

 winmostar tutorial

Modeling Crystal Slab Model

V11.5.6

05 January, 2024 X-Ability Co., Ltd.

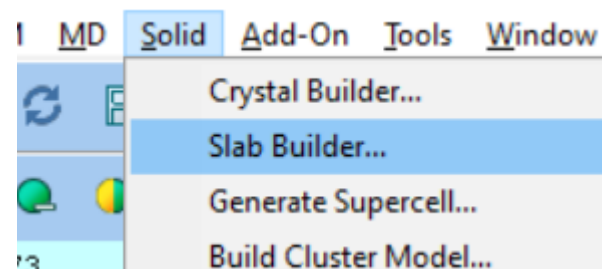
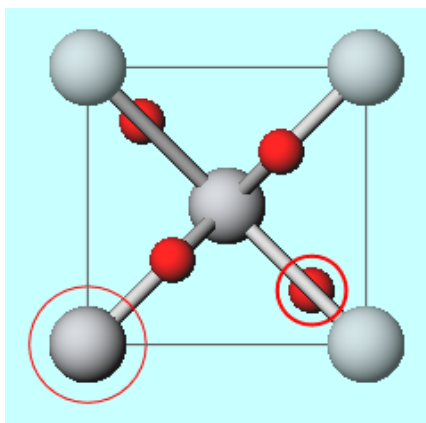
About This Document

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult [Beginner's Guide](#).
- For those who wish to explore the details of each feature, please refer to [Winmostar User Manual](#).
- If you are unable to proceed with the operations as outlined in this manual, please first consult [Frequently asked questions](#).
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us from [Contact](#). Attach files generated at the time of the issue and provide steps to reproduce the problem.
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A. Loading the Unit Cell

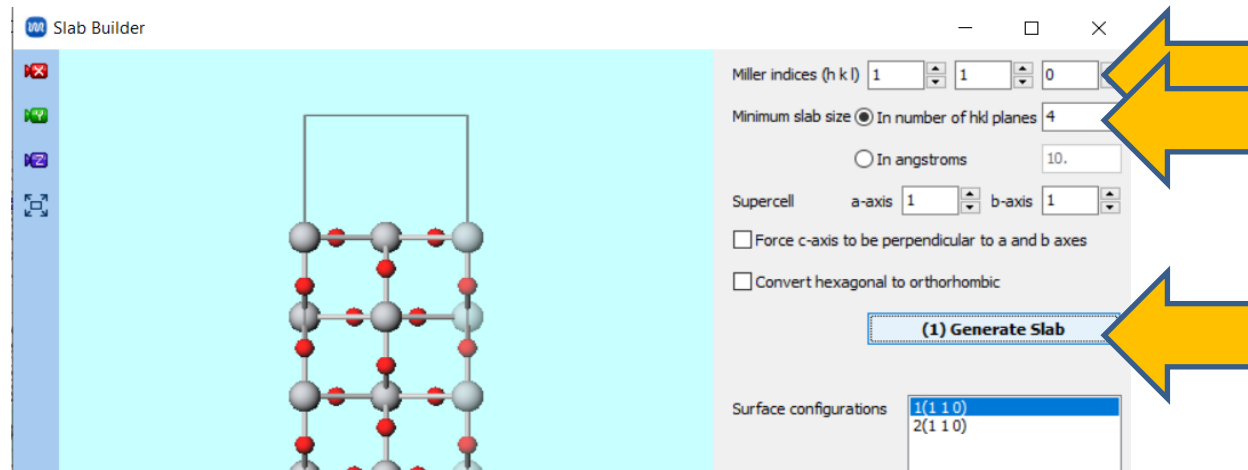
For detailed methods on creating a unit cell, please refer to [Crystal Modeling Unit Cell Edition tutorial](#). Here, we will load an existing molecular structure file.

- A. Click **File | New File, New Project**, or **Edit | Reset Structure**.
- B. Click **File | Import | Samples File | tio2_rutile.cif**.
 - If you wish to load a specific file, use **File | Import File** at this stage instead.
- C. In **Import File** dialog, click **Discard and Import**.
 - If necessary, perform structure optimization calculations at this stage (omitted in this manual).
- D. Click **Solid | Slab Builder**, and after 'Analyzing symmetry using Spglib...' is displayed for a few seconds, **Slab Builder** window will appear.



