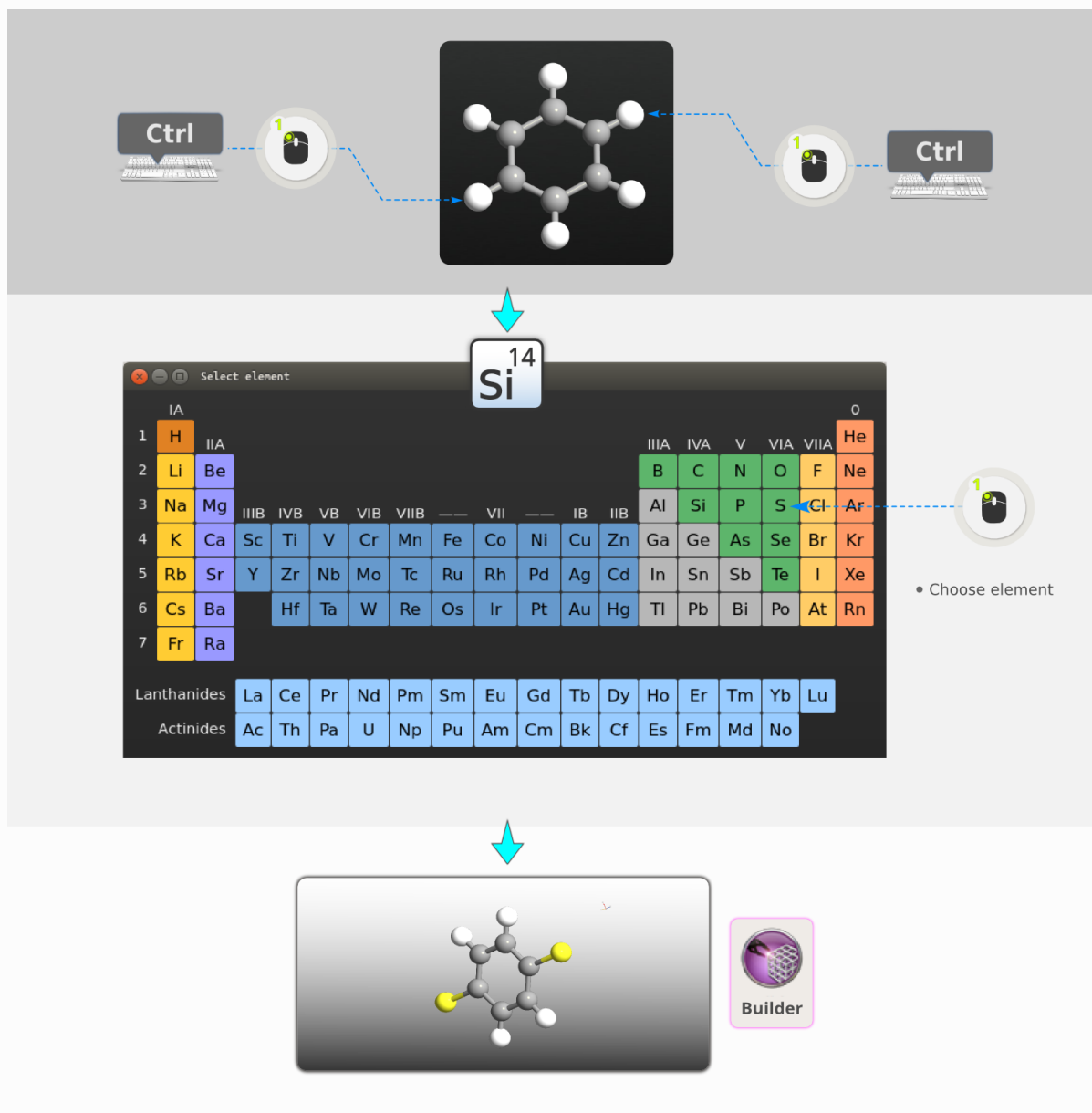
## Benzene to DTB: Building the molecule

- **Step 1:** Click Add ► Add From Database and from the menu select Databases ► Molecules. Locate

benzene, and click the + icon in the lower right-hand corner to add the molecule to the stash.



