Visualization and post-processing tools for SIESTA

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Lyon, June 22, 2006

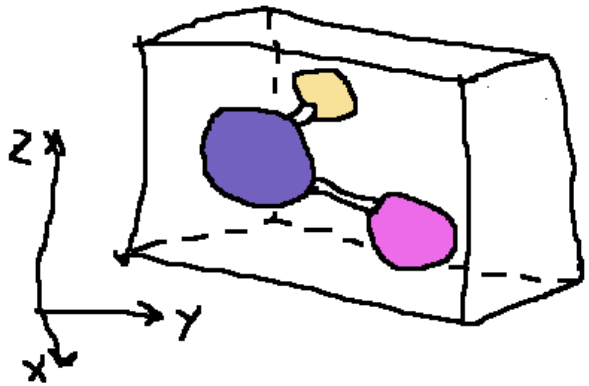
What to visualize..?

- 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 **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").

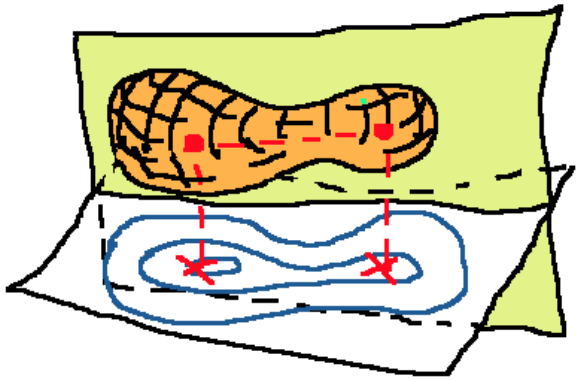


Since the input format is quite flexible (a big advantage!), it is difficult to organize a simple viewer of *input* structure data, without using the fdf routines. However, the .XV file (created after the completion of electronic structure loop) contains all necessary information, as it was *really* 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 vizualization 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 givel level. Both representations are possible with XCrySDen.

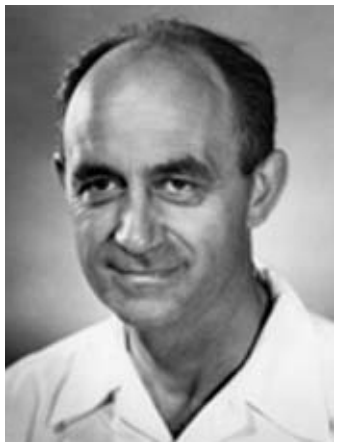
Kohn-Sham wavefunctions

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

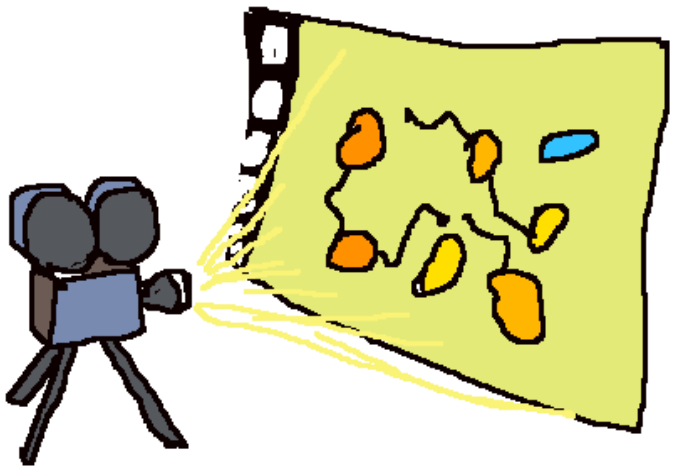
can be calculated using the energy dispersion data $E(\mathbf{k})$, available from any band structure code. The difficulty of purely technical character is, how to construct energy isosurfaces and conveniently manipulate them (to choose viewpoint, select different sheets of the Fermi surface, etc.) This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



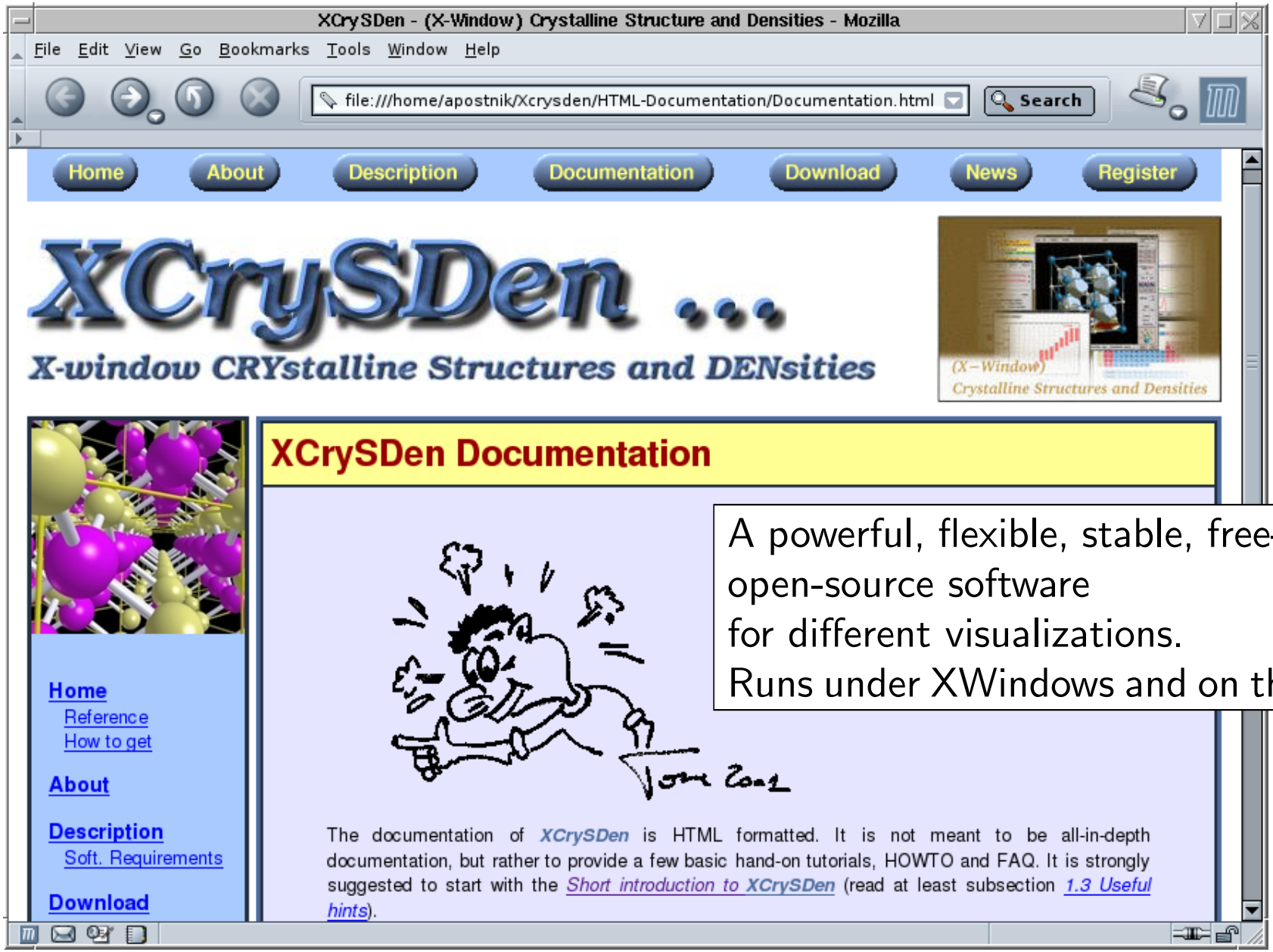
Phonon modes

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 by Tone Kokalj, http://www.xcrysden.org



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

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

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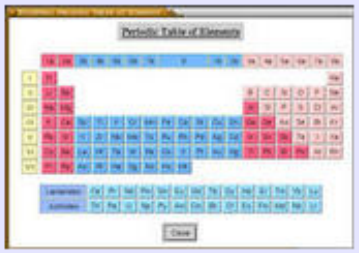
file:///home/apostnik/Xcrysden/HTML-Documentation/doc/intro.html Search

1.1 What *XCrySDen* can do?

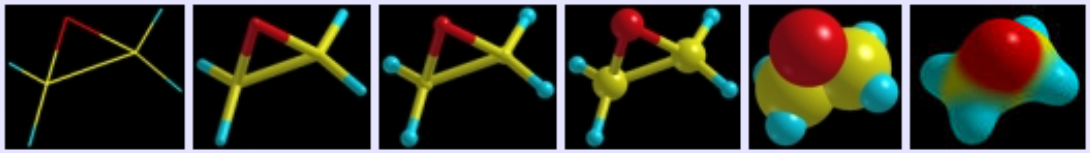
In short: *XCrySDen* is a crystalline and molecular structure render program, with additional capabilities of rendering contours, isosurfaces, Wigner-Seitz cells (also Brillouin zone), Fermi surfaces and so on. Some of its features are the following:

- widget with periodic table of elements:

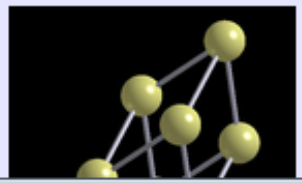


Enables different presentations
of atoms and bonds (colors, shadows, ...),
measuring distances and angles ...

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



- displaying crystal and Wigner-Seitz cells:



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

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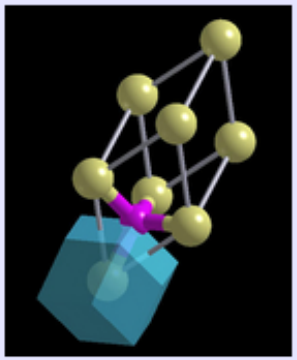
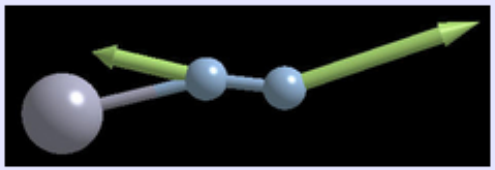
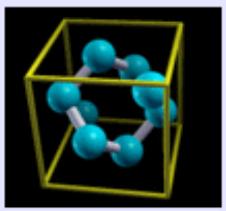
- displaying crystal and Wigner-Seitz cells:



- 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 fictituous atoms) and make animations ...

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

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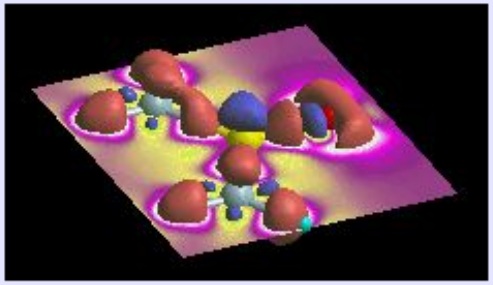
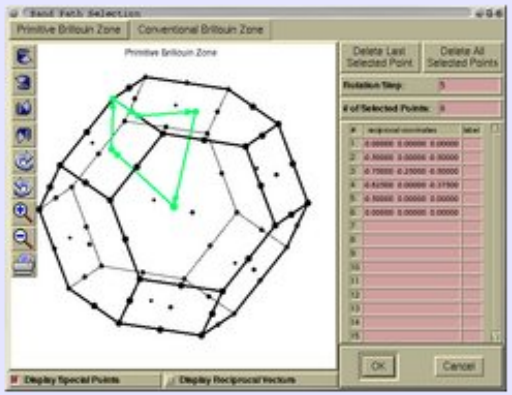
file:///home/apostnik/Xcrysden/HTML-Documentation/doc/intro.html Search

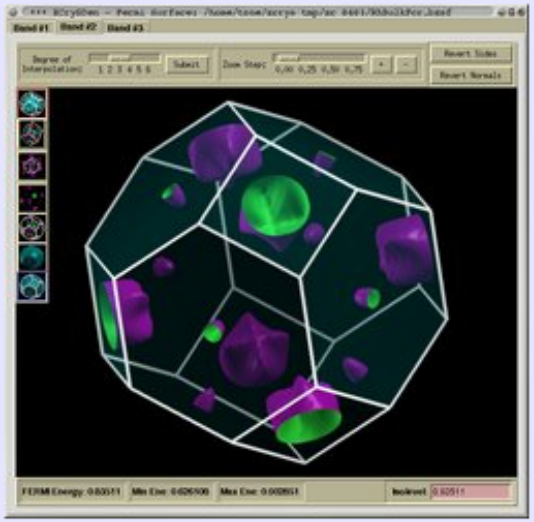
- displaying contours and colorplanes
- displaying isosurfaces:



