

Introduction to VESTA for Material Modeling and Visualization

Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften

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Garching bei München | 2025

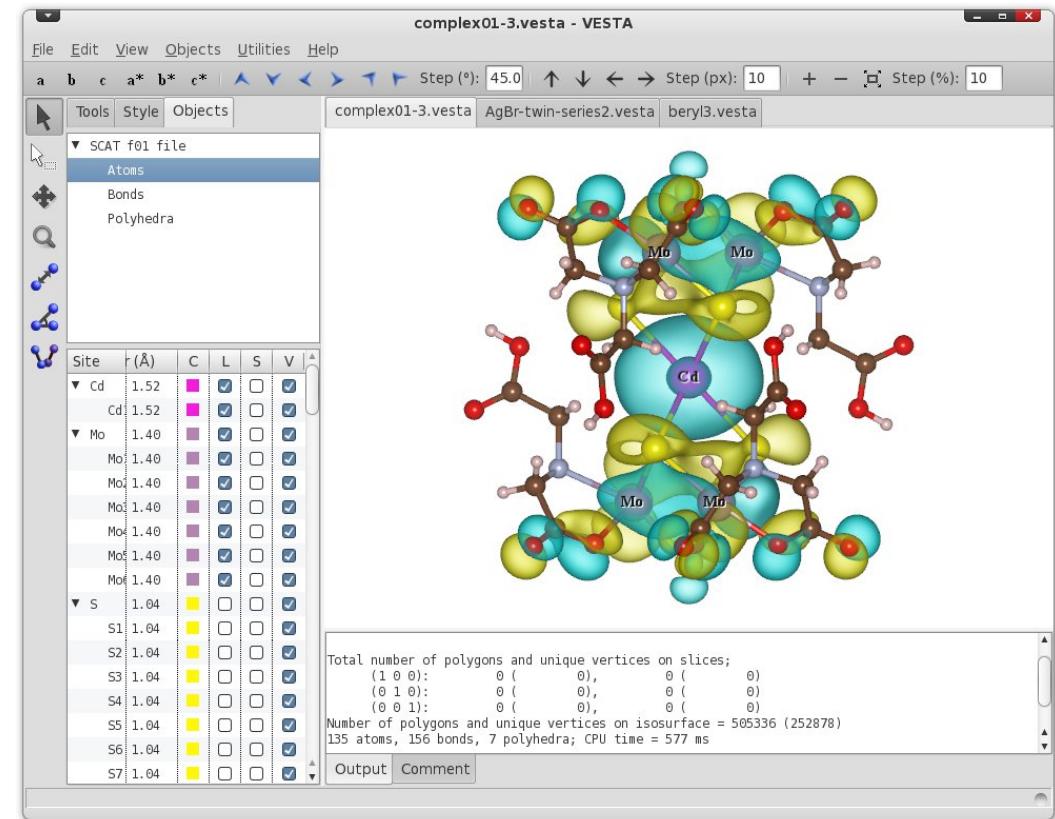
What is VESTA?

3D visualization program by JP-Minerals.

Handles:

- Structures (CIF, POSCAR, PDB)
- Volumetrics (Cube, XSF)
- Crystal faces

Free for academic users; supports Windows, Mac and Linux



<https://jp-minerals.org/vesta/en/gallery.html>

Installation

- Download on <https://jp-minerals.org/vesta/en/download.html>
- Extract archive and run executable (no installer required)
- Available for Win/Mac/Linux

Latest stable versions



Windows

- [VESTA.zip](#) (ver. 3.5.8, built on Aug 11 2022, 14.3MB)
For 32-bit version of Windows.
- [VESTA-win64.zip](#) (ver. 3.5.8, built on Aug 11 2022, 17.2MB)
For 64-bit version of Windows.



macOS

- [VESTA.dmg](#) (ver. 3.5.8, built on Aug 11 2022, 25.3MB)
Requires OS X 10.9 or newer, Intel CPUs that are capable of 64 bit instruction sets.



Linux x86_64

- [VESTA-gtk3.tar.bz2](#) (ver. 3.5.8, built on Aug 11 2022, 23.8MB)
Requires GTK 3.22 or newer.
Distributions where VESTA is known to work:
 - Redhat Enterprise Linux 7 or later
 - Ubuntu 18.04 or later

- [VESTA-gtk2.tar.bz2](#) (ver. 3.5.8, built on Aug 11 2022, 23.1MB)
Requires GTK 2.10 or newer.
Distributions where VESTA is known to work:
 - Fedora 10 or later
 - openSUSE 11.2 or later
 - Redhat Enterprise Linux 5 or later
 - Ubuntu 9.10 or later

