

Visualization and post-processing tools for SIESTA

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What to visualize..?

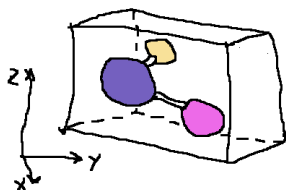
- The structure (unit cell, positions of atoms)
- Charge (spin) density $\rho(\mathbf{r})$, or “local density of states”: properties on the grid
- Kohn-Sham wavefunctions: properties expanded over the basis functions
- Fermi surfaces (or other isoenergy surfaces in \mathbf{k} -space)
- Molecular dynamics or relaxation: how the atoms moves (a movie)
- Phonon vibration modes (after a **Vibra/vibrator** run)

What to visualize..?

Atomic structure

The error-free choice of structure (unit cell, positions of atoms) is the full responsibility is on the user; only minimal checks are done by SIESTA (e.g., “atoms too close”).

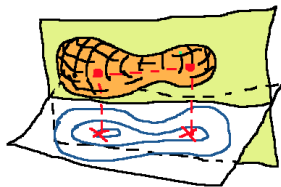
Since the input format is quite flexible (a big advantage!), it is difficult to organize a simple viewer of *input* structure data, without using the *fdf* routines. However, the *.XV* file (created after the completion of electronic structure loop) contains all necessary information, as it was *really* understood by SIESTA, in a fixed format: unit cell vectors and atom coordinates (all in Bohr). This file can be easily transformed to, e.g. *.xyz* format which is read by many visualization programs (*xmakemol*, ...). In the following examples, we'll use XCrySDen.



What to visualize..?

Charge/spin density; local density of states

These are scalar fields available, after a SIESTA run, on a 3-dim. mesh (the number of divisions along three lattice vectors is governed by the `MeshCutoff` parameter). A typical graphical representation of such scalar fields is by contour plots in 2-dim. cutting planes, and/or isosurfaces of a given level. Both representations are possible with XCrySDen.



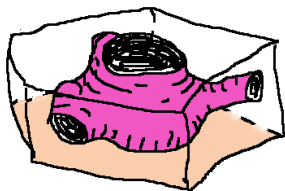
Kohn-Sham wavefunctions

These are also scalar functions of spatial coordinates, but obtained in SIESTA as expression over basis functions. Their visual representation (as 2-dim. contours in a chosen plane, or 3-dim. isosurfaces) is handled by the `denchar` code. `denchar` allows export of data in the Gaussian cube format, which can be read in by XCrySDen.

What to visualize..?

Fermi surfaces

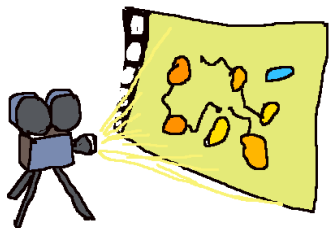
can be calculated using the energy dispersion data $E(\mathbf{k})$, available from any band structure code. The difficulty of purely technical character is, how to construct energy isosurfaces and conveniently manipulate them (to choose viewpoint, select different sheets of the Fermi surface, etc.) This job is done within XCrySDen, provided the $E(\mathbf{k})$ data are passed in a right format.



What to visualize..?

Molecular dynamics or relaxation

leave the atomic positions in .MD and/or .ANI files (with and without unit cell information, correspondingly). From sequences of atomic positions can be animated using different software, including XCrySDen.



Phonon modes

from [Vibra/vibrator](#) calculation after a `MD.TypeOfRun` `FC`

SIESTA run: they can be represented by arrows (in a static figure), or as animations (a sequence of vibration snapshots).

XCrySDen - (X-Window) Crystalline Structure and Densities - Mozilla

file:///home/apostnik/Xcrysden/HTML-Documentation/Documentation.html

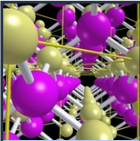
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XCrySDen ...

X-window CRYstalline Structures and DENsities

(X-Window) Crystalline Structures and Densities

XCrySDen Documentation




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A powerful, flexible, stable, free-to-use, open-source software for different visualizations. Runs under XWindows and on the Mac.

The documentation of *XCrySDen* is HTML formatted. It is not meant to be all-in-depth documentation, but rather to provide a few basic hand-on tutorials, HOWTO and FAQ. It is strongly suggested to start with the [Short introduction to XCrySDen](#) (read at least subsection [1.3 Useful hints](#)).

A.Postnikov (Université Metz) Visualization and post-processing tools June 2007 3 / 11

1.1 What *XCrySDen* can do?

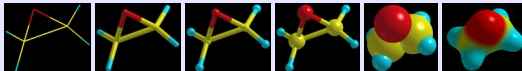
In short: *XCrySDen* is a crystalline and molecular structure render program, with additional capabilities of rendering contours, isosurfaces, Wigner-Seitz cells (also Brillouin zone), Fermi surfaces and so on. Some of its features are the following:

- widget with periodic table of elements:

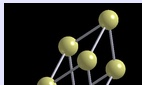


Enables different presentations of atoms and bonds (colors, shadows, ...), measuring distances and angles ...

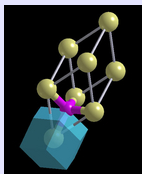
- displaying molecular and crystalline structure in several different display modes:



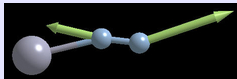
- displaying crystal and Wigner-Seitz cells:



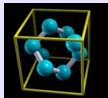
- displaying crystal and Wigner-Seitz cells:



- displaying smaller or bigger portion of crystal (multiplying the unit cells)
- visualizing the forces as vectors:



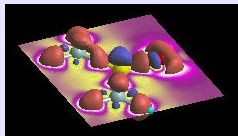
- animations



- displaying contours and colorplanes

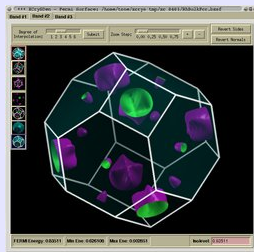
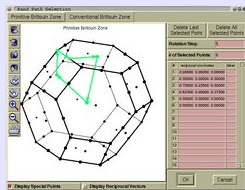
Allows to set arrows on atoms
(or, on fictitious atoms)
and make animations ...