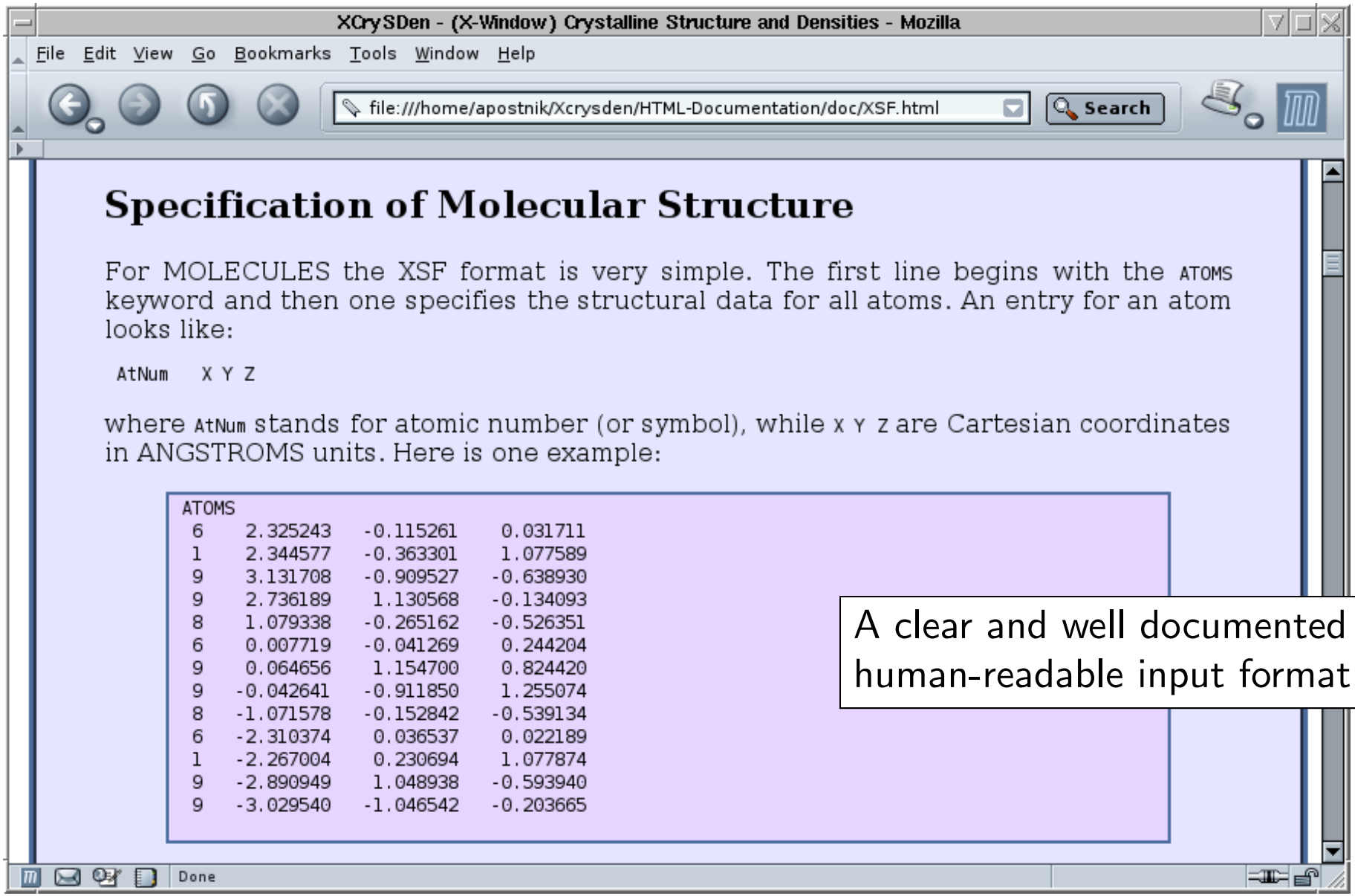
Allows to make contour plots,
to draw isosurfaces,
to choose path through the Brillouin zone,
to use different modi
of presenting the Fermi surfaces

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





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



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

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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 Fx Fy Fz 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:

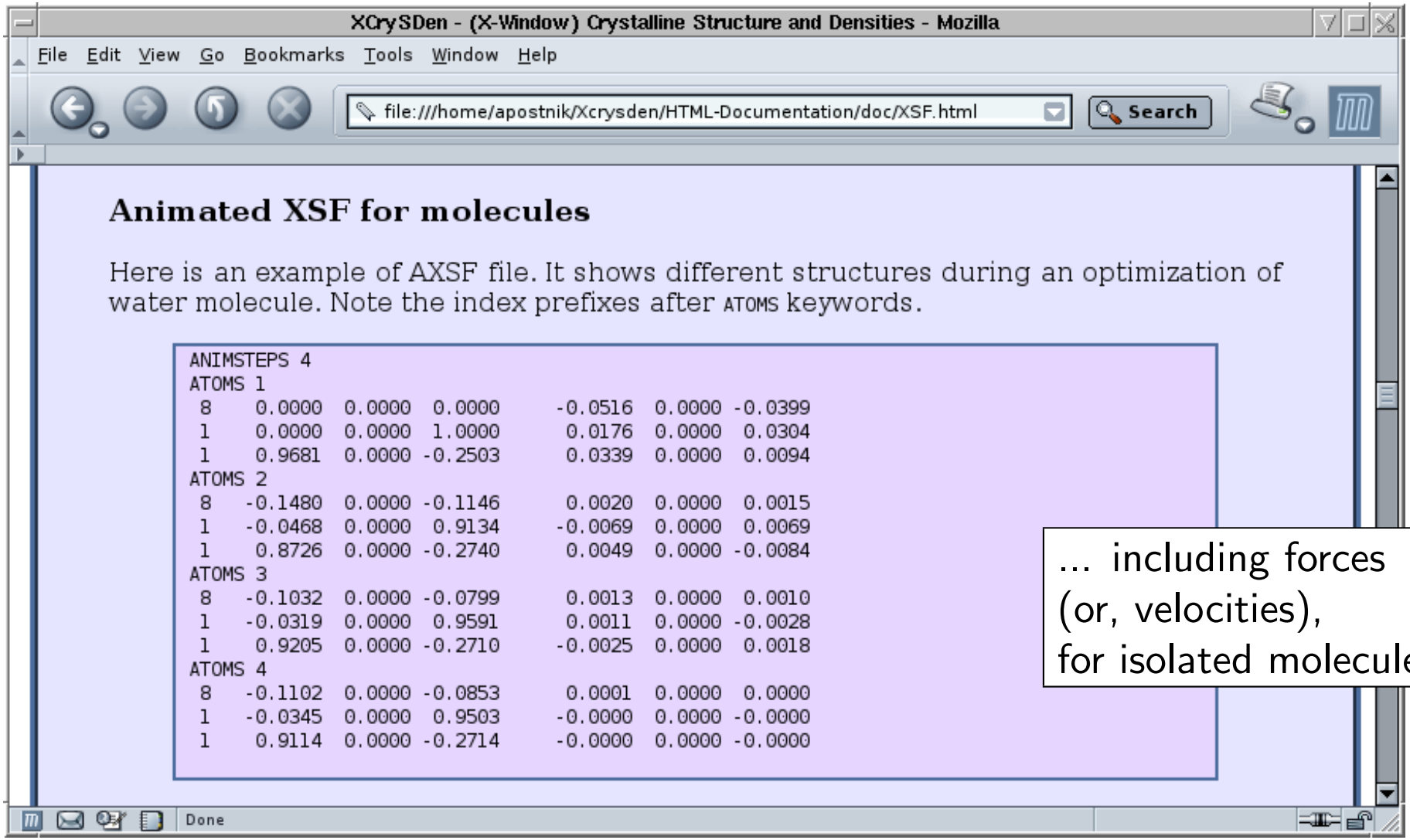
```
ATOMS
 8   0.00000  0.00000  0.00000   -.05164  .00000 -.03999
 1   0.00000  0.00000  1.00000    .01769  .00000  .03049
 1   0.96814  0.00000 -0.25038    .03395  .00000  .00949
```

And here is an example for the periodic structure structure:

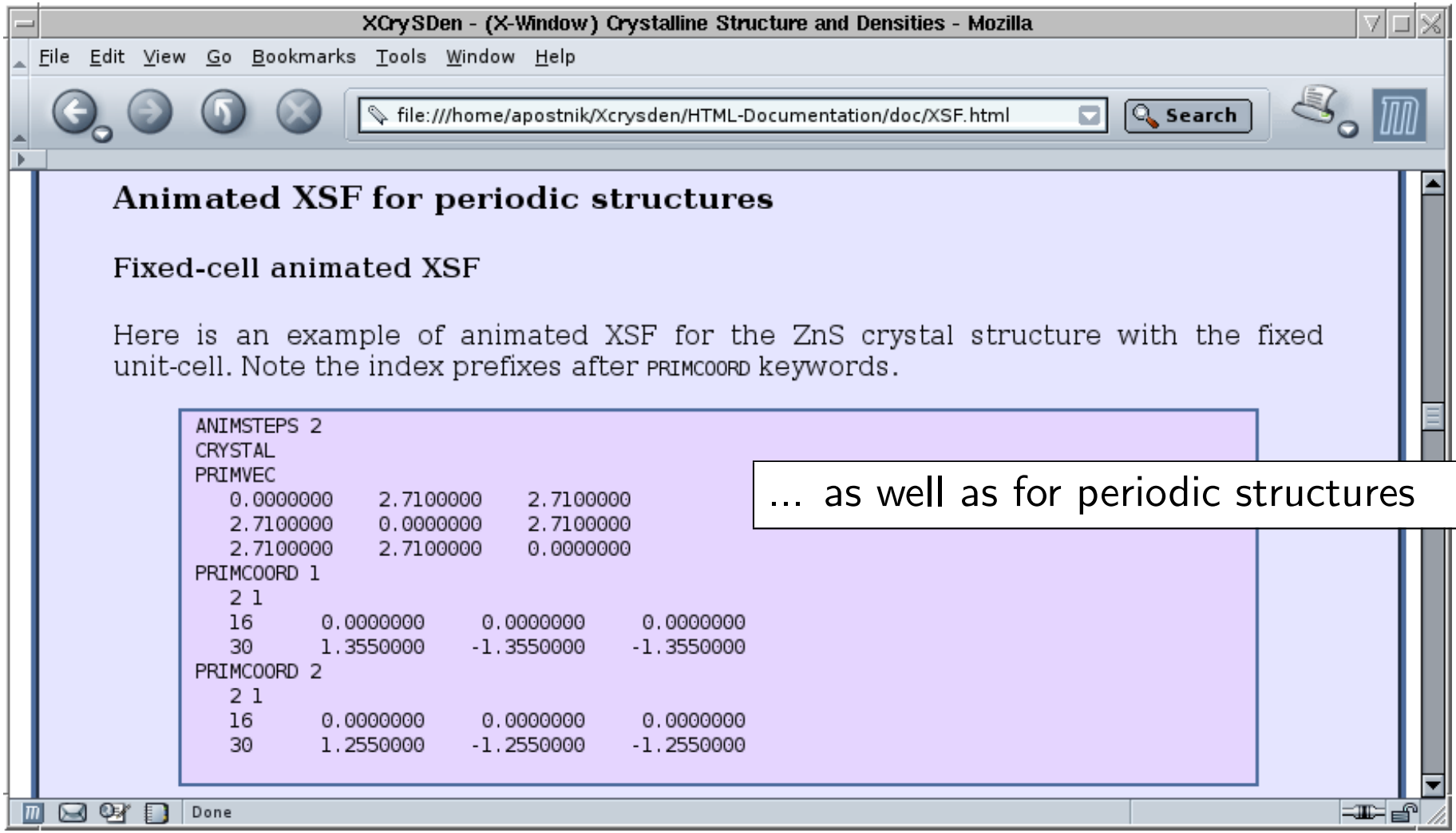
```
SLAB
PRIMVEC
  5.8859828533     0.0000000000     0.0000000000
  0.0000000000     5.8859828533     0.0000000000
  0.0000000000     0.0000000000     1.0000000000
PRIMCOORD 1
11 1
 6    3.674759   2.942992  -3.493103     -0.021668   0.000000  -0.057324
 1    4.121990   3.816734  -4.007689     -0.000478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



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



Sies2xsf utilities

Where to find them:

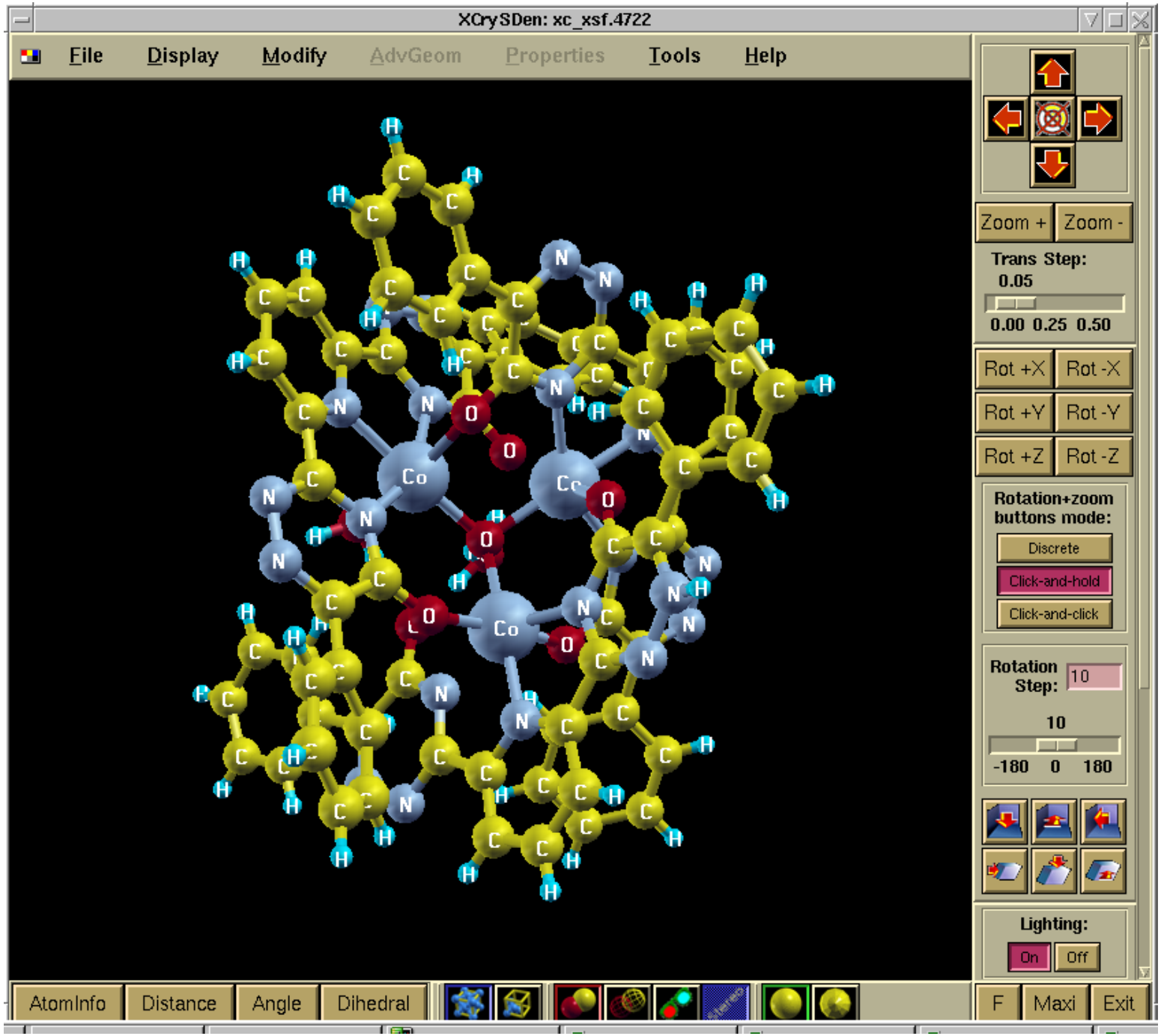
- `··· siesta-2.0/Util/Contrib/APostnikov/`
- http://www.home.uni-osnabrueck.de/apostnik/Downloads ,
  or mailto apostnik@uos.de or postnikov@univ-metz.fr

What are they:

- **xv2xsf**: .XV → .XSF (view structure + cell)
- **rho2xsf**: .XV, .RHO or .LDOS → .XSF
  (atoms within a selected box + data grids)
- **md2axsf**: .XV, .ANI or .MD → .AXSF
  (animations of structure with fixed or variable cell)
- **eig2bxsf**: .XV, .KP and .EIG → .BXSF (Fermi surfaces)
- **vib2xsf**: .XV and .vectors → .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 defned 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 to generated grid.
5. Choice isosurface parameters, cutting planes, isolines on the cutting planes, colors, lighting etc. by means of XCrySDen.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File
Display
Modify
AdvGeom
Properties
Tools
Help
Zoom +
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Trans Step:
0.05
0.00 0.25 0.50
Rot +X
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Rot +Y
Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
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-180 0 180
Lighting:
On
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AtomInfo
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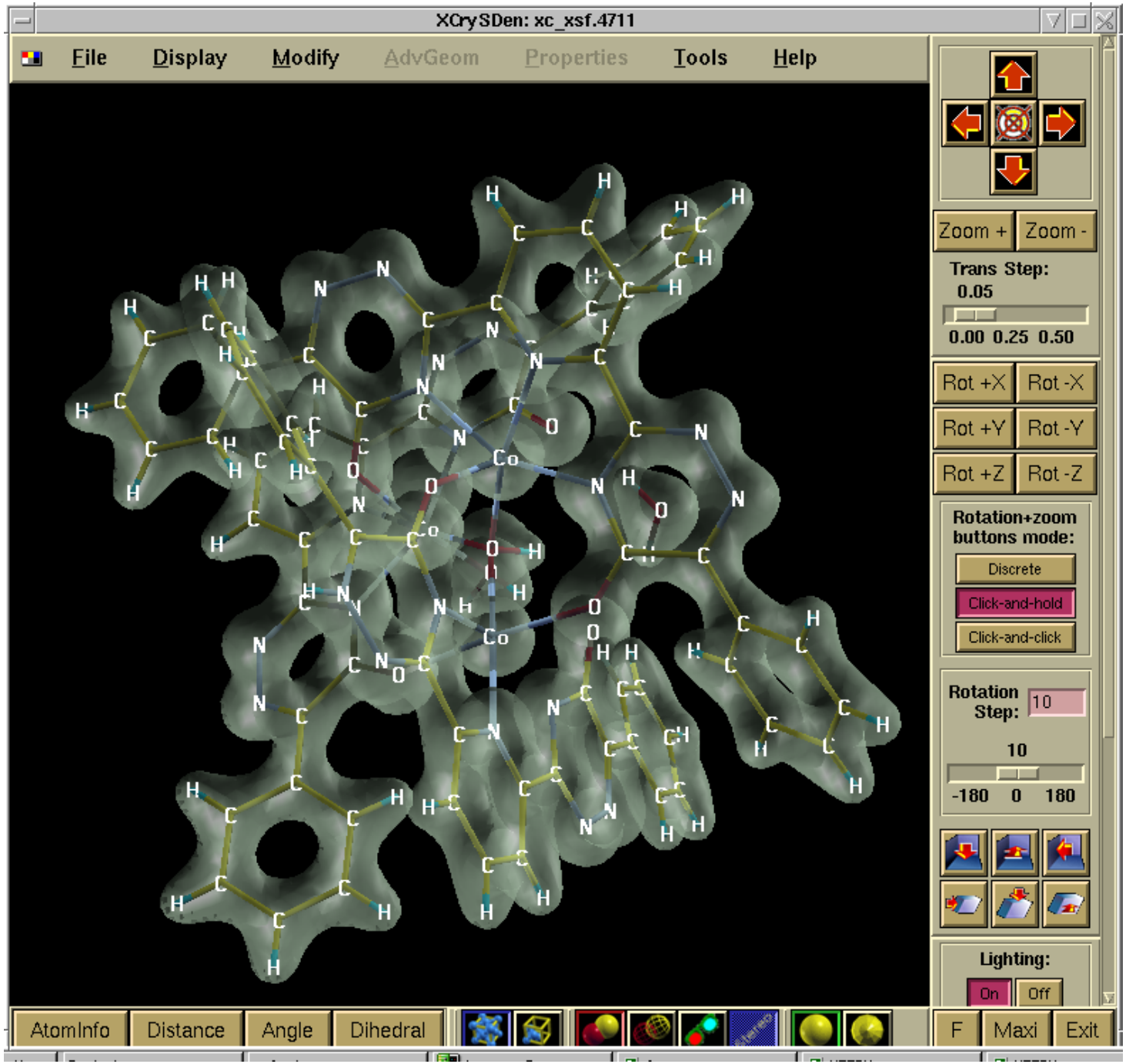
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Zoom -
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Rot +X
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Rot +Y
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Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
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-180 0 180
Lighting:
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AtomInfo
Distance
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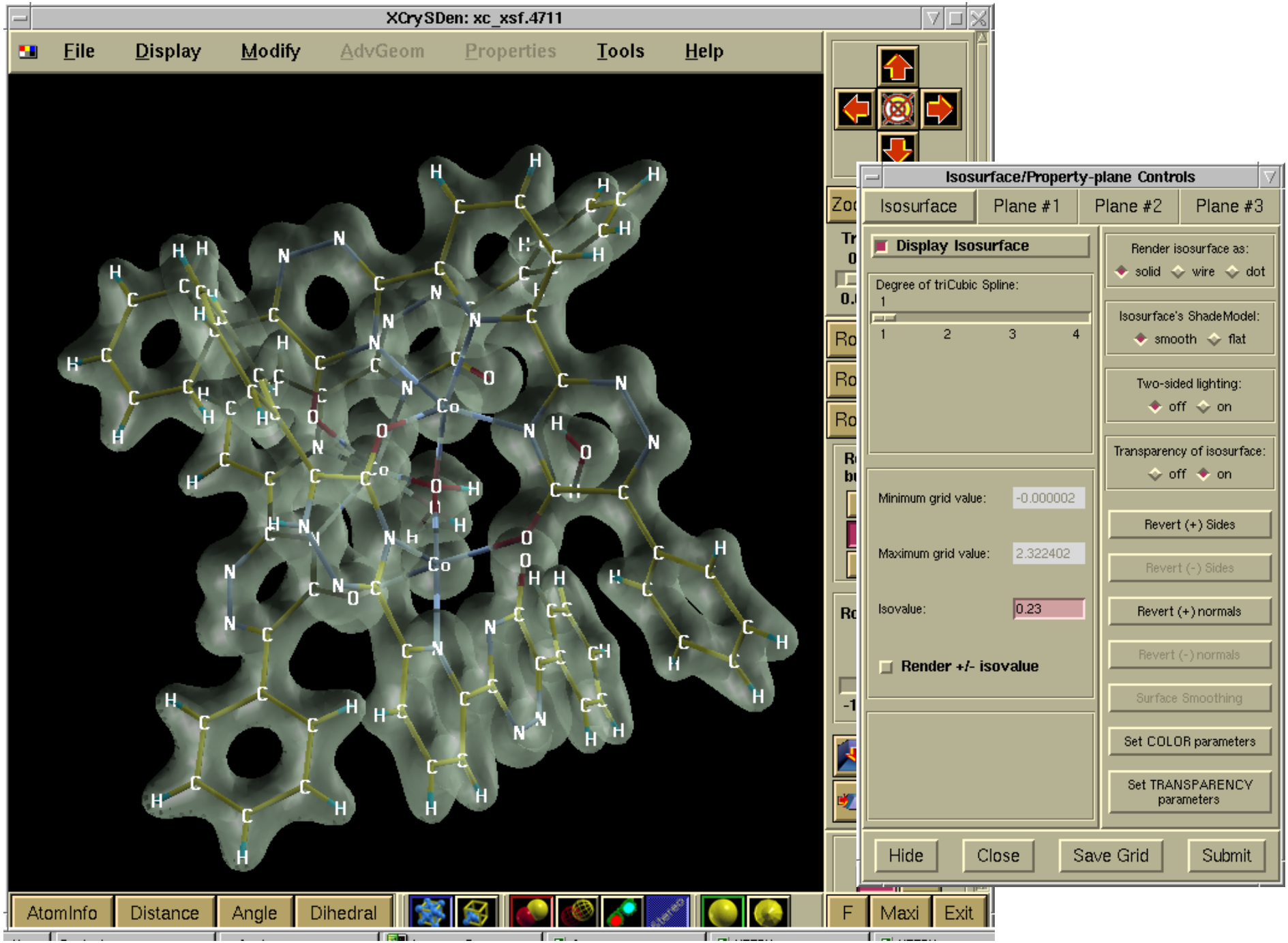
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Display
Modify
AdvGeom
Properties
Tools
Help
Isosurface/Property-plane Controls
Isosurface
Plane #1
Plane #2
Plane #3
Display Isosurface
Degree of triCubic Spline:
1
1 2 3 4
Render isosurface as:
solid wire dot
Isosurface's ShadeModel:
smooth flat
Two-sided lighting:
off on
Transparency of isosurface:
off on
Minimum grid value:
-0.000002
Maximum grid value:
2.322402
Isovalue:
0.23
Render +/- isovalue
Revert (+) Sides
Revert (-) Sides
Revert (+) normals
Revert (-) normals
Surface Smoothing
Set COLOR parameters
Set TRANSPARENCY parameters
Hide
Close
Save Grid
Submit
AtomInfo
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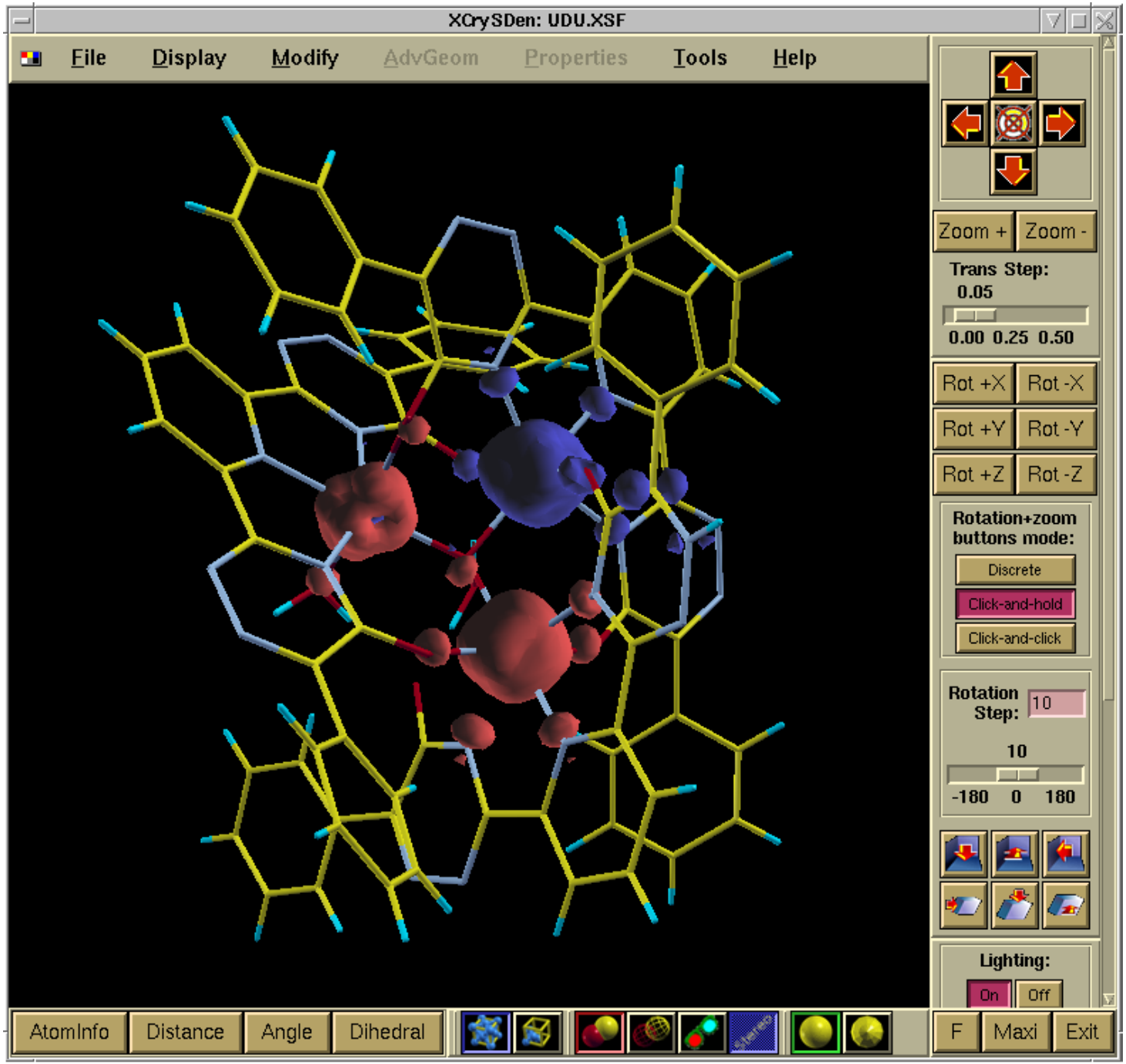