VESTA: Components of the Main Window

Horizontal Toolbar

Menu Bar

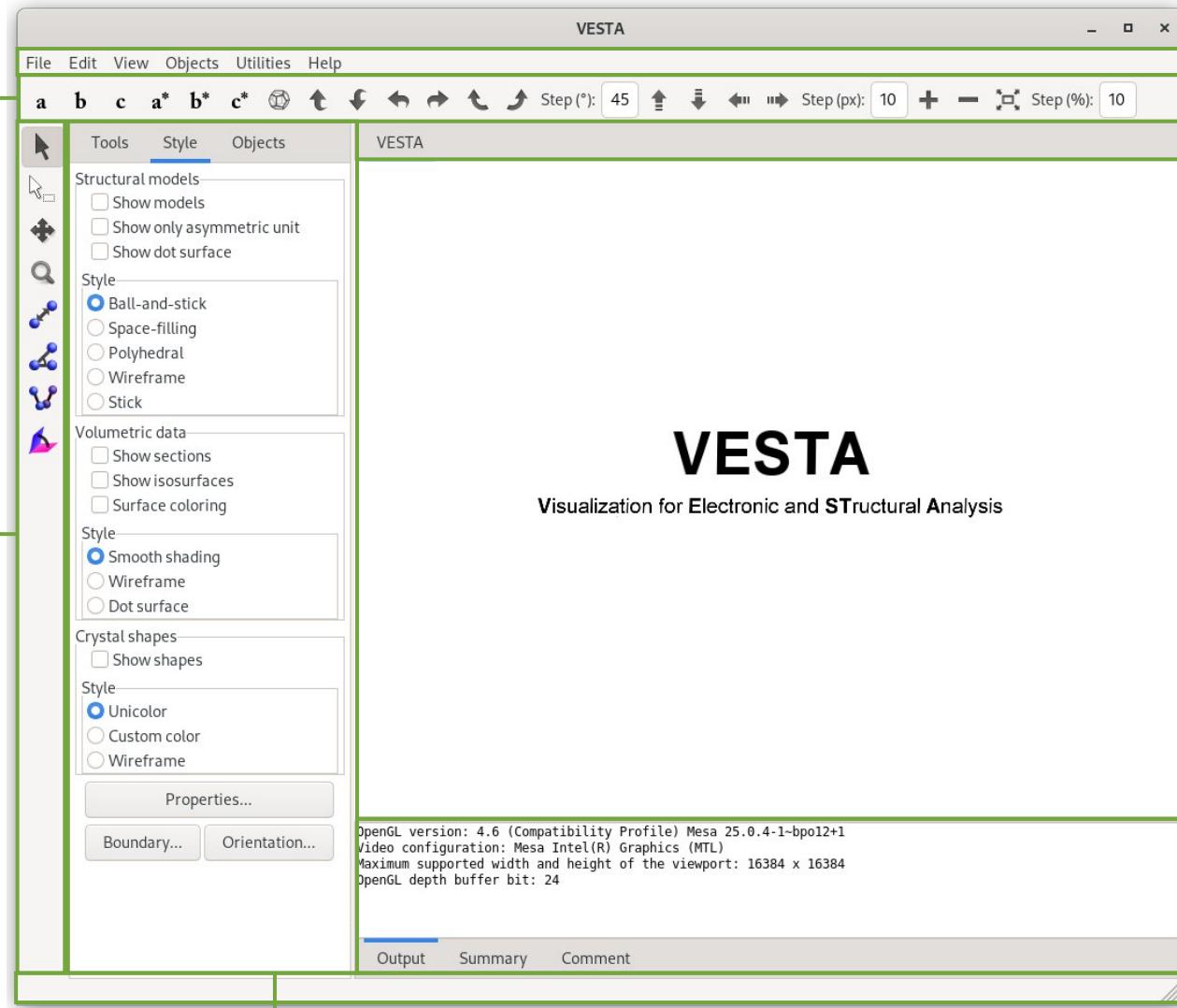
Vertical Toolbar

Graphics Area

Side Bar

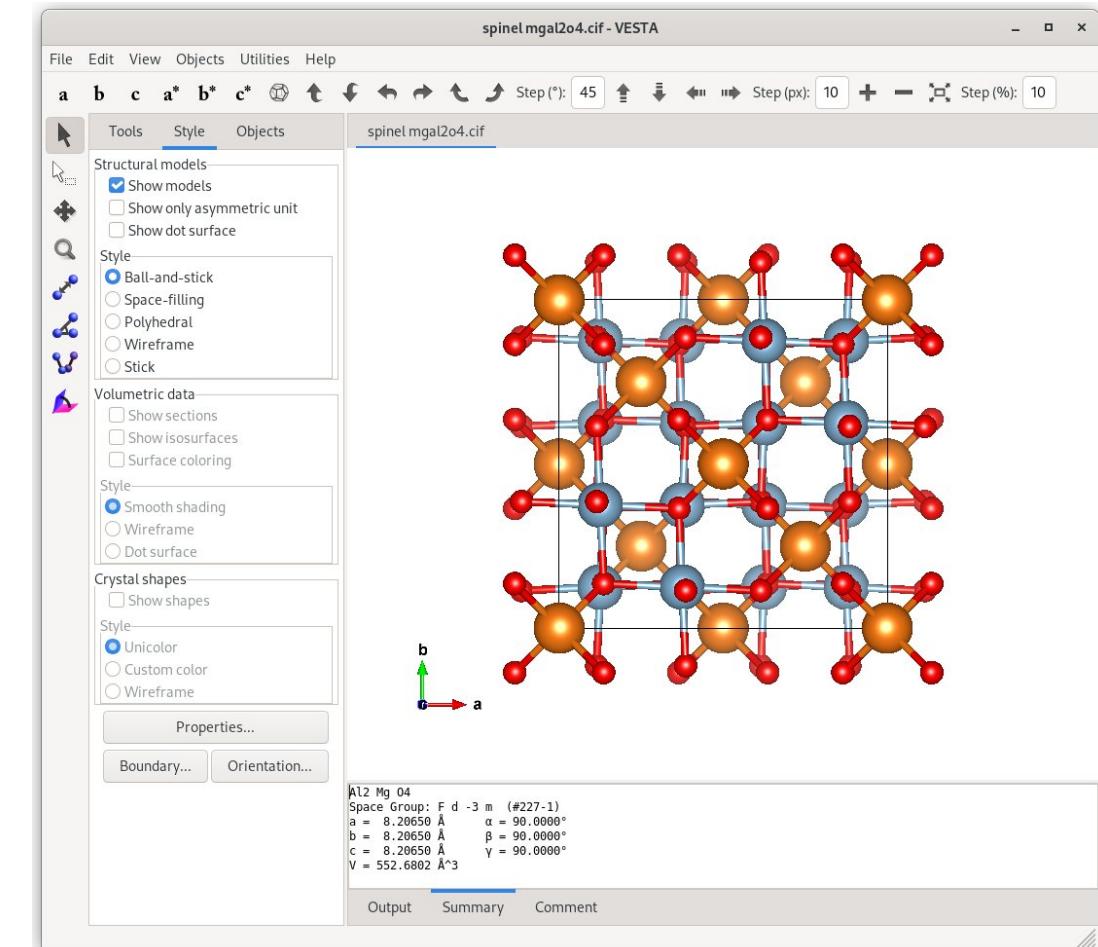
