Post-processing tools for SIESTA crystal structure, vibrations, and grid properties : `Sies2xsf` and `Sies2vesta`

SIESTA school, Barcelona, June 2021

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Sies2xsf suite

Recently discussed in :

The Journal of Chemical Physics ARTICLE scitation.org/journal/jcp

SIESTA: Recent developments and applications

Cite as: J. Chem. Phys. **152**, 204108 (2020); doi: 10.1063/5.0005077
Submitted: 18 February 2020 • Accepted: 20 April 2020 •
Published Online: 27 May 2020

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3. Other post-processing and visualization utilities

The body of utilities contributed by non-core developers and other SIESTA users has continued to expand. In particular, we feature in this section two suites of utilities: one dealing with alternate visualization tools for some SIESTA results and another one specifically dealing with lattice dynamics.

For structures, the `xv2xsf` and `xv2vesta` converters process data from the SIESTA `.XV` file into the native formats of XCrySDen[134] and VESTA,[135] respectively. Each of these two codes offers many options of graphical representation of structures, adding translations, clipping fragments, etc. Three-dimensional spatial functions (e.g., charge density and local density of states integrated throughout the chosen energy range) are computed by SIESTA on a real-space grid. Tools are provided for interpolating the data from the SIESTA output grid (fixed by the unit cell dimensions and the `MeshCutoff` parameter) onto an arbitrarily cut (and possibly rotated or resampled) parallelepipedic box. XCrysDen provides a number of display options, including contour lines over grid planes or isosurfaces. A special feature available in XCrySDen is plotting the Fermi surfaces. A special script, `eig2bxsf`, serves to analyze the list of **k**-points handled by SIESTA, expanding it onto a regular sequence and writing the respective band energies in the necessary format.

Earlier tutorials:

`https://siesta-project.org/SIESTA_MATERIAL/Docs/Tutorials/Lyon-2007/Postnikov-visual.pdf`
`https://siesta-project.org/SIESTA_MATERIAL/Docs/Tutorials/Barcelona-2007/Postnikov-visual.pdf`

Sies2xsf suite

Fortran codes, to be compiled and linked with a provided `Makefile`

Tool	Visualises	Needs	Creates
`xv2xsf`	structure	`.XV`	`.XSF`
`rho2xsf`	grid property	`.XV` and (`.RHO` | `.IORHO` | `.VH` | `.VT` | `.IOCH` | `.TOCH` | `.LDOS`)	`.XSF`
`vib2xsf`	zone-center vibration modes, statically (arrows) or dynamically (animation)	`.XV` and `.vectors` (from `Vibra`)	`.XSF` and (optionally) `.AXSF`
`md2axsf`	molecular dynamics or structure relaxation	`.XV` and (`.MD` | `.ANI`)	`.AXSF`
`eig2bxsf`	Fermi surfaces	`.XV`, `.EIG` and `.KP`	`.BXSF`

`.XSF` is an input format of XCrySDen, which is also read by Vesta.

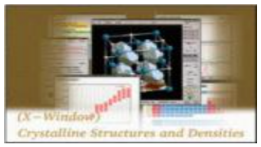
`.AXSF` is a XCrySDen format for animations, `.BXSF` – for Fermi surfaces.

XCrySDen software by Tone Kokalj

Not Secure | xcrysden.org

XCrySDen ...

X-window CRYstalline Structures and DENsities



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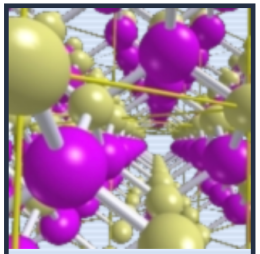

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XCrySDen

XCrySDen is a **crystalline and molecular structure visualisation program** aiming at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. It runs on GNU/Linux.

XCrySDen has been also ported to Mac OS (requires X11) and Windows (requires either CYGWIN or WSL).

The name of the program stands for *Crystalline Structures and Densities* and *X* because it runs under the X-Window environment.

Read more... | See screenshots ...

Latest version: 1.6.2

XCrySDen mailing list

XCrySDen mailing list is an open mailing list where XCrySDen related issues can be discussed among users.

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News

[28 Oct 2019] *XCrySDen*-1.6.2 released.

XCrySDen software by Tone Kokalj

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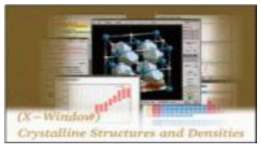
XCrySDen ...