- **Step 2:** To convert the molecule to DTB, select two hydrogen atoms on opposite sides of the molecule by clicking them while holding down Ctrl. Then open the periodic table tool , and click **Sulfur (S)** element:



- **Step 3:** Deselect all atoms by pressing Esc or clicking the background.
- **Step 4:** The C-S bond lengths need to be adjusted. Select one pair of bonded C-S atoms, taking care to **select the carbon atom first**. So, Open Coordinate Tools ► Z-matrix and set the bond length to 1.75 Å. Note that the second selected atom moves, i.e. the S atom.

Coordinate Tools Builder

set the C-S bond length

Z-matrix

Select atoms in the 3D-View to view their [Z-matrix](#) in the table below. Use ctrl-left mouse click to select multiple atoms.

	Element	d (Å)	θ (°)	φ (°)
10	Carbon			
11	Sulfur	1.75		

- **Step 5:** Do the same for the other Carbon-Sulfur bond!

## Cleaving gold into two surfaces

- **Step 6:** Click Add ► Add from Database... and this time select Databases ► Crystals from the menu. Locate Gold and add it to the stash.

Builder

Stash

Add  
Copy  
Delete

New Configuration

From Files ...  
From Database ...  
From Plugin  
From Clipboard

Database - Crystal Opened

Gold

Au (Gold)

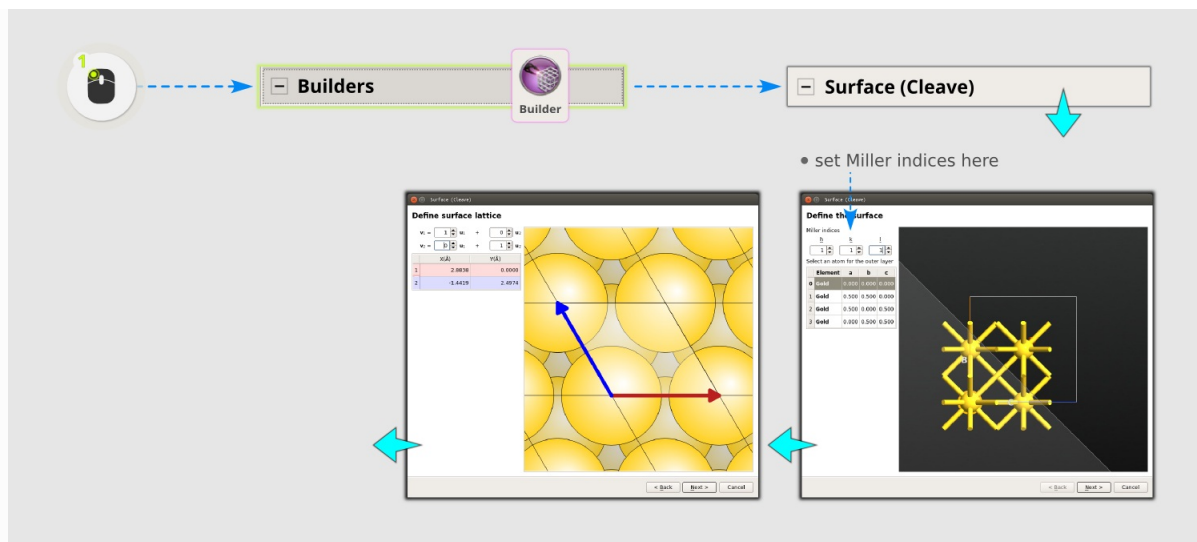
Chemical formula: Au  
Lattice  
• Face centered cubic (fcc)  
• a = 4.07825 Angstrom

