

Introduction to VESTA for Material Modeling and Visualization

Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften

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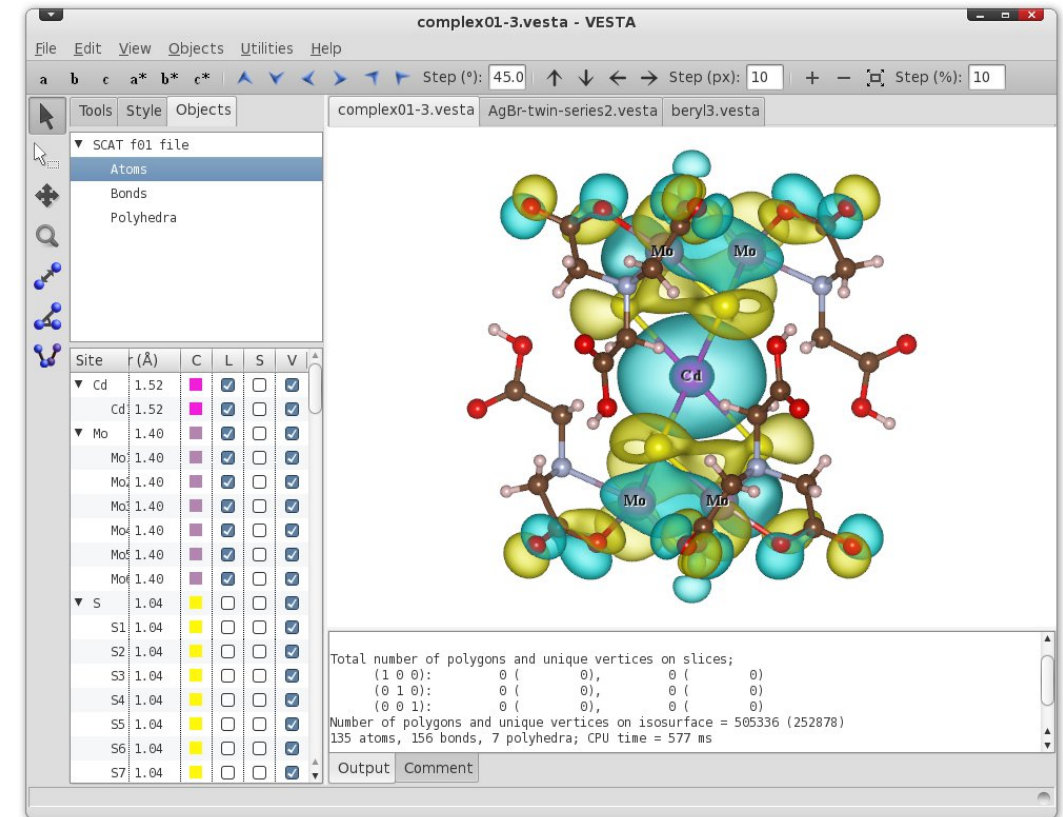
What is VESTA?

