

 winmostar tutorial

Modeling Crystal Unit Cell

V11.5.6

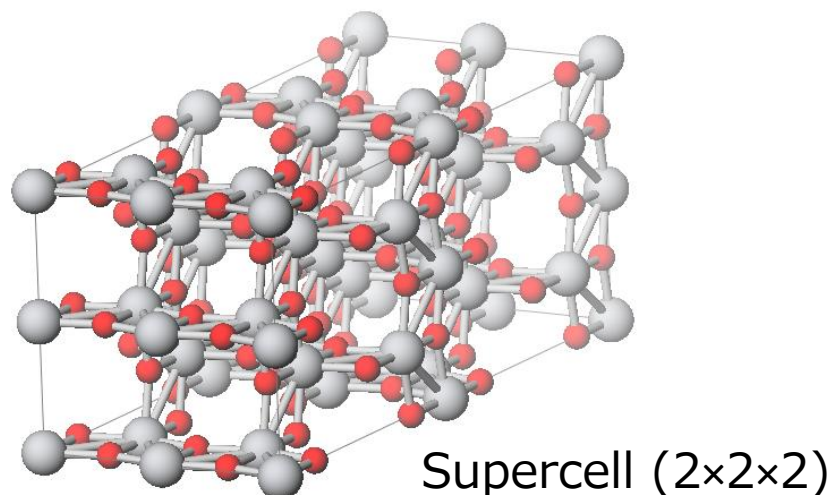
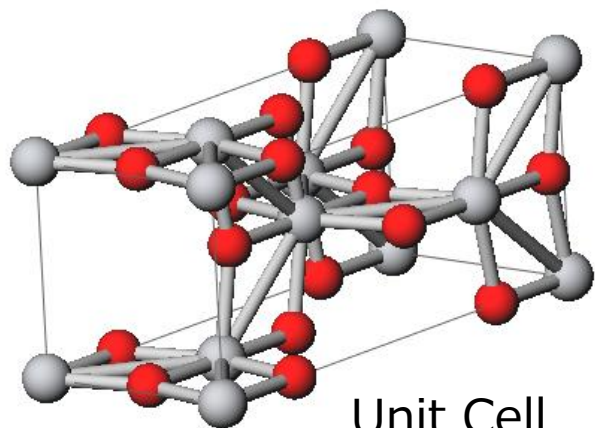
05 January, 2024 X-Ability Co., Ltd.

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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Overview

- In Winmostar, crystal structures can be created using the following two methods:
 - A. Load files created in other software or obtained from various databases.
 - Supports formats such as pdb, cif, xyz.
 - For detailed procedures, refer to the [Molecular Modeling Organic Molecules Edition tutorial](#).
 - B. Direct modeling of 3D crystal structures.
- In this tutorial, we will introduce the procedure using anatase-type TiO₂ crystal as an example under 'B. Direct Modeling of 3D Crystal Structures'. The method for creating a supercell will also be shown.



A. Creation of Unit Cell

- Click **File | New File, New Project**, or **Edit | Reset Structure**.
- Click **Solid| Crystal Bulder**.
- Set **Crystal System** to **Tetragonal** and **Space Group** to **141**. Change **Lattice Constants** with **a** to '3.7842' and **c** to '9.5146', then press Enter key.

The screenshot shows the Crystal Builder software interface. A yellow arrow points to the 'Solid' menu, which is open, showing 'Crystal Builder...' and 'Slab Builder...'. Another yellow arrow points to the 'Crystal System' dropdown menu, which is set to '[075-142]: Tetragonal'. A third yellow arrow points to the 'Lattice Constants' section, where the 'c' length is set to 9.5146. The 'Lattice Constants' section also shows 'a' and 'b' lengths set to 3.784200. The 'Asymmetric unit' table below shows the coordinates for the unit cell.

Element	X	Y	Z
C	0.000000	0.000000	0.000000


A. Creation of Unit Cell

- A. Click **Add atom** in **Asymmetric unit**.
- B. Double-click the first cell in the first row and change **Element** from **C** to **Ti**.
- C. Similarly, change **Element** in the second row from **C** to **O**.
- D. Change **Z** value in the second row to '**0.2081**'.
- E. Click **OK**.