- displaying contours and colorplanes
- displaying isosurfaces:

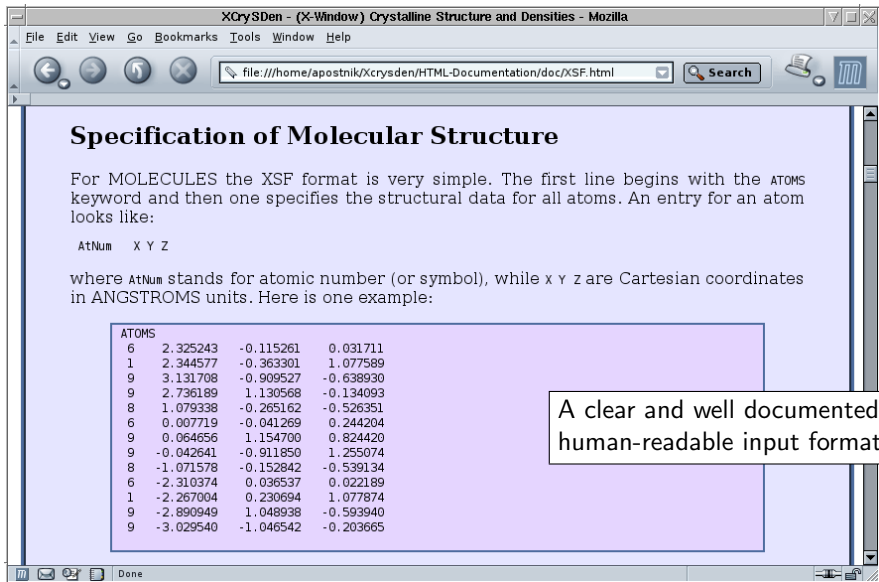


Allows to make contour plots,
to draw isosurfaces,
to choose path through the Brillouin zone,
to use different modi
of presenting the Fermi surfaces

- reciprocal-space analysis:
 - + selecting a k-path inside the Brillouin-zone
 - + visualizing Fermi surfaces



Format of XCrySDen input files (.xsf, .axsf, .bxsf)



XCrySDen - (X-Window) Crystalline Structure and Densities - Mozilla

File Edit View Go Bookmarks Tools Window Help

file:///home/apostnik/Xcrysden/HTML-Documentation/doc/XSF.html Search

Specification of Molecular Structure

For MOLECULES the XSF format is very simple. The first line begins with the ATOMS keyword and then one specifies the structural data for all atoms. An entry for an atom looks like:

```
AtNum X Y Z
```

where AtNum stands for atomic number (or symbol), while x y z are Cartesian coordinates in ANGSTROMS units. Here is one example:

```
ATOMS
6 2.325243 -0.115261 0.031711
1 2.344577 -0.363301 1.077589
9 3.131708 -0.909527 -0.638930
9 2.736189 1.130568 -0.134093
8 1.079338 -0.265162 -0.526351
6 0.007719 -0.041269 0.244204
9 0.064656 1.154700 0.824420
9 -0.042641 -0.911850 1.255074
8 -1.071578 -0.152842 -0.539134
6 -2.310374 0.036537 0.022189
1 -2.267004 0.230694 1.077874
9 -2.890949 1.048938 -0.593940
9 -3.029540 -1.046542 -0.203665
```

A clear and well documented human-readable input format...

Done

File Edit View Go Bookmarks Tools Window Help

file:///home/apostnik/Xcrysden/HTML-Documentation/doc/XSF.html Search

Specification of Forces

All that is needed to specify the forces acting on atoms is to supplement the appropriate coordinate section (ATOMS or PRIMCOORD). Now an entry for an atom would look like:

```
AtNum X Y Z Fx Fy Fz
```

where F_x F_y F_z stands for force components in X, Y and Z direction, respectively. The force components are expressed in Cartesian coordinate system in Hartree/ANGSTROM unit.

Here is an example of water molecule:

```
ATOMS
8  0.00000  0.00000  0.00000  -.05164  .00000  -.03999
1  0.00000  0.00000  1.00000  .01769  .00000  .03049
1  0.96814  0.00000  -0.25038  .03395  .00000  .00949
```

And here is an example for the periodic structure structure:

```
SLAB
PRIMVEC
5.8859828533  0.0000000000  0.0000000000
0.0000000000  5.8859828533  0.0000000000
0.0000000000  0.0000000000  1.0000000000
PRIMCOORD 1
11 1
6  3.674759  2.942992  -3.493103  -0.021668  0.000000  -0.057324
1  4.121990  3.816734  -4.007689  -0.000478  0.001204  0.006657
1  4.121990  2.069250  -4.007689  -0.000478  -0.001204  0.006657
6  2.211226  2.942992  -3.493103  0.021668  0.000000  -0.057324
```

Done

Format of XCrySDen input files (.xsf, .axsf, .bxsf)

Animated XSF for molecules

Here is an example of AXSF file. It shows different structures during an optimization of water molecule. Note the index prefixes after ATOMS keywords.

```
ANIMSTEPS 4
ATOMS 1
8 0.0000 0.0000 0.0000 -0.0516 0.0000 -0.0399
1 0.0000 0.0000 1.0000 0.0176 0.0000 0.0304
1 0.9681 0.0000 -0.2503 0.0339 0.0000 0.0094
ATOMS 2
8 -0.1480 0.0000 -0.1146 0.0020 0.0000 0.0015
1 -0.0468 0.0000 0.9134 -0.0069 0.0000 0.0069
1 0.8726 0.0000 -0.2740 0.0049 0.0000 -0.0084
ATOMS 3
8 -0.1032 0.0000 -0.0799 0.0013 0.0000 0.0010
1 -0.0319 0.0000 0.9591 0.0011 0.0000 -0.0028
1 0.9205 0.0000 -0.2710 -0.0025 0.0000 0.0018
ATOMS 4
8 -0.1102 0.0000 -0.0853 0.0001 0.0000 0.0000
1 -0.0345 0.0000 0.9503 -0.0000 0.0000 -0.0000
1 0.9114 0.0000 -0.2714 -0.0000 0.0000 -0.0000
```

... including forces
(or, velocities),
for isolated molecules

Format of XCrySDen input files (.xsf, .axsf, .bxsf)