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Modify
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Properties
Tools
Help
Zoom +
Zoom -
Trans Step:
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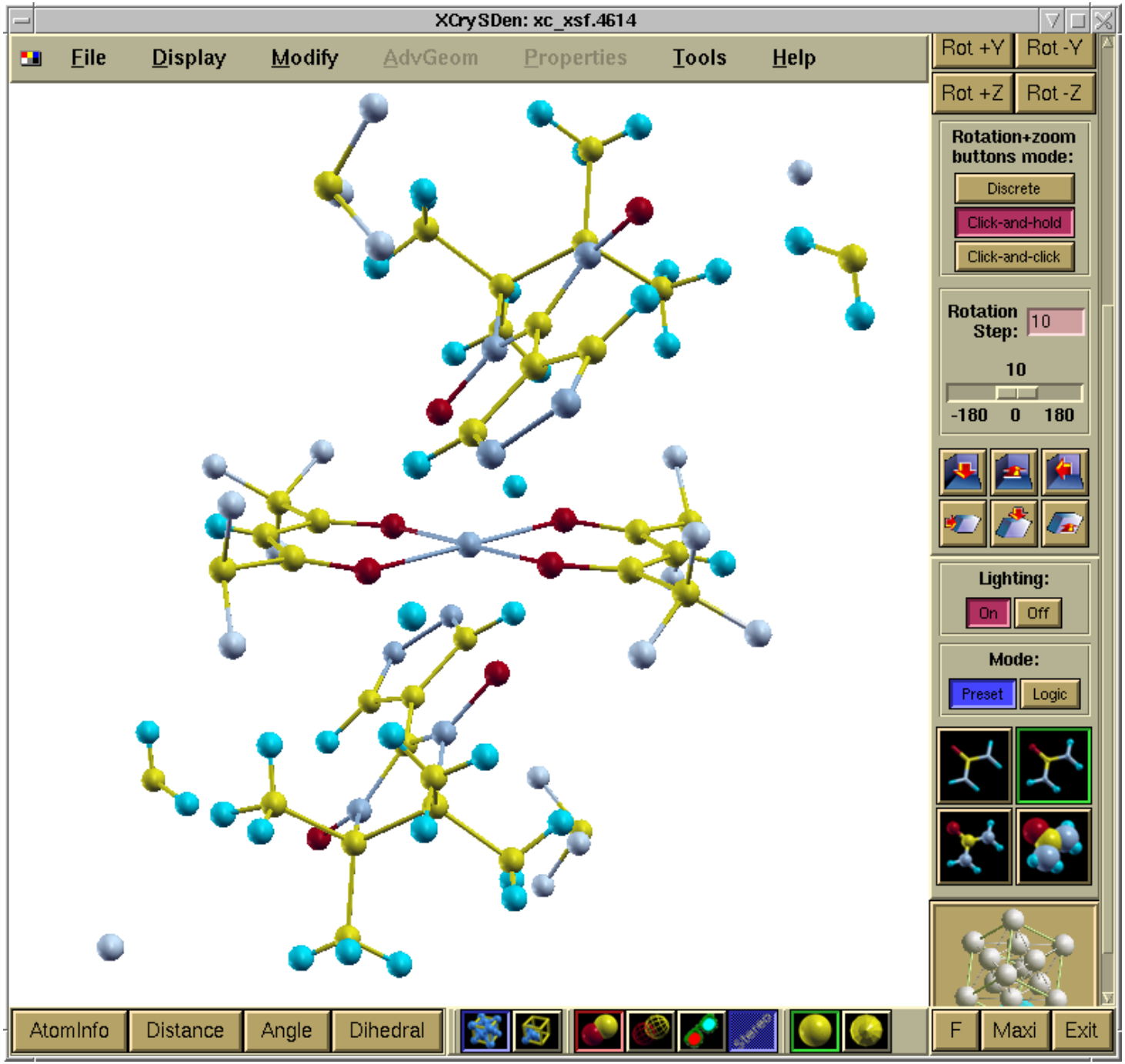
0.00 0.25 0.50
Rot +X
Rot -X
Rot +Y
Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
10
10
-180 0 180
Lighting:
On
Off
AtomInfo
Distance
Angle
Dihedral
F
Maxi
Exit

Visualization of Wave Functions

1. Use Denchar, define output box there, save result as Gaussian98 Cube file.
2. Read this Gausian98 Cube file into XCrySDen. Save in the XCrySDen format .xsf ($\rightarrow$ 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 ($\rightarrow$ 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 Gausian Cube) into a single .xsf file.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File
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Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
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Mode:
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AtomInfo
Distance
Angle
Dihedral
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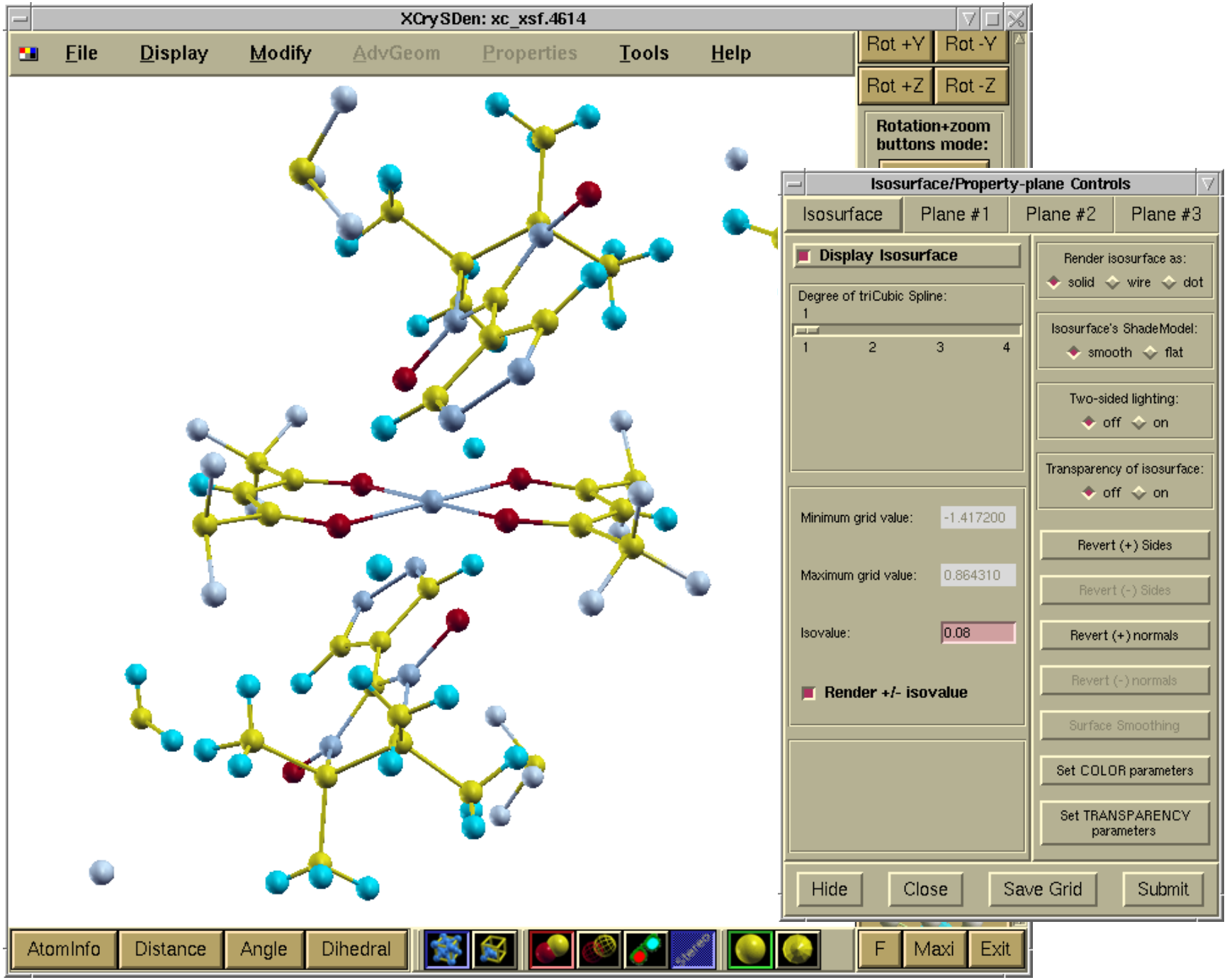
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Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Isosurface/Property-plane Controls
Isosurface
Plane #1
Plane #2
Plane #3
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Degree of triCubic Spline:
1
1 2 3 4
Render isosurface as:
solid wire dot
Isosurface's ShadeModel:
smooth flat
Two-sided lighting:
off on
Transparency of isosurface:
off on
Minimum grid value:
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Maximum grid value:
0.864310
Isovalue:
0.08
Render +/- isovalue
Revert (+) Sides
Revert (-) Sides
Revert (+) normals
Revert (-) normals
Surface Smoothing
Set COLOR parameters
Set TRANSPARENCY parameters
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Distance
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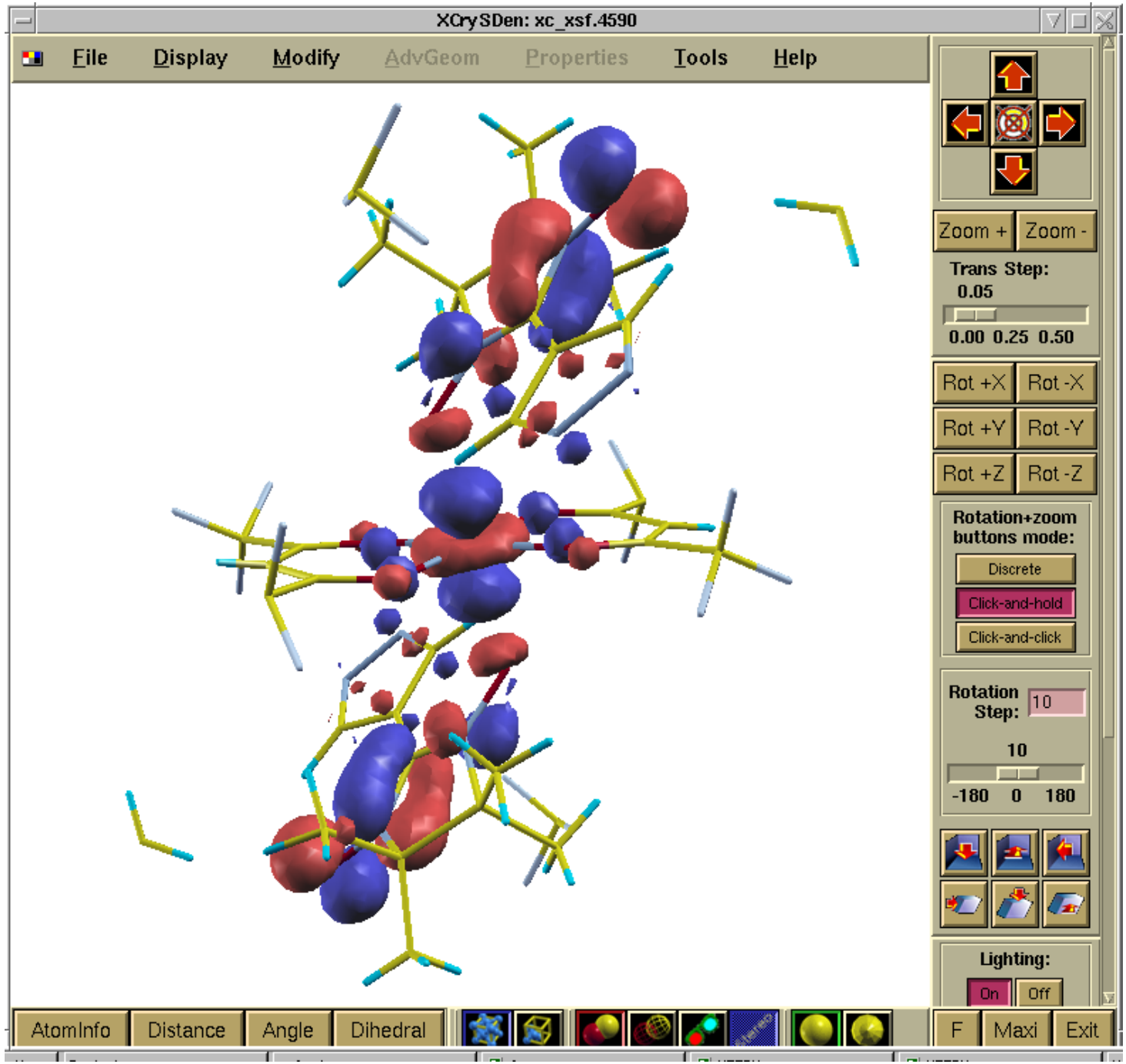
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Zoom +
Zoom -
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Rotation+zoom buttons mode:
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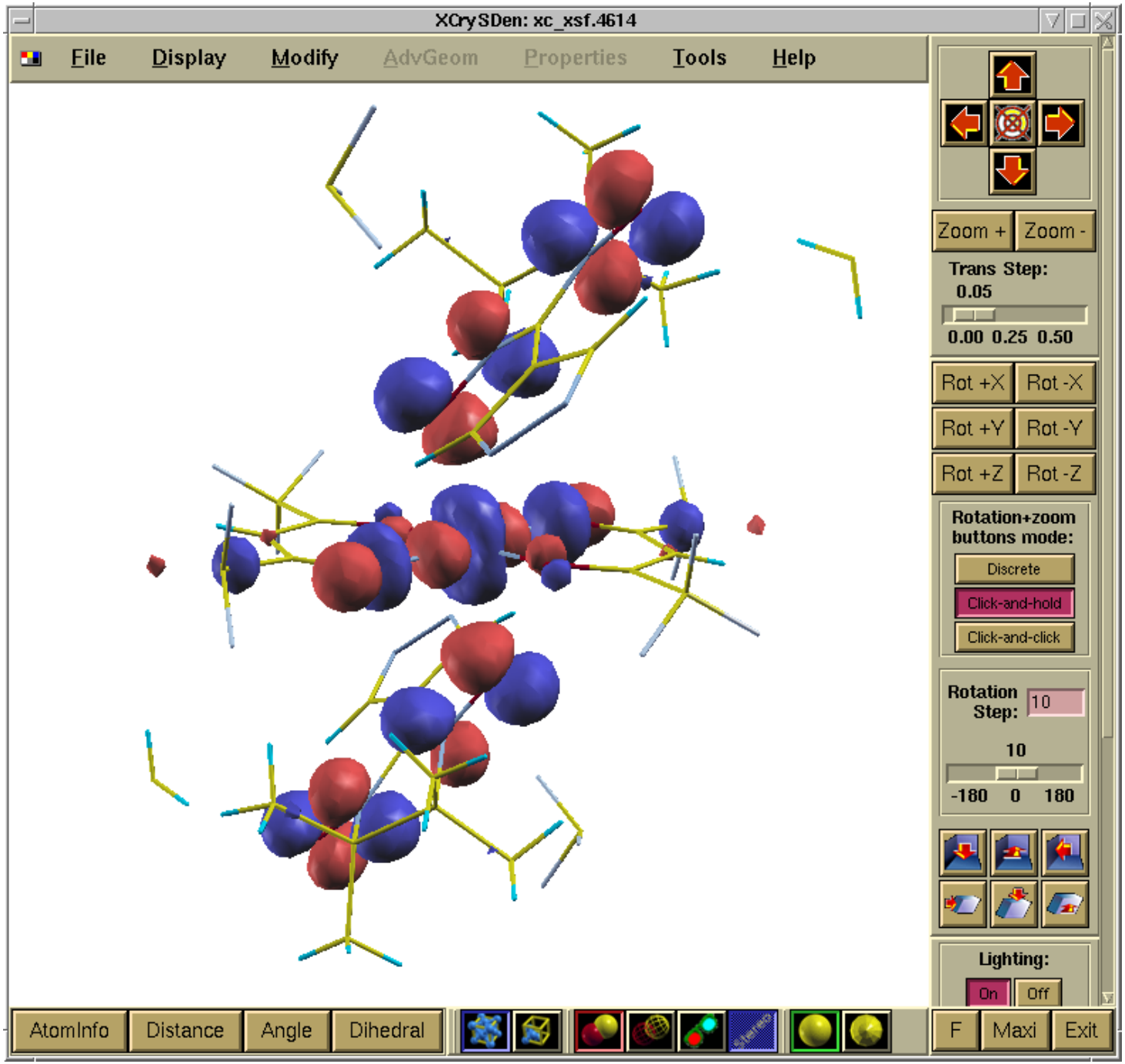
XCrySDen: xc_xsf.4614
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Tools
Help
Zoom +
Zoom -
Trans Step:
0.05
0.00 0.25 0.50
Rot +X
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Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
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-180 0 180
Lighting:
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AtomInfo
Distance
Angle
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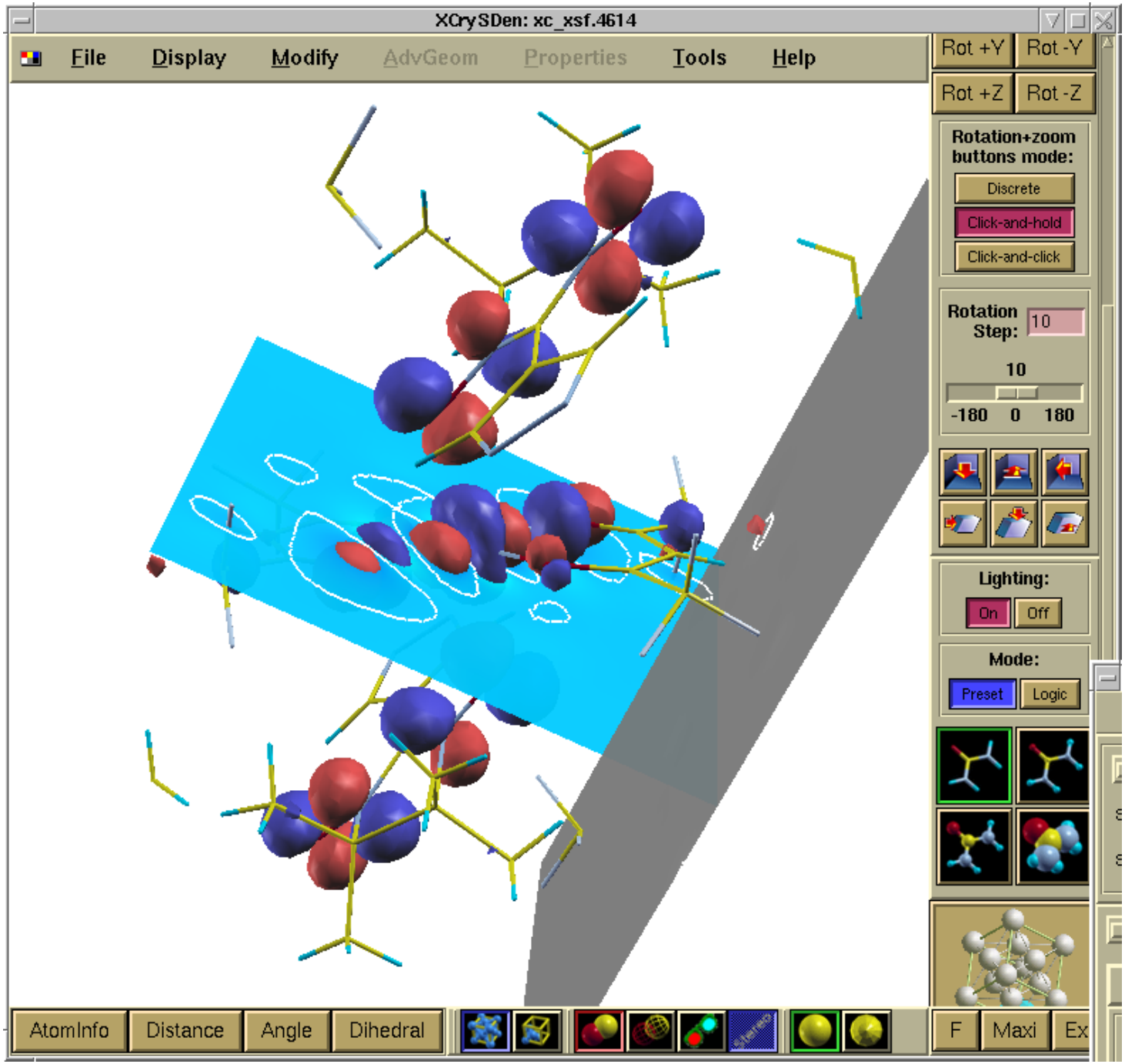
Maxi
Exit


XCrySDen: xc_xsf.4614
File
Display
Modify
AdvGeom
Properties
Tools
Help
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
Mode:
Preset
Logic
AtomInfo
Distance
Angle
Dihedral
F
Maxi
Ex

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
```