Symmetry information

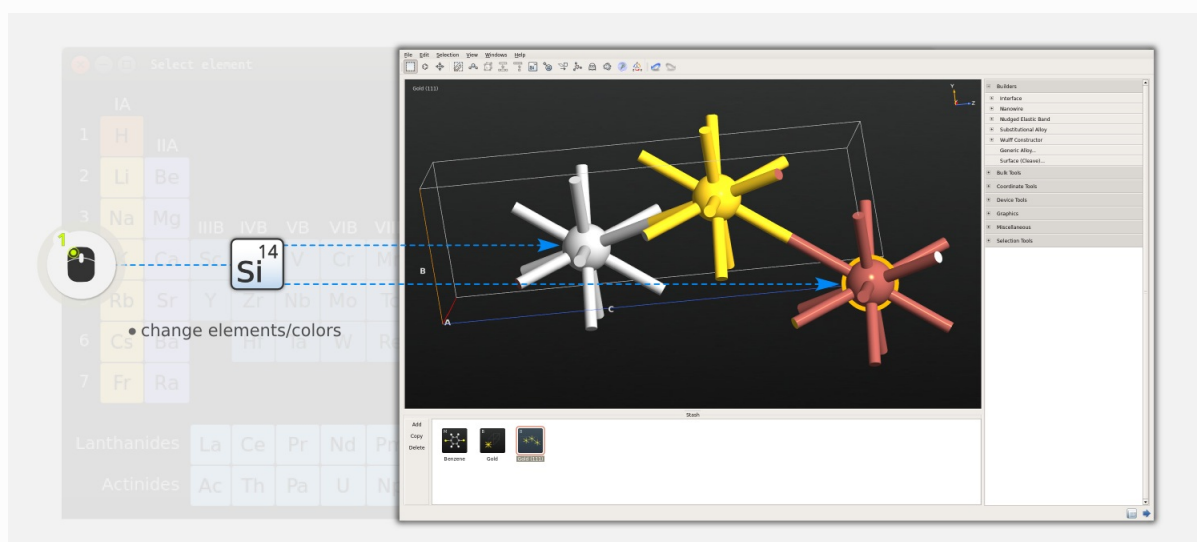
• Space group: 225  
• Crystal system: cubic  
• Pearson: cF4  
• Hermann-Mauguin: Fm-3m  
• Schoenflies:  $o_h$

Atoms and positions (primitive cell)

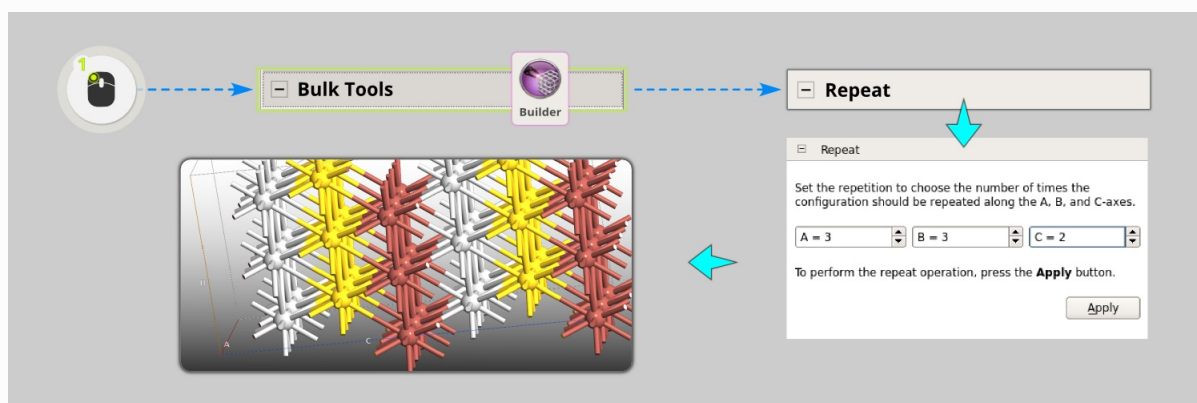
- **Step 7:** To cleave the gold crystal, open Builders ► Surface (Cleave). Enter Miller indices h=1, k=1, l=1 and click Next ► Next ► Finish.



- **Step 8:** To make it easier to visually identify the three layers (ABC) in the fcc stacking sequence, change the gold atom in layer A to Ag and the one in layer C to Tl (these elements are just chosen to give nice colors).