Animated XSF for periodic structures

Fixed-cell animated XSF

Here is an example of animated XSF for the ZnS crystal structure with the fixed unit-cell. Note the index prefixes after PRIMCOORD keywords.

```
ANIMSTEPS 2
CRYSTAL
PRIMVEC
  0.0000000  2.7100000  2.7100000
  2.7100000  0.0000000  2.7100000
  2.7100000  2.7100000  0.0000000
PRIMCOORD 1
  2 1
  16  0.0000000  0.0000000  0.0000000
  30  1.3550000  -1.3550000  -1.3550000
PRIMCOORD 2
  2 1
  16  0.0000000  0.0000000  0.0000000
  30  1.2550000  -1.2550000  -1.2550000
```

... as well as for periodic structures

Where to find them:

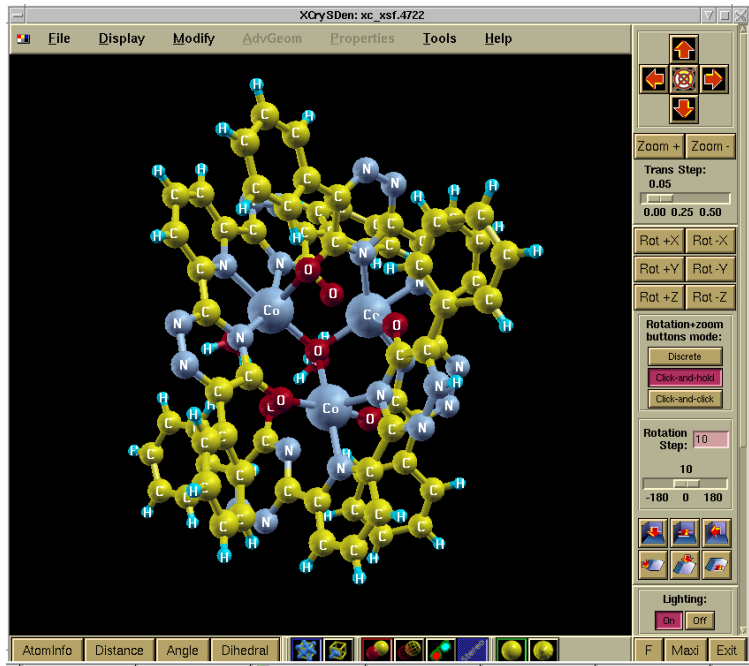
- ... [siesta-2.0/Util/Contrib/APostnikov/](#)
- <http://www.home.uni-osnabrueck.de/apostnik/Downloads> ,
or mailto apostnik@uos.de or postnikov@univ-metz.fr

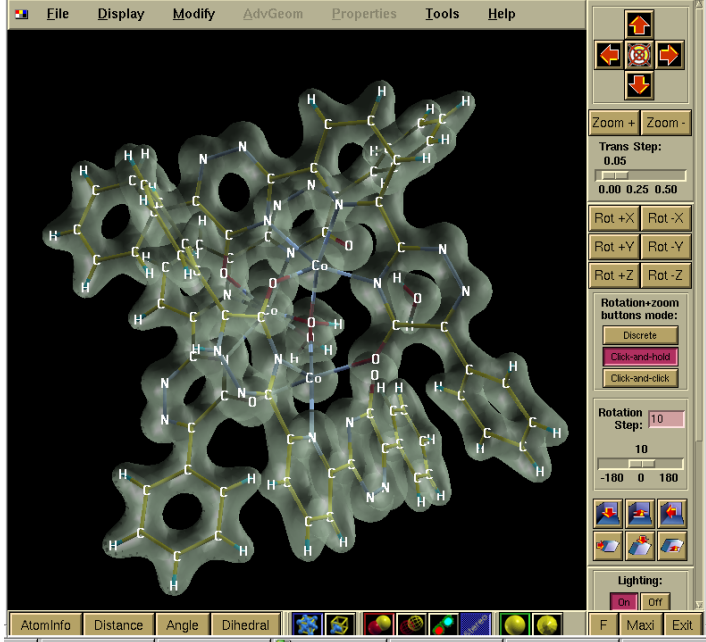
What are they:

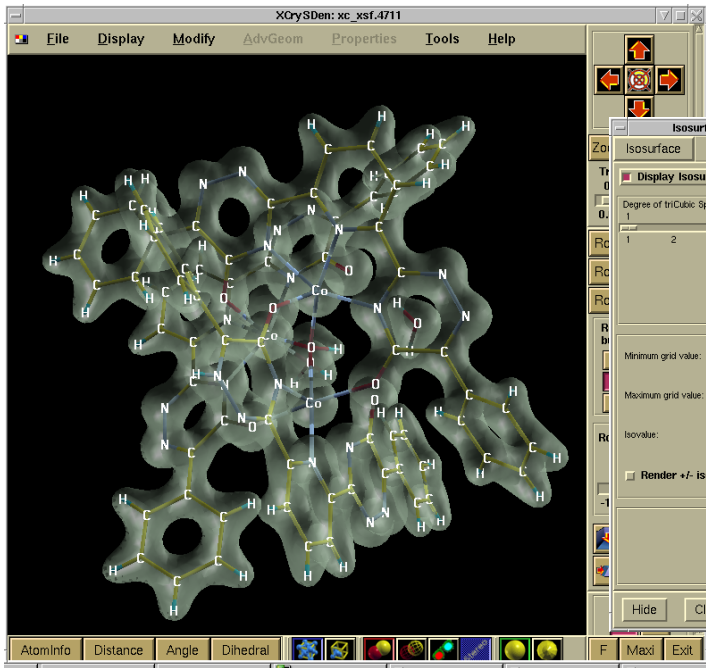
- **xv2xsf**: .XV \rightarrow .XSF (view structure + cell)
- **rho2xsf**: .XV, .RHO or .LDOS \rightarrow .XSF
(atoms within a selected box + data grids)
- **md2axsf**: .XV, .ANI or .MD \rightarrow .AXSF
(animations of structure with fixed or variable cell)
- **eig2bxsf**: .XV, .KP and .EIG \rightarrow .BXSF (Fermi surfaces)
- **vib2xsf**: .XV and .vectors \rightarrow .XSF and .AXSF
for each selected phonon mode; static (with arrows to indicate
dilacement patterns) and dynamic (animated phonon).