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

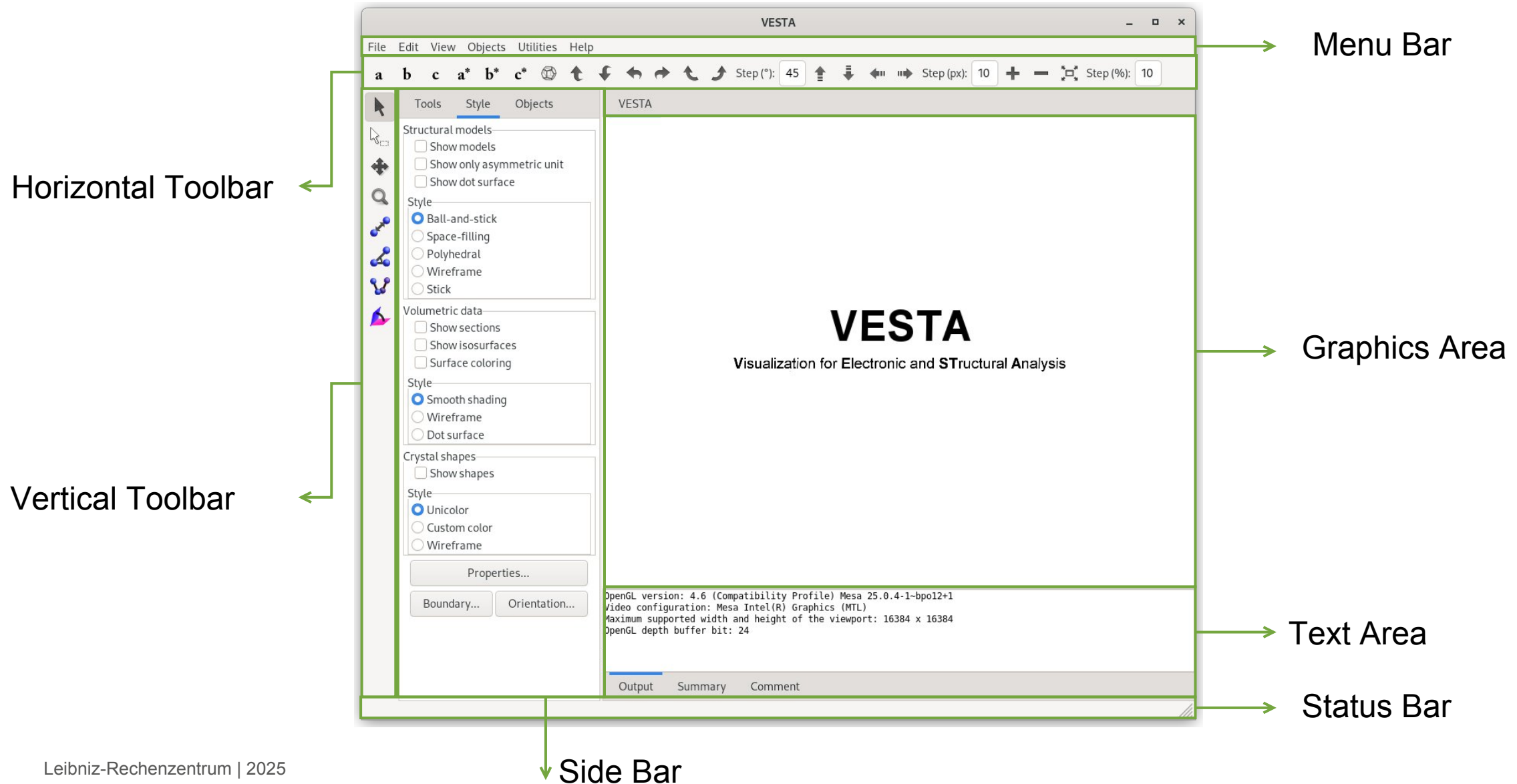
- [VESTA.dmg](#) (ver. 3.5.8, built on Aug 11 2022, 25.3MB)
Requires OS X 10.9 or newer, Intel CPUs that are capable of 64 bit instruction sets.