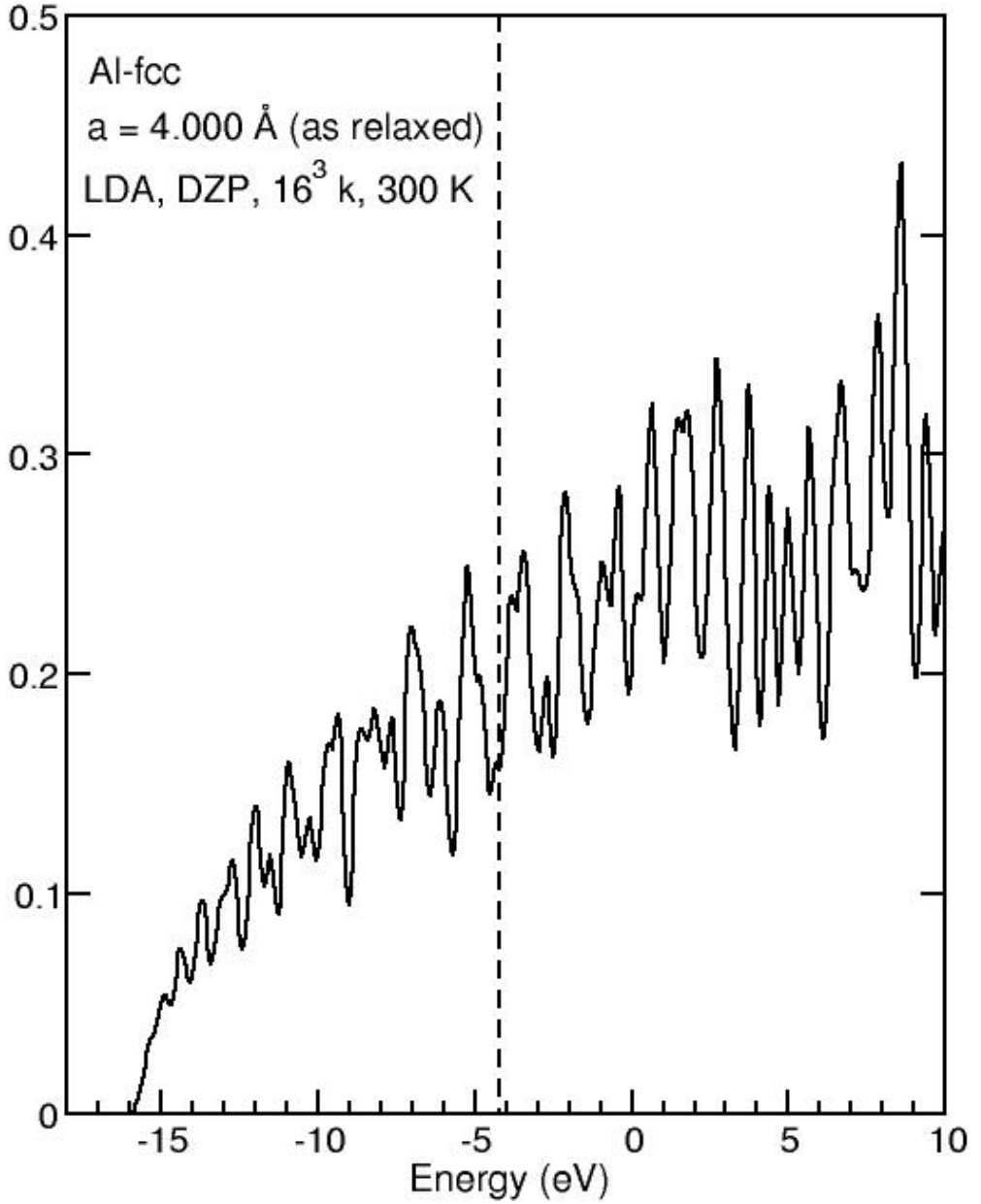
2. get files .XV, .KP, .EIG,
run eig2bxsf $\longrightarrow$ creates .BXSF
(or .BXSF_1 and .BXSF_2
for spin-polarized case).