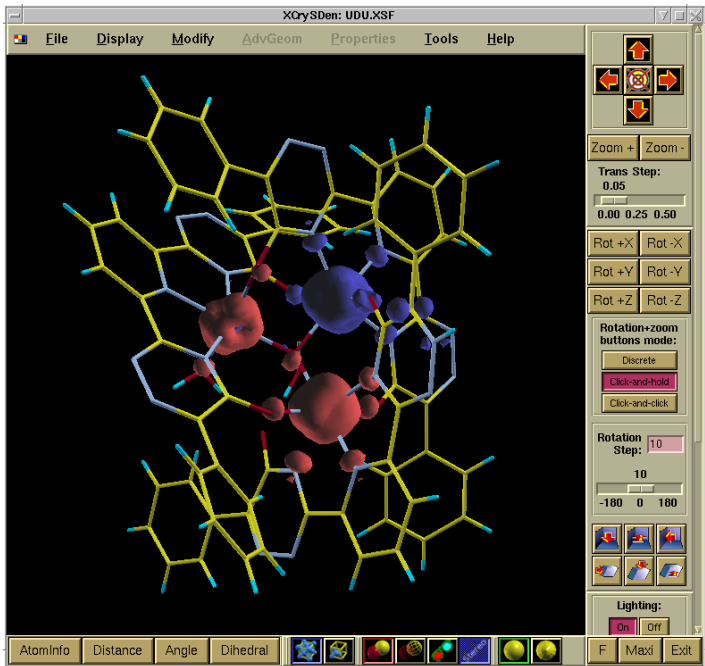
Visualization of Charge/spin densities, or of LDOS

- 1 An input file for XCrySDen is created by **rho2xsf**.
- 2 Accept the same approach as in Denchar: define the output box (by origin point and three spanning vectors, not necessarily orthogonal) and grid size along each grid direction. The values of a Siesta property defined on the internal Siesta grid are (linearly) interpolated onto the grid of the output box.
- 3 The output box may be also 2-dimensional (No. of divisions =1 along one spanning vector).
- 4 The output box may coincide with the Siesta box. XCrySDen can apply translations to the generated grid.
- 5 Choice isosurface parameters, cutting planes, isolines on the cutting planes, colors, lighting etc. by means of XCrySDen.



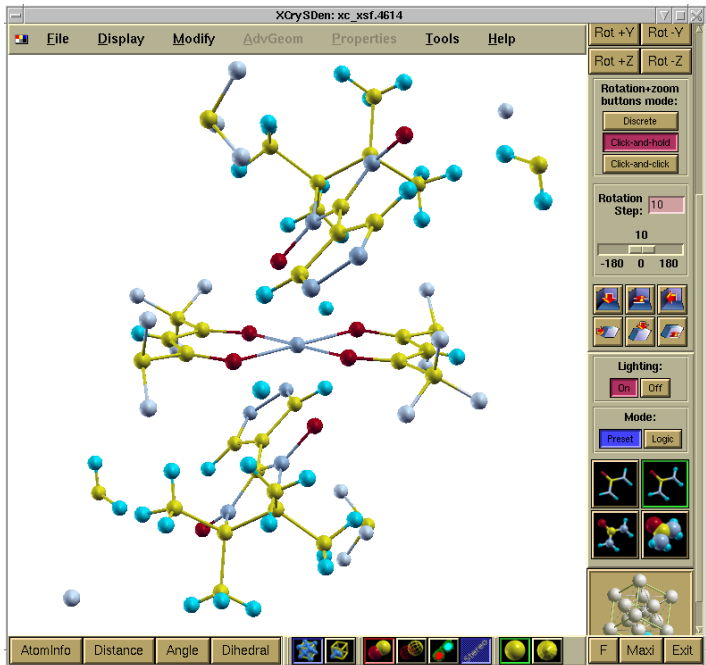






Visualization of Wave Functions

- 1 Use Denchar, define output box there, save result as Gaussian98 Cube file.
- 2 Read this Gaussian98 Cube file into XCrySDen. Save in the XCrySDen format .xsf (→ A).
- 3 A bug (or a feature?) in Denchar: it correctly translates the WF images (grid) over the output box, but not atoms.
- 4 How to fix: run **rho2xsf**, define the same output box as in Denchar. Save the atom part in the XCrySDen format .xsf (→ B).
- 5 Insert (by hand) the “correct” atom part from (B) into the place of “incomplete” atom part from (A).
- 6 If needed, merge many grid blocks (which reside in different .xsf files, each exported from its own Gaussian Cube) into a single .xsf file.



XCrystal: xc_xsf.4614

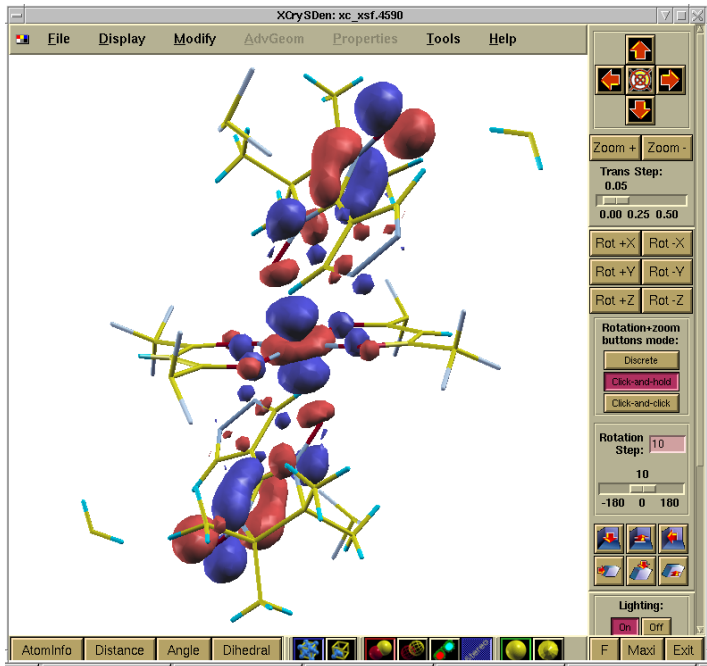
File Display Modify AdvGeom Properties Tools Help

