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Building molecule–surface systems: Benzene on Au(111)

Version: 2017.0

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In this tutorial you will learn how to use **QuantumATK (QuantumATK)** to construct two different adsorption configurations of a benzene molecule adsorbed on the gold (111) surface, here denoted Bz@Au(111). In particular, you will:

- Create the structure of bulk Au using the value of the lattice constant reported by Lui *et al.* in Ref. [\[LRZ+13\]](#);
- Construct a slab model for the Au(111) surface according to the parameters reported in [\[LRZ+13\]](#);
- Attach a benzene molecule to the Au(111) surface slab model;
- Modify the atomic coordinates of the Bz molecule to construct configurations of Bz@Au(111) using the advanced building tools in the QuantumATK **Builder**.

Tip

Once you have constructed these geometries, you can optimize them using one of the computational methods implemented in QuantumATK, and perform further analysis.

Note

Many of the QuantumATK functions described in this tutorial are rather general, and can be used to build complex geometries other than molecules on surfaces, see for example the tutorial on [Building a molecular junction](#).



Summary of workflow

The following is a summary of the main steps needed for building the Bz@Au(111) configurations. These steps are also shown in the short **video** available below. If needed, more detailed instructions are given in the sections after the video.

1. Create a new QuantumATK project and open the  **Builder**.
2. Use the **Builder Database** to import the bulk gold primitive unit cell.
3. Use the **Lattice Parameters** plugin to change the gold lattice parameter to $a = 4.159 \text{ \AA}$, as reported in Ref. [LRZ+13] using DFT and the PBE density functional.
4. Open the **Surface (Cleave)** plugin, and create the 3×3 Au(111) slab with 6 metal layers and 20 \AA vacuum above it.
5. Use the  **Molecular Builder** tool to add the benzene molecule to the slab configuration.
6. Select the Bz atoms, and use the **Rotate** plugin to rotate the molecule 90° around the y-axis such that the molecule can adsorb parallel to the slab surface plane.
7. Click the  icon to add a new atom in at the geometrical center of the molecule.
8. Use the  **Move** tool to move the molecule into the hcp-30° adsorption site. The extra atom added in the previous step is used to “snap” the molecule into position, and is afterwards removed from the configuration.
9. **Rename** the configuration and create a **copy** of it in the Stash.
10. **Rename** the copy, and use the **Rotate** plugin to rotate the Bz 30° around the z-axis to create the hcp-0° adsorption geometry.

Many more **video tutorials** are available on the [QuantumWise YouTube](#) channel.

Detailed instructions

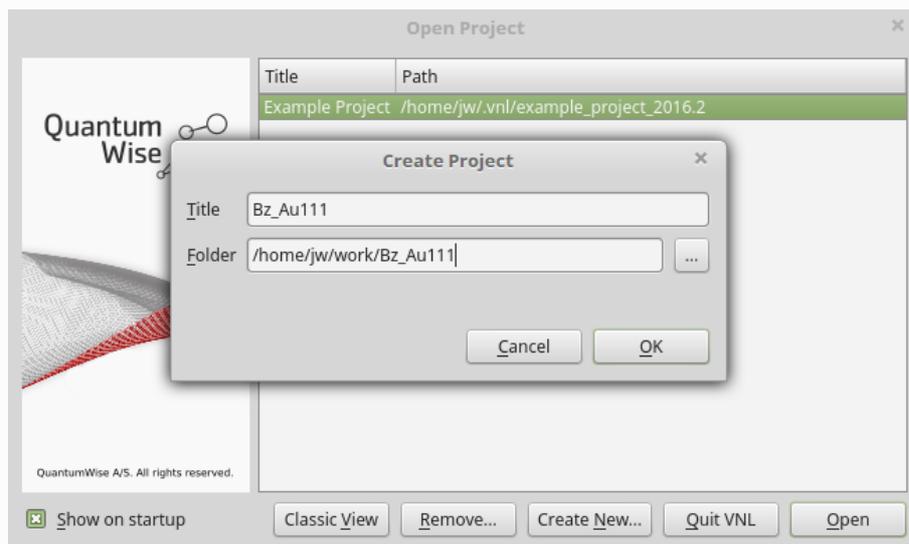
Building the Au(111) surface

You will here construct a slab model for the Au(111) surface starting from the gold primitive unitcell.