- **Step 9:** To make a large enough surface cell for the molecule, repeat the structure 3x3x2 times using Bulk Tools ► Repeat. The 2x repetition in the C direction is needed so that we later can extract the electrode from the central region.



- **Step 10:** You need to make some room for the molecule on the surface by adding vacuum. Open Bulk Tools ► Lattice Parameters, select to keep Cartesian coordinates, and increase the C vector to 45 Å (still pointing along Z, as is necessary for a device).

**1** Bulk Tools Builder Lattice Parameters

Choose the lattice type from the dropdown menu.  
Lattice type: Unit cell  
Keep Cartesian coordinates constant when changing the lattice

Lattice Parameters  
Adjust the lattice parameters of the selected lattice type. Only parameters relevant for the lattice type can be changed. Lattice parameters can be exported to the clipboard by right-clicking.

a (Å) 8.65127  $\alpha$  90  
b (Å) 8.65127  $\beta$  90 b/a 1  
c (Å) 45  $\gamma$  120 c/a 5.20155

Primitive Vectors  
Manipulate the Primitive Vectors directly. This is only possible if UnitCell was chosen from the dropdown menu.

	x (Å)	y (Å)	z (Å)
A	8.65127	0	0
B	-4.32564	7.49222	0
C	0	0	45

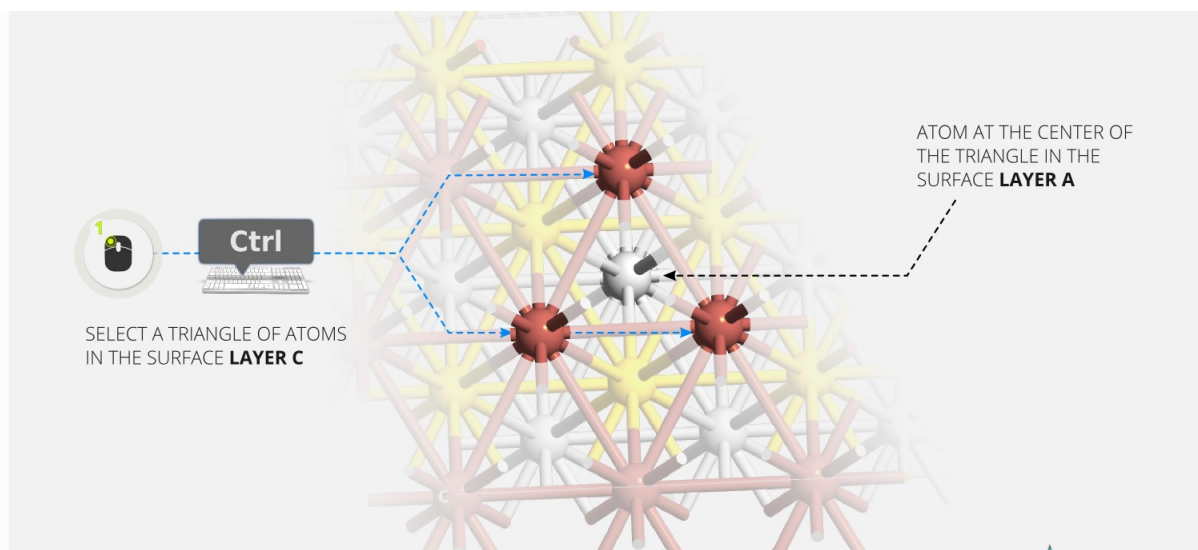
Volume = 2916.77 Å<sup>3</sup>

Gold (111)

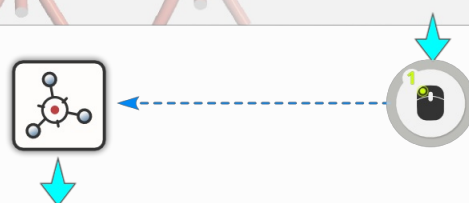
**ROTATE THE STRUCTURE SO THAT THE Z AXIS POINTING OUT OF THE SCREEN**

You will now create an alignment point on the surface where we can attach the molecule.

