Visualization and post-processing tools for SIESTA

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CECAM tutorial, Lyon, June 22, 2007

Outline

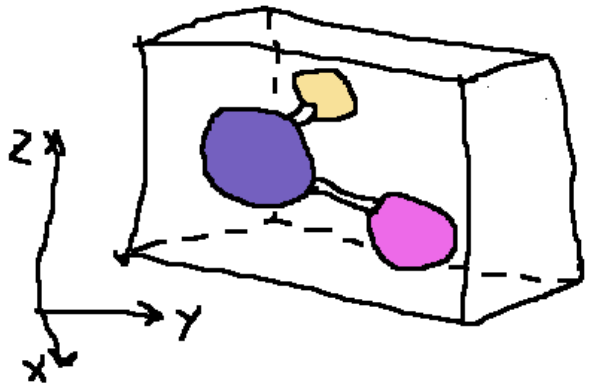
What to visualize..?

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

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").

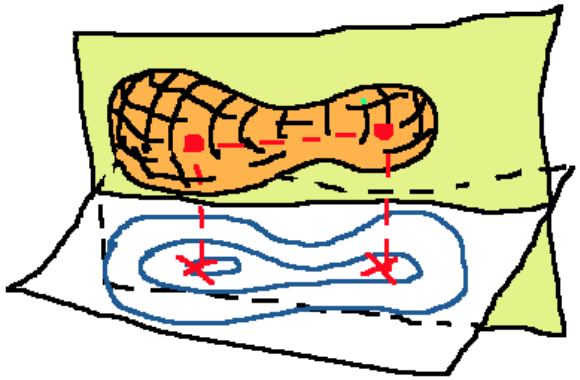


Since the input format is quite flexible (a big advantage!), it is difficult to organize a simple viewer of *input* structure data, without using the fdf routines. However, the .XV file (created after the completion of electronic structure loop) contains all necessary information, as it was *really*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

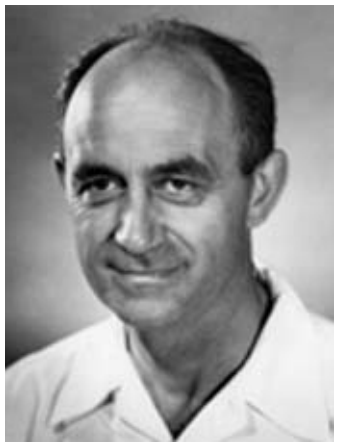
Kohn-Sham wavefunctions

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

What to visualize..?

Fermi surfaces

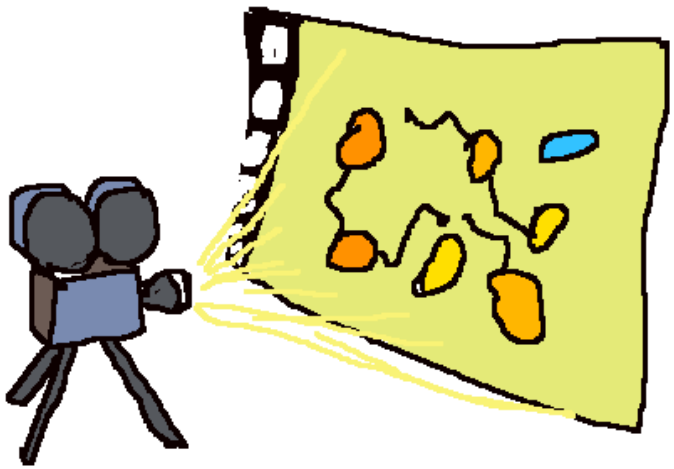
can be calculated using the energy dispersion data $E(\mathbf{k})$, available from any band structure code. The difficulty of purely technical character is, how to construct energy isosurfaces and conveniently manipulate them (to choose viewpoint, select different sheets of the Fermi surface, etc.) This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



What to visualize..?

Molecular dynamics or relaxation

runs store the atomic positions in .MD and/or .ANI files (with and without unit cell information, correspondingly). Such sequences of atomic positions can be animated using various software packages, including XCrySDen.



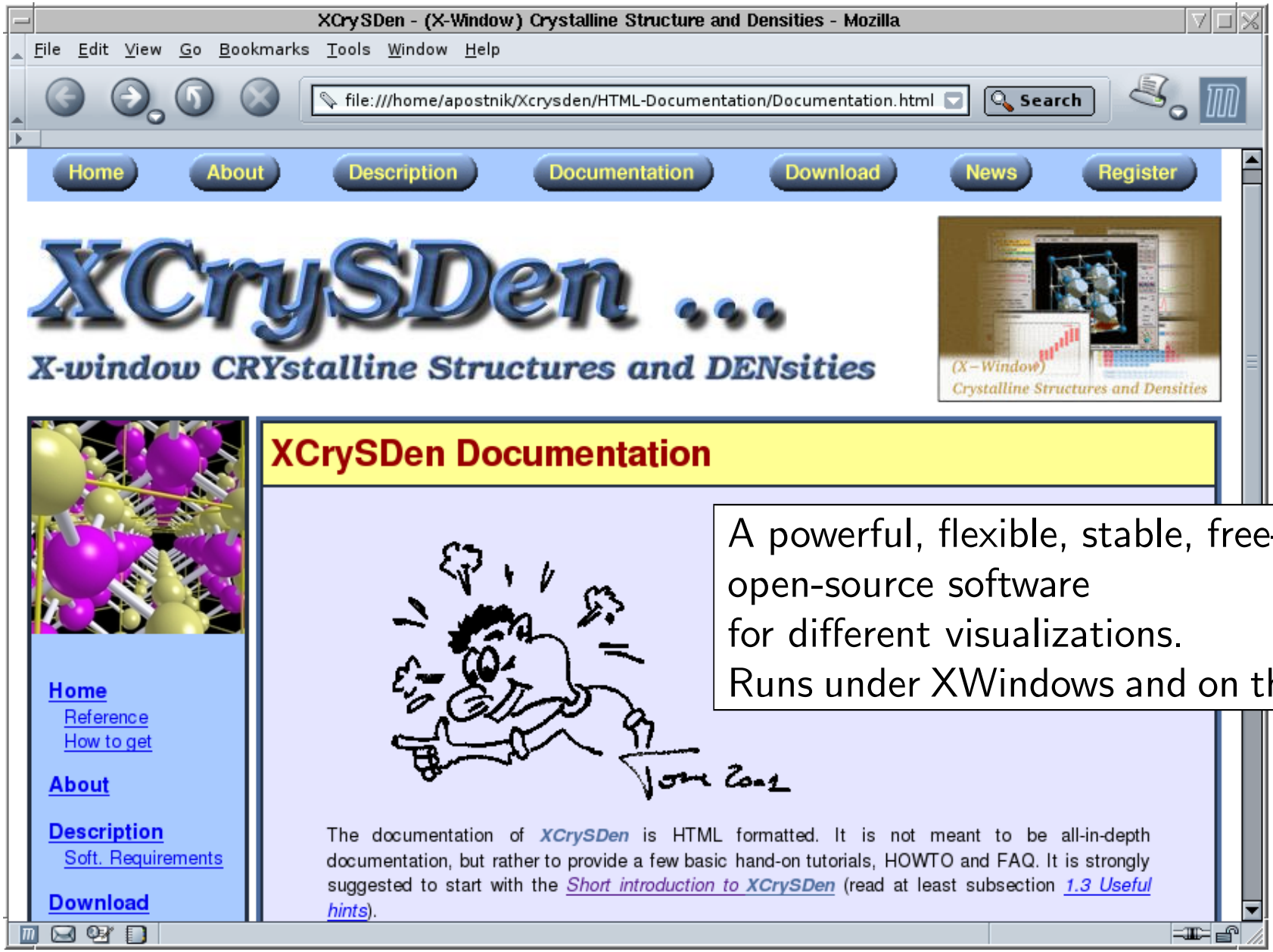
Phonon modes

from `Vibra/vibrator` calculation after a

`MD.TypeOfRun FC`

SIESTA run 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

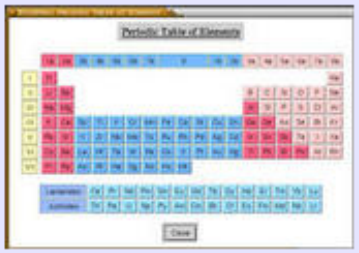
File Edit View Go Bookmarks Tools Window Help

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

1.1 What *XCrySDen* can do?

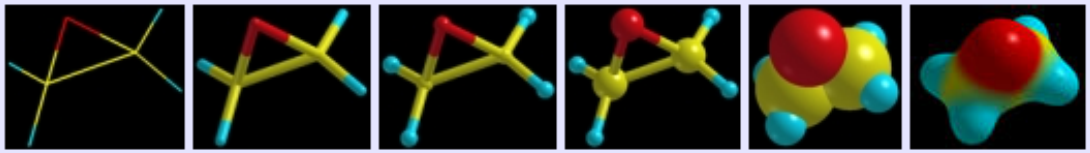
In short: *XCrySDen* is a crystalline and molecular structure render program, with additional capabilities of rendering contours, isosurfaces, Wigner-Seitz cells (also Brillouin zone), Fermi surfaces and so on. Some of its features are the following:

- widget with periodic table of elements:

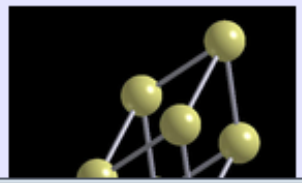


It enables different presentations
of atoms and bonds (colors, shadows, ...),
measuring distances and angles ...