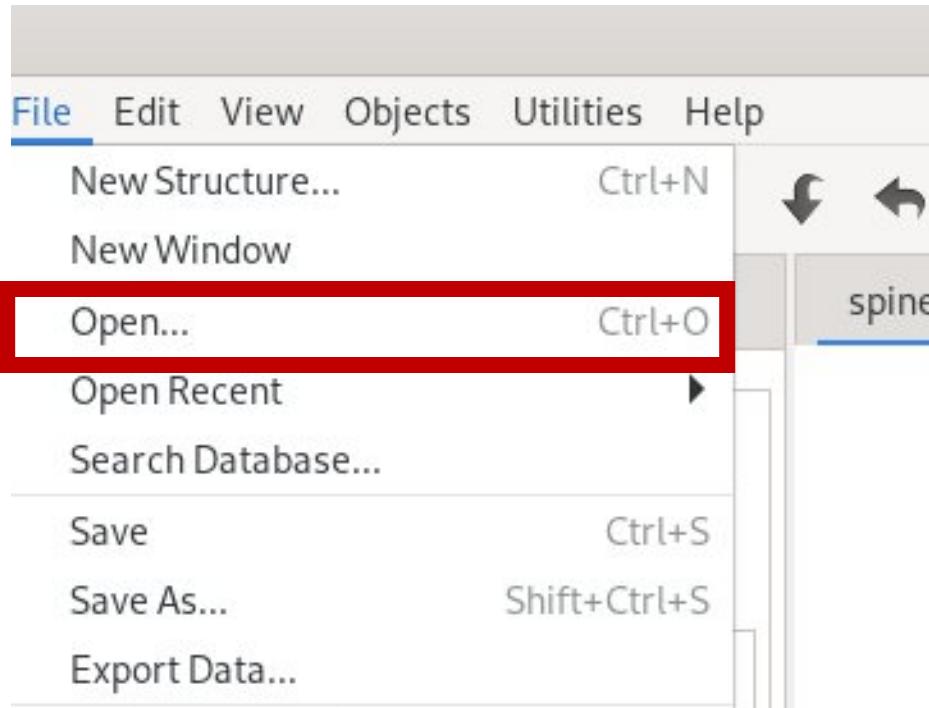
Text Area

Status Bar



Opening a Structure

- **File → Open** (e.g., CIF file)
- Drag and drop
- Interface autofocus and quick visualization