Bulk gold

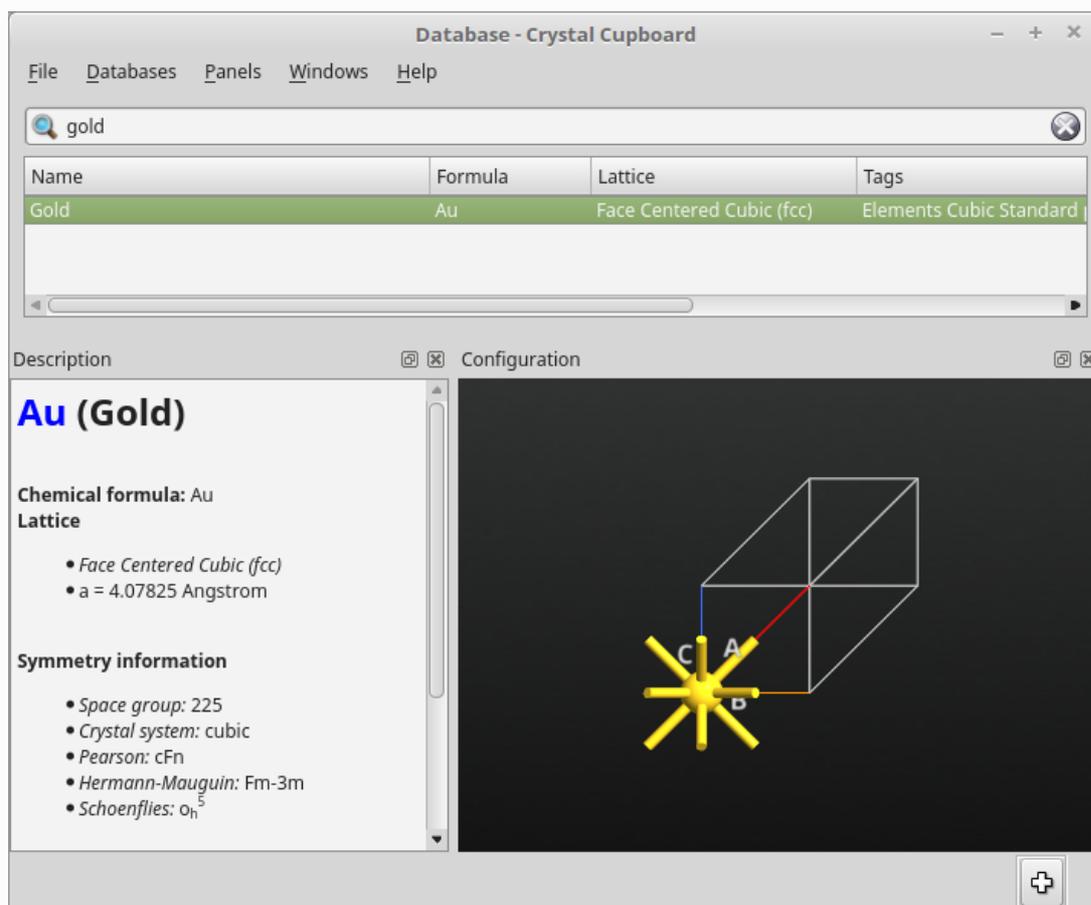
Open **QuantumATK** and create a new project. Give the project a title (here: “*Bz_Au111*”), select the folder where the project files should be stored (scripts, data files, etc.), and click **OK** to create the project.

click **Open** to open the project and start your QuantumATK session.



In the QuantumATK main window, open the **Builder**, and click **Add** ► **From Database** next to the **Stash** to open a database of common materials in their experimental structures.