- **Step 11:** Select three atoms in a triangle in the surface layer C (the Ti atoms), such that the center of the triangle is above a silver atom in the A layer. Press the centroid tool to insert another atom in the average position of the three selected atoms. By choosing these particular atoms, the inserted atom sits in an fcc site, which is where we want to attach the molecule.
- **Step 12:** Use Coordinate Tools ► Translate to move this atom 1.71 Å in the Z direction. (The value 1.71 Å gives an Au-S distance of 2.39 Å, taken from <sup>[1]</sup>).



- click the centroid tool to insert an atom in an fcc arrangement



1

Coordinate Tools

Builder

Translate

Translate

To input the translation vector using fractional coordinates, check the **Fractional** box below.

☐ Fractional

To translate the configuration, first define the translation vector using the input fields below.

x (Å) y (Å) z (Å)

0.0 0.0 1.71

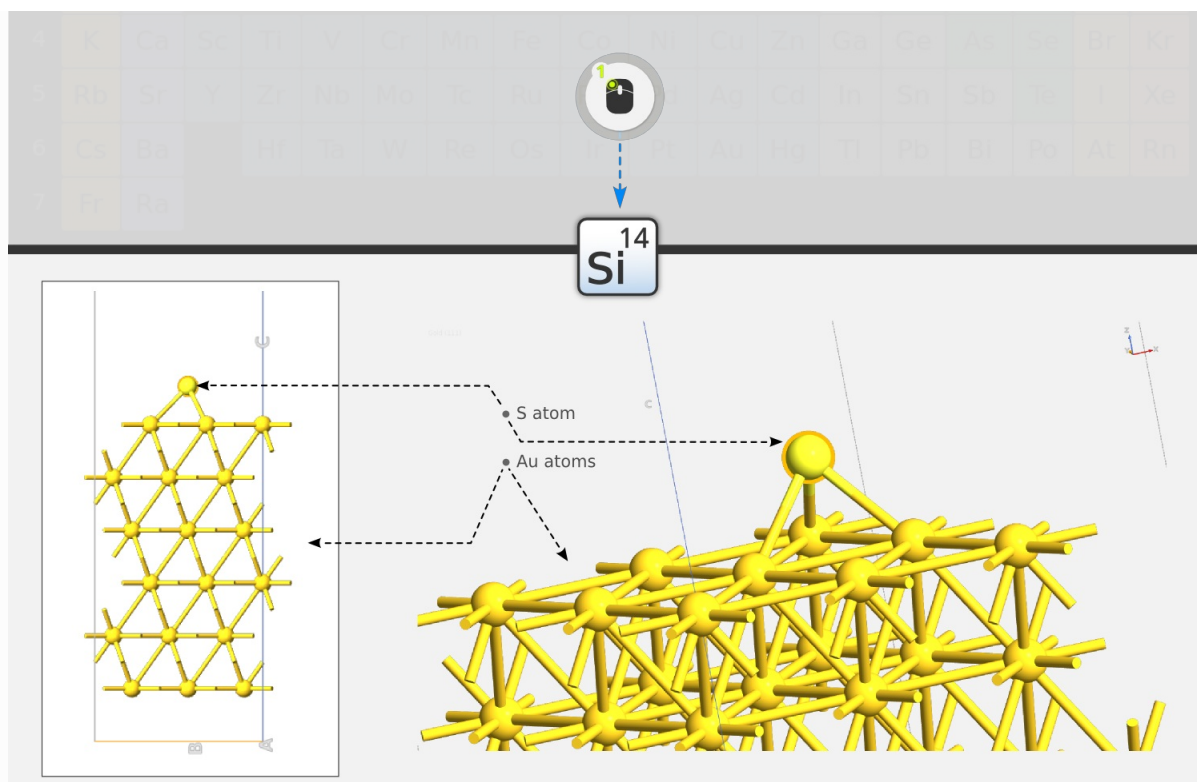
Check the **Copy** box, if you want the translated atoms to be copied. Finally, press **Apply** in order to perform the actual translation.