Navigating Unit Cells

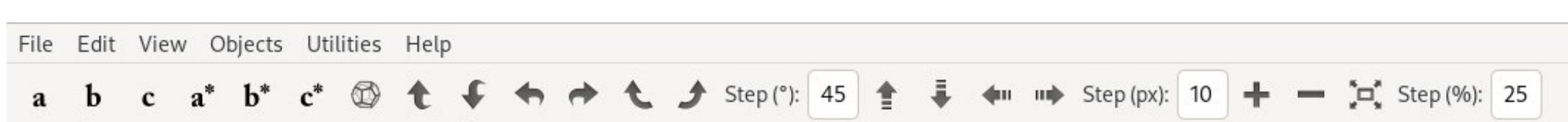
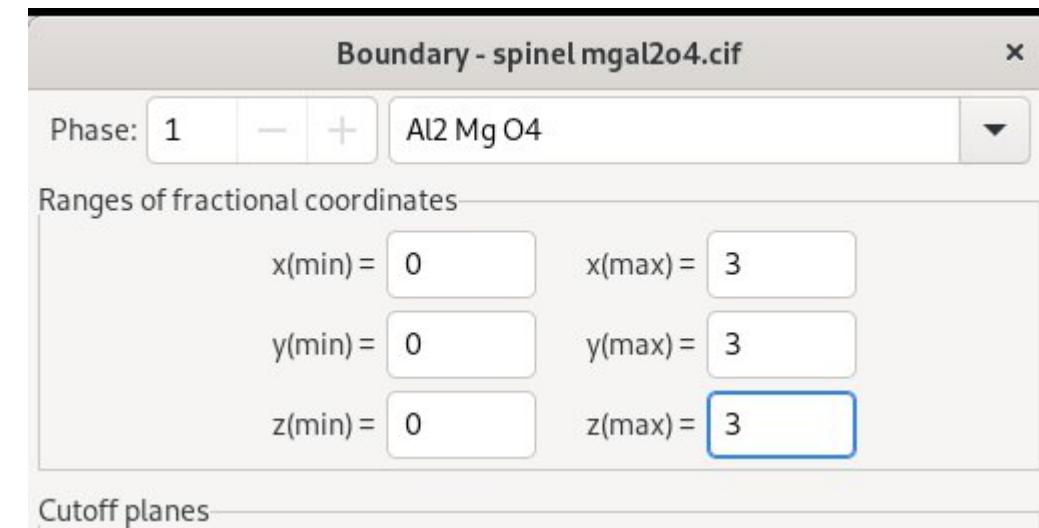
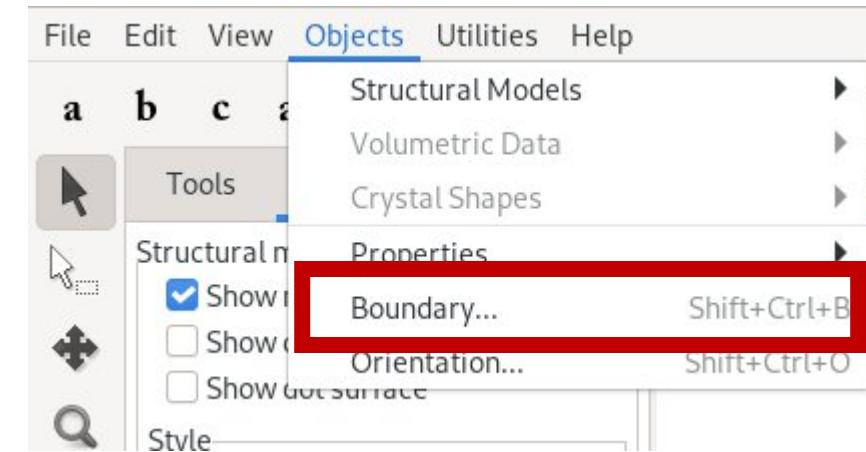
- Rotate via mouse drag, zoom with scroll
- Realign axes via toolbar (a, b, c)
- Display supercell via **Objects** → **Boundary**, set repeat counts



: Rotate freely

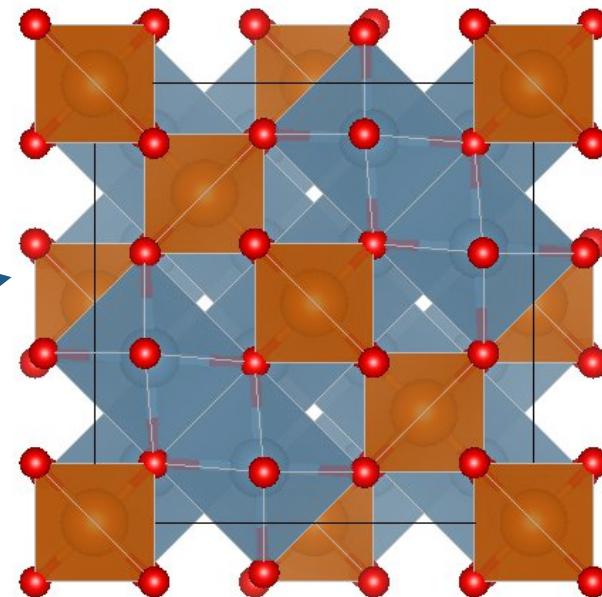
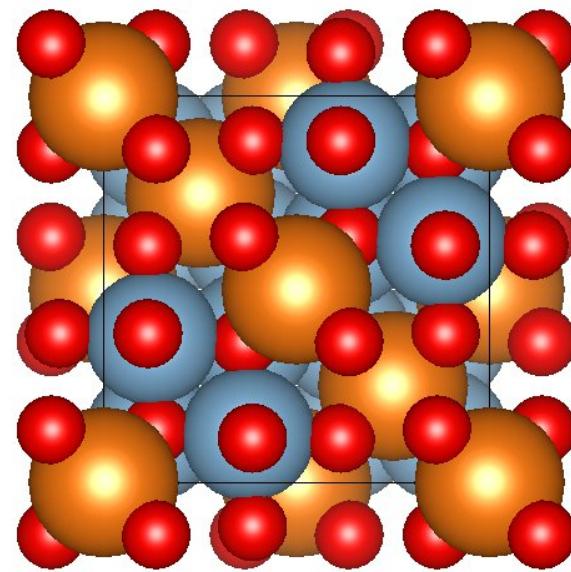
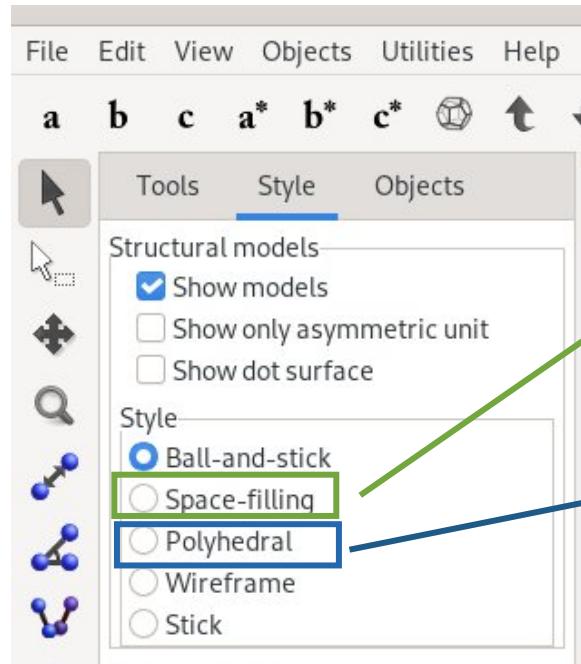