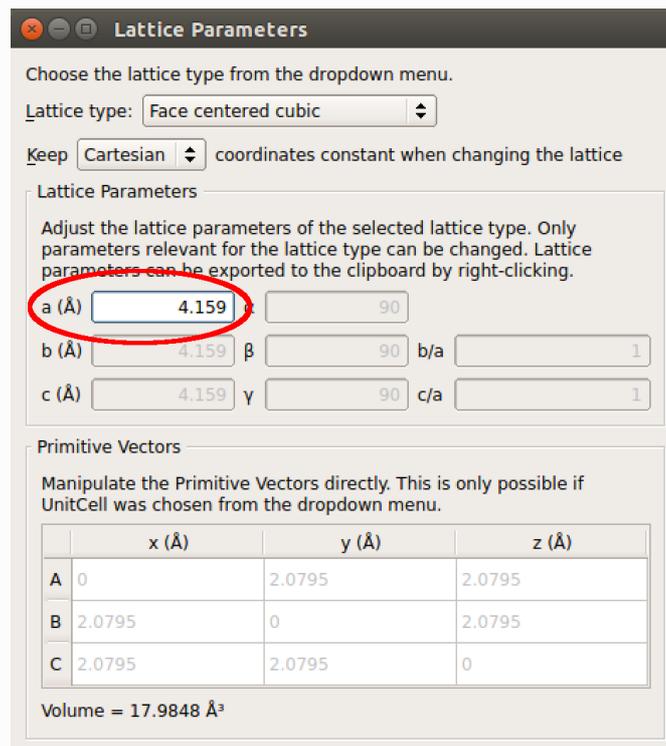
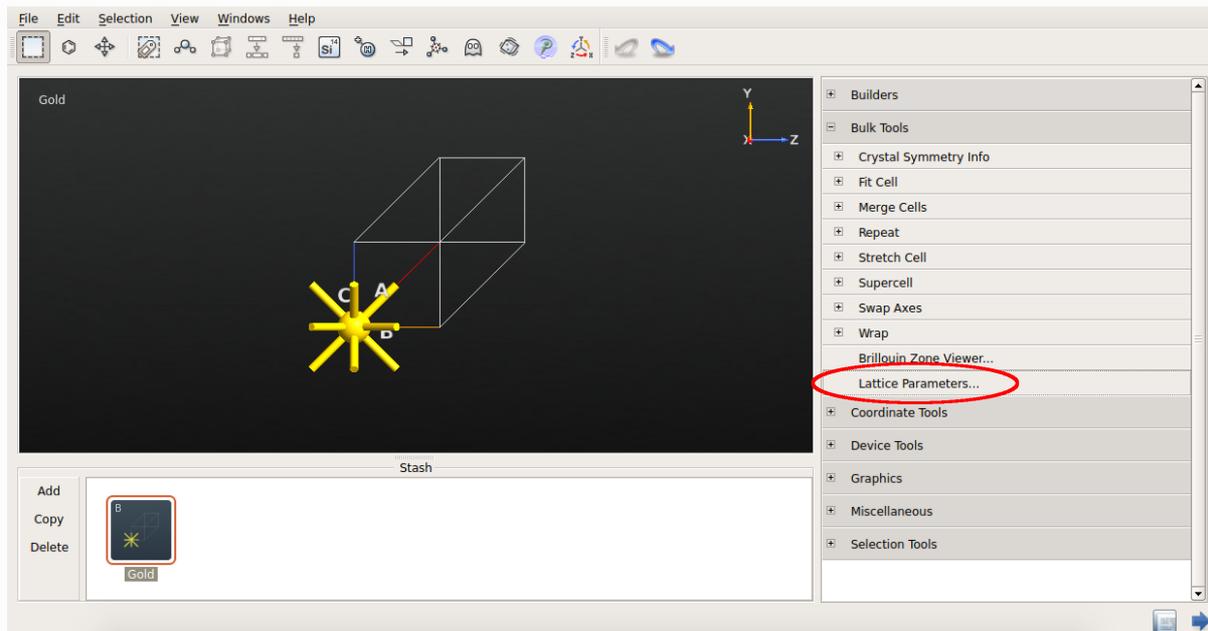
Search for “gold” using the search bar, and import the structure to the **Stash** by clicking the search result and then clicking the  icon:



The gold primitive cell has been added as a **Stash** item, and may now be modified using the **Builder** plugins.

In this case, use the **Bulk Tools** ► **Lattice Parameters** plugin to change the lattice parameter to that

reported in Ref. [LRZ+13] using DFT and the PBE functional, $a = 4.159 \text{ \AA}$.



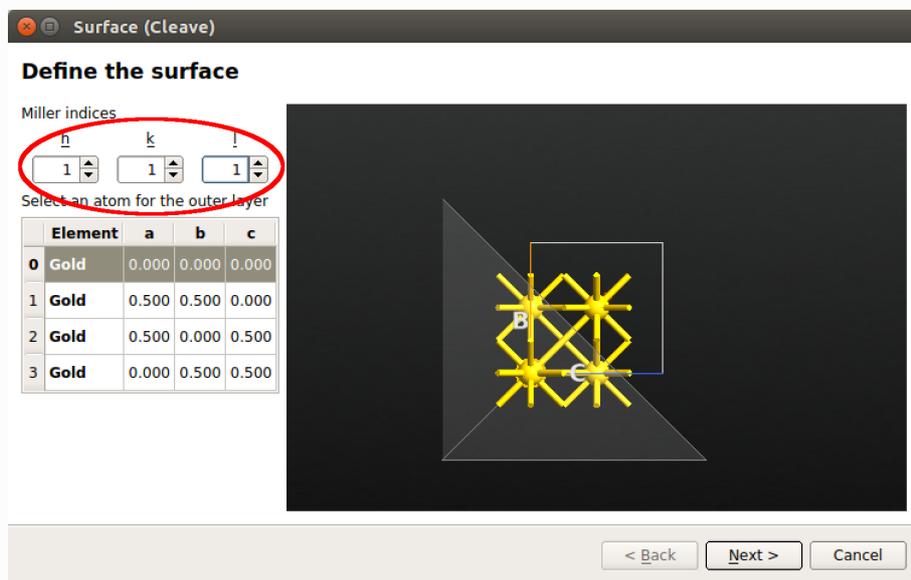
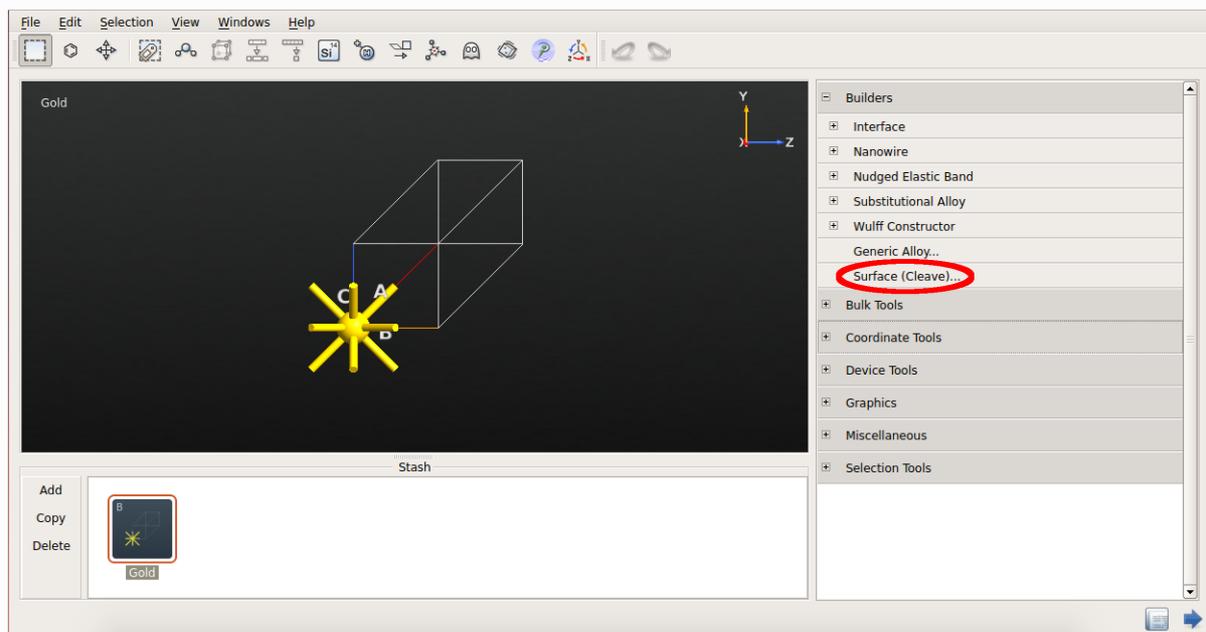
When you are done, close the plugin widget and go back to the Builder.