B. Creation of Slab

- A. Change **Miller indices** to the desired surface Miller indices '1', '1', '0'.
- B. To change the thickness, alter **In number of hkl planes** in **Minimum slab size** to '4'.
 - If you want to create steps or other features later as per the procedure on page 7, set a slightly larger size.
- C. (Not needed in this manual) To expand the cell in the surface direction, modify the values in **Supercell**.
- D. (Not needed in this manual) If necessary, click **Force c-axis to be perpendicular to a and b axes** or **Convert hexagonal to orthorhombic**.
- E. Click **Generate Slab** and wait a few seconds for the process to complete, and the slab structure will appear on the left. If you want to change Miller indices, thickness, surface size, or cell shape, return to steps 1-4, make the changes, and click **Generate Slab** again.

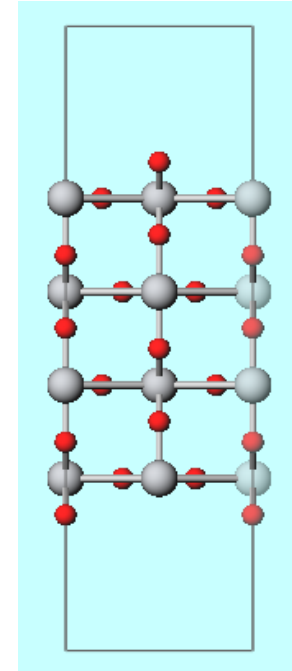
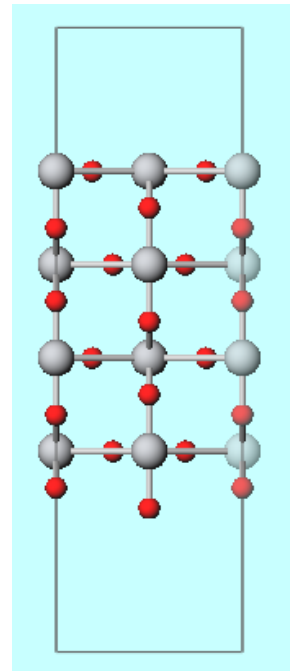
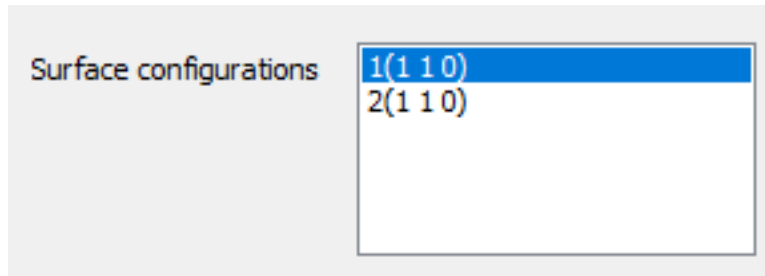


B. Creation of Slab

- A. (Not needed in this manual) To change the position where the surface is cut, modify the options in **Surface configurations**. Note that some crystals may have only one option available.
- If you wish to create a slab with a changed composition overall, such as a symmetric slab, use the procedures from page 7 onwards. Therefore, it is not a problem if only one side of the slab initially matches the structure you ultimately want to create.

For 1(1 1 0) case

For 2(1 1 0) case

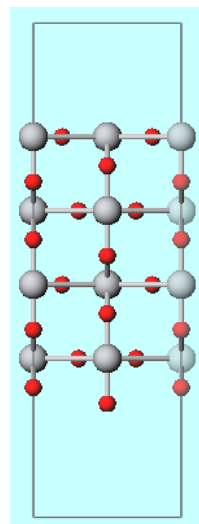


B. Creation of Slab

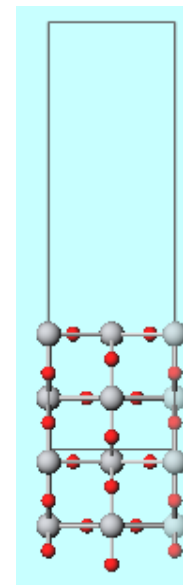
- (Not needed in this manual) If you want to change the thickness of the vacuum layer, modify the values of **Vacuum** or **Total width**.
- (Not needed in this manual) To change the position of the slab, adjust **Position** (refer to the diagram below).
- Finally, click **OK**. If 'Successfully generated slab' is displayed, click **OK** again.