X-window CRYstalline Structures and DENsities



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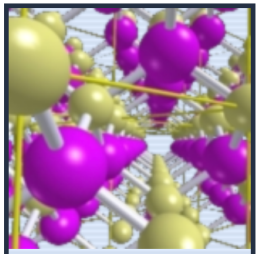

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because it runs

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License

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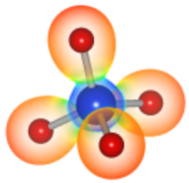
[28 Oct 2(

*The documentation of **XCrySDen** is available only in HTML format. For the beginners, it is strongly suggested to start with the Short introduction to XCrySDen (read at least subsection 1.3 Useful hints).*

VESTA software by Koichi Momma

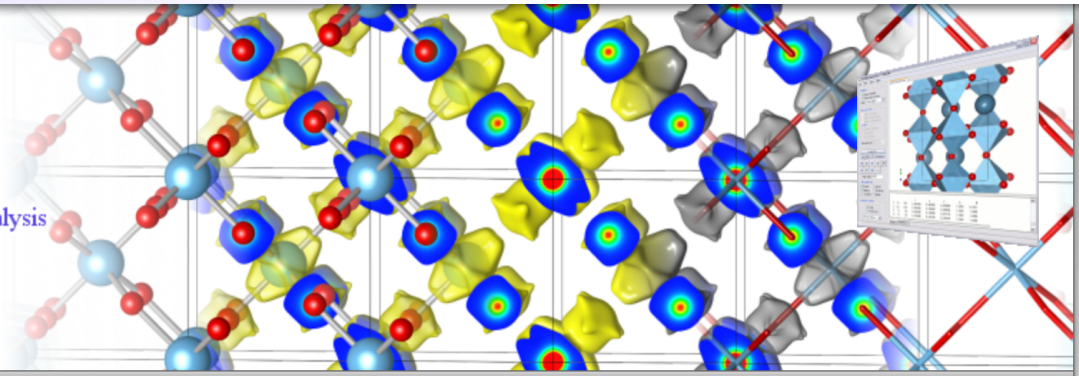
jp-minerals.org/vesta/en/

rals | | English | Japanese |



VESTA

Visualization for Electronic and STructural Analysis



Software > VESTA

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1. Introduction

VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. Some of the novel features of VESTA are listed below.

- Deal with multiple structural models, volumetric data, and crystal morphologies in the same window.
- Support multiple tabs corresponding to files.
- Support multiple windows with more than two tabs in the same process.
- Deal with virtually unlimited number of objects such as atoms, bonds polyhedra, and polygons on isosurfaces (theoretical limit on 32bit operating system is 1,073,741,823)
- Support lattice transformation from conventional to non-conventional lattice by using matrix. The transformation matrix is also used to create superlattice and sublattice.
- Visualize interatomic distances and bond angles that are restrained in Rietveld analysis with RIETAN-FP.
- Transparent isosurfaces can be overlap with structural models.
- Isosurface can be colored on the basis of another physical quantity.
- Arithmetic operations among multiple volumetric data files.
- High quality smooth rendering of isosurfaces and sections.
- Export high-resolution graphic images exceeding Video card limitation.

VESTA is a successor to two 3D visualization programs, VICS and VEND, in the VENUS (Visualization of Electron/NUclear and Structures) software package.

VESTA runs on Windows, Mac OS X, and Linux. It is contributed free of charge for non-commercial users.

A short "howto" on the `Sies2xsf` suite

All scripts are started from the command line, without specifying any parameters. The necessary information is passed by responding the queries on the command line as well. A short `README` is provided along with the distribution.

`rho2xsf` and `vib2xsf` require to define a visualisation box, which needs not to be related to the unit cell. The box is defined as a cuboid, constructed via a reference point (3 coordinates), three orthogonal axes passing through this point, and max. $+/-$ distances (not necessarily identical) along each axis, measured from the reference point. Defining this box may demand answering too many questions; if done repeatedly, it might make sense to organise the "answers" into an input file.

For Fermi surface calculation, band energies need to be calculated beforehand on a fine enough unshifted k-mesh (i.e., that containing the Γ point). The corresponding `.EIG` and `.KP` files must be available for calculation, along with the `.XV` file.

A "sister suite" Sies2vesta

Only two scripts are so far provided in it, `xv2vesta` and `vib2vesta`. The first one is rather straightforward and does not offer anything beyond `xv2xsf`, the result of which (just the crystallographic information) can be read directly into `Vesta` in the `.XSF` format.

`vib2vesta` was needed because the control over arrows (decorating the atoms in order to mark their displacements within a given vibration mode), which were placed using the "Forces" feature of XCrySDen, does not seem to be readable by Vesta. Therefore, the native language of Vesta is used to define these arrows. `vib2vesta` allows more control over the shapes, colors etc. of arrows. Possible choices are offered for selection on the command line while running the `vib2vesta` script.

In the following, we go through several examples how to run the scripts so far discussed and how to visualise the results with the help of XCrySDen and Vesta.