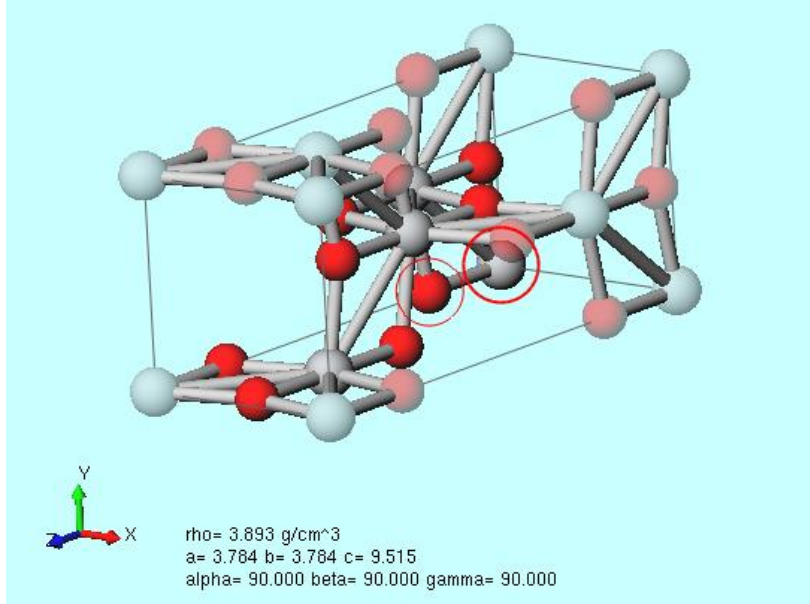
Element	X	Y	Z
Ti	00	0.000000	0.000000
O	00	0.000000	0.2081

- The first click is for selection
- The second click is for editing

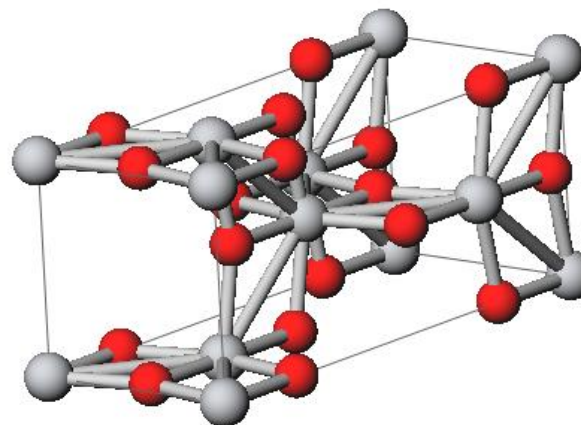
Supplement: Adjusting the Display Method of Crystals

Atoms on the cell boundaries, other than asymmetric elements, are displayed semi-transparently by default. To display these atoms opaquely, click  (**View Preset**) button and select 'Winmostar Report'. Alternatively, adjust the settings in **Tools | Preference | View | Replicated atoms at cell edge on both sides**.

Winmostar N= 12 Ti4O8 M= 319.46
Marked Order: 1 - 2 - 0 - 0
Marked Atom: X= 0 Y= 0 Z= 0
Length= 1.98 Angle= * Dihedral= * Lper= *