☐ Copy

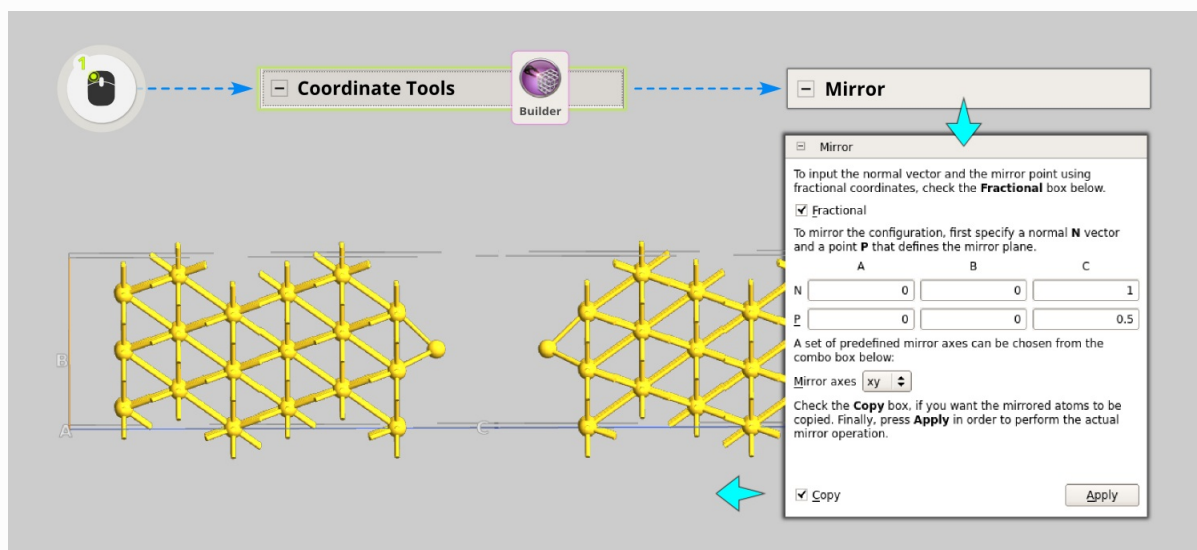
Apply

• set the translation here

- **Step 13:** Press Ctrl+A to select all atoms, and switch them back to gold.
- **Step 14:** Also, to make it easier to handle the alignment atom later on, convert it to sulfur.



- **Step 15:** So far there is only one gold surface - there should be two. Therefore, press Ctrl+A again and open Coordinate Tools ► Mirror . Select "Fractional" coordinates and set P=[0,0,0.5]. Tick "Copy", then press Apply.



## Combining the molecule and the surfaces

- **Step 16:** Add the benzene to the gold structure by dragging it from the stash onto the main window (where the gold surfaces are displayed). When the molecule is added, the Builder automatically activates **Move mode**.

### Note

All atoms in the molecule are selected (indicated by the yellow circles around the atoms); in **Move mode**, you cannot change this selection, but you can appoint so-called **anchor atoms** which are used to translate and rotate the selection. **Anchor atoms will be indicated by red circles.**