Au(111) slab

Next step is to cleave the bulk gold along the (111) direction in order to create a slab model of the Au(111) surface.

In the **Builder**, use the Builders \triangleright Surface (Cleave) plugin to cleave the Au crystal using the Miller indices

$$(h, k, l) = (1, 1, 1):$$



The default supercell lateral size is 1×1 . This is sometimes sufficient, but in the present case we aim for a 3×3 slab in order to minimize in-plane interactions between neighboring Bz molecules.

Therefore, increase the lengths of the lattice vectors v_1 and v_2 , such that

- $v_1 = 3u_1 + 0u_2$
- $v_2 = 0u_1 + 3u_2$

Surface (Cleave)

Define surface lattice

$v_1 = 3 u_1 + 0 u_2$
 $v_2 = 0 u_1 + 3 u_2$

	X(Å)	Y(Å)
1	8.8226	0.0000
2	-4.4113	7.6406

< Back Next > Cancel

Tip

You can also modify the lattice vectors **interactively** by using the mouse to manually displace the red and blue vectors in the right-hand window showing the in-plane cell.

Finally, use the drop-down menu to select the out-of-plane cell vector v_3 to be **Non-periodic and slab-like** such as to model a surface with vacuum above and below it. Also increase the **Top vacuum** to 20 Å and the slab **Thickness** to 6 layers, as shown in the figure below.

Surface (Cleave)

Finalize output configuration

Automatically update 3D view

Out-of-plane cell vector v_3 is

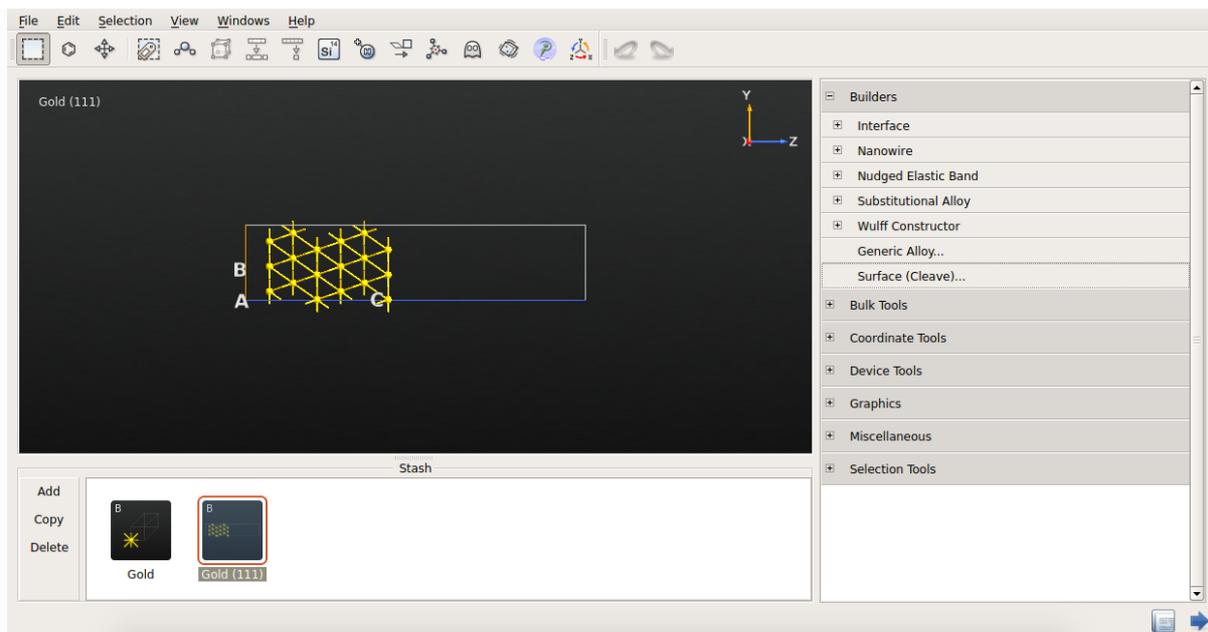
Non-periodic and normal (slab)