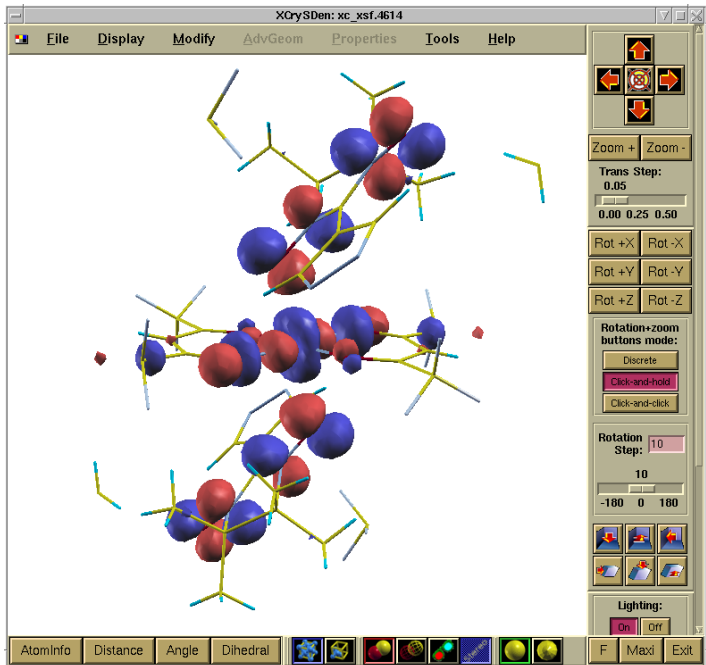
Rot +Y Rot -Y
Rot +Z Rot -Z
Rotation+zoom buttons mode:

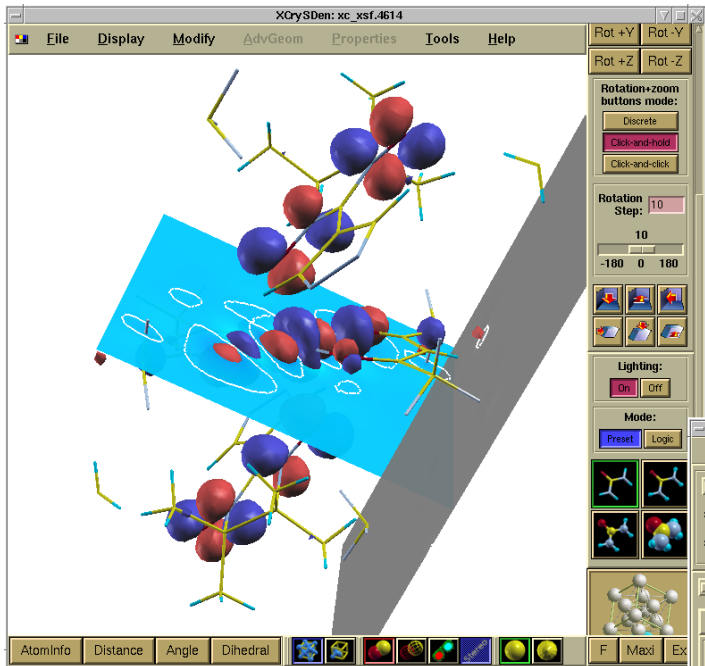
Isosurface/Property-plane Controls

Isosurface	Plane #1	Plane #2	Plane #3
<input checked="" type="checkbox"/> Display Isosurface			
Degree of triCubic Spline: 1			
<input type="radio"/> 1 <input type="radio"/> 2 <input type="radio"/> 3 <input type="radio"/> 4			
Minimum grid value: -1.417200			
Maximum grid value: 0.864310			
Isovalue: 0.08			
<input checked="" type="checkbox"/> Render +/- isovalue			
Render isosurface as: <input checked="" type="radio"/> solid <input type="radio"/> wire <input type="radio"/> dot			
Isosurface's ShadeModel: <input checked="" type="radio"/> smooth <input type="radio"/> flat			
Two-sided lighting: <input checked="" type="radio"/> off <input type="radio"/> on			
Transparency of isosurface: <input checked="" type="radio"/> off <input type="radio"/> on			
Revert (+) Sides			
Revert (-) Sides			
Revert (+) normals			
Revert (-) normals			
Surface Smoothing			
Set COLOR parameters			
Set TRANSPARENCY parameters			
Hide Close Save Grid Submit			

AtomInfo Distance Angle Dihedral F Maxi Exit







Visualization of Fermi surfaces

- 1 Calculate eigenvalues on a sufficiently fine, *undicplaced* k-mesh, i.e.

```
%block kgrid_Monkhorst_Pack
 16  0  0  0.
  0 16  0  0.
  0  0 16  0.
%endblock kgrid_Monkhorst_Pack
```

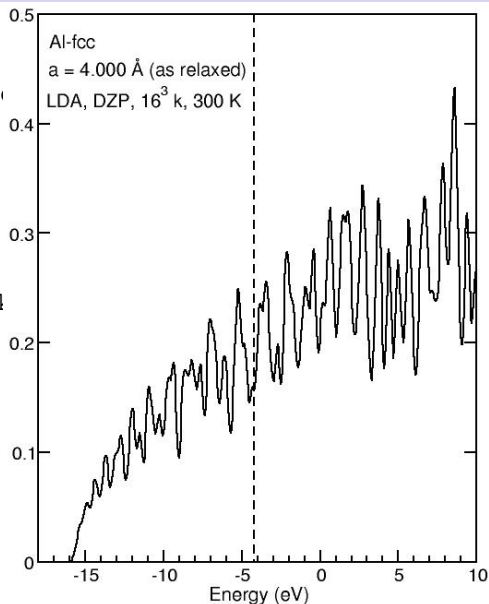
- 2 get files .XV, .KP, .EIG,
run eig2bxsf → creates .BXSf
(or .BXSf_1 and .BXSf_2
for spin-polarized case).