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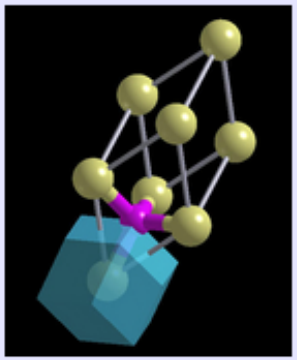
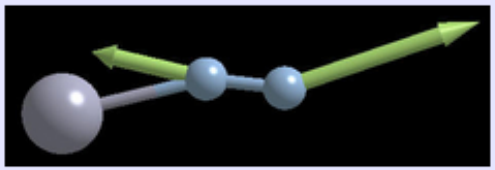
file:///home/apostnik/Xcrysden/HTML-Documentation/doc/intro.html Search

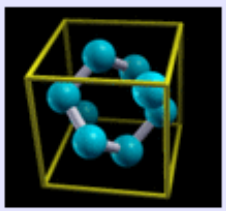
- displaying crystal and Wigner-Seitz cells:



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



- animations



- displaying contours and colorplanes

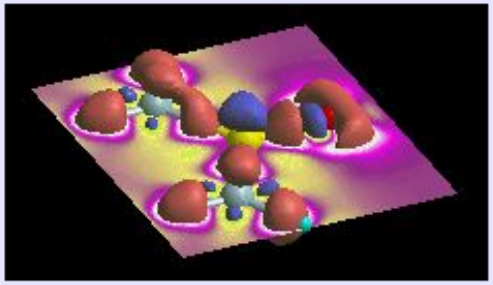
... allows to set arrows on atoms
(or, on fictituous atoms)
and make animations ...

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

File Edit View Go Bookmarks Tools Window Help

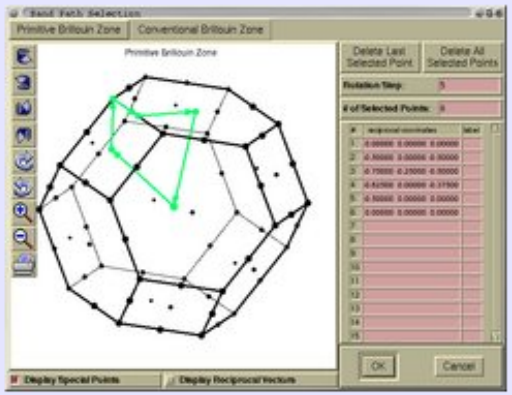
file:///home/apostnik/Xcrysden/HTML-Documentation/doc/intro.html Search

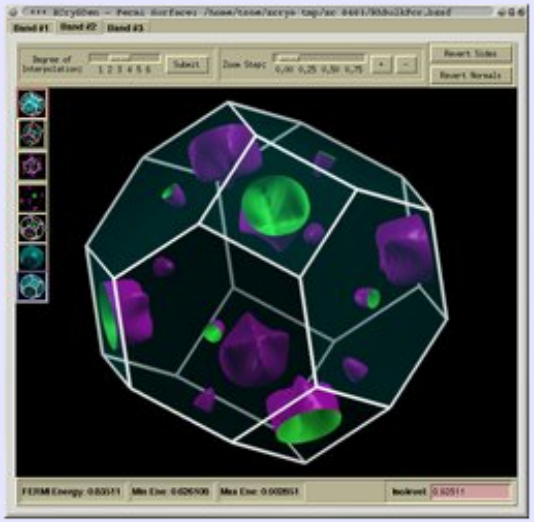
- displaying contours and colorplanes
- displaying isosurfaces:



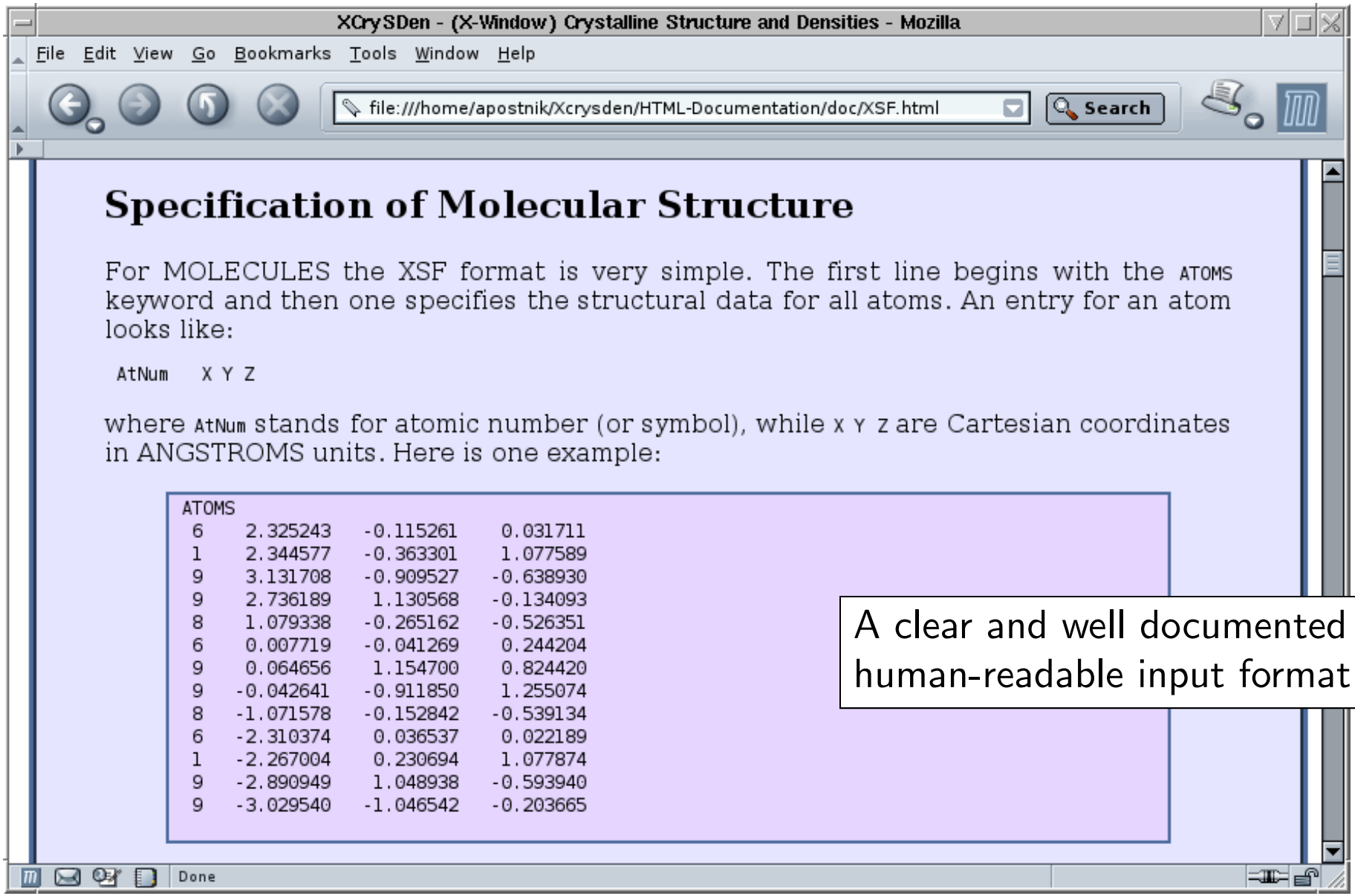
... allows to make contour plots,
to draw isosurfaces,
to choose path through the Brillouin zone,
to use different modi
of presenting the Fermi surfaces

- 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...

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 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
```

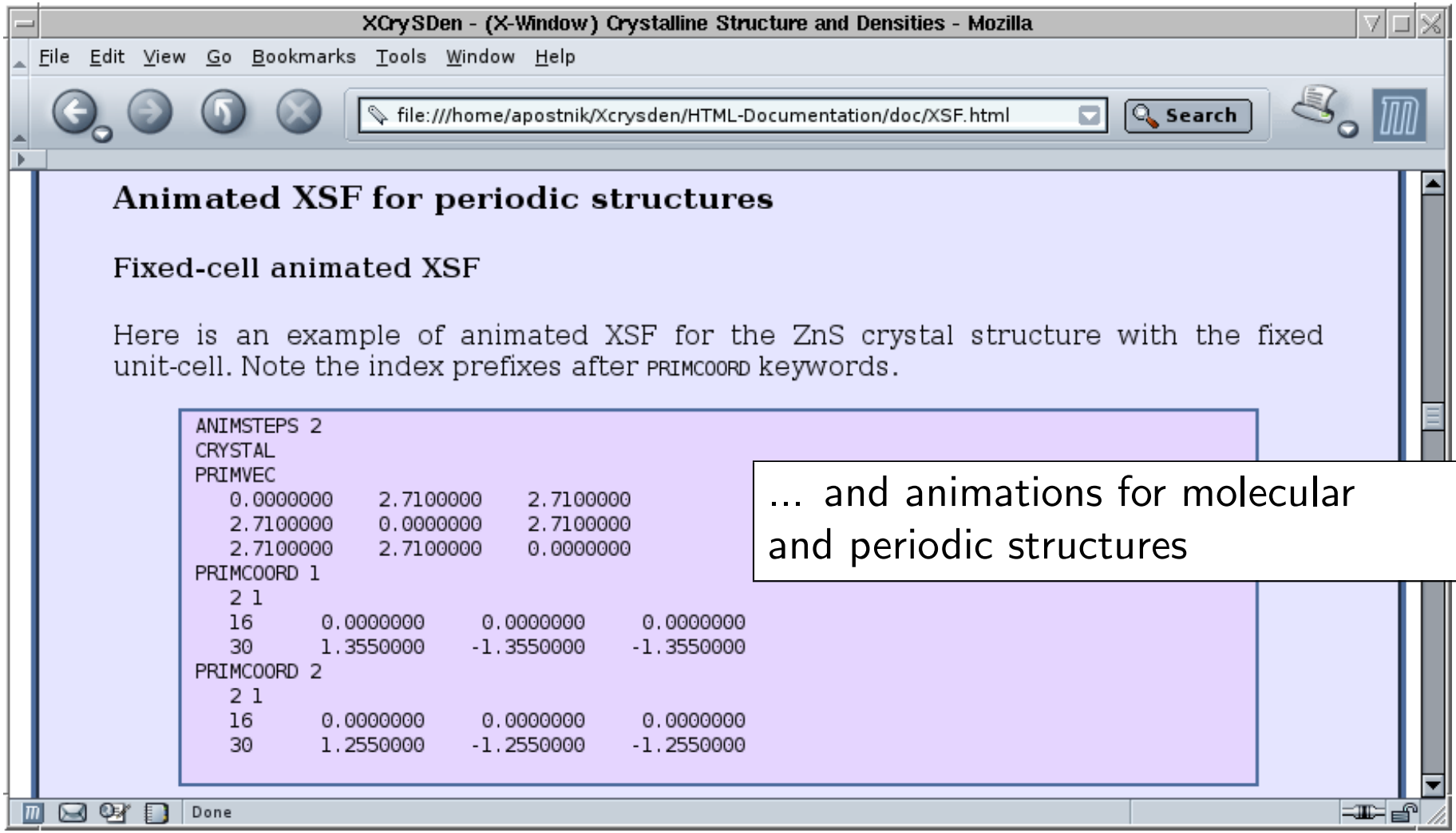
And here is an example for the periodic structure structure:

```
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
```

... including forces (or, velocities)

Done

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



Sies2xsf utilities

Where to find them:

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

What do they make out of what:

- **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).

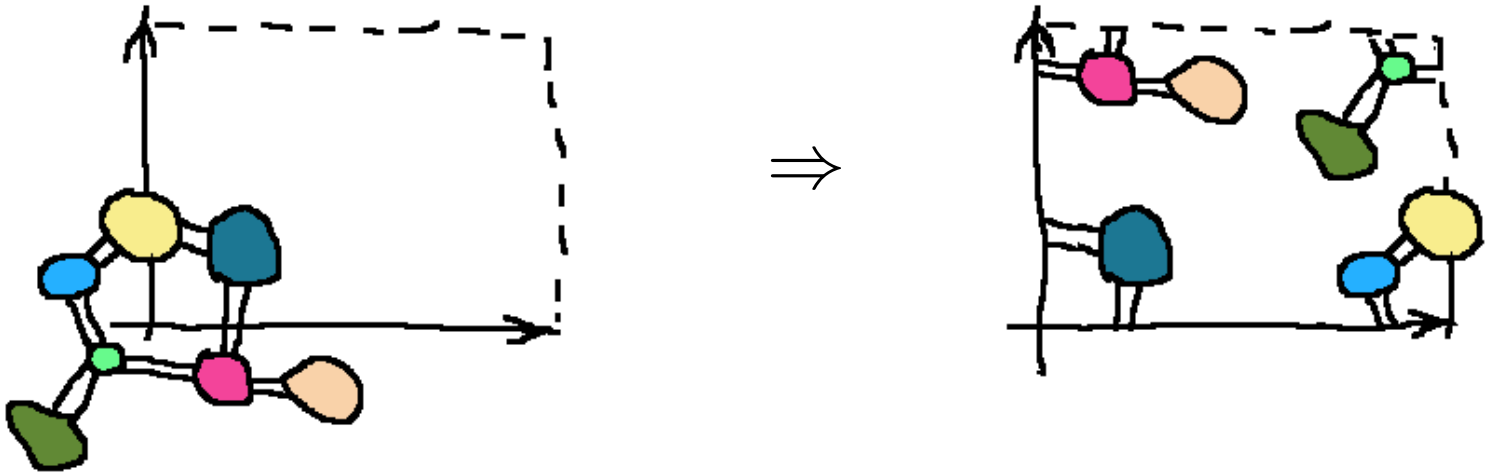
Visualization of atomic positions

xv2xsf asks for a .XV file and transforms it into .XSCF

I know my structure already, why visualize it? $\longrightarrow$ two reasons:

1. **xv2xsf** uses .XV file, i.e. the structure information *as is was understood* by SIESTA, including possible input errors (messed up units etc.)
2. **xv2xsf** allows to draw the simulation cell, which is useful in case of molecules or slabs: is there enough space around? Is it not too much?

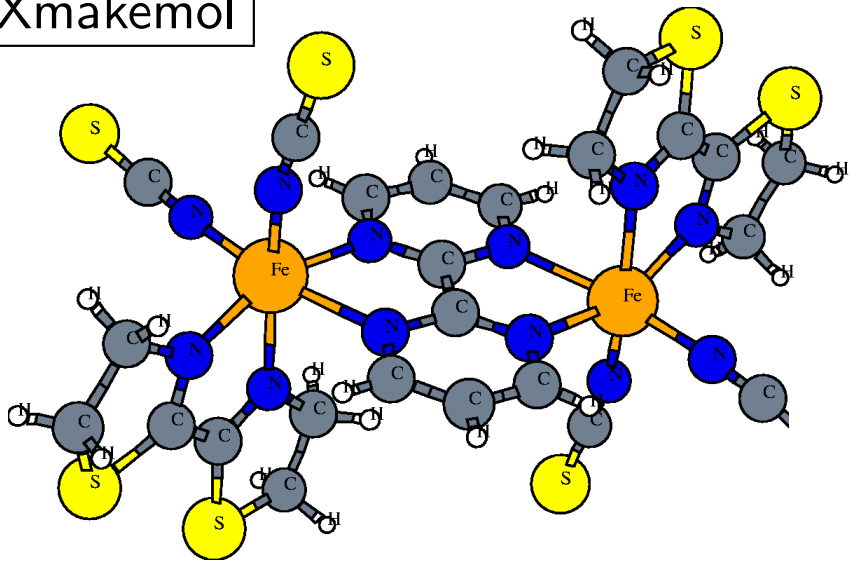
Note: XCrySDen draws all atoms *inside* the simulation box, irrespectively of their given positions. So you might want to see replicated cells ...



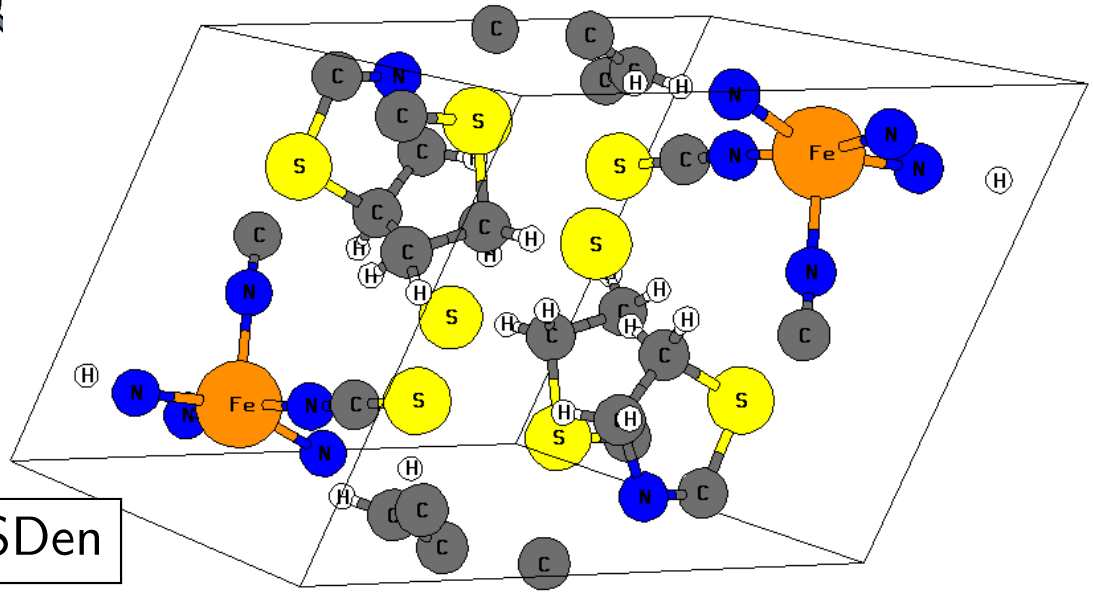
Visualization of atomic positions

Example of for a crystal of Fe-binuclear units:

Xmakemol

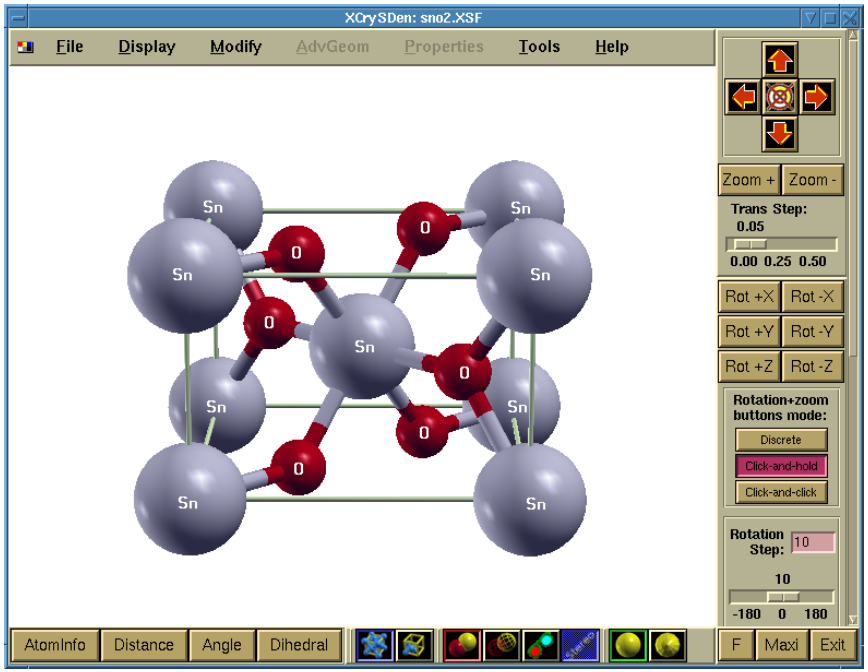


This is "Lighting Off" mode of XCrySDen: no shadows or isosurfaces, but fast manipulations with a structure, and possibilty of vectorial PostScript optput.



XCrySDen

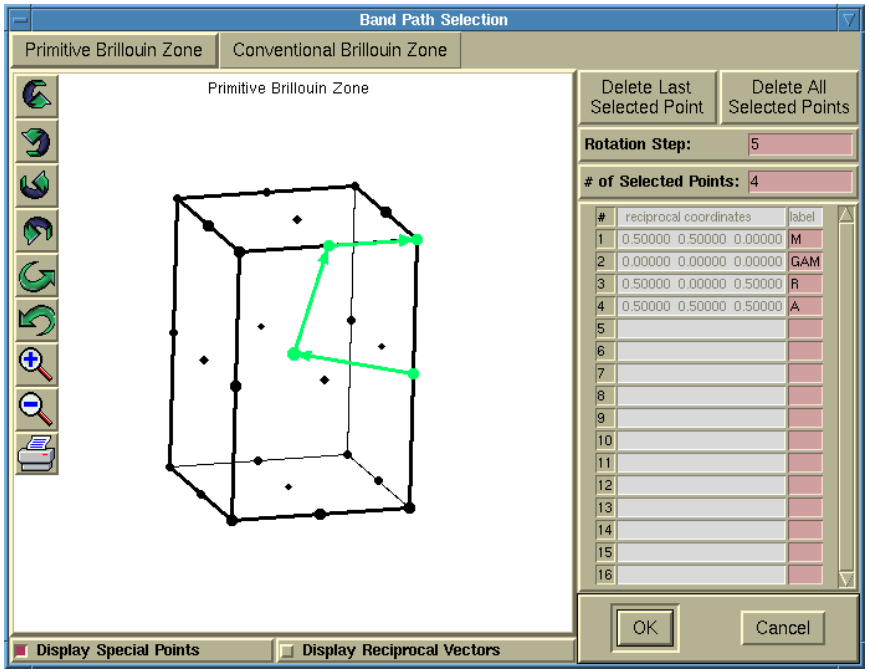
Visualization of atomic positions



SnO_2 (rutile structure)

An unexpected bonus for SIESTA users: XCrySDen constructs the Brillouin zone from structure information in the .XCF file and allows to select k-path for plotting band structurse. Go to

Tools → k-path Selection



Putting arrows on atoms

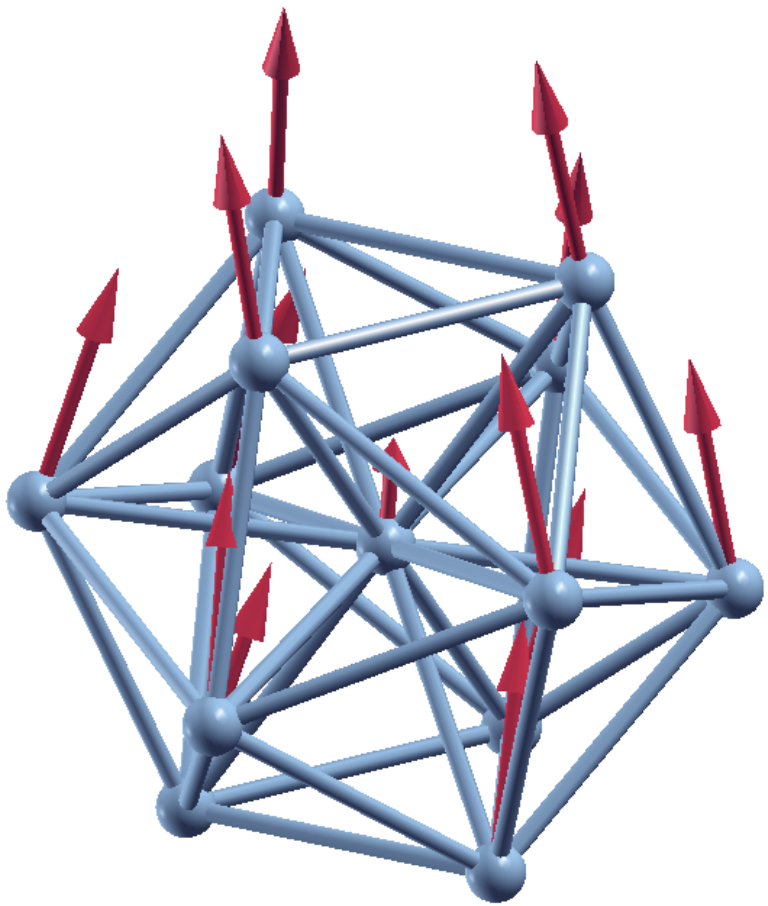
Suppose we have local (e.g., non-collinear) magnetic moments. Can we show them with XCrySDen?
→ Yes, we can use "Forces" entry in the XCrySDen input file format, columns #5 – 7. (But, there is no special tool for this. You should do it by hand, or write your own script). An example:

```
ATOMS
  27    6.00000011    6.00000011    6.00000011    0.6220    0.6280    0.8430
  27    7.24176814    7.94065215    6.00000011    1.1770    1.0700    0.8980
  27    4.75823209    7.94065215    6.00000011    1.3540    0.7410    1.0070
  27    7.24176814    4.05934808    6.00000011    0.4440    1.0860    1.4230
  27    4.75823209    4.05934808    6.00000011    0.6370    0.7360    1.5460
  27    6.00000011    7.24176814    7.94065215    1.1860    1.1880    0.7810
  27    6.00000011    7.24176814    4.05934808    1.0440    0.4820    1.4290
  27    6.00000011    4.75823209    7.94065215    0.7380    1.3350    1.0180
  27    6.00000011    4.75823209    4.05934808    0.6020    0.6130    1.6410
  27    7.94065215    6.00000011    7.24176814    0.8070    1.3540    0.9490
  27    4.05934808    6.00000011    7.24176814    1.2290    1.0180    0.8930
  27    7.94065215    6.00000011    4.75823209    0.5630    0.8130    1.5400
  27    4.05934808    6.00000011    4.75823209    0.9880    0.4610    1.4830
```

Putting arrows on atoms

Suppose we have local (e.g., non-collinear) magnetic moments. Can we show them with XCrySDen?

→ Yes, we can use "Forces" entry in the XCrySDen input file format, columns #5 – 7. (But, there is no special tool for this. You should do it

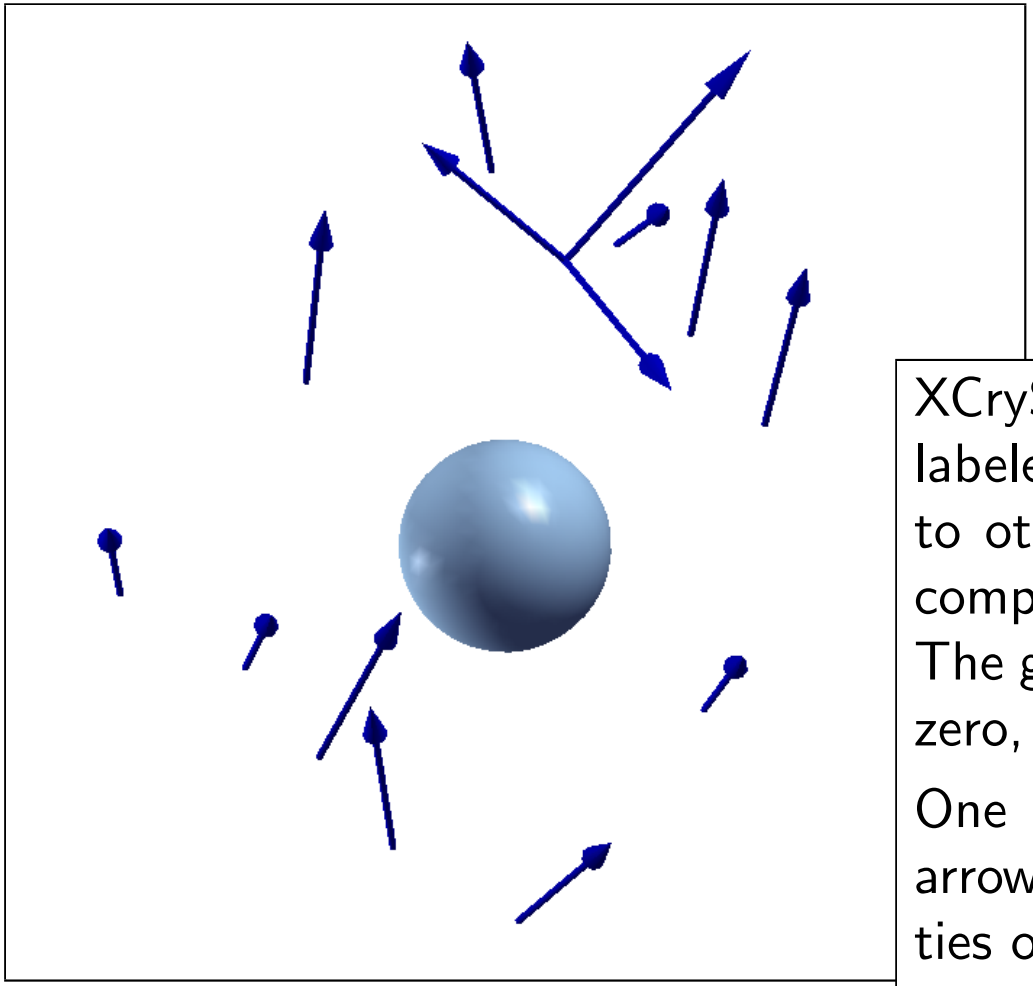


After opening this .XSF file,
do not forget to activate
Display → Forces,
and optionally do
Modify → Force settings

1.1860	1.1880	0.7810
1.0440	0.4820	1.4290
0.7380	1.3350	1.0180
0.6020	0.6130	1.6410
0.8070	1.3540	0.9490
1.2290	1.0180	0.8930
0.5630	0.8130	1.5400

An icosahedral Co_{13} cluster
with non-collinear setting of spin moments

Putting arrows where there are no atoms



XCrySDen allows to declare ghost atoms, labeled 'X'. They can be set very close to other atoms, so that XCrySDen won't complain – even at exactly the same place. The ghost atoms may have any radius, e.g. zero, and yet carry arrows.

One can make quite diferent use of such arrows. The only limitation: the properties of *all* arrows are fixed by

Modify → Force settings

and cannot be diversified.

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, or not. XCrySDen can apply translations to to generated grid.
5. Choice isosurface parameters, cutting planes, isolines on the cutting planes, colors, lighting etc. from the means of XCrySDen.

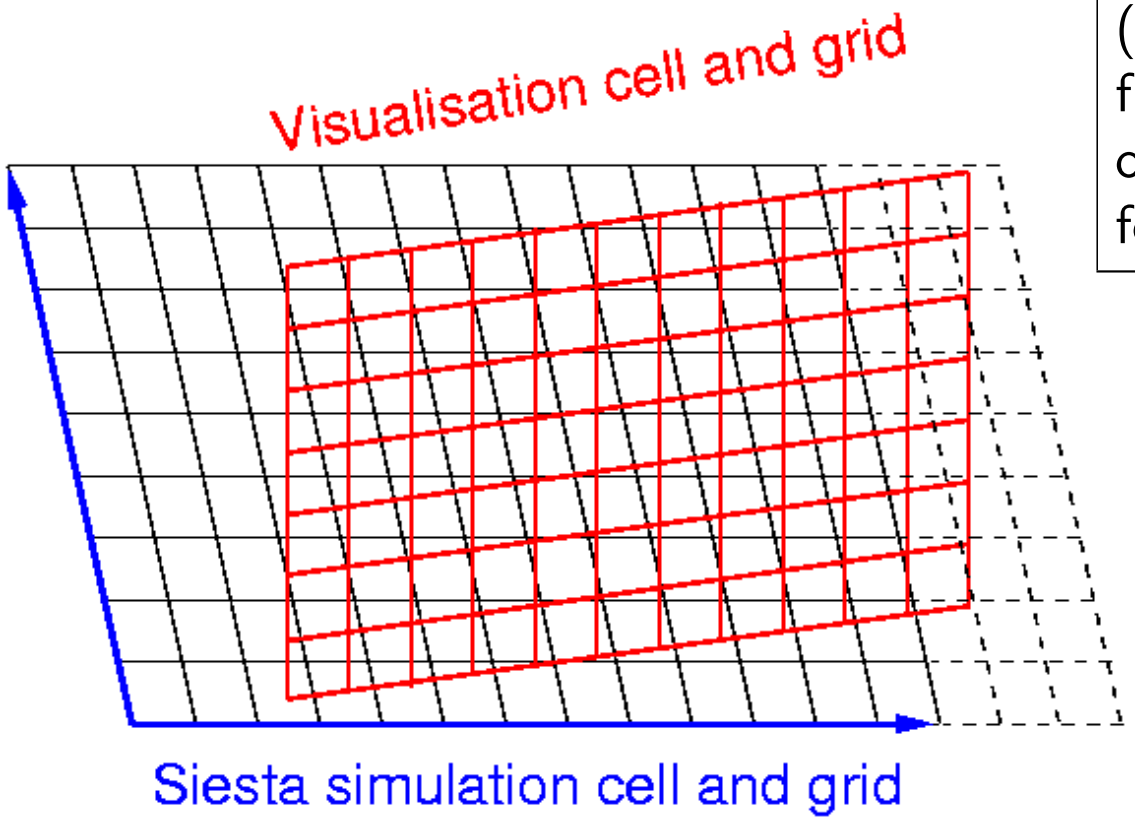
Visualization of Charge/spin densities, or of LDOS

XTERM