: Zoom in and out



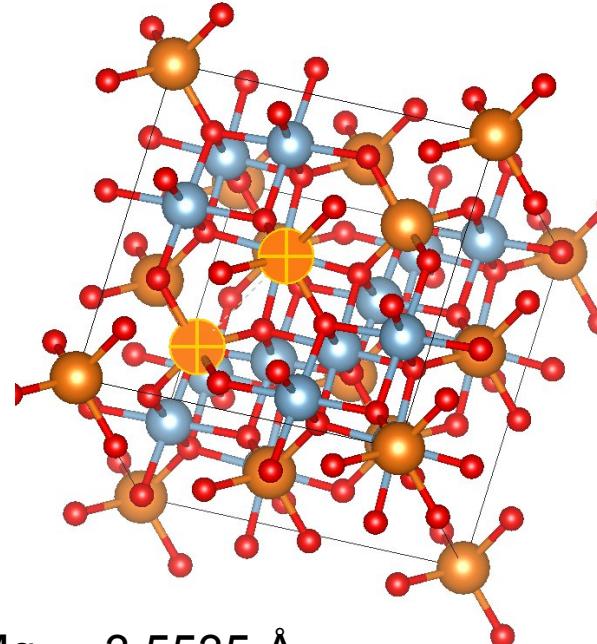
Representation Styles

- Options include: Ball-and-stick, space-filling, polyhedral, wireframe
- From **Objects → Style**, apply per site or bond type



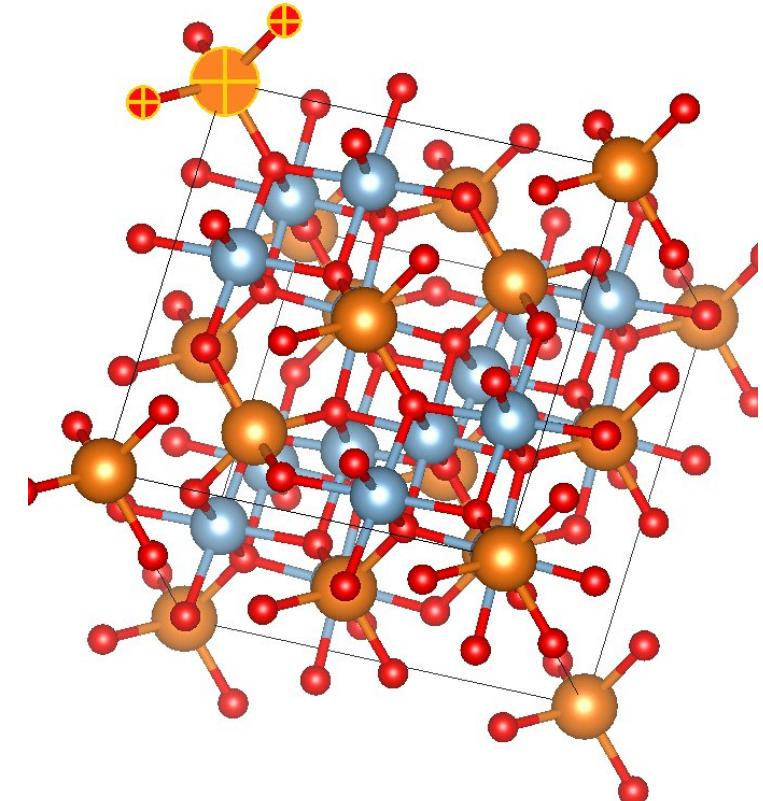
Measuring Geometry

- Select atoms to measure bond distances, angles
- Tools available in measurement toolbar