Visualization of Fermi surfaces

- 1 Calculate eigenvalues on a sufficient *undicplaced* k-mesh, i.e.

```
%block kgrid_Monkhorst_Pack
 16  0  0  0.
  0 16  0  0.
  0  0 16  0.
%endblock kgrid_Monkhorst_Pack
```

- 2 get files .XV, .KP, .EIG,
run eig2bxsf → creates .BXSF
(or .BXSF_1 and .BXSF_2
for spin-polarized case).

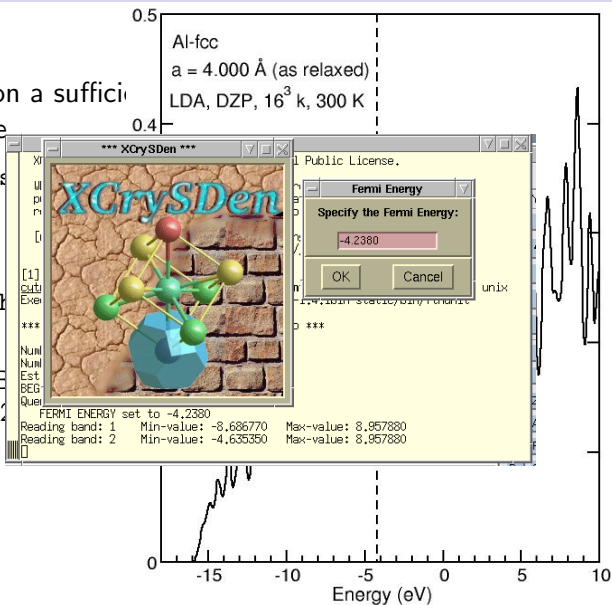


Visualization of Fermi surfaces

- 1 Calculate eigenvalues on a sufficient *undicplaced* k-mesh, i.e.

```
%block kgrid_Monkhorst-Pack
16 0 0 0.
0 16 0 0.
0 0 16 0.
%endblock kgrid_Monkhorst-Pack
```

- 2 get files .XV, .KP, .EIG, run eig2bxsf → creates .EIGSF (or .BXSF_1 and .BXSF_2 for spin-polarized case).

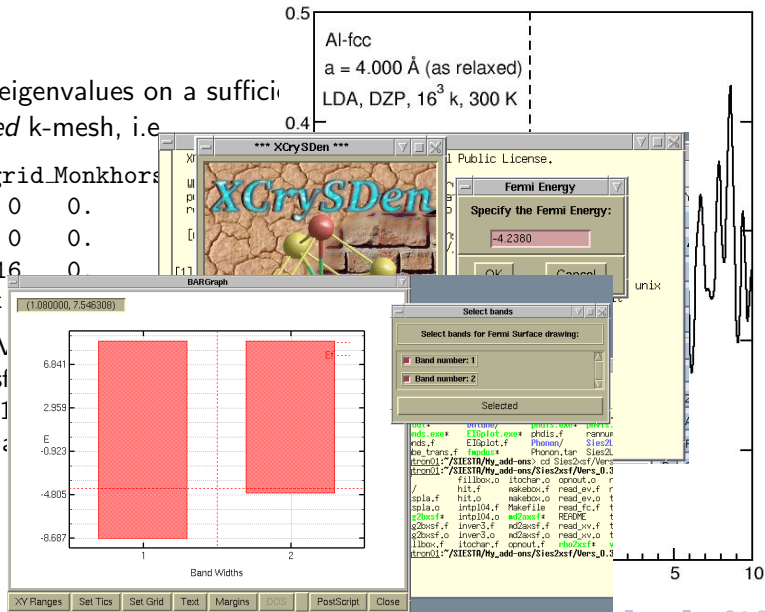


Visualization of Fermi surfaces

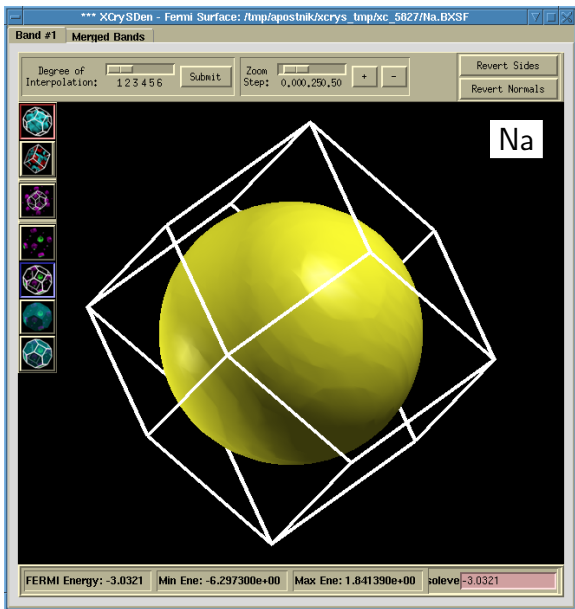
- 1 Calculate eigenvalues on a sufficient *undisplaced* k-mesh, i.e.

```
%block kgrid_Monkhors  
16 0 0 0.  
0 16 0 0.  
0 0 16 0.  
%endblock
```

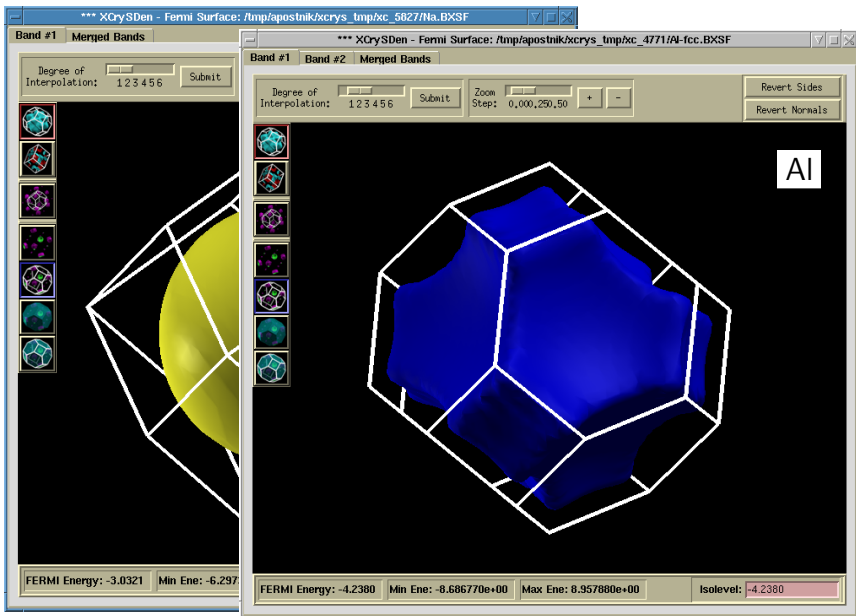
- 2 get files .XV
run eig2bxsf
(or .BXSF_1
for spin-polar