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).

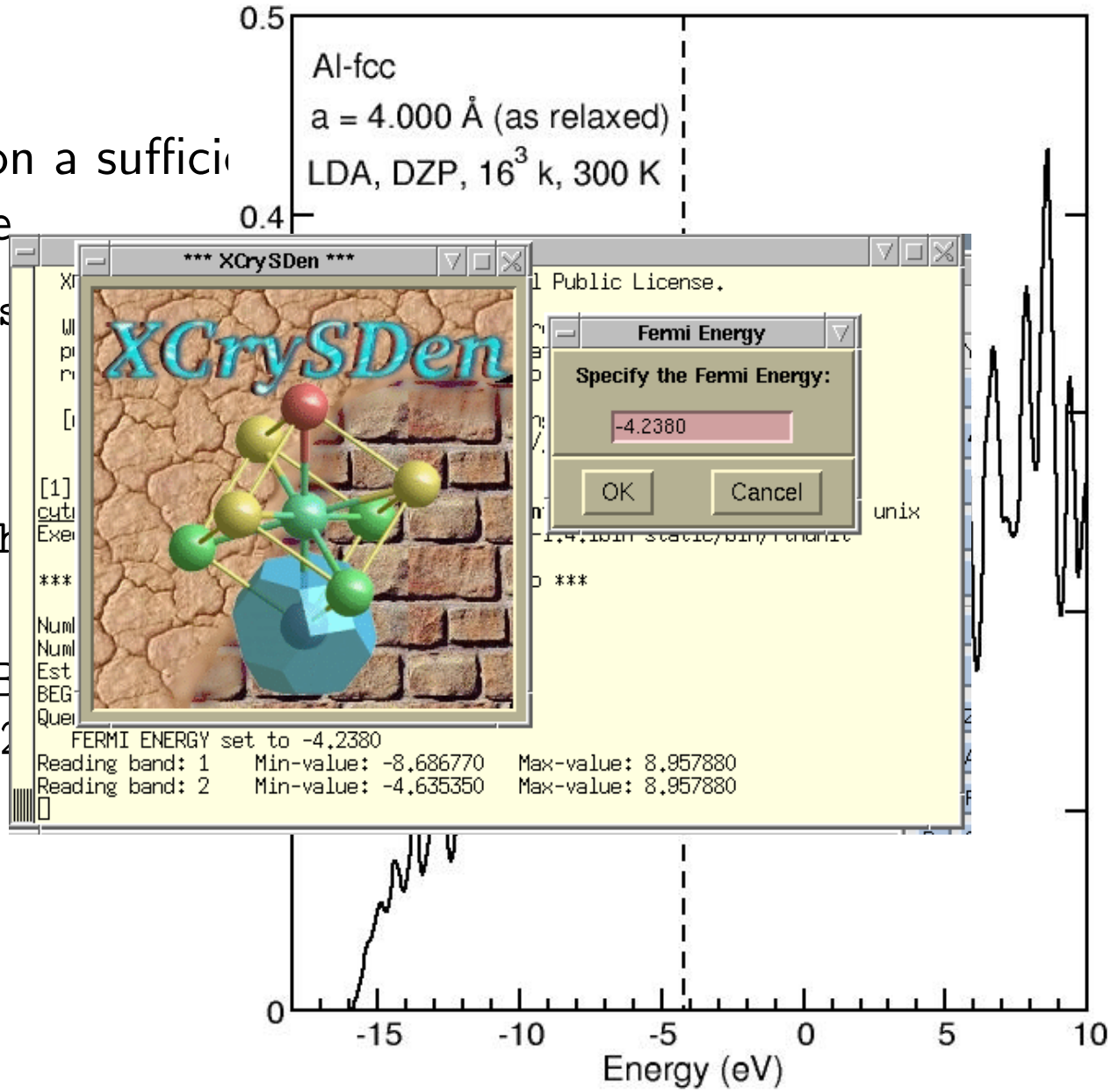


Visualization of Fermi surfaces

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

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

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

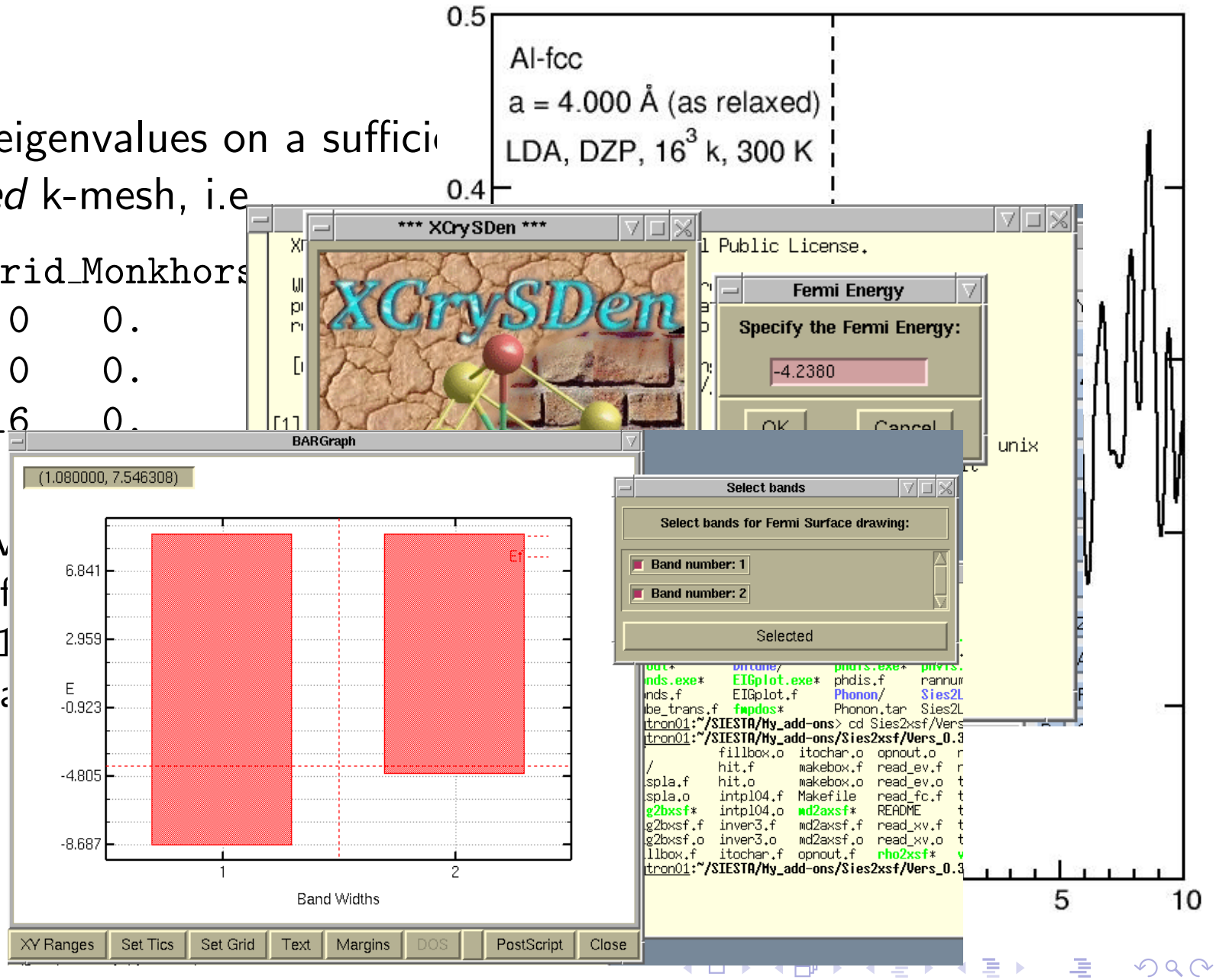


Visualization of Fermi surfaces

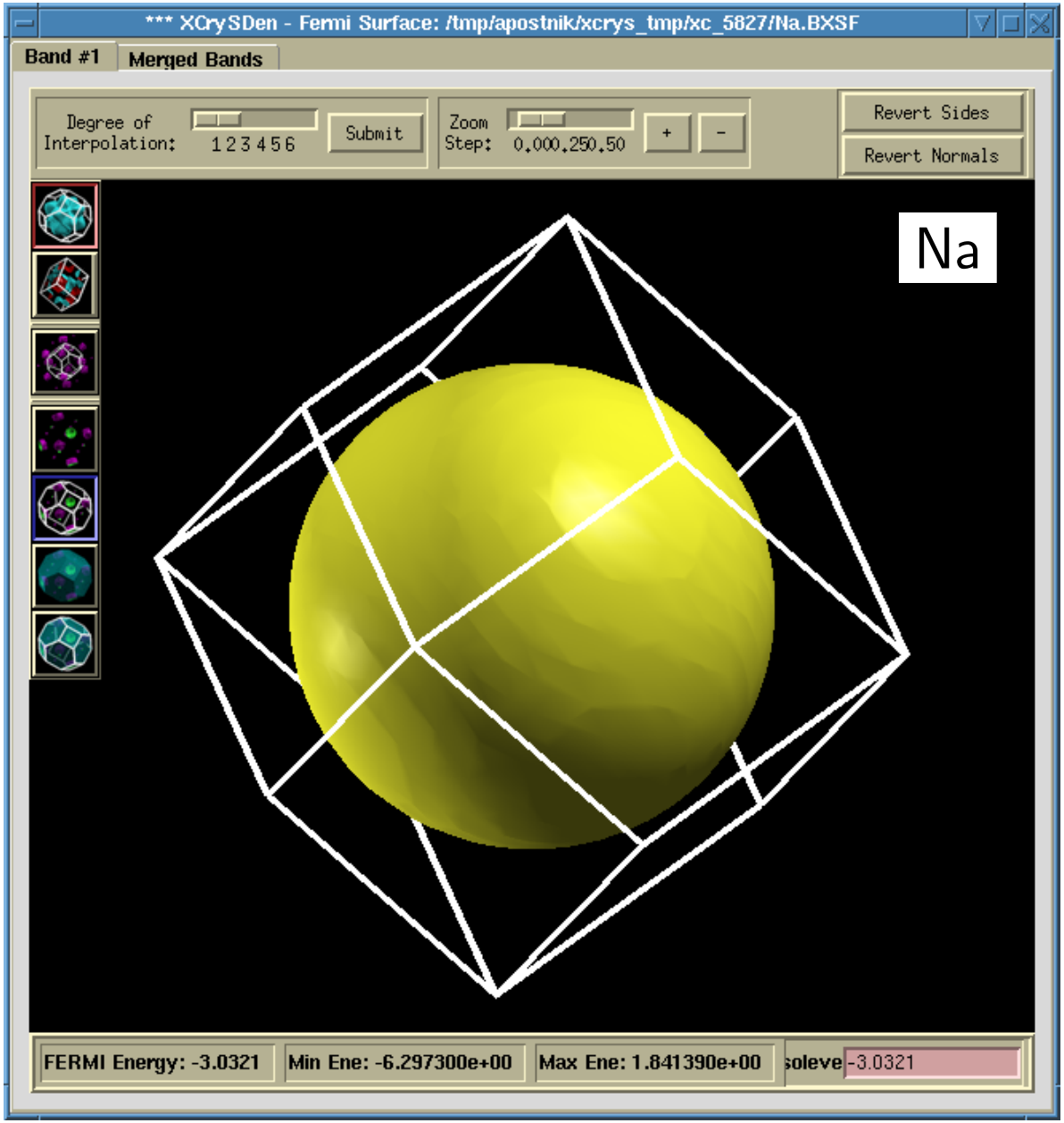
1. Calculate eigenvalues on a sufficie
   undicplaced k-mesh, i.e

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

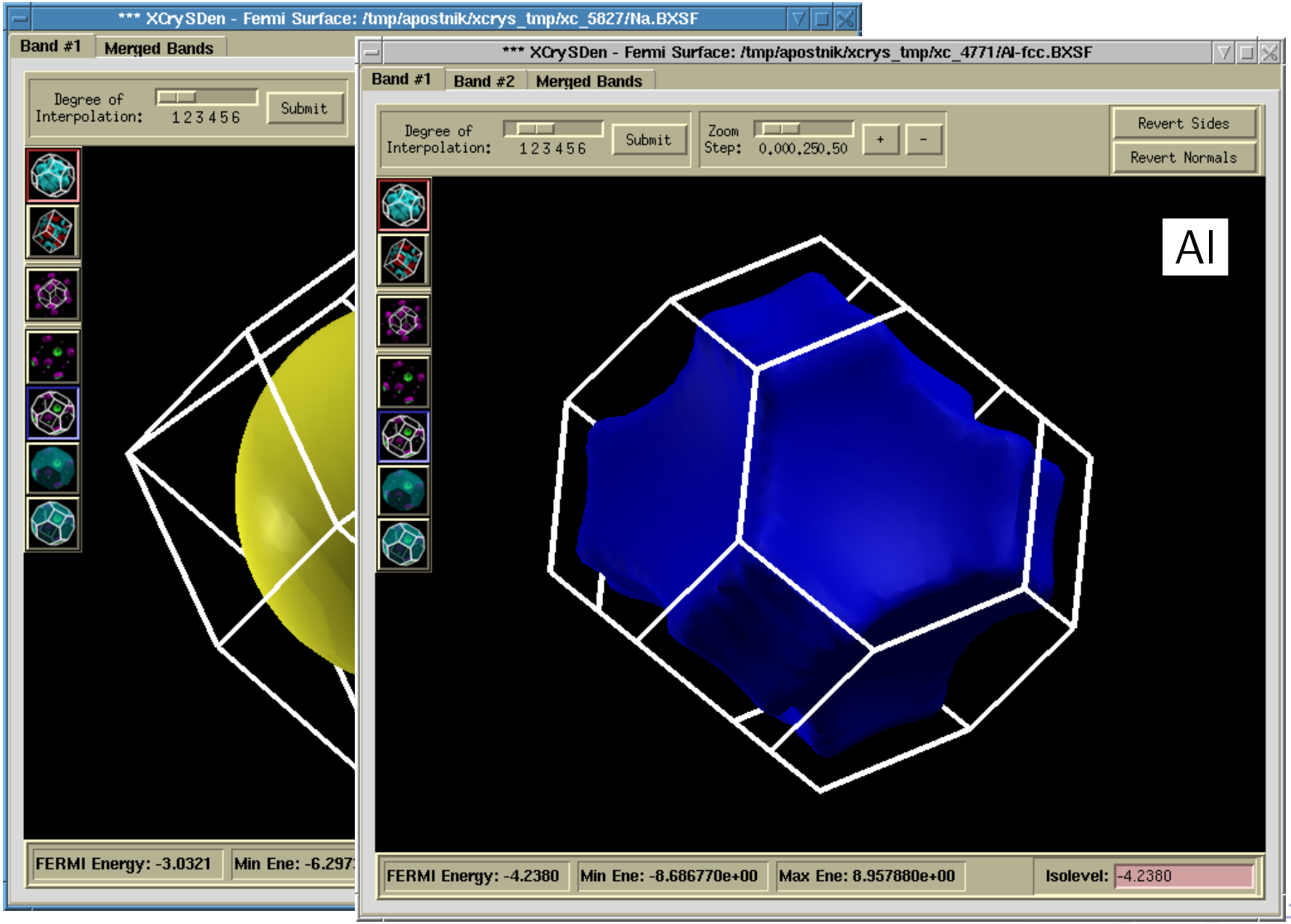
2. get files .XV
   run eig2bxsf
   (or .BXSF_1
   for spin-pola