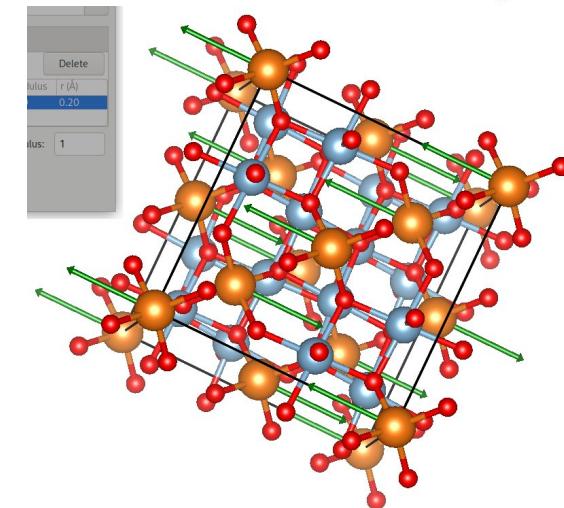
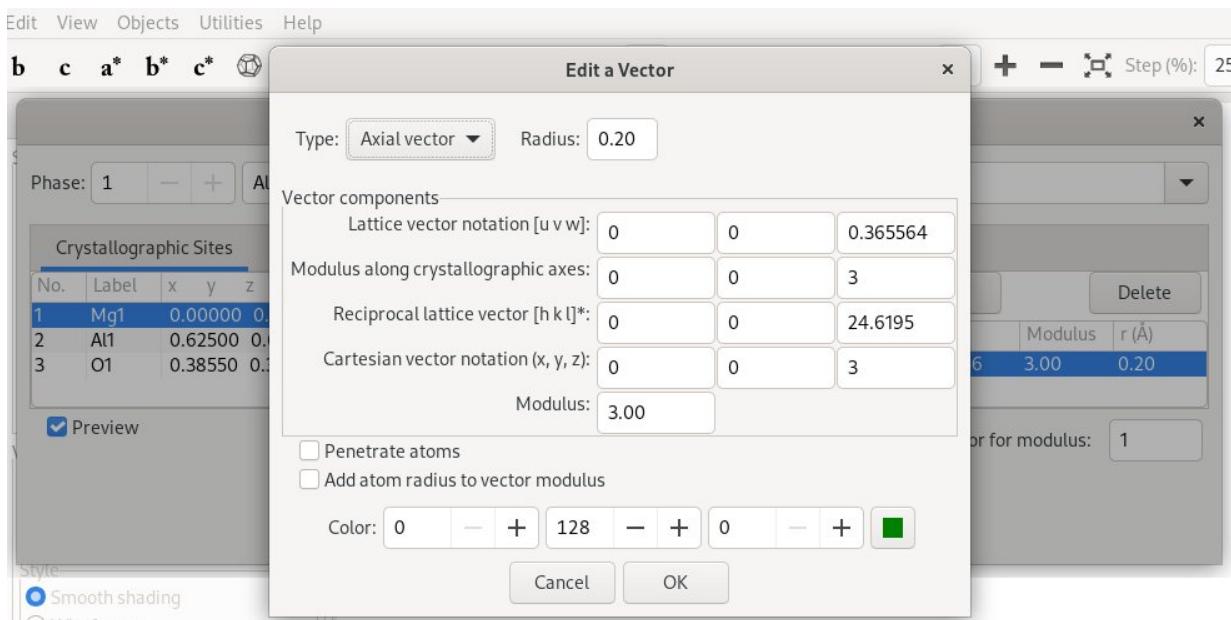
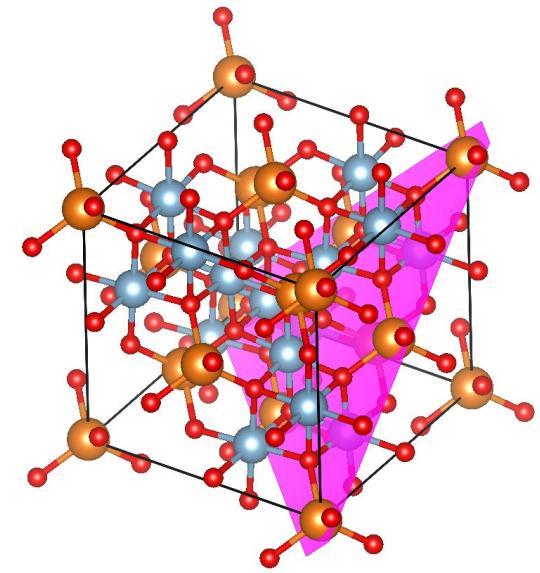
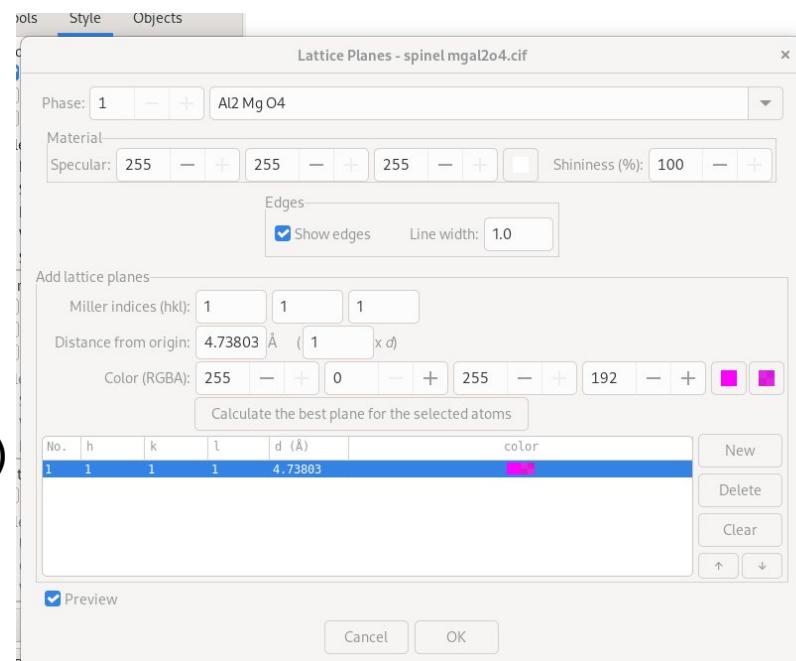
- Free movement
- Select
- Translate
- Magnify
- Distance
- Angle
- Dihedral angle
- Interfacial angle

O-Mg-O = 109.4712 deg.