	Layers	Å
Top vacuum	8.3292	20.000
Thickness	6.0000	14.4072
Bottom vacuum	0.0000	0.0000

Update

< Back Finish Cancel

Once you are done, click **Finish** to add the Au(111) slab configuration to the **Stash** and close the plugin widget.



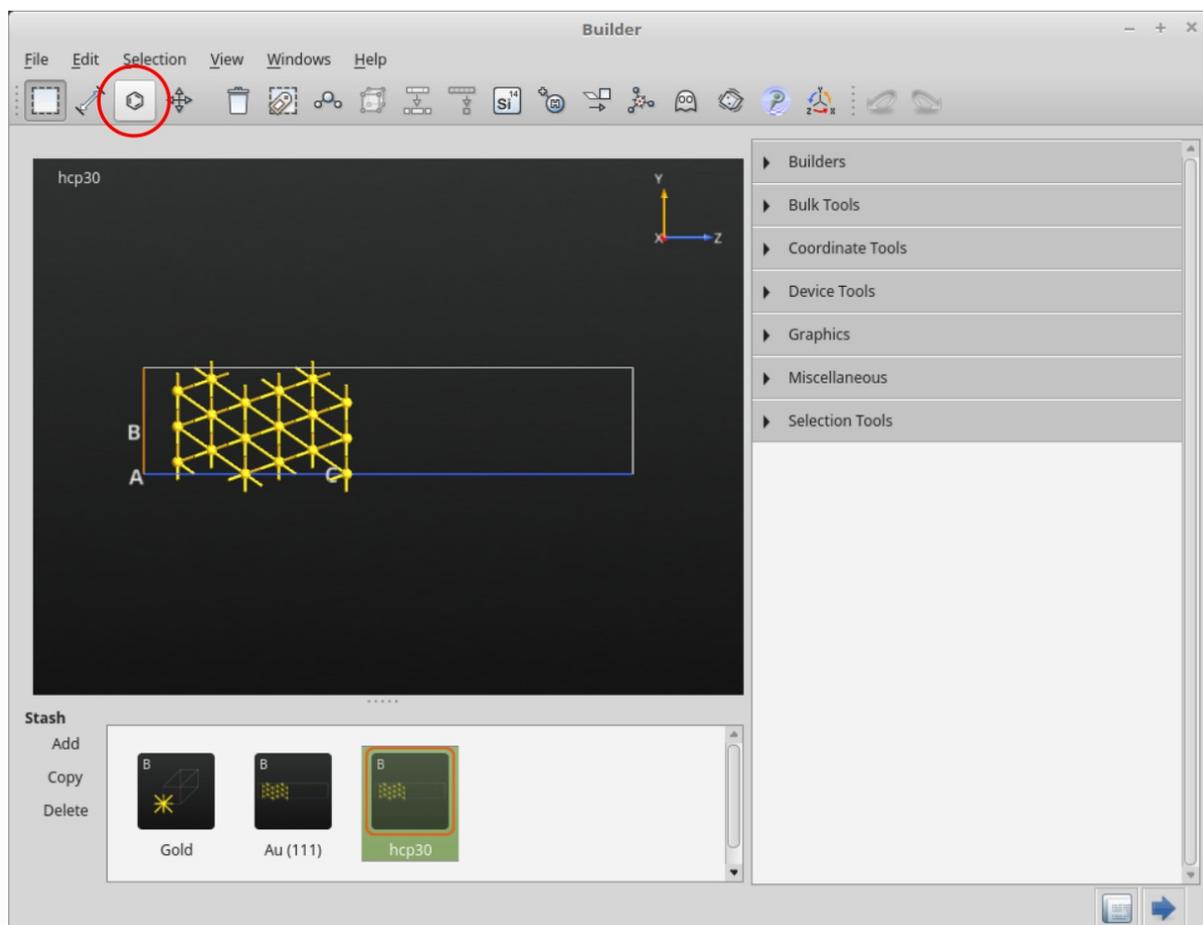
Attaching benzene to Au(111)