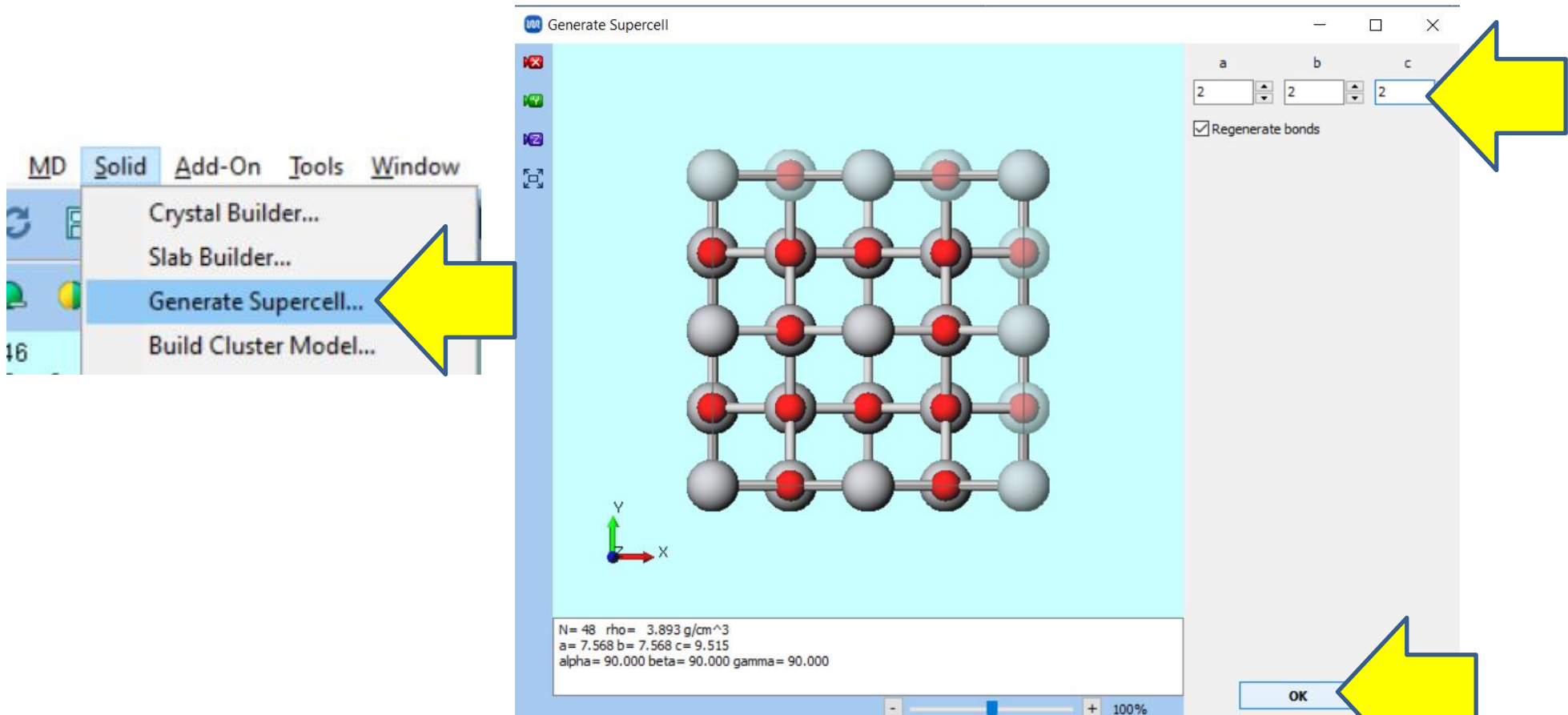
Winmostar Modeling (Default)



Winmostar Report

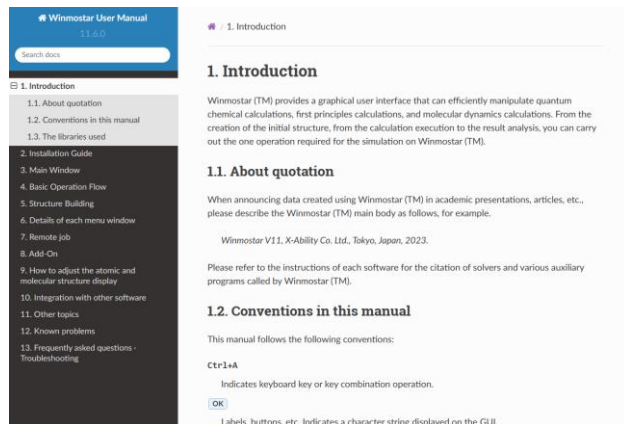
B. Construction of a Supercell

- A. Click **Solid** | **Generate Supercell**.
- B. Change **a**, **b**, and **c** each to '2' and click **OK**.



Troubleshooting and Additional Resources

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



[Winmostar User Manual](#)

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