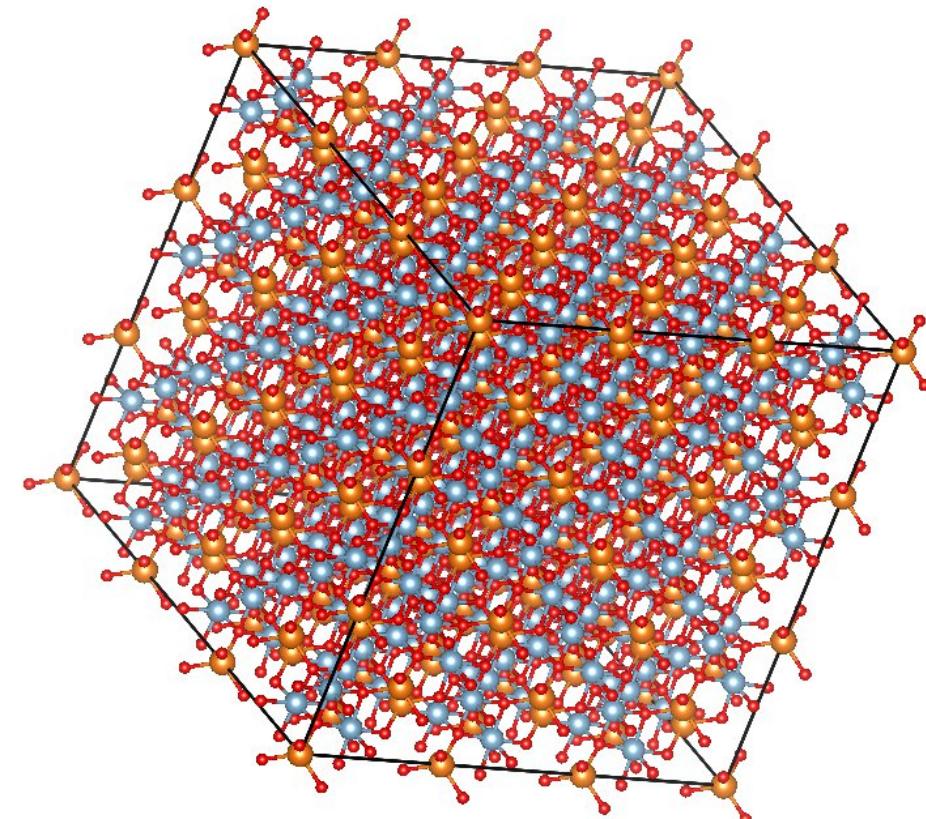
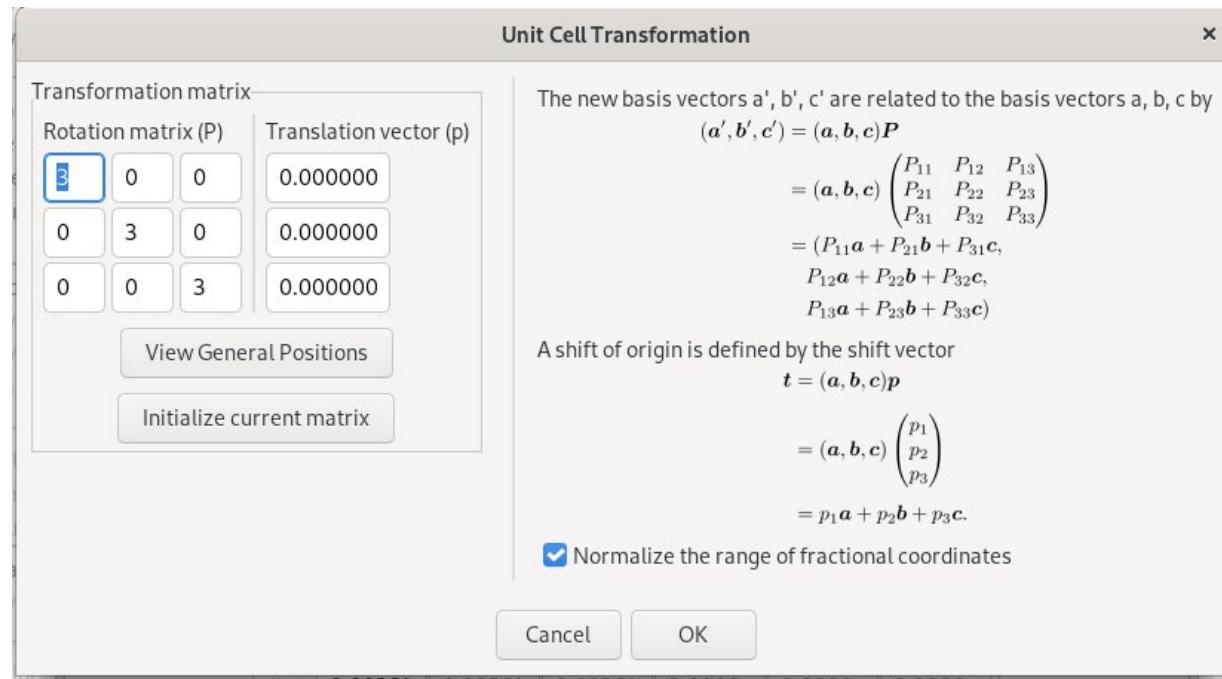
Lattice Planes & Vectors