DBT

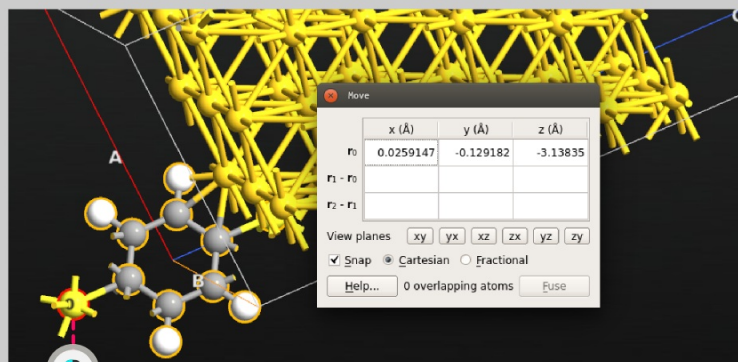


drag 'n' drop



Electrodes

THE **MOVE** TOOL/WINDOW APPEARS AUTOMATICALLY

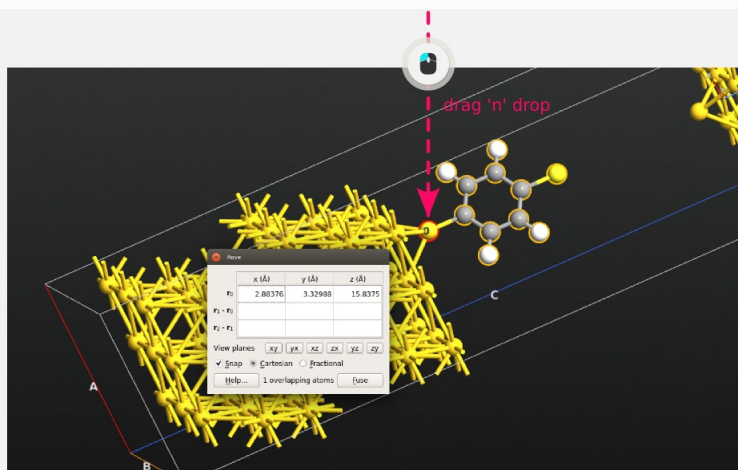


drag 'n' drop

- **Step 17:** Click one of the sulfur atoms - it will become an anchor atom. Then drag it so that it ends up on top of the sulfur alignment atom on the left surface. Since "Snap" is on, it will latch on to the exact position of the alignment atom, indicated by the selection marker turning blue when the two atoms are on top of each other.

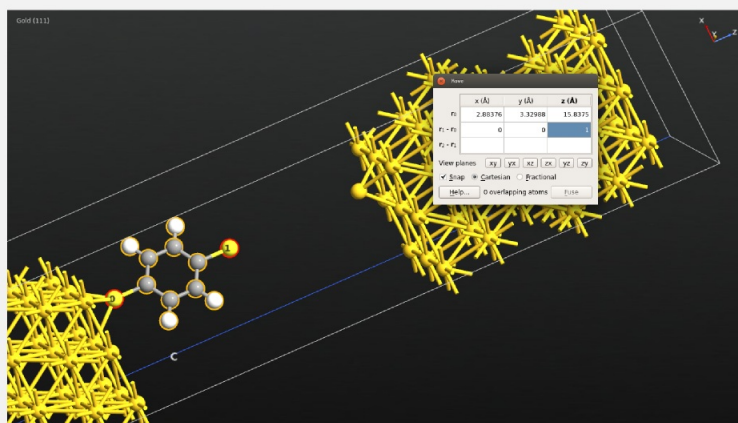
**DRAG 'N' DROP** THE C ATOM OF THE MOLECULE ON THE ATOME OF THE GRID