The final step is of course to attach a benzene molecule to the Au(111) slab. We will first aim for the hcp-30

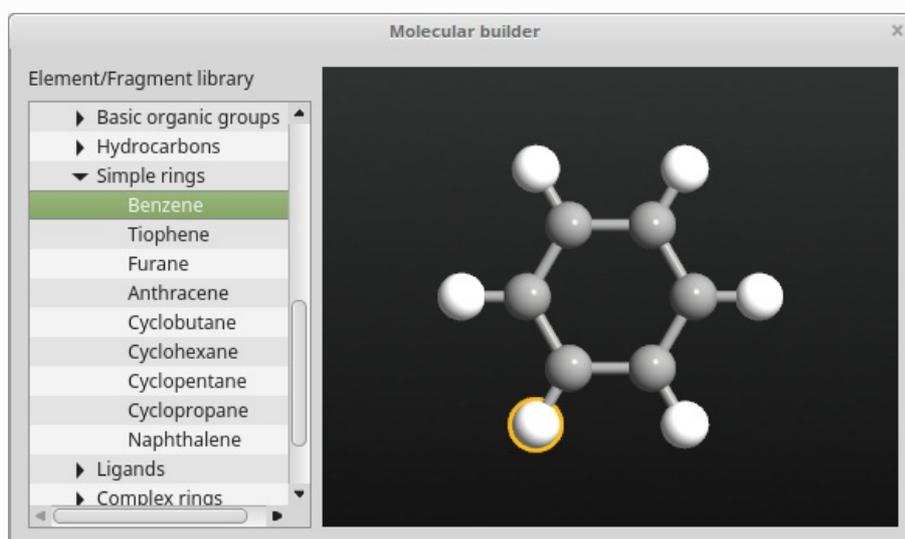
° configuration reported in [\[LRZ+13\]](#).

Select the "Gold(111)" Stash item and rename it to "Au(111)" by using mouse right-click or F2 on the keyboard. Then create a copy of the item, again using mouse right-click. Rename the copy "hcp30".

In the  Builder, click the  icon to open the Molecular Builder.



In the **Molecular Builder**, select Fragments ▶ Simple rings ▶ Benzene from the drop-down menu.



You can now insert the benzene molecule into the Au(111) configuration: Click somewhere in the Au(111) vacuum region to place the molecule there. Then close the Molecular Builder widget.

⚠ Warning

Take care to click only once to add the Bz molecule to Au(111). For each click, a new molecule will be added at exactly the same position, so that it's atoms will overlap with those of the already existing molecule!

Remember that you can always check for the presence of overlapping atoms by using the Selection Tools ► Close Neighbors plugin and choosing a relatively small threshold (for example, 0.001 Å).

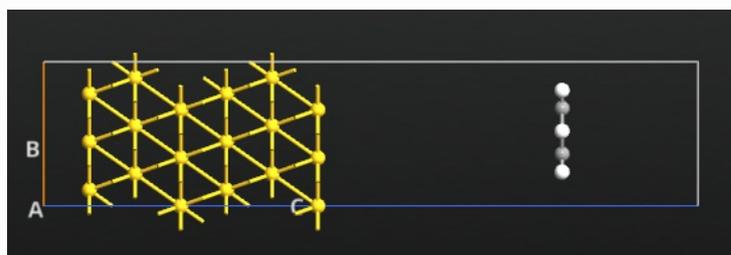
You will then need to rotate the molecule 90

- First select all Bz atoms by using the mouse to draw a rectangle around the molecule. Then open the Coordinate Tools ► Rotate plugin. Set the rotation axis to "y" and the rotation angle to 90
- , and make sure the check-box *Rotate around selection center* is ticked. Click **Apply** to perform the rotation.

The screenshot shows the Builder software interface. The main window displays a 3D model of a surface (hcp30) and a molecule (Bz). The Rotate plugin is active, and the following settings are shown:

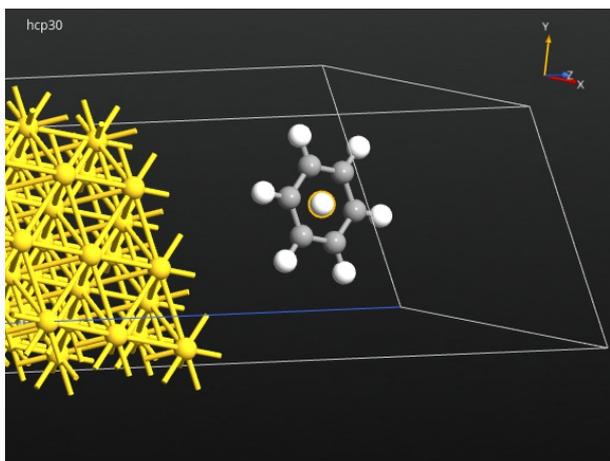
- Coordinate Tools** ► **Rotate**
- To input the normal vector and the center using fractional coordinates, check the **Fractional** box below.
 Fractional
- To rotate the configuration, first define the vector **V** and the center **C** that defines the rotation axis.
x (Å) y (Å) z (Å)
V 0 1 0
C 1.44188 3.54689 27.9412
- A set of predefined rotation axes can be chosen from the combo box below:
Rotation axes: y
- Then choose the rotation angle using the input fields below.
Angle (°): 90.0
- Rotate around selection center
- Check the **Copy** box, if you want the rotated atoms to be copied. Finally, press **Apply** in order to perform the actual rotation.
 Copy

The Stash panel at the bottom left shows the current state of the simulation, with the hcp30 surface and the Bz molecule selected.