Linux x86_64

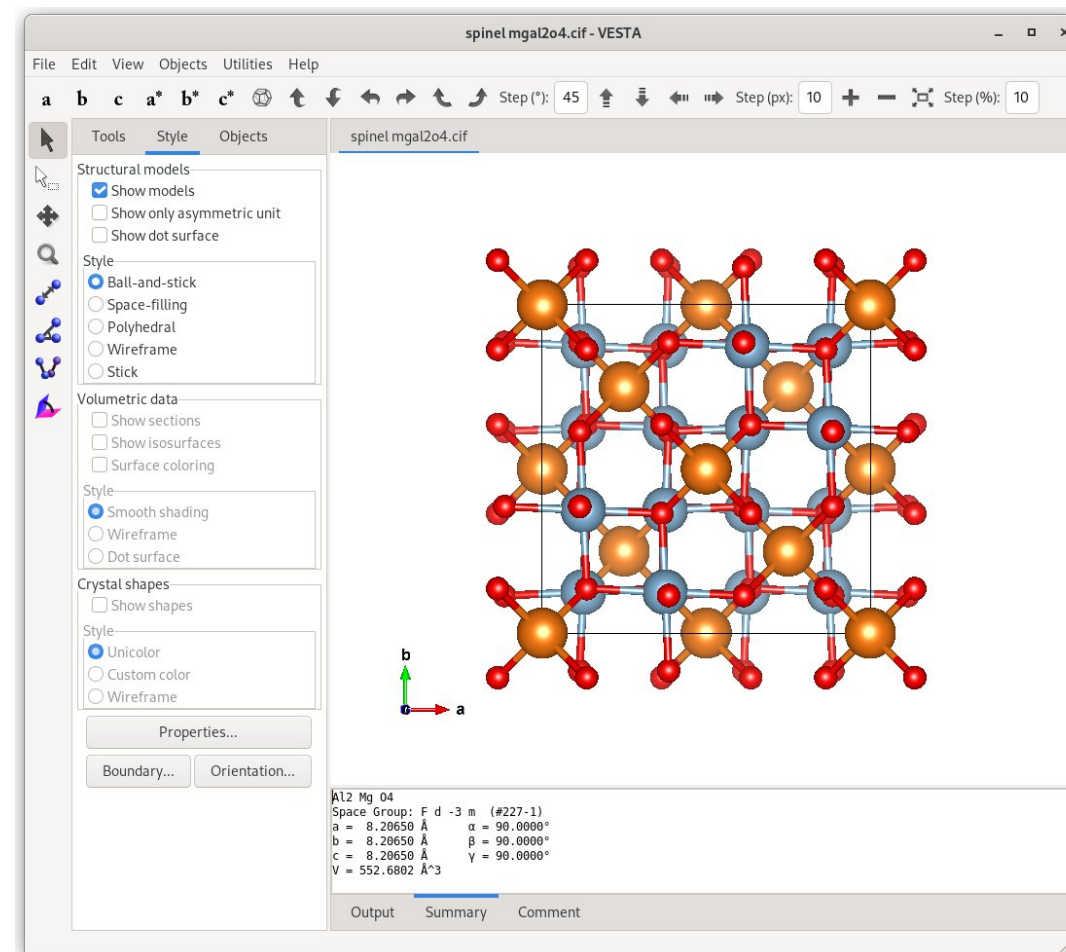
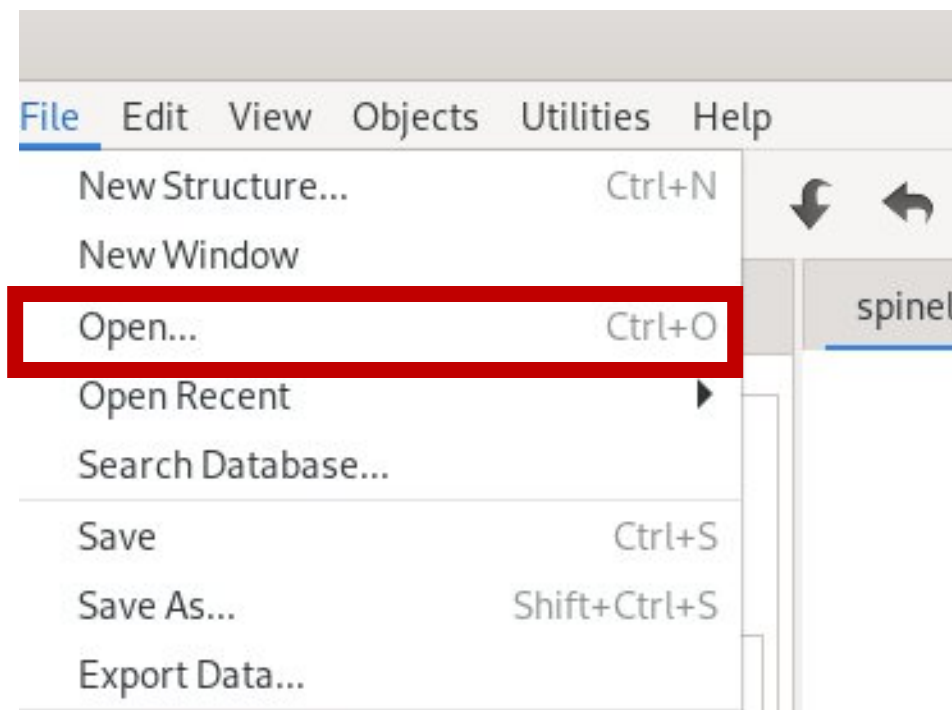
- [VESTA-gtk3.tar.bz2](#) (ver. 3.5.8, built on Aug 11 2022, 23.8MB)
- [vesta-3.5.8-1.x86_64.rpm](#) (built on Aug 11 2022, 40.9MB)
Requires GTK 3.22 or newer.
Distributions where VESTA is known to work:
 - Redhat Enterprise Linux 7 or later
 - Ubuntu 18.04 or later
- [VESTA-gtk2.tar.bz2](#) (ver. 3.5.8, 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