```
cytron01:~/Conferences/2007-LyonSIESTA/Examples/Fe2/Cryst-AFM> rho2xsf
 Specify  SystemLabel (or 'siesta' if none): AFM
 Now define the grid cell for your XCrysDen plot.
 Note that it can be arbitrarily chosen with respect to the Siesta simulation ce
ll, and it needs not to be orthogonal. We'll define it by the origin point and t
hree spanning vectors. They can be given in Bohr or Ang.
 Would you use Bohr (B) or Ang (A) ? A
 Enter origin point in Ang  :  1.2 -3   0.6
 Enter 1st spanning vector in Ang  : 1   -2.3   9
 Enter 2nd spanning vector in Ang  : 0    8    -2
 Enter 3rd spanning vector in Ang  :  -9    0    2
  File AFM.XSF exists. Overwrite? (Y/N)
y
 The box contains           46  atoms.
 Now define the grid. If you want it two-dimensional,
 give 1 as number of grid points along one spanning vector.
 Enter number of grid points along three vectors: 80 80 90
 Add grid property (LDOS, RHO, ...; or BYE if none): RHO
 Found and opened: AFM.RHO
 mesh0 = (          80          80         120 ),   nspin=           2
 For is=1: max. grid value = 6.79048E-01 at iix,iiy,iiz=  18  66  75
 For is=1: min. grid value = 5.77762E-07 at iix,iiy,iiz=  48  53  50
 For is=2: max. grid value = 6.67557E-01 at iix,iiy,iiz=  79  53  32
 For is=2: min. grid value = 5.68289E-07 at iix,iiy,iiz=  48  53  50
 Add grid property (LDOS, RHO, ...; or BYE if none): q
  A wild guess! There is no file AFM.q; close XSF and quit.
cytron01:~/Conferences/2007-LyonSIESTA/Examples/Fe2/Cryst-AFM>
```

Start **rho2xsf** from a console and type in the answers (marked in red) to the queries set by the system

Visualization of Charge/spin densities, or of LDOS



A linear interpolation
(over the four nearest points)
from the SIESTA real-space grid
onto the visualization grid
for XCrySDen

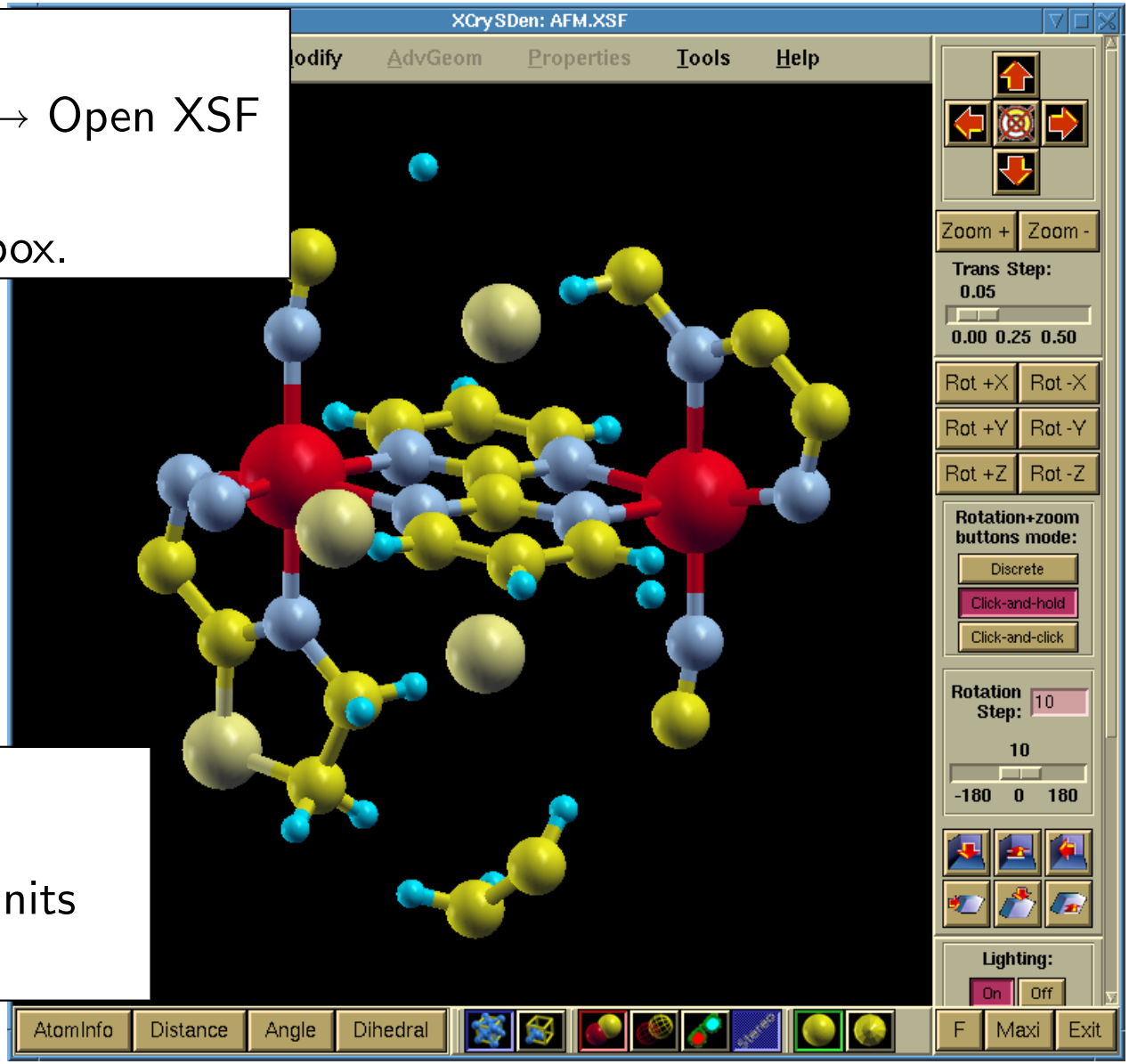
- The fineness of the visualization is limited by the sparciest one of the two grids.
- The cutting planes in XcrySDen may only be those of the visualization grid.

Plotting of grid properties