Slab [A]	Vacuum [A]	Total width [A]
11.724834	+ 10	= 21.724834
Position	Adjust center of slab to center of cell <input checked="" type="checkbox"/>	
(2) OK		

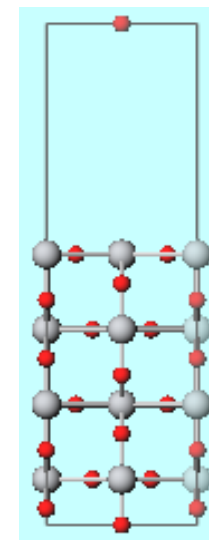
Adjust center
of slab to
center of cell



Adjust center
of slab to
origin of cell



Adjust origin of
slab to origin
of cell



C. Adjusting the Structure

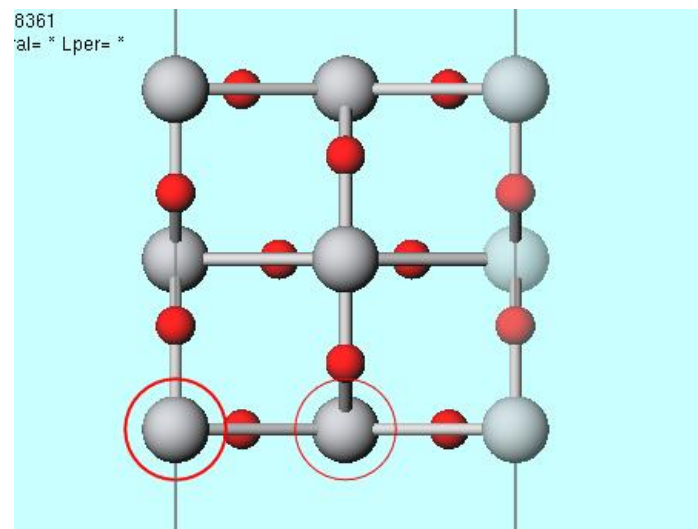
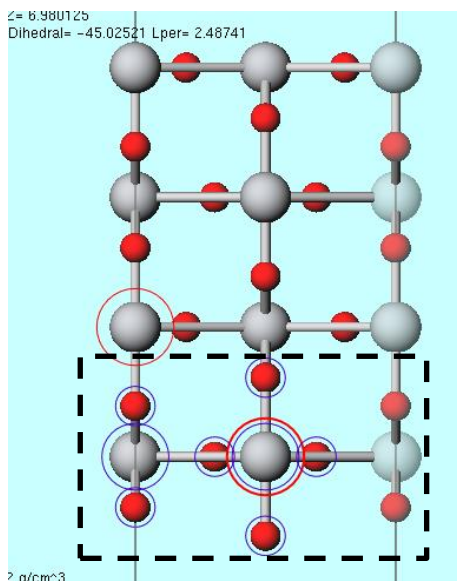
Here, we adjust the structure to create a symmetric slab. Steps and other features can be created using a similar procedure.

A. Click  (**Align View to X-Axis**) .

B. Select the area indicated by the dotted line in the diagram by Ctrl+dragging to create a rectangle.

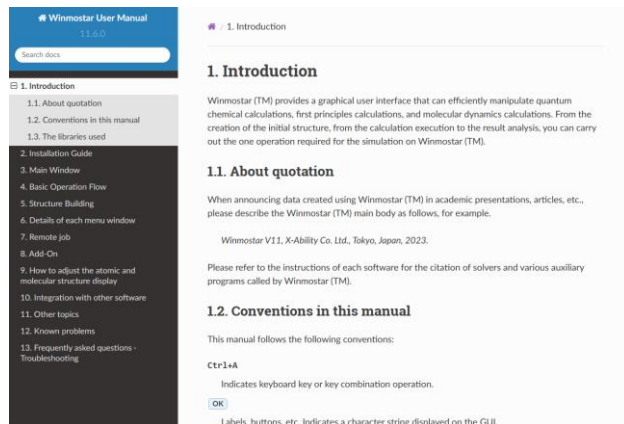
- For atoms that are replicated and displayed on both sides of the cell, blue circles will appear on only one side.

C. Click  (**Delete Atom**), then click **Delete**.



Troubleshooting and Additional Resources

- For detailed information on each feature, please refer to [Winmostar User Manual](#).



[Winmostar User Manual](#)

- If you are unable to proceed as instructed in this guide, please first refer [Frequently asked questions](#).
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through [Contact](#), detailing the steps to reproduce the issue and attaching any generated files at that time.