Next step is to move the Bz molecule into position in the hcp-30

- adsorption site. First, make sure all Bz atoms are selected. Then click the  icon to add a new atom in at the geometrical center of the molecule. You will use this anchor atom to "snap" the molecule into position above the surface.



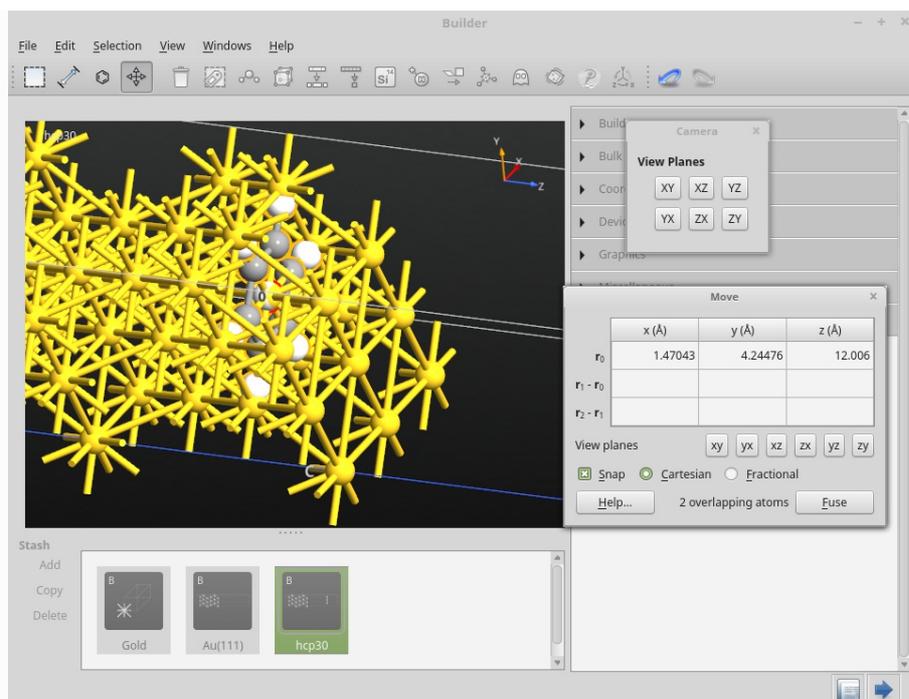
Select again all benzene atoms, including the extra atom, and rotate the view such that you see a top-view of the configuration.

Tip

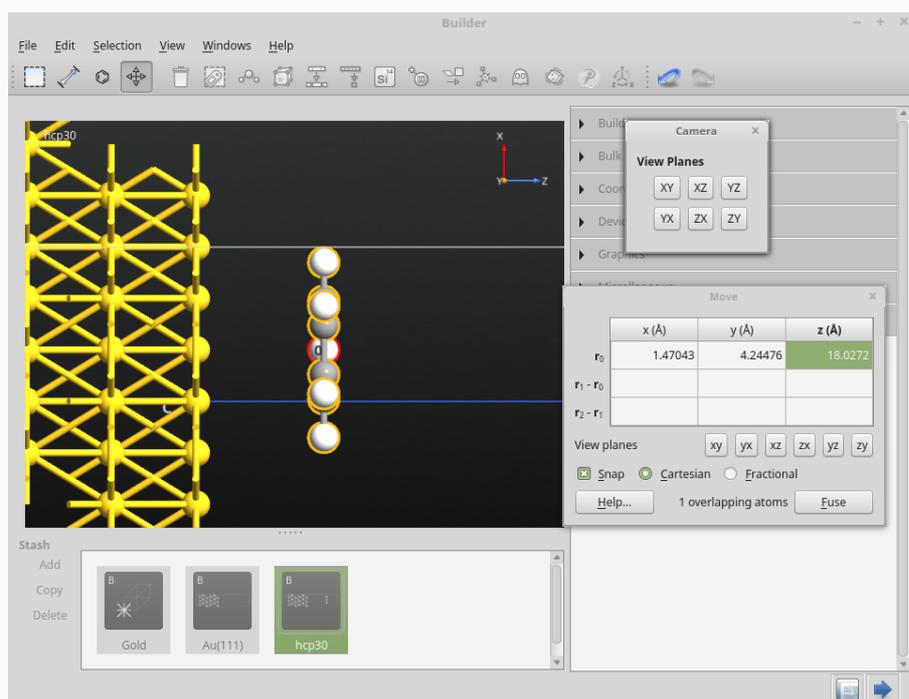
The  Camera tool may be useful: Select the **XY** view plane to get a perfect view down along the z-axis.