Opening a Structure

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



Navigating Unit Cells

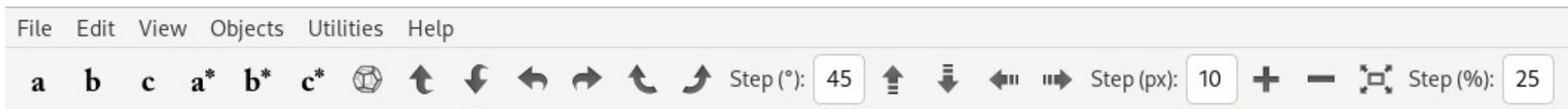
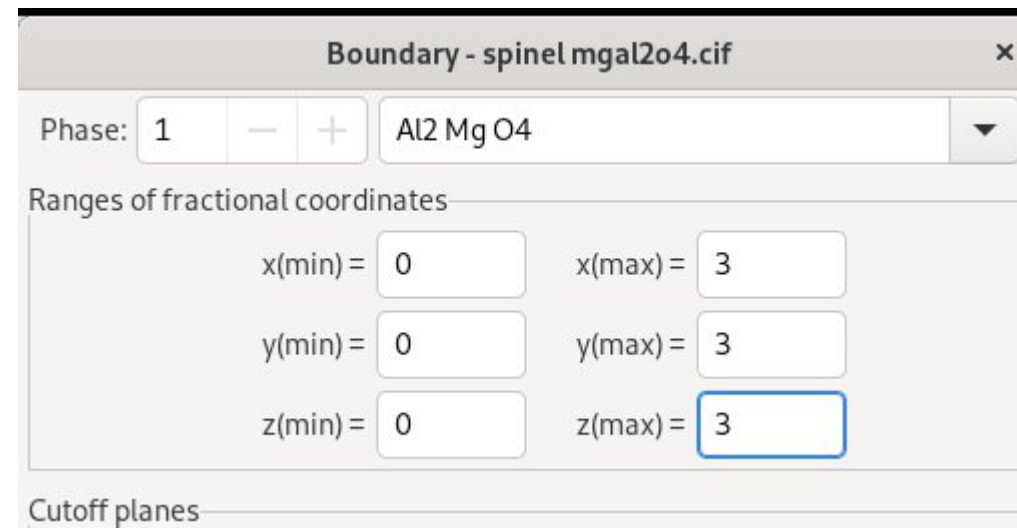
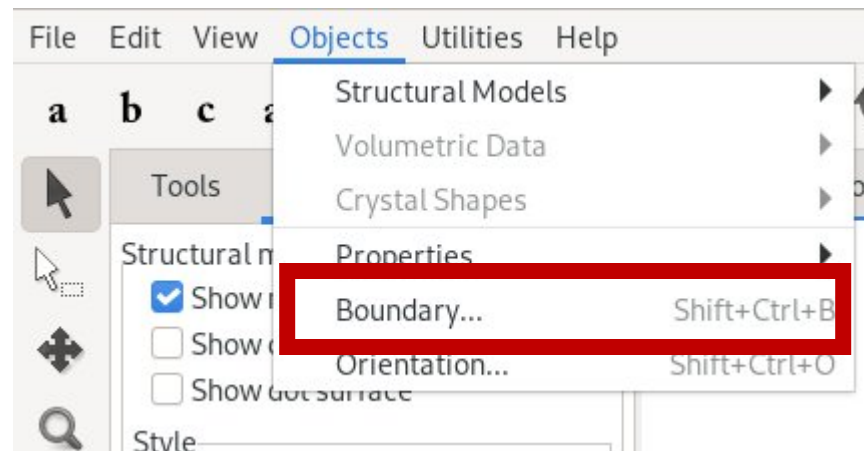
- Rotate via mouse drag, zoom with scroll
- Realign axes via toolbar (a, b, c)
- Display supercell via **Objects** → **Boundary**, set repeat counts