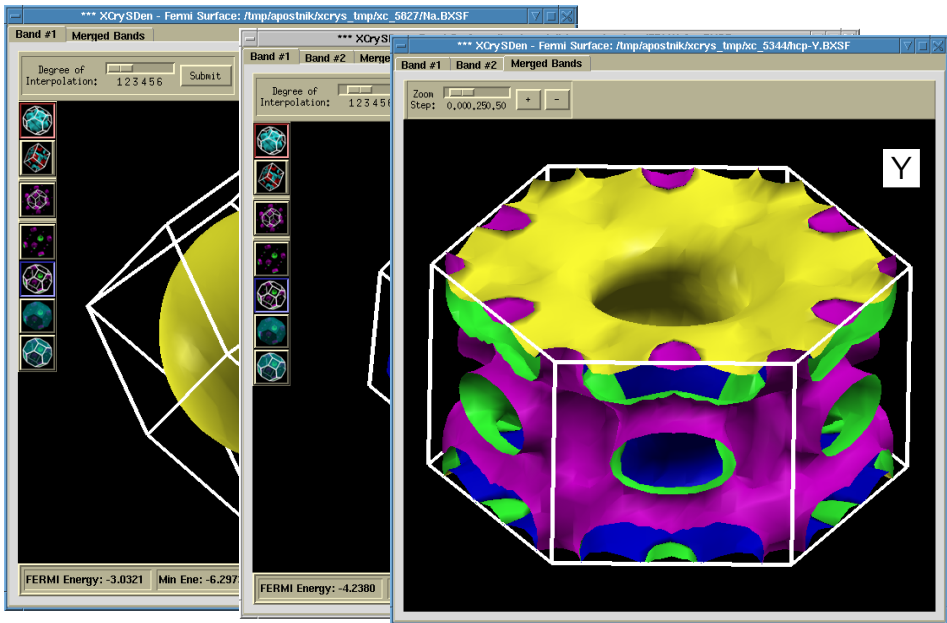
Fermi surfaces of some elemental metals



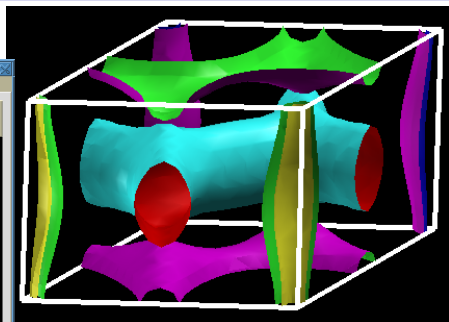
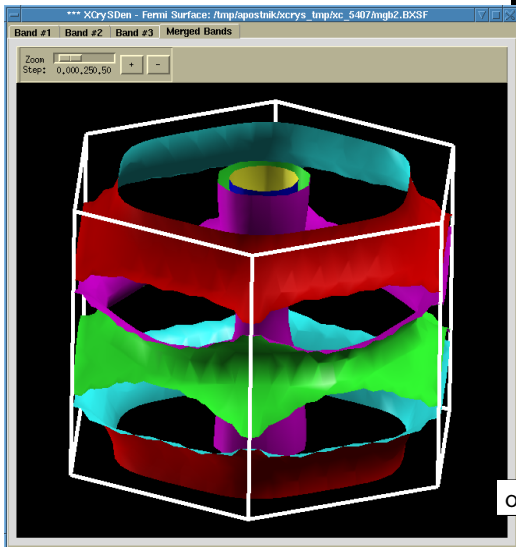
Fermi surfaces of some elemental metals



Fermi surfaces of some elemental metals



Fermi surface of MgB₂



over the reciprocal cell

over the Brillouin zone

① Calculate MD history:

`WriteMDhistory T`
writes (updates existing) *unformatted* .MD file,
either with or without variable cell;

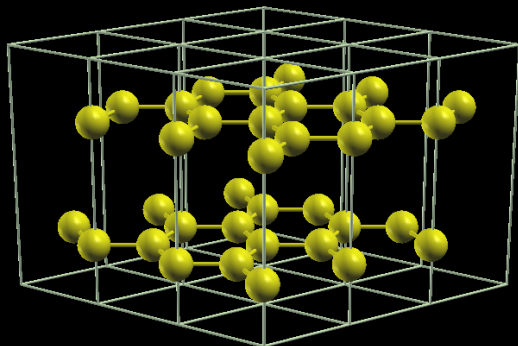
`WriteMDXmol T`
writes (updates existing) *formatted* .ANI file
(coordinates only, no variable cell information).

② Having .XV, and either .MD, or .ANI

run `md2axsf`, answering questions about the (optional) choice of output box
and the MD steps to visualize (first #; last #; keep only each #'s)
→ creates .AXSF.

Hopefully, variable or fixed cell will be recognized automatically.
If cell information from .MD is not available, the .XV will be used
(assuming fixed cell).