Click the  icon to open the **Move** tool, and then click the extra “snap-atom” in the middle of the molecule to select it as an anchor atom. The selection shade should change color to red.

In the **Move** panel, make sure that the **Snap** option is selected. Use then the mouse to drag the molecule by the anchor atom, and drop it such that the anchor atom snaps onto a gold atom in the second slab layer.



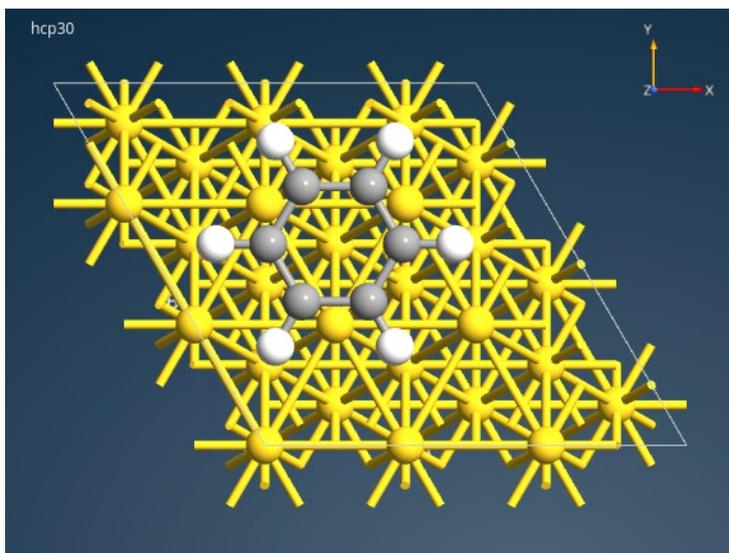
Finally, adjust the molecule–surface distance such that it matches the 3.62 Å reported in [LRZ+13]: In the **Move** panel, enter 18.0272 Å for the z-coordinate of the anchor atom position r_0 , as shown in the figure below.



Note

In general, to set the desired molecule–surface distance, you of course need to first know the cartesian coordinate Z of the Au topmost layer. This can be done by simply hovering the pointer above one of the atoms of the Au(111) topmost layer.

Finally, remove the anchor atom by selecting it and deleting it. Your “*hcp30*” configuration should now look like this:



Tip

You may save the configuration as an ATKPython script, or **export** it to a range of popular file formats.

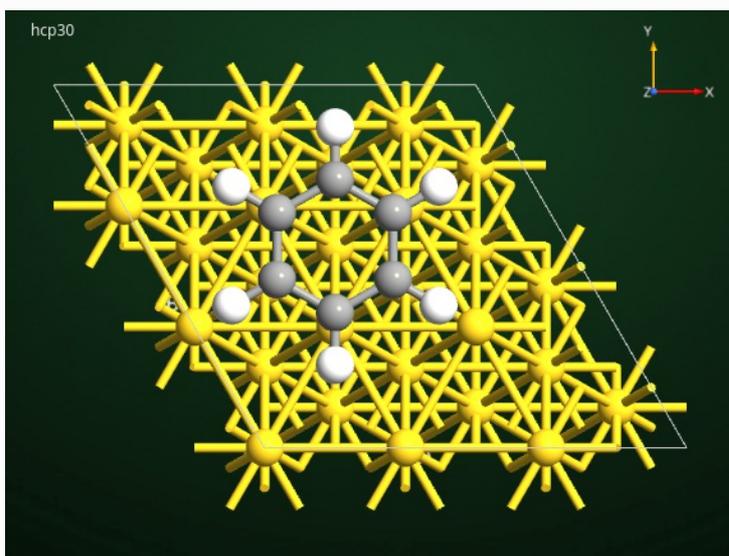
Creating the hcp-0 configuration

- The hcp-0
- adsorption configuration is simply related to the hcp-30
- one by a 30
- rotation of the benzene adsorbate (assuming constant Bz–Au(111) distance).

First, **copy** the “hcp30” Stash item and **rename** the copy to “hcp0”. Then select all benzene atoms in the newly created copy, and open once again the Coordinate Tools ▶ Rotate plugin.

Apply a rotation of 30

- around the z-axis, which is normal to the surface plane. The “hcp0” configuration should now look like this:



References

[LRZ+13] (1, 2, 3, 4, 5, 6) Wei Liu, Victor G Ruiz, Guo-Xu Zhang, Biswajit Santra, Xinguo Ren, Matthias Scheffler, and Alexandre Tkatchenko. Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. *New Journal of Physics*, 15(5):53046, 2013. URL: <http://stacks.iop.org/1367-2630/15/i=5/a=053046>.

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