: Rotate freely

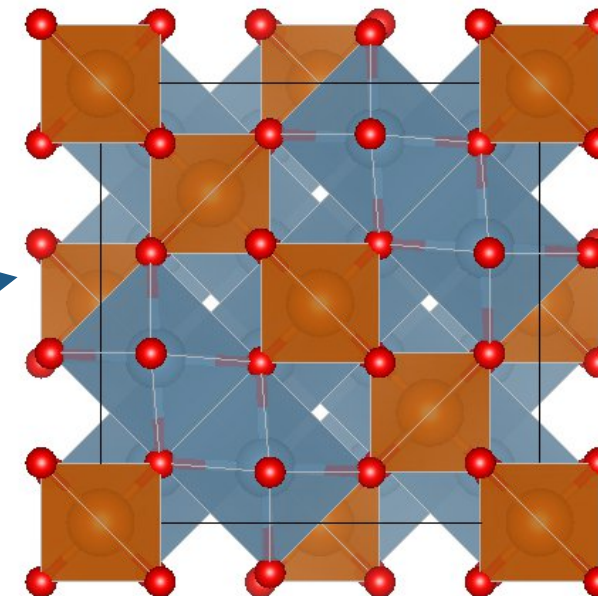
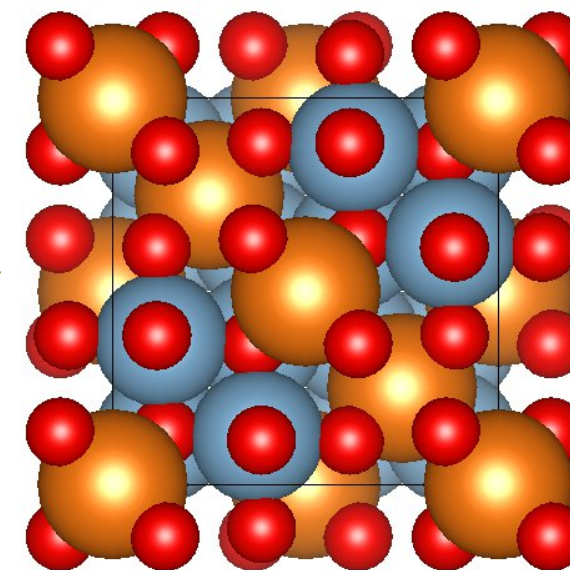
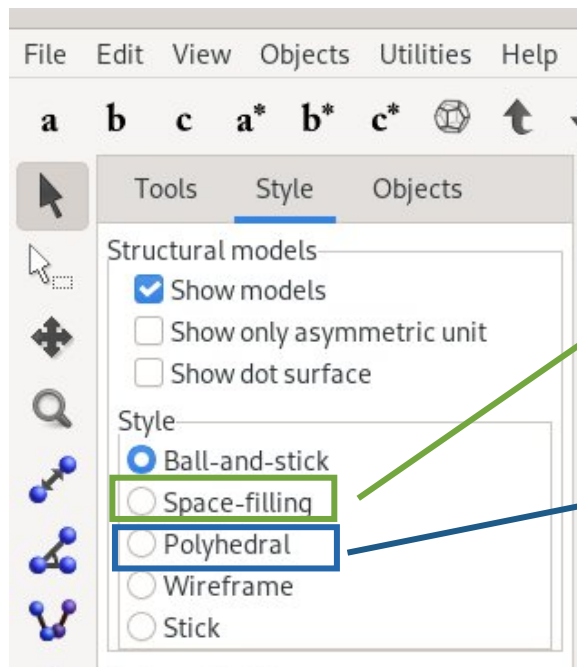