- **Edit → Lattice Planes → add miller indices**
(e.g., (111) plane)
- **Edit → Vectors → specify indices (e.g., [111])**
to visualize geometry



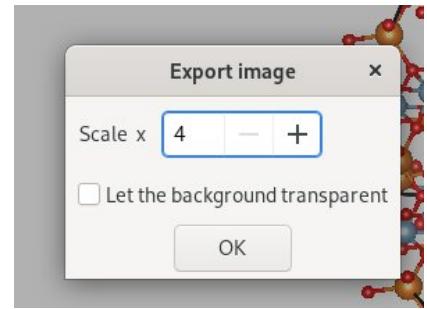
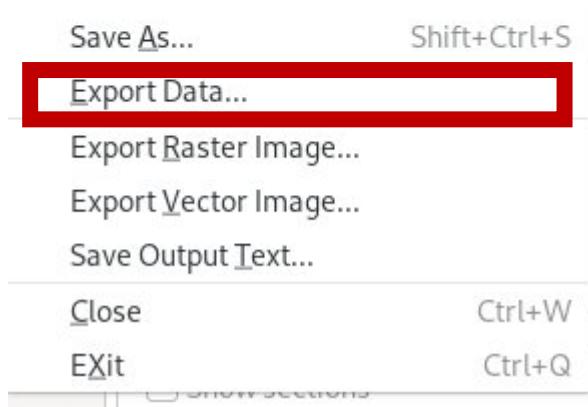
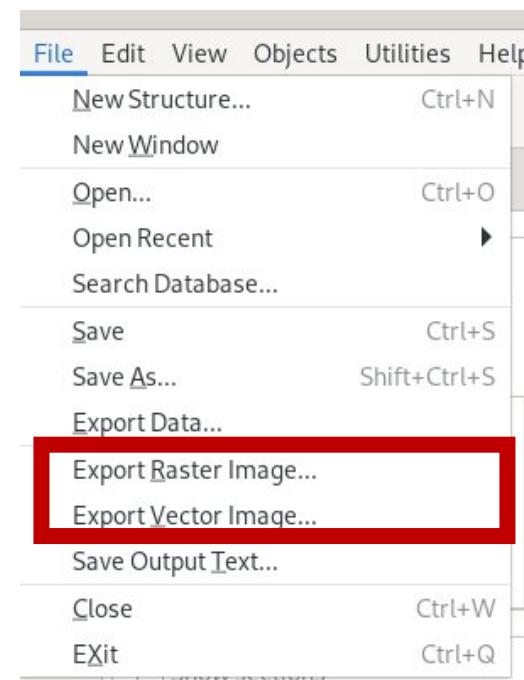
Lattice Transforms & Supercells

- Under **Edit Data**, apply lattice lattice matrix
- Generate super- or sub-lattice cells
- Useful for analyzing symmetry variations



Export Options

- **File → Export Raster/Vector Image:** choose EPS, PDF, SVG, PNG, TIFF, etc.
- Export beyond screen resolution for publication quality
- **File → Export Data:** CIF, POSCAR, PDB, STL, etc.



Learning Resources

- **Official manual:**
 - <https://jp-minerals.org/vesta/en/doc.html>
- **PDF tutorials:**
 - Many university-hosted guides and quick-start files
(search „VESTA tutorial PDF“)
- **Youtube walkthroughs**
- **Community Q&A and help:**
 - Look at forums like ResearchGate, Crystallography Reddit, or the VESTA Google Group



The screenshot shows the VESTA software documentation page. At the top is a logo featuring a 3D molecular model of a crystal structure. To the right of the logo, the word "VESTA" is written in large blue letters, with "Visualization for Electronic and Structural" in smaller text below it. Below the logo is a breadcrumb navigation bar: "Software > VESTA > Documentation". The main content area is divided into two columns. The left column, under "Home", includes links to "About", "History", and "Donate". The right column, under "Manual", is titled "For VESTA 3 series" and contains a link to "VESTA_Manual.pdf". Below this, text explains that the manual can be opened by placing the binary file of VESTA in a specific directory on Linux. Further down, it mentions an "Online manual" and "Other information about VESTA". On the far left, there is a vertical sidebar with links to "RIETAN-FP", "VESTA" (which is expanded to show "Change Log", "Features", and "Gallery"), and "Documentation" (which is also expanded to show "Online Manual").

Thank You!

- **Contact:**
 - Dr. Birkan Emrem at LRZ-CXS Group
(Birkan.Emrem@lrz.de)
- **Special Thanks:**
 - JP-Minerals for VESTA
 - Computational X Support Group at LRZ
 - Everyone attending today!