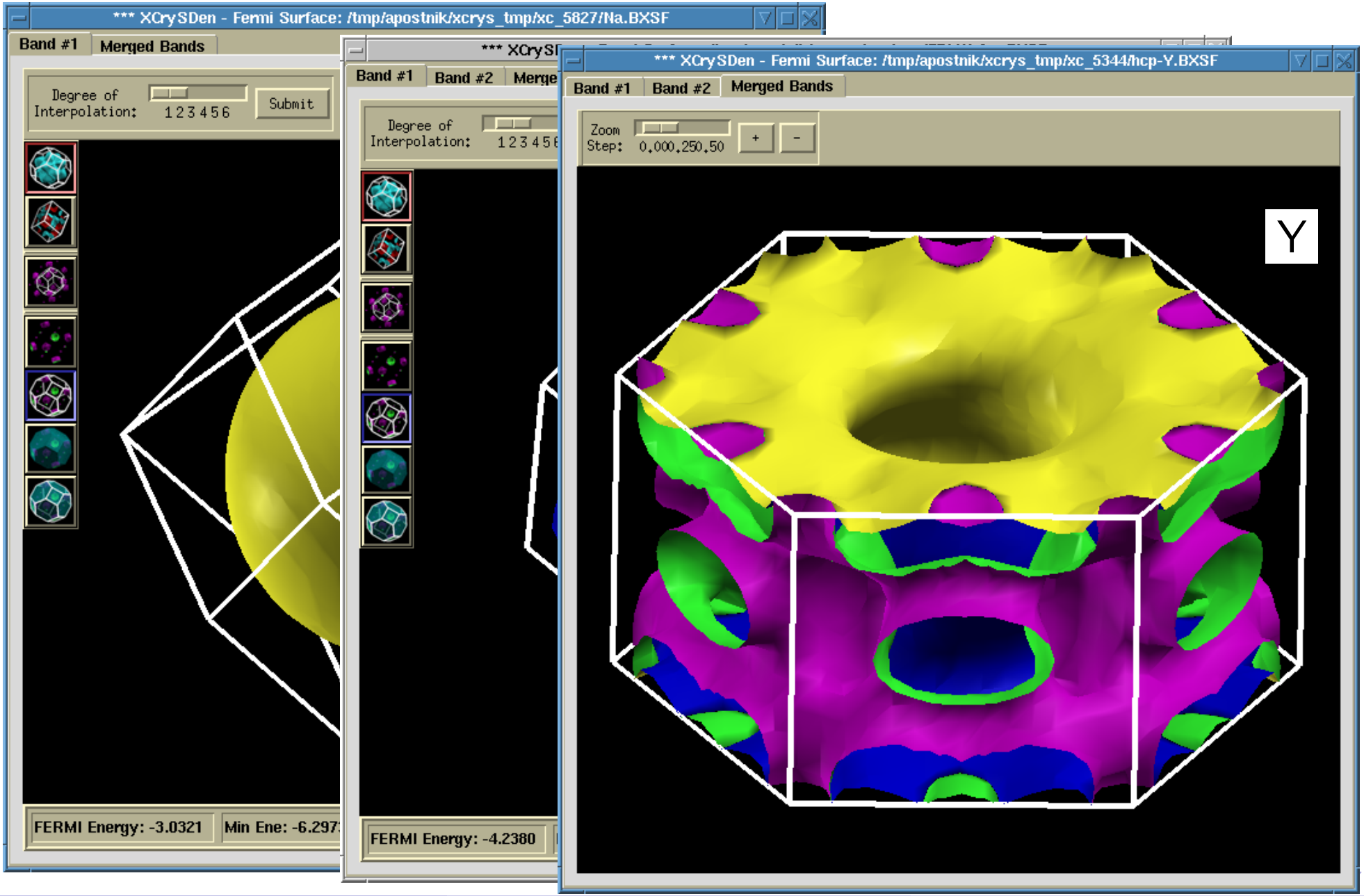
Fermi surfaces of some elemental metals



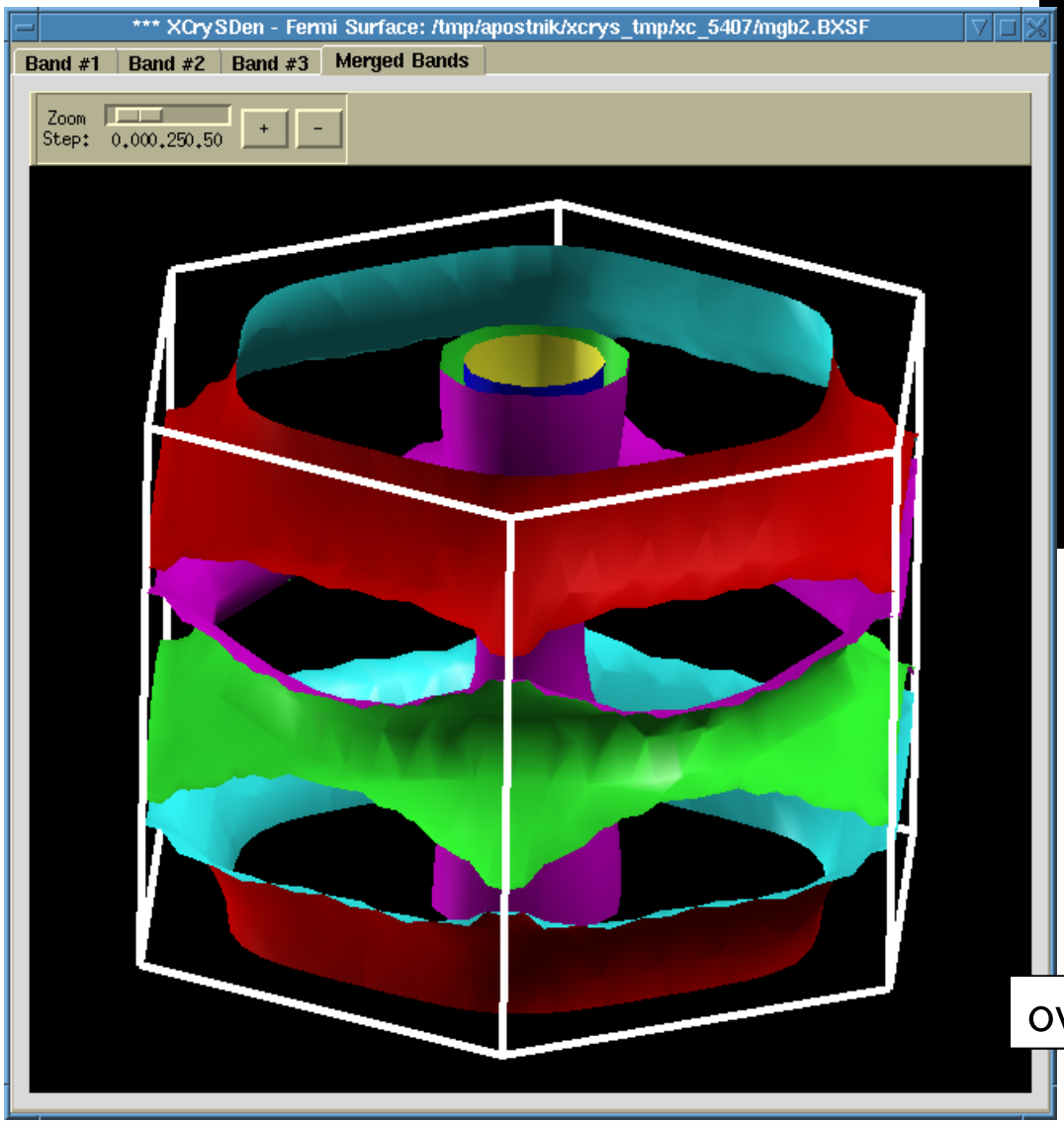
Fermi surfaces of some elemental metals

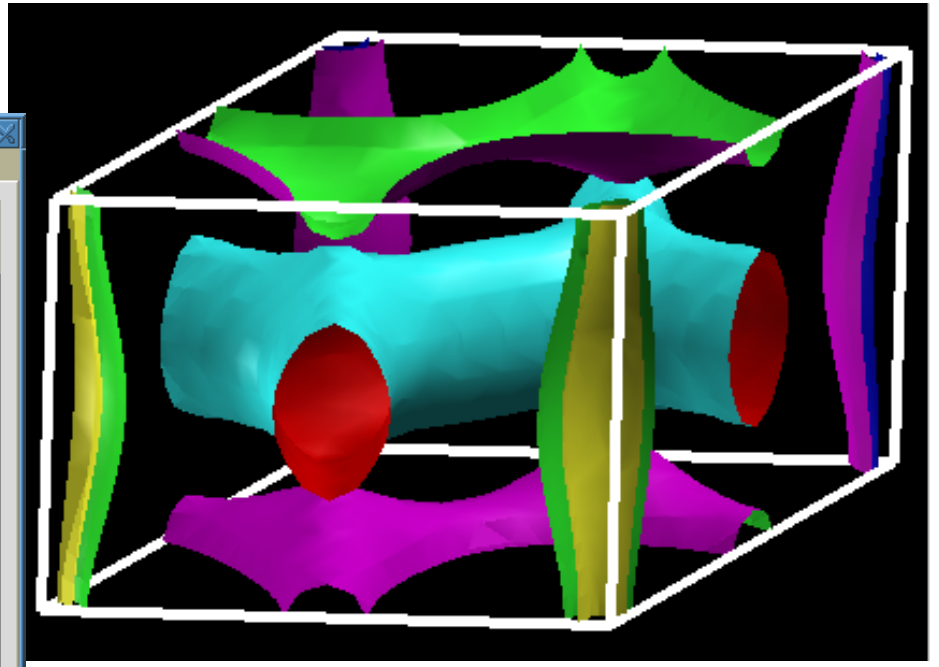


Fermi surfaces of some elemental metals



Fermi surface of MgB_2





over the reciprocal cell

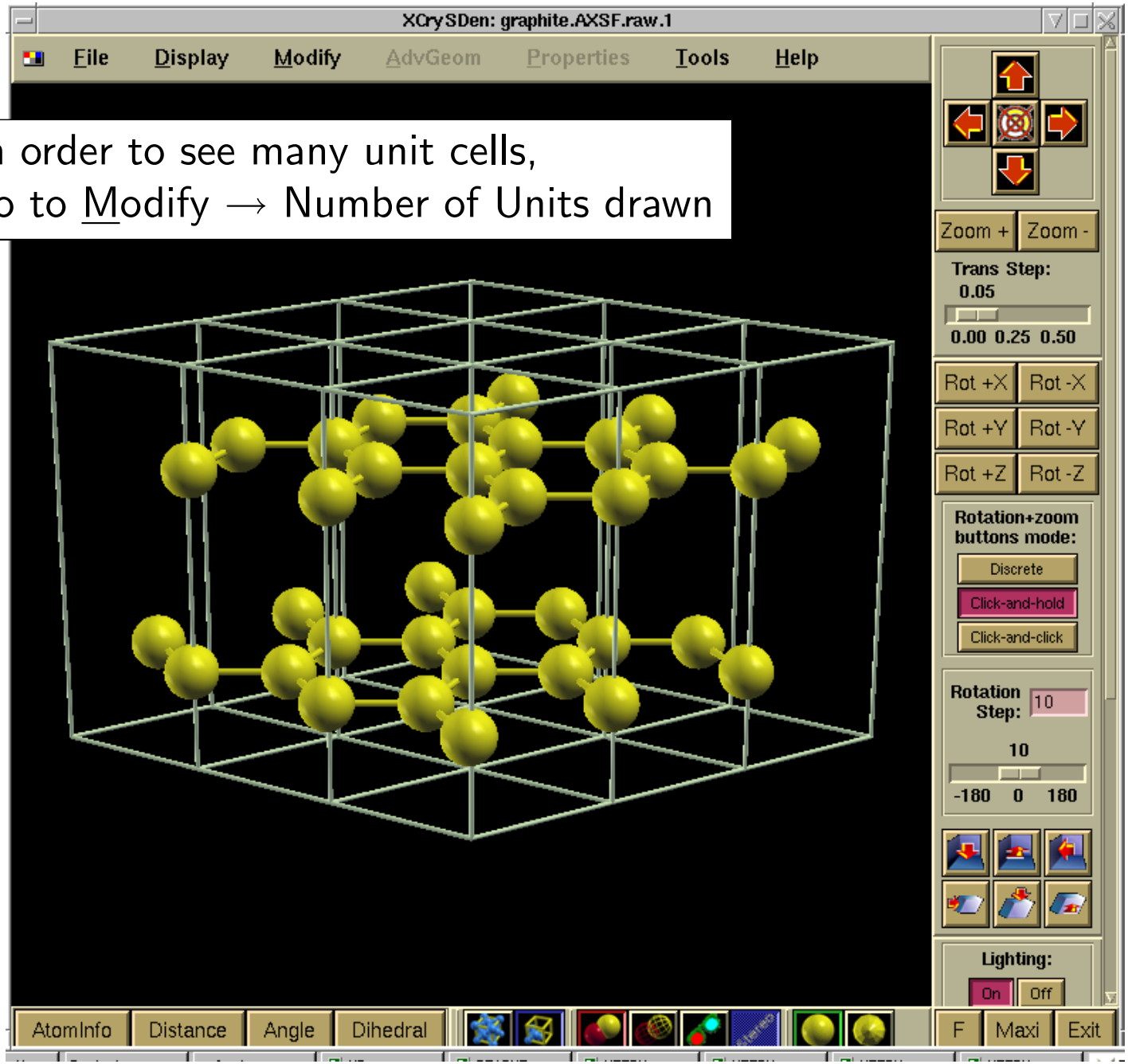
over the Brillouin zone

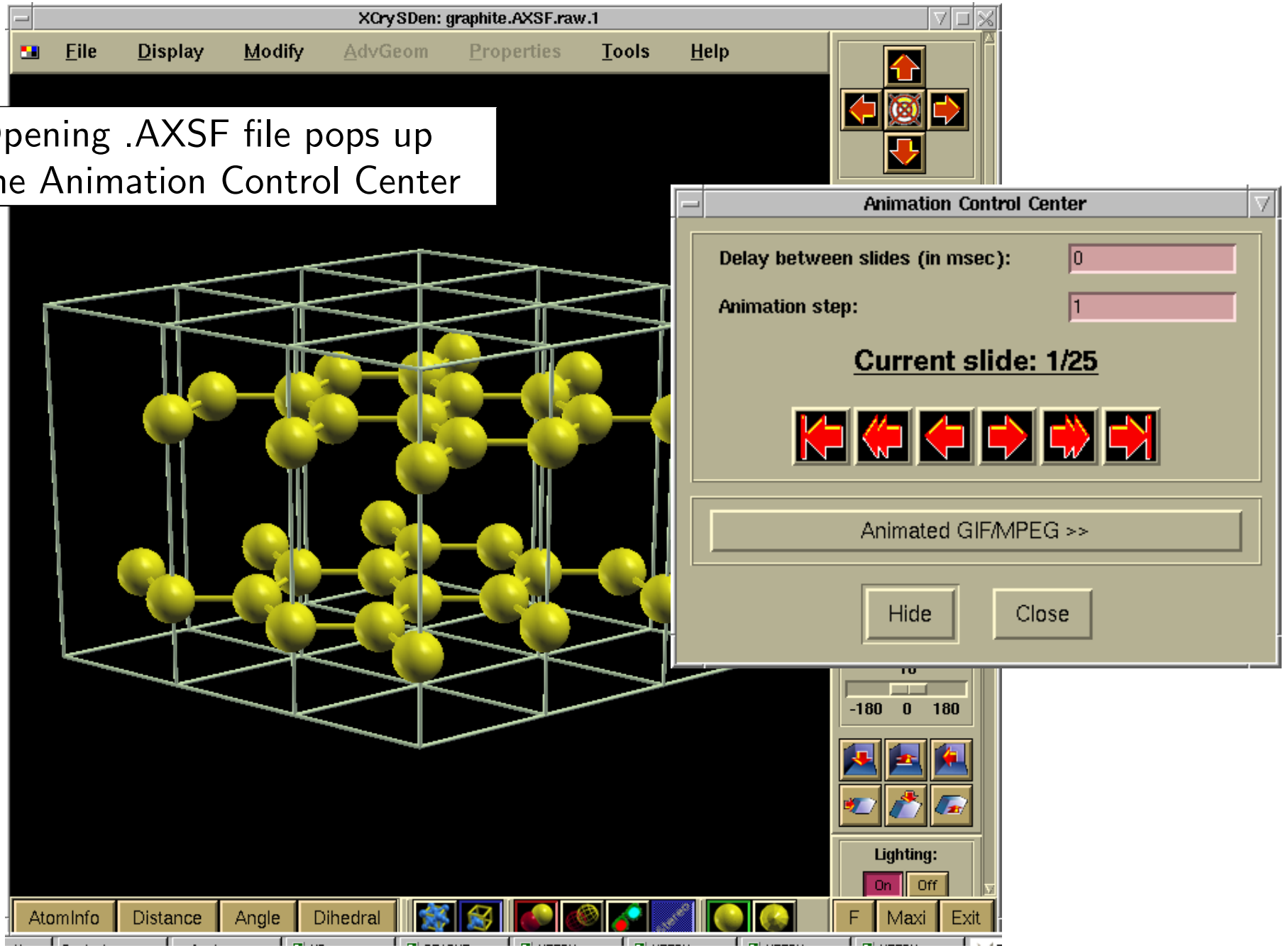
Molecular Dynamics or Relaxation

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).