: Zoom in and out



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

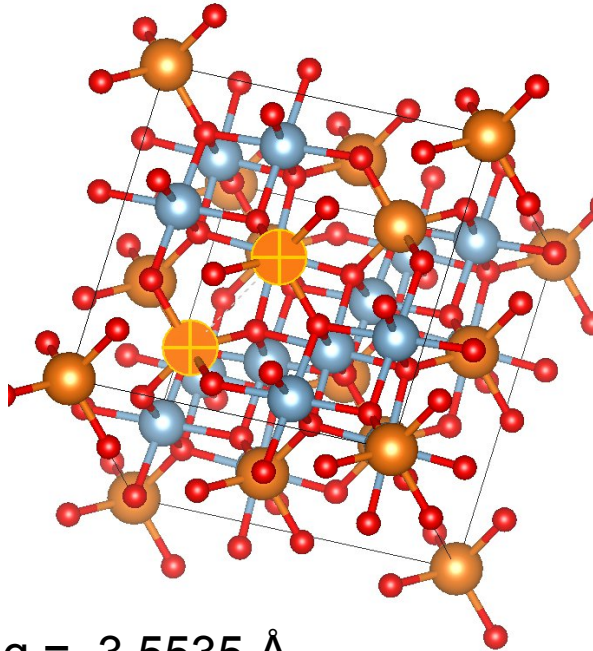
Magnify

Distance

Angle

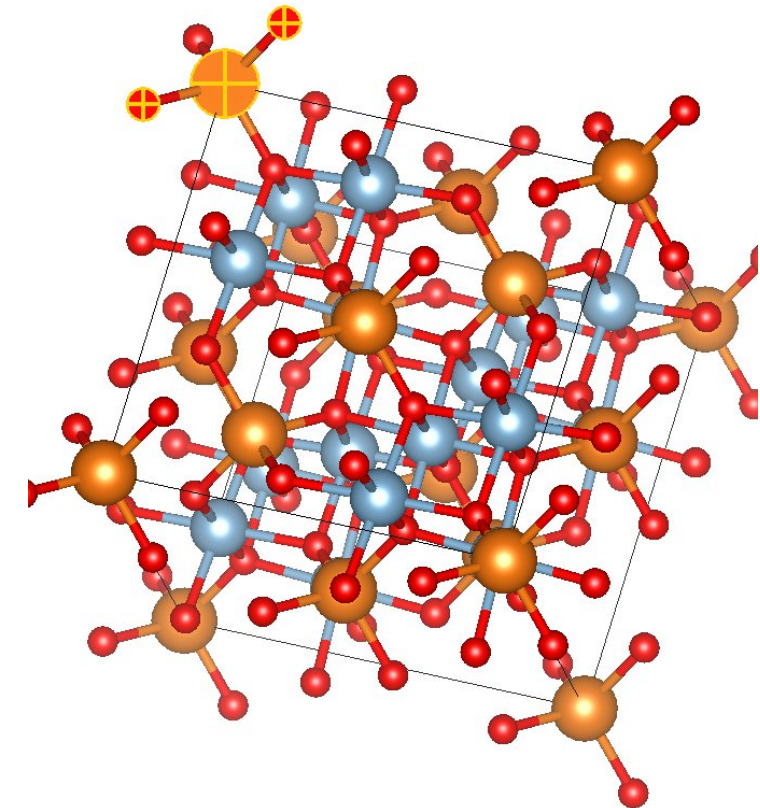
Dihedral angle