Loading the .XSF file

File → Open Structure → Open XSF

shows the atoms
within the visualization box.



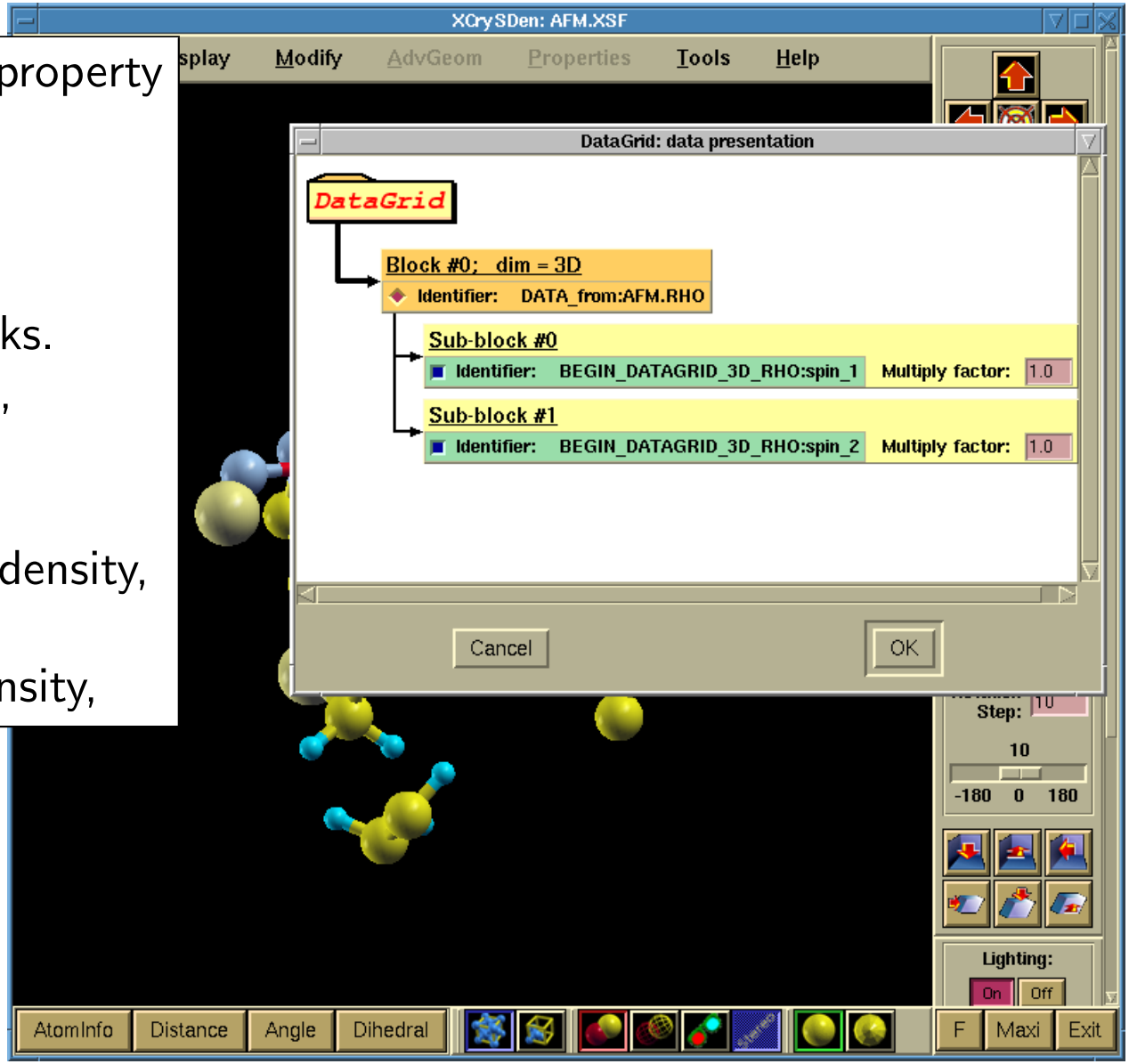
This is a cut
out of molecular crystal
formed by Fe-binuclear units
(shown earlier)

Plotting of grid properties

For loading a grid property (RHO), go to

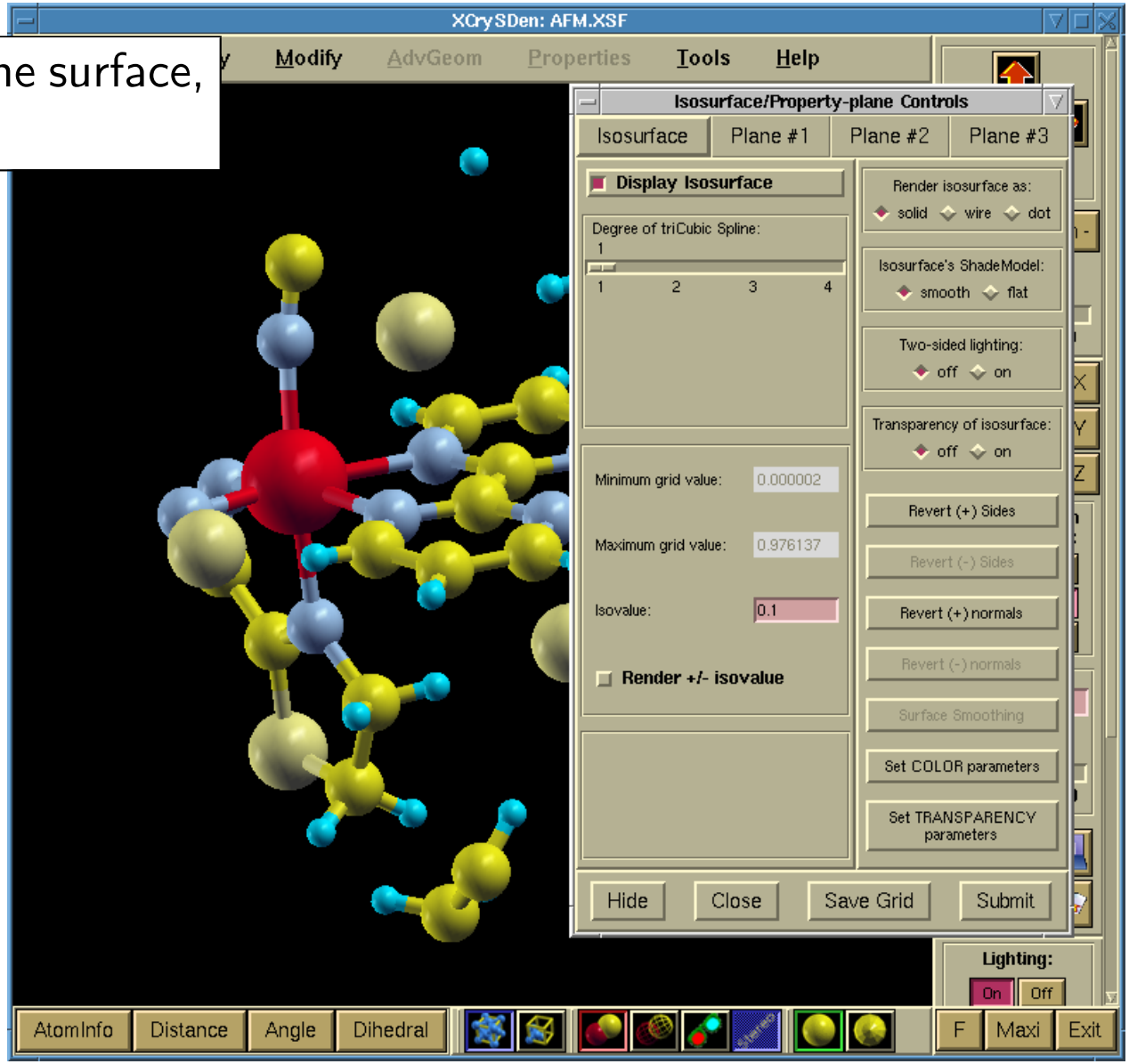
Tools → Data Grid

and set the weights
of the different subblocks.
In a spin-polarized case,
there are two.
Choose 1.0 and 1.0
for plotting the charge density,
1.0 and −1.0
for plotting the spin density,



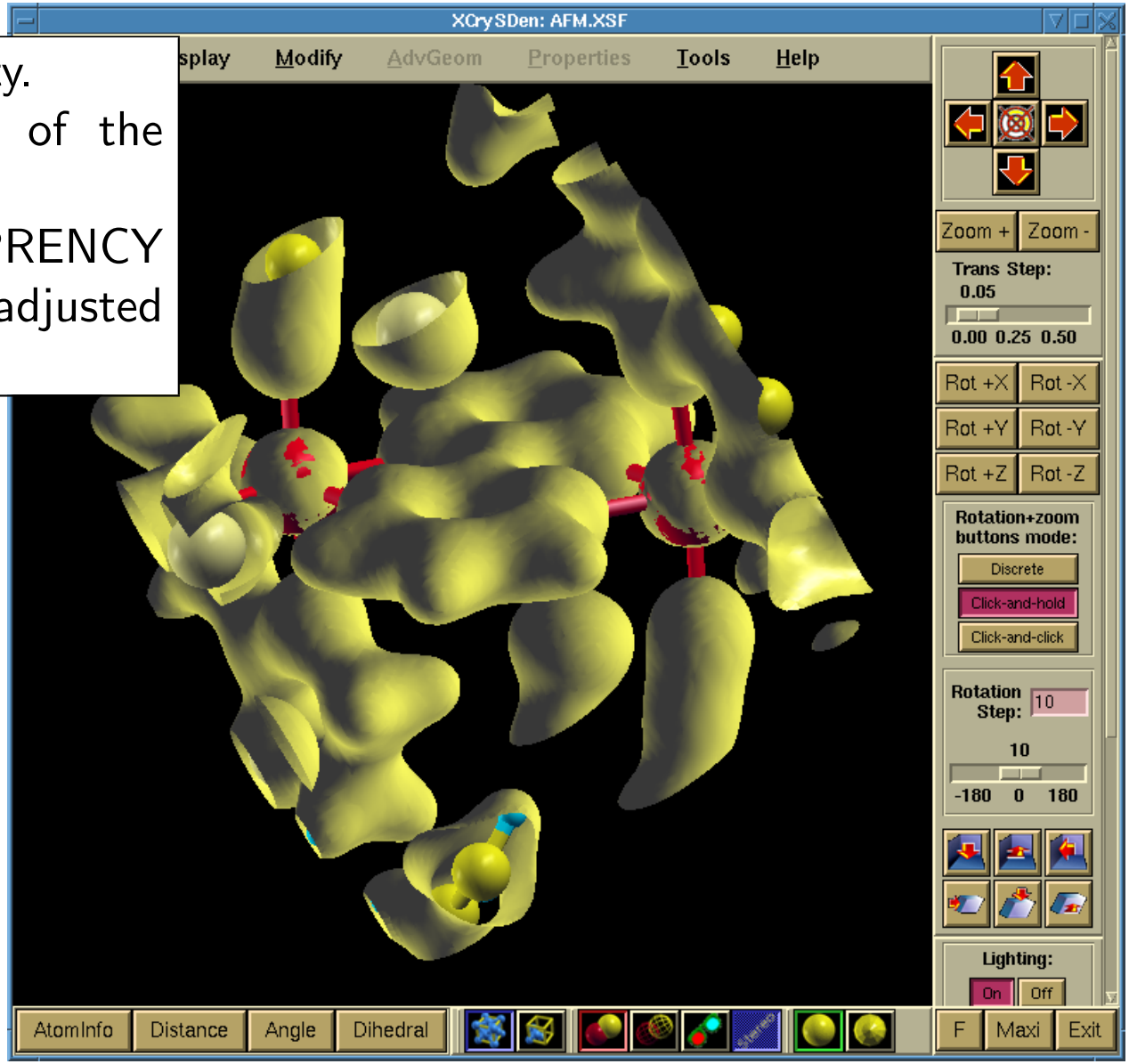
Plotting of grid properties

Set the isovalue to plot the surface, and press "Submit"



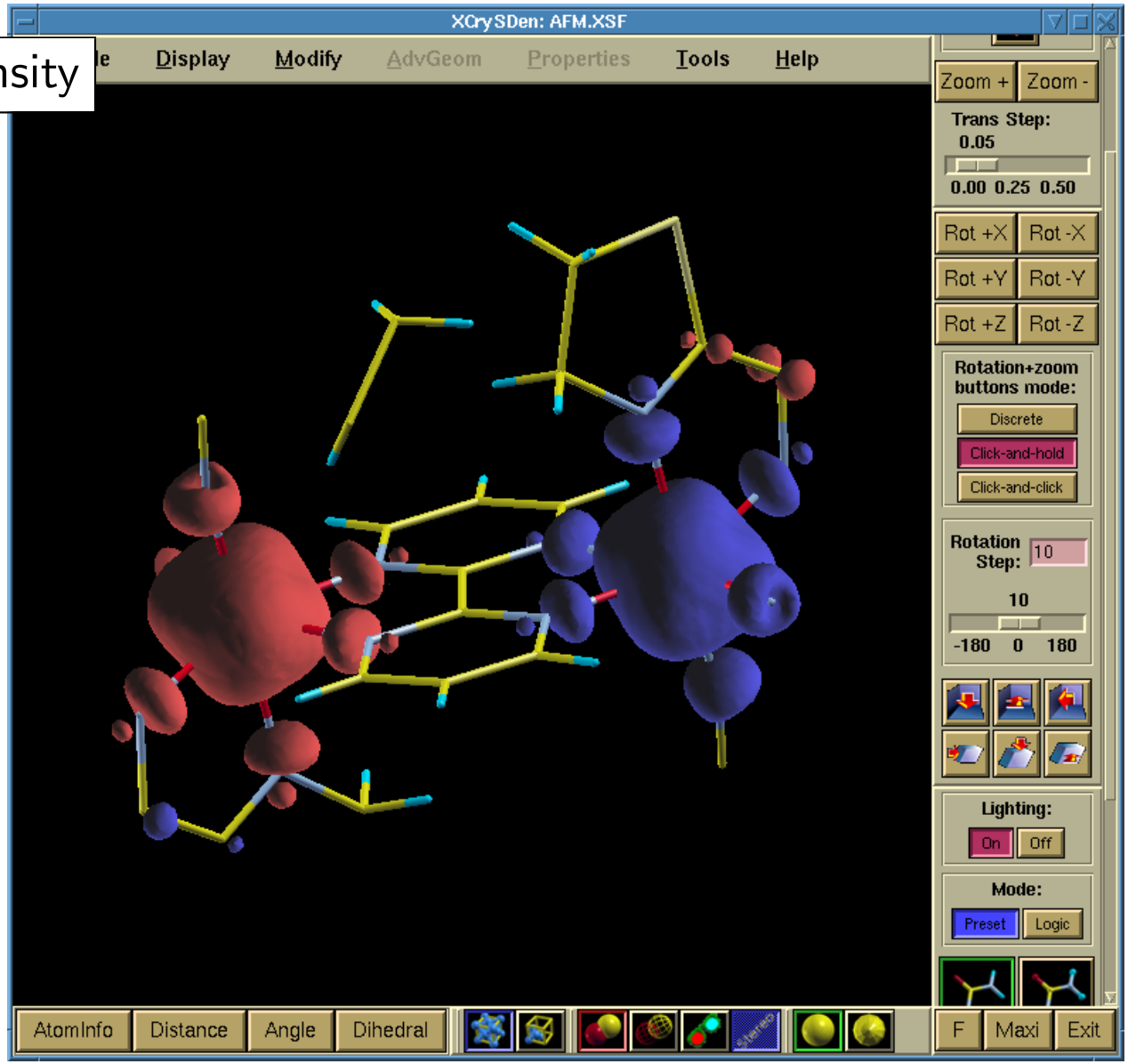
Plotting of grid properties

Here is the charge density.
It is cut at the edges of the visualization box.
COLOR and TRANSPRENCY parameters can be adjusted within broad limits.



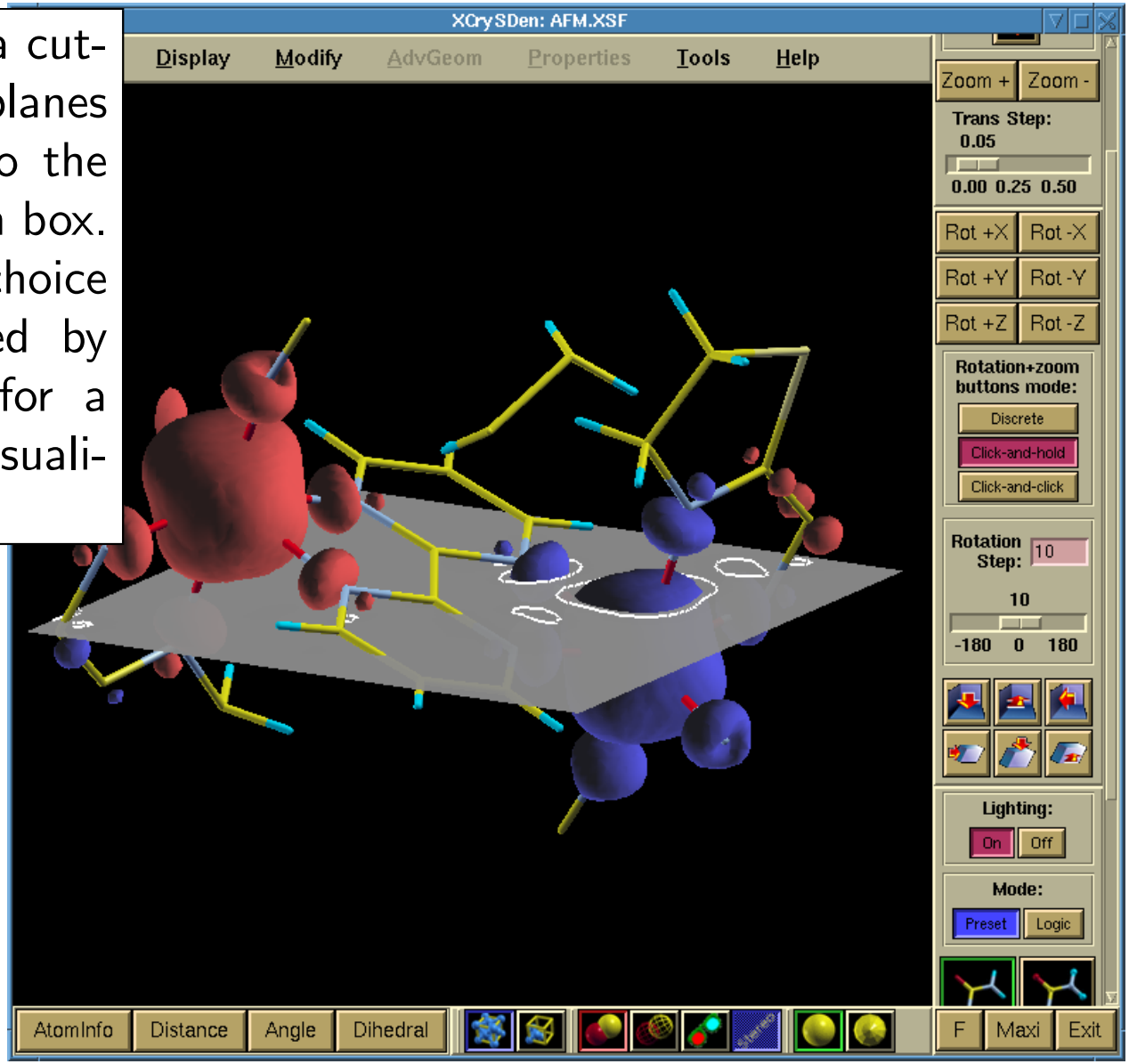
Plotting of grid properties

Similar, for the spin density