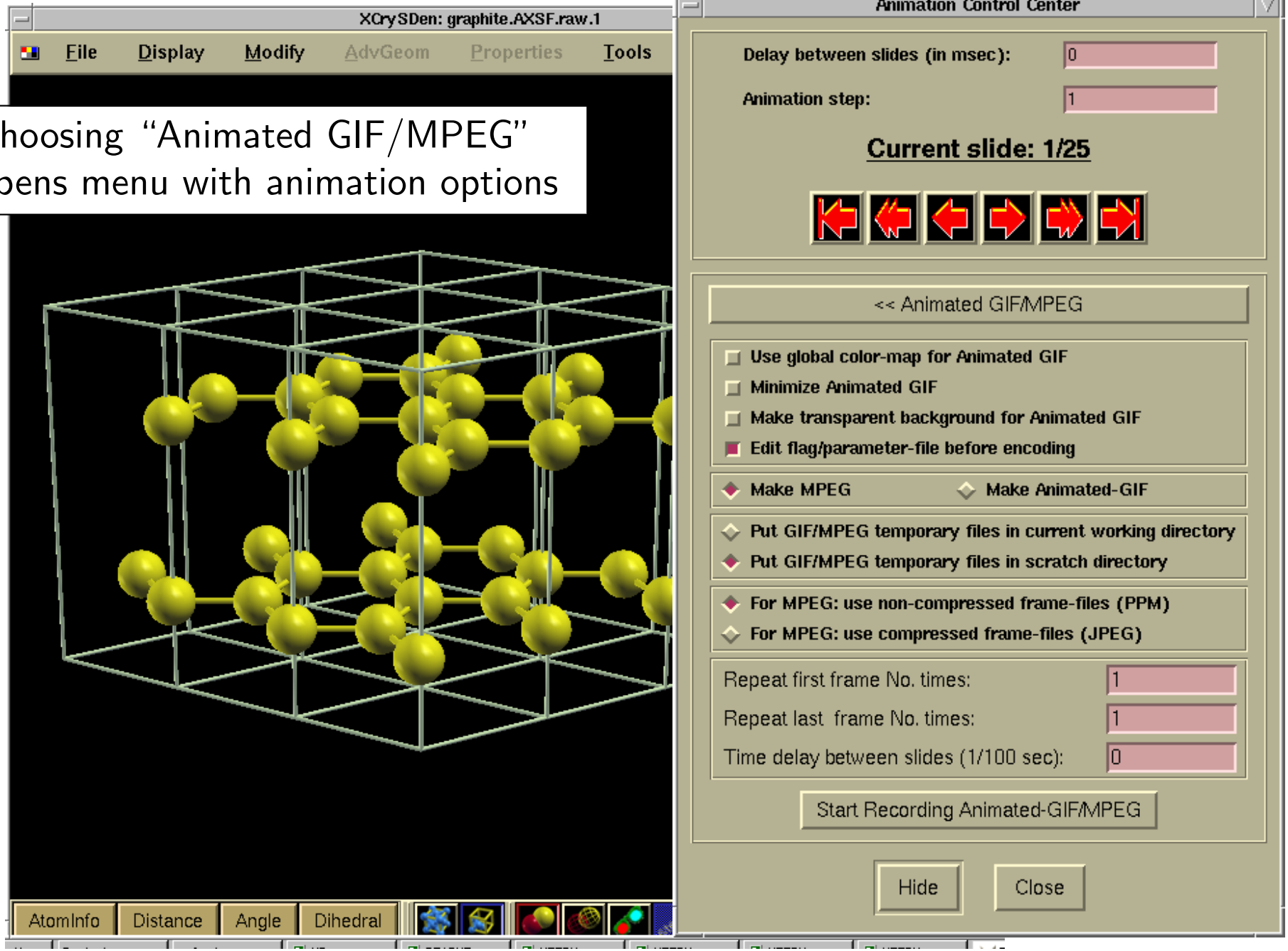
2. Having .XV, and either .MD, or .ANI
   run md2axsf, answering questions about the (optional) choice of output box
   and the MD steps to visualize (first #; last #; keep only each #'s)
   $\longrightarrow$ creates .AXSF.

   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).

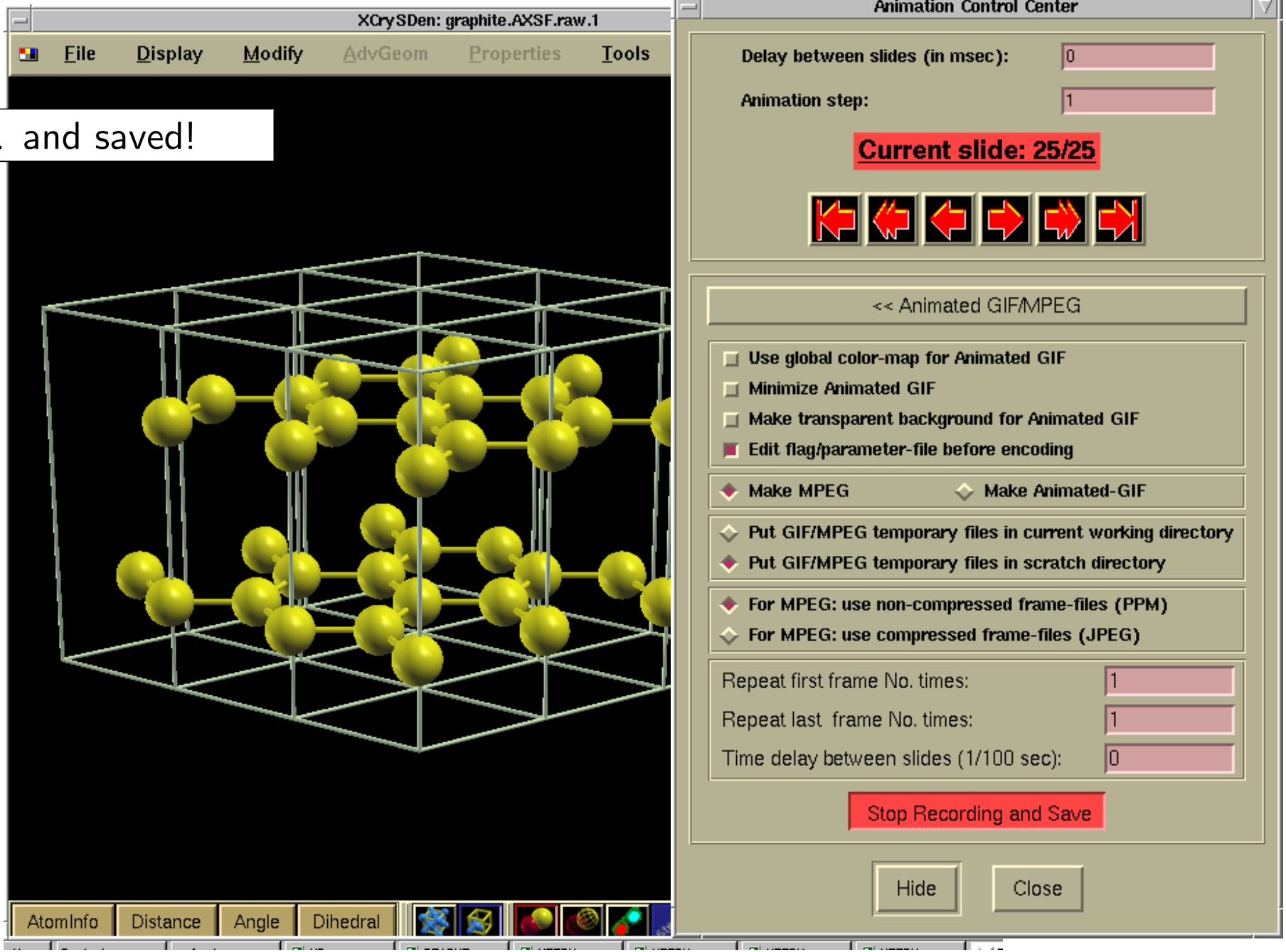

XCrySDen: graphite.AXSF.raw.1
File
Display
Modify
AdvGeom
Properties
Tools
Help
In order to see many unit cells,
go to Modify → Number of Units drawn
Zoom +
Zoom -
Trans Step:
0.05
0.00 0.25 0.50
Rot +X
Rot -X
Rot +Y
Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
10
10
-180 0 180
Lighting:
On
Off
AtomInfo
Distance
Angle
Dihedral
F
Maxi
Exit


XCrySDen: graphite.AXSF.raw.1
File
Display
Modify
AdvGeom
Properties
Tools
Help
Opening .AXSF file pops up the Animation Control Center
Animation Control Center
Delay between slides (in msec):
0
Animation step:
1
Current slide: 1/25
Animated GIF/MPEG >>
Hide
Close
-180
0
180
Lighting:
On
Off
AtomInfo
Distance
Angle
Dihedral
F
Maxi
Exit

Choosing “Animated GIF/MPEG” opens menu with animation options



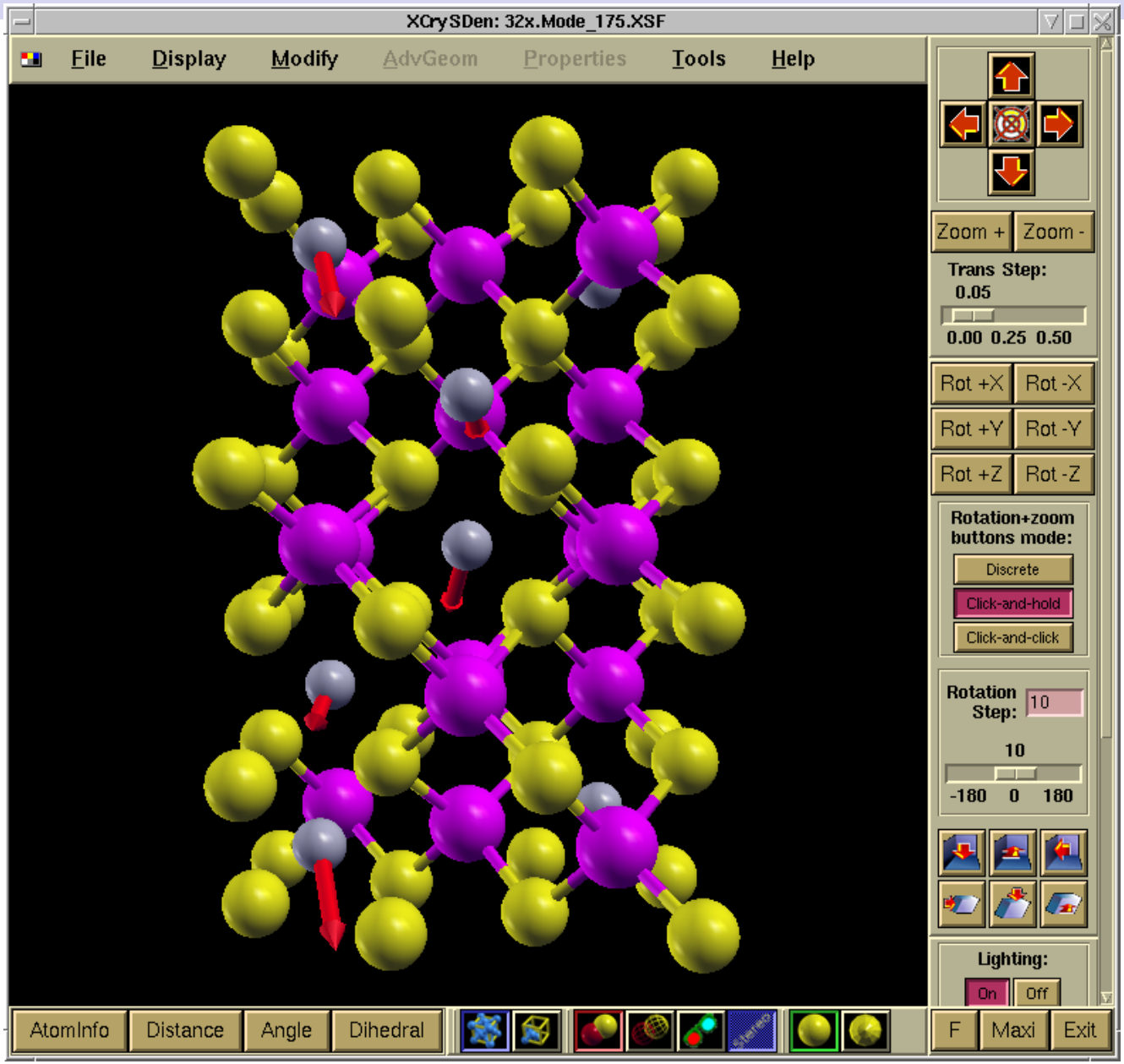
... and saved!


XCrySDen: graphite.AXSF.raw.1
File
Display
Modify
AdvGeom
Properties
Tools
AtomInfo
Distance
Angle
Dihedral
Animation Control Center
Delay between slides (in msec):
0
Animation step:
1
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:
1
Repeat last frame No. times:
1
Time delay between slides (1/100 sec):
0
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 vizualize. For each selected mode, a separate .XSF file and an .AXSF file are created.
   .XSF contains a static structures (as in .XV), with arrors 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