Interfacial angle



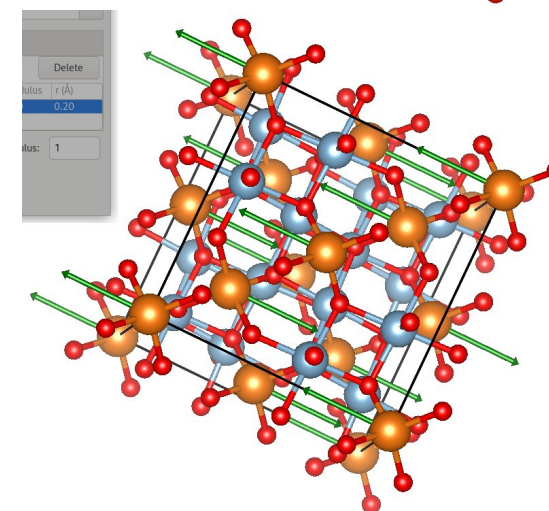
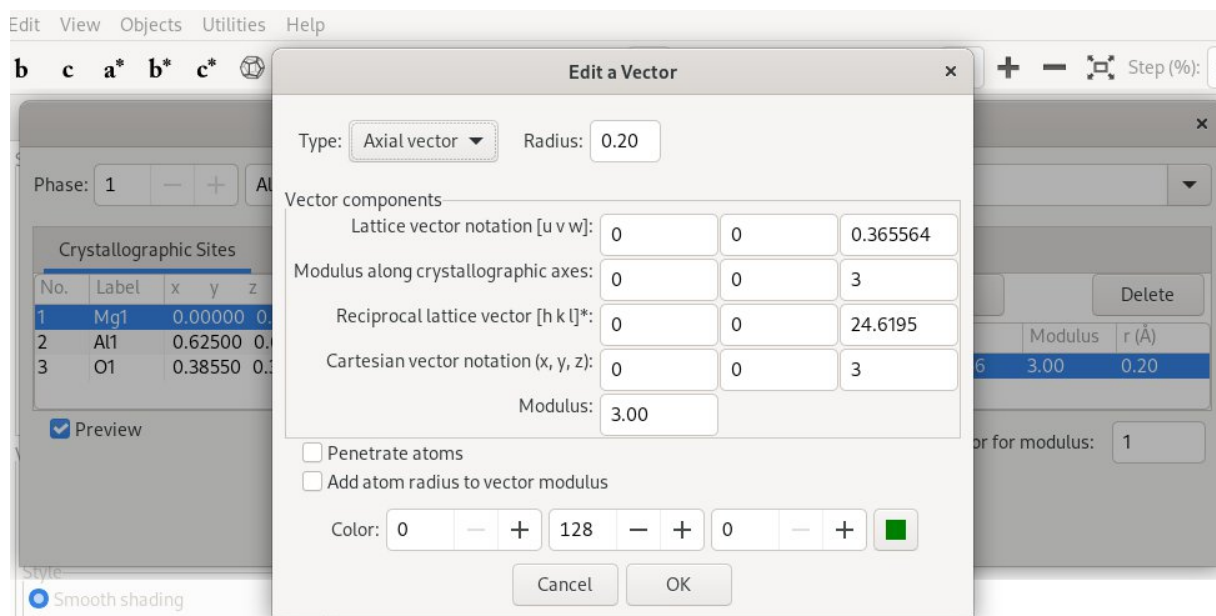
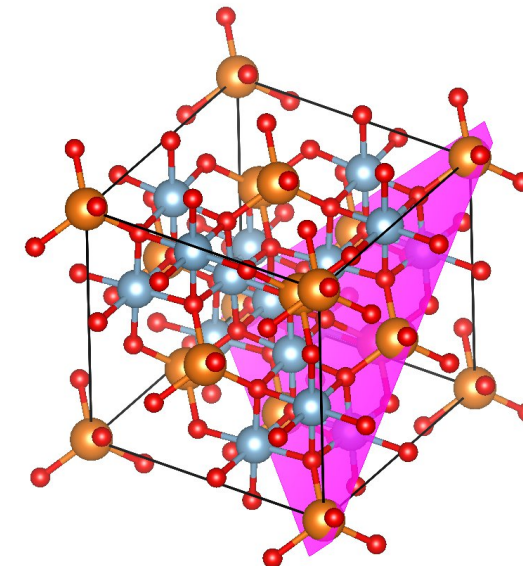
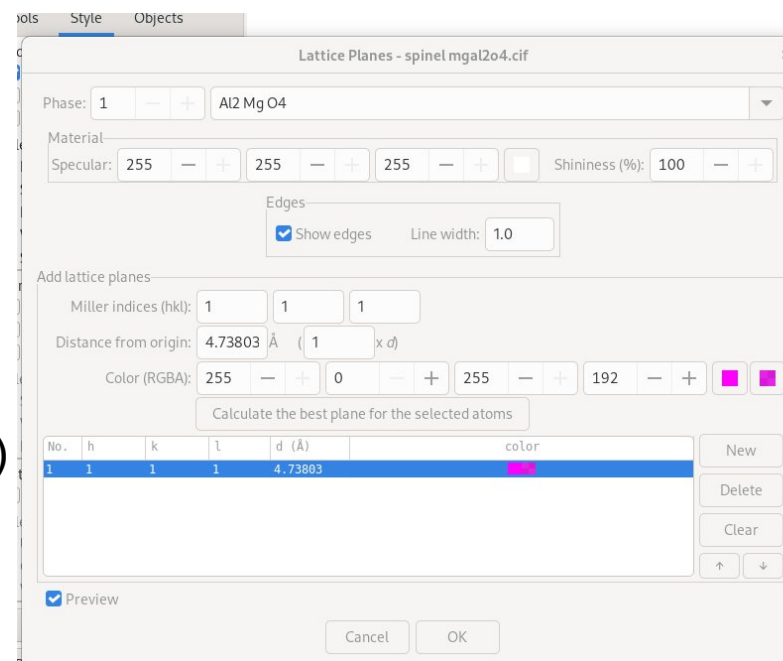
Mg-Mg = 3.5535 Å