In order to see many unit cells,
go to Modify → Number of Units drawn



Zoom + Zoom -

Trans Step:

0.05

0.00 0.25 0.50

Rot +X Rot -X

Rot +Y Rot -Y

Rot +Z Rot -Z

Rotation+zoom
buttons mode:

Discrete

Click-and-hold

Click-and-click

Rotation

Step: 10

10

-180 0 180



Lighting:

On Off

AtomInfo

Distance

Angle

Dihedral



F

Maxi

Exit

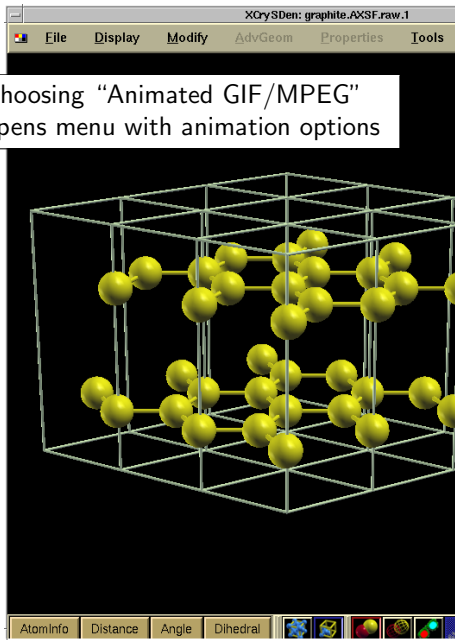
Opening .AXSF file pops up
the Animation Control Center

The screenshot displays the XCrystal software interface. The main window, titled "XCrySDen: graphite.AXSF.raw.1", features a menu bar with "File", "Display", "Modify", "AdvGeom", "Properties", "Tools", and "Help". The central area shows a 3D ball-and-stick model of a graphite crystal structure, with yellow spheres representing atoms and grey rods representing bonds, all contained within a white wireframe unit cell. An "Animation Control Center" dialog box is overlaid on the right side of the window. This dialog box includes the following elements:

- Input fields for "Delay between slides (in msec):" set to 0 and "Animation step:" set to 1.
- A status indicator showing "Current slide: 1/25".
- A set of six navigation buttons: two left-pointing arrows, a double left-pointing arrow, two right-pointing arrows, and a double right-pointing arrow.
- A button labeled "Animated GIF/MPEG >>".
- "Hide" and "Close" buttons at the bottom.

The bottom of the XCrystal window contains a toolbar with buttons for "AtomInfo", "Distance", "Angle", "Dihedral", and several visualization icons. A "Lighting:" section with "On" and "Off" buttons is also visible. The Windows taskbar at the bottom shows the system tray with icons for help, search, and other background processes.

Choosing "Animated GIF/MPEG" opens menu with animation options




Animation Control Center

Delay between slides (in msec):

Animation step:

Current slide: 1/25



<< Animated GIF/MPEG

- Use global color-map for Animated GIF
- Minimize Animated GIF
- Make transparent background for Animated GIF
- Edit flag/parameter-file before encoding

Make MPEG Make Animated-GIF

Put GIF/MPEG temporary files in current working directory

Put GIF/MPEG temporary files in scratch directory

For MPEG: use non-compressed frame-files (PPM)

For MPEG: use compressed frame-files (JPEG)

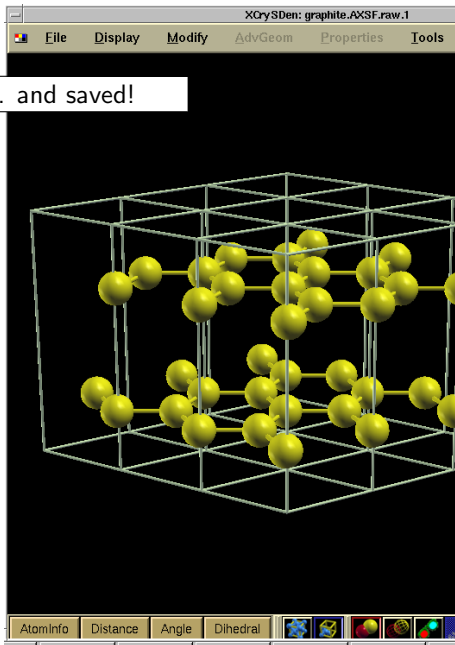
Repeat first frame No. times:

Repeat last frame No. times:

Time delay between slides (1/100 sec):

Start Recording Animated-GIF/MPEG

Hide Close



Animation Control Center

Delay between slides (in msec):

Animation step:

Current slide: 25/25

<< Animated GIF/MPEG

- Use global color-map for Animated GIF
- Minimize Animated GIF
- Make transparent background for Animated GIF
- Edit flag/parameter-file before encoding

◆ Make MPEG ◆ Make Animated-GIF

- ◆ Put GIF/MPEG temporary files in current working directory
- ◆ Put GIF/MPEG temporary files in scratch directory

- ◆ For MPEG: use non-compressed frame-files (PPM)
- ◆ For MPEG: use compressed frame-files (JPEG)

Repeat first frame No. times:

Repeat last frame No. times:

Time delay between slides (1/100 sec):

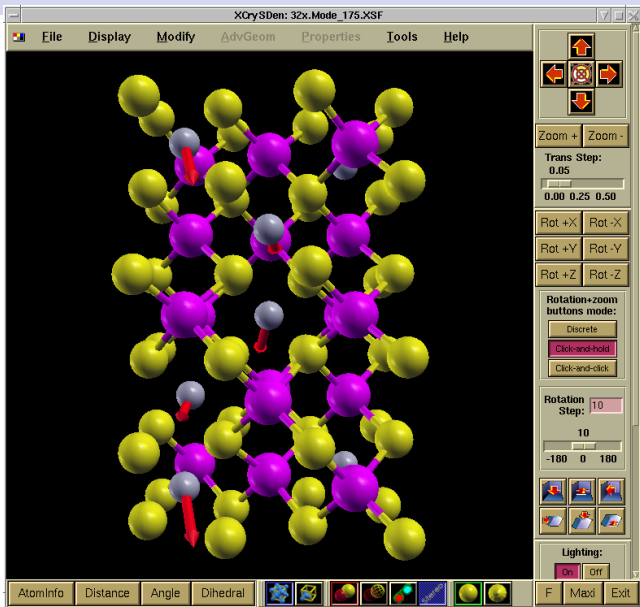
Stop Recording and Save

Hide Close

Frozen phonons (zone-center only)

- 1 get `.vectors` (calculated by `vibrator`) and `.XV` (from Siesta)
- 2 run `vib2xsf`, select # modes (first ... last) to visualize. For each selected mode, a separate `.XSF` file and an `.AXSF` file are created. `.XSF` contains a static structures (as in `.XV`), with arrows added to each atom to indicate displacement pattern. `.AXSF` contains the animation of a phonon, for a (user-chosen) amplitude and number of steps.

An example of phonons



An example of phonons