PRESS **FUSE** TO CORRECT THE OVERLAPPING

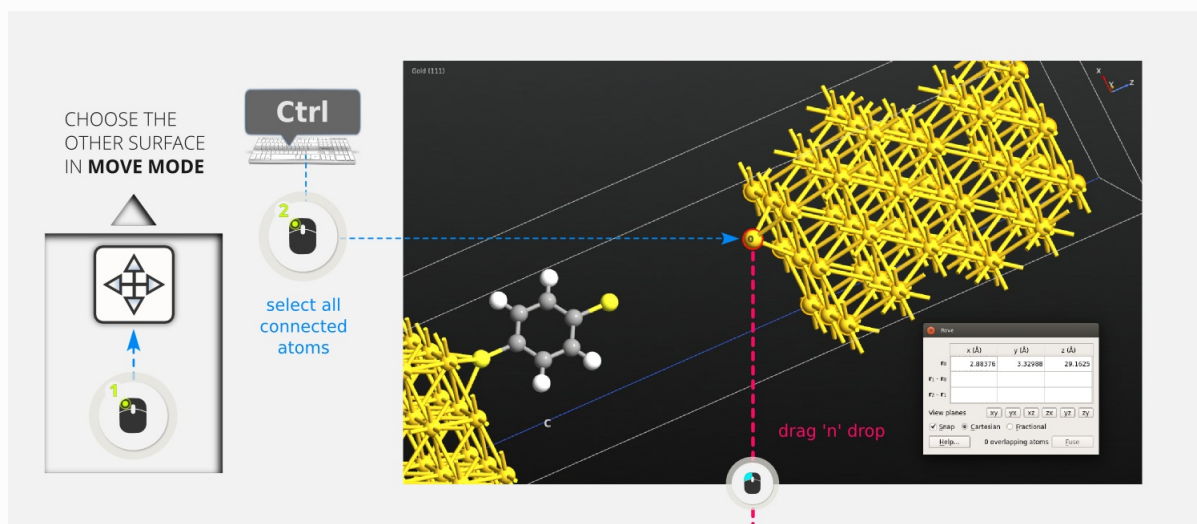


- **Step 18:** Press Fuse - this removes one of the two overlapping sulfur atoms (the one in the surface is removed; atoms in the active selection are always kept when fusing).
- **Step 19:** Now click the other S atom (the first one will remain selected). Then enter [0,0,1] on the r1-r0 row of the Move tool widget. This aligns the two atoms - and hence the molecule along the Z axis. Close the Move tool widget.

CHOOSE THE OTHER  
S ATOM OF MOLECULE  
AND **ALIGN** IT!



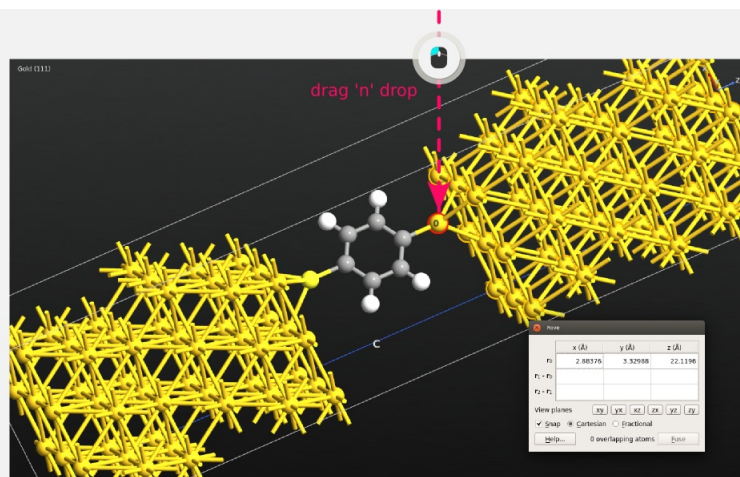
- **Step 20:** Select the second surface by holding down Ctrl while double-clicking one of the atoms in it. This selects all connected atoms.
- **Step 21:** Enter **Move mode**  again and click the sulfur alignment atom in the second surface to make it an anchor atom.



- **Step 22:** Drag the right surface so that the anchor/alignment atom ends up on top of the sulfur atom on the free end of the DTB molecule.
- **Step 23:** Press **Fuse** to remove one of the two overlapping sulfur atoms (the one in the molecule, this time). Close the Move tool widget.


**DRAG 'N' DROP** THE C ATOM  
OF THE MOLECULE ON THE  
ATOME OF THE GRID

PRESS **FUSE** TO CORRECT  
THE OVERLAPPING



You now have a complete central region, and the only thing remaining is to convert it to a device configuration.

## Converting the central region to a device configuration

- **Step 24** Open Devices Tools ► Device from Bulk. The tool automatically figures out the size of the electrodes, since we repeated the gold (111) surface cell 2x in C.
- **Step 25:** This is however a very large central region, which will take a long time to calculate. Therefore, reduce the left and right surfaces to four layers by clicking  twice for each surface (left and right). Press OK and you are done!

### Note

In order to optimize the geometry of the device you can read the [Advanced device relaxation - manual workflow](#) tutorial.

## References

[1]

M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro. Density-functional method for nonequilibrium electron transport. *Phys. Rev. B*, 65:165401, Mar 2002. [doi:10.1103/PhysRevB.65.165401](https://doi.org/10.1103/PhysRevB.65.165401).

 Previous

Next 