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 matrix
- Generate super- or sub-lattice cells
- Useful for analyzing symmetry variations

Unit Cell Transformation

Transformation matrix

Rotation matrix (P)			Translation vector (p)
<input checked="" type="checkbox"/>	0	0	0.000000
0	3	0	0.000000
0	0	3	0.000000

The new basis vectors a', b', c' are related to the basis vectors a, b, c by

$$(a', b', c') = (a, b, c)P$$

$$= (a, b, c) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

$$= (P_{11}a + P_{21}b + P_{31}c, P_{12}a + P_{22}b + P_{32}c, P_{13}a + P_{23}b + P_{33}c)$$

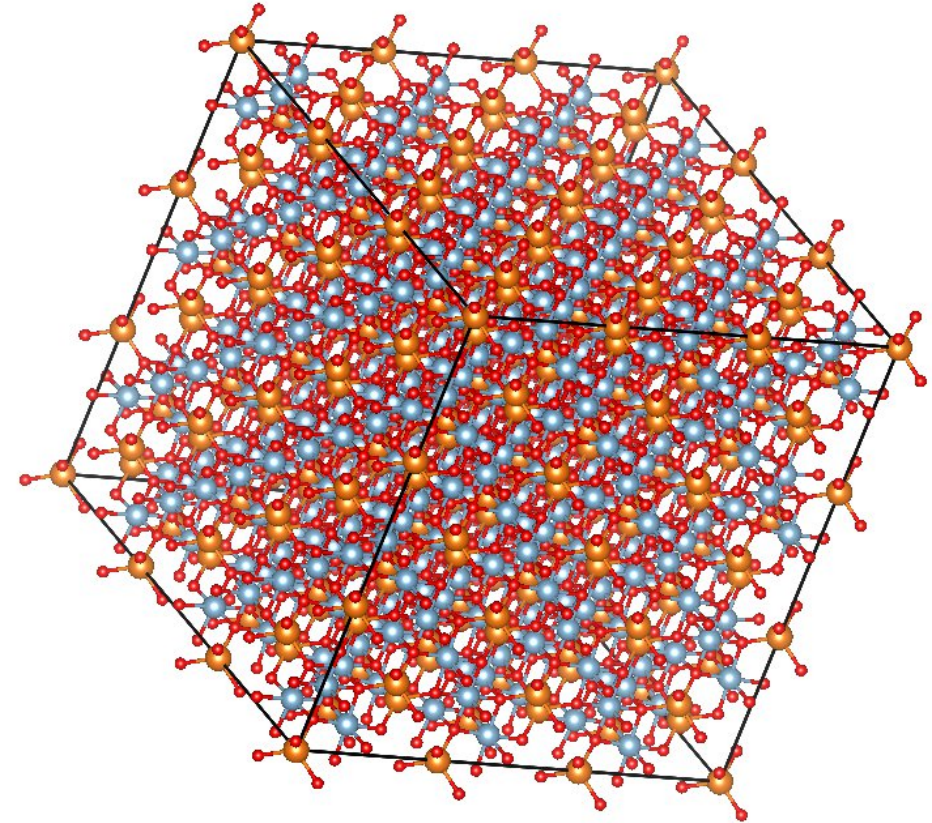
A shift of origin is defined by the shift vector

$$t = (a, b, c)p$$

$$= (a, b, c) \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

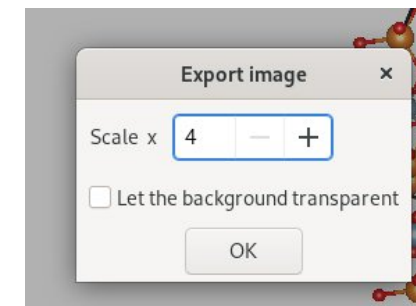
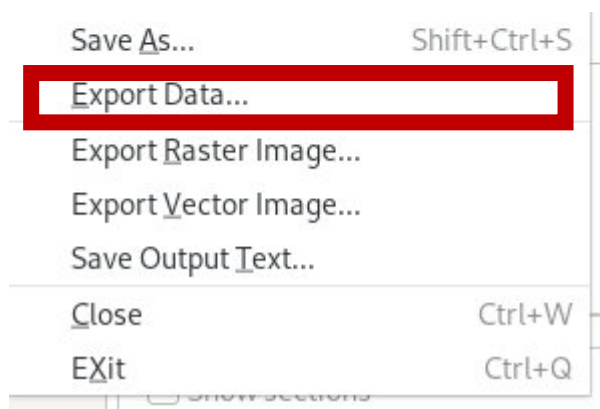
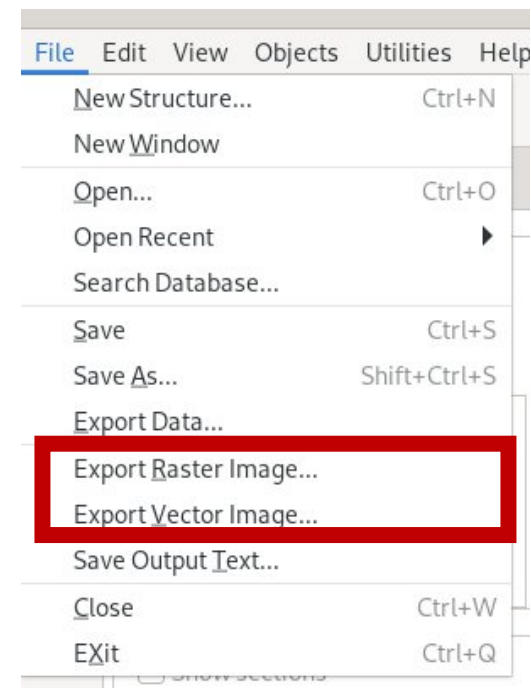
$$= p_1a + p_2b + p_3c.$$

☒ Normalize the range of fractional coordinates



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.



CUBE file (*.cube)
VASP file (*.vasp;POSCAR)
STL file (*.stl)
VRML file (*.wrl)
CIF file (*.cif)
PDB file (*.pdb)
SHELX (*.ins)
RIETAN (*.ins)
XYZ file (*.xyz)
Chem3D file (*.cc1)
DL_POLY CONFIG file
MADEL input file (*.pme)
STRUCTURE TIDY input file (*.stin)
P1 Structure (*.p1)
Fractional Coordinate (*.xtl)

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



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!