Plotting of grid properties

Similar, with isolines in a cutting plane. Cutting planes can only pass parallel to the edges of the visualization box. Therefore, the initial choice of the box (as rendered by **rho2xsf**) is important for a physically meaningful visualization.

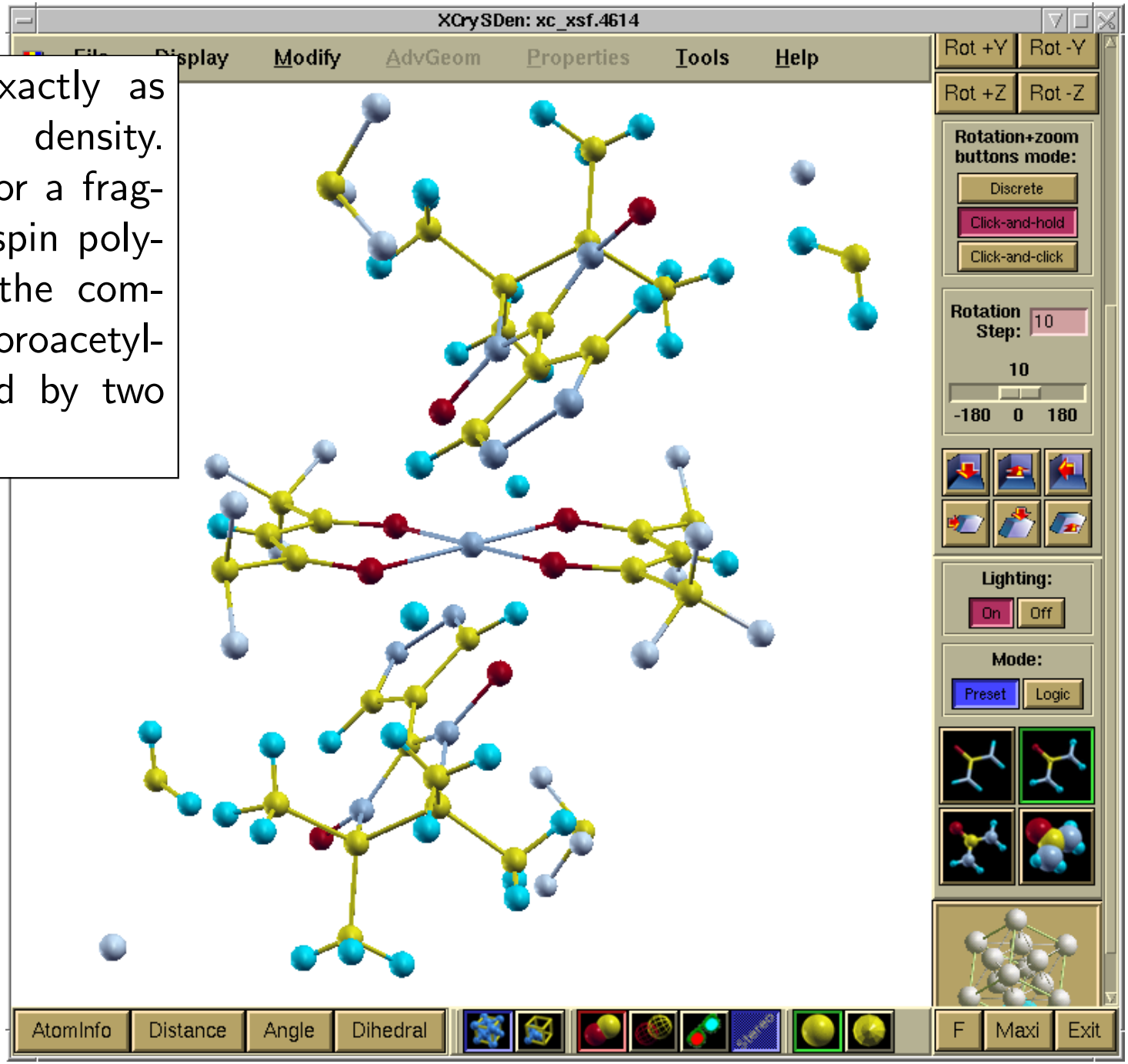


Visualization of Wave Functions

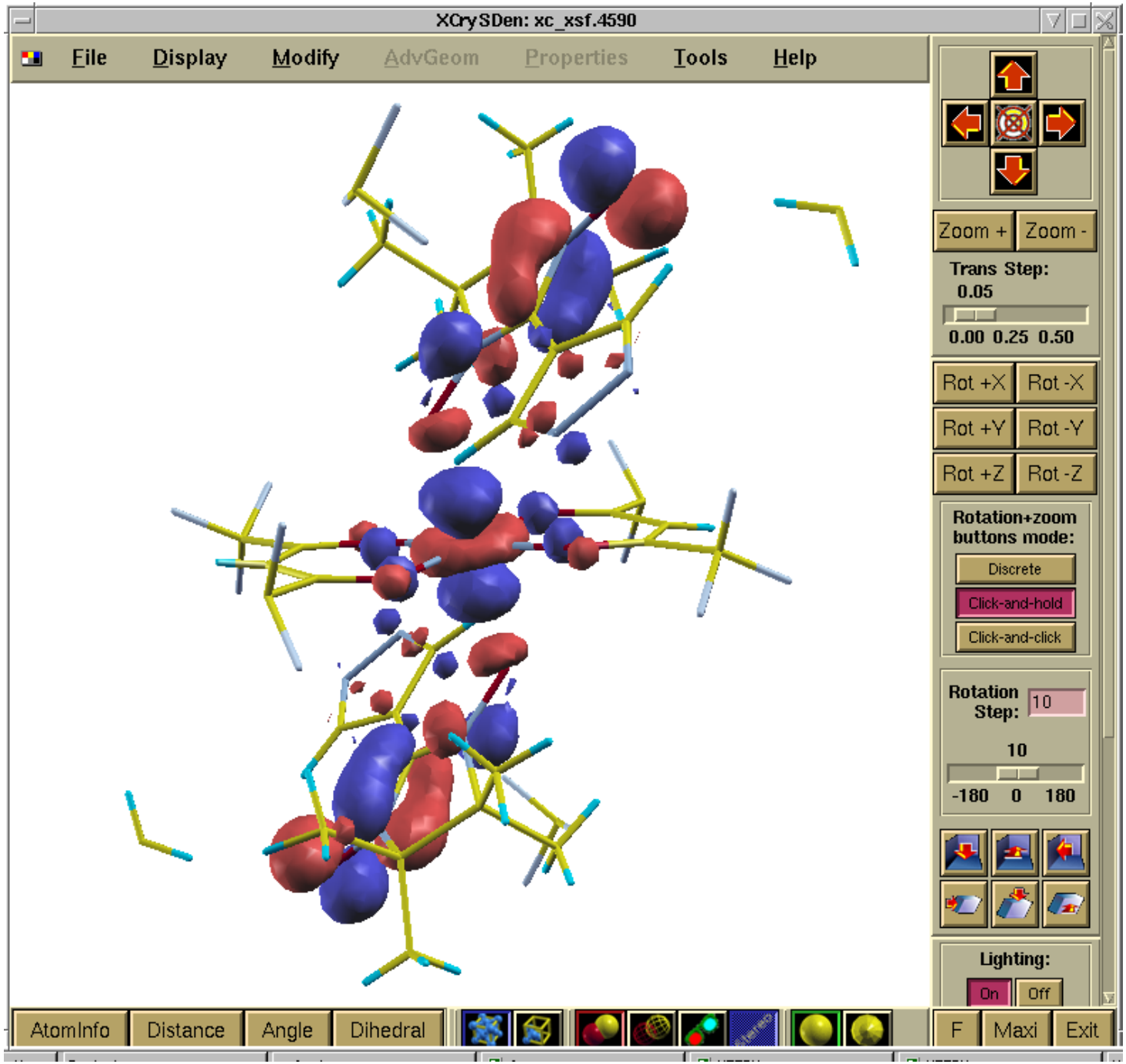
In principle, **Denchar** does this job quite fine. However, we'd like to have an interface to XCrySDen. To this end:

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 ($\longrightarrow$ 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 ($\longrightarrow$ 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.

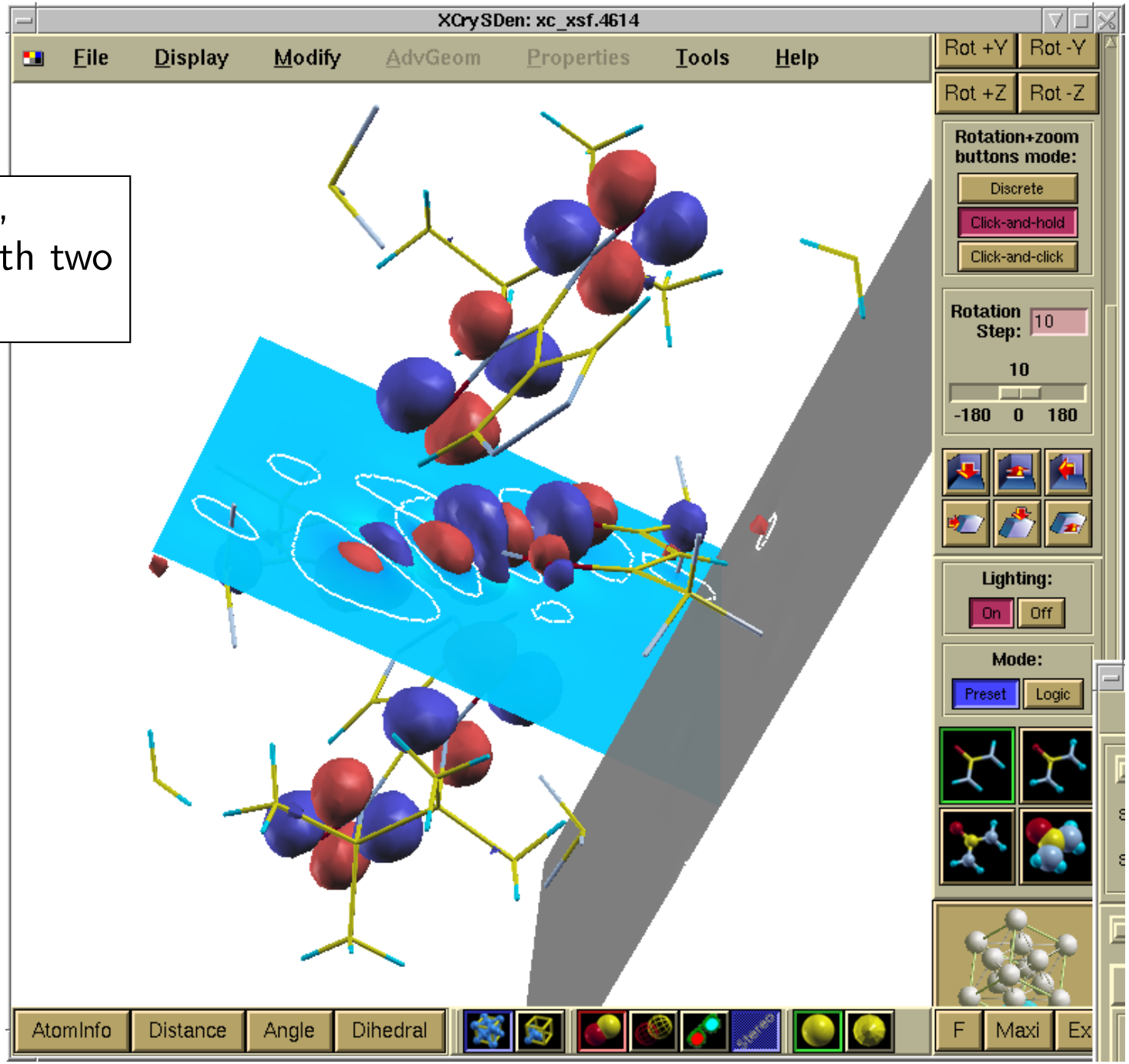
The rest goes exactly as with the charge density. This example is for a fragment of a heterospin polymer (Cu ion in the complex with hexafluoroacetylacetonate, flanked by two free radicals).



one orbital...


XCrySDen: xc_xsf.4590
File
Display
Modify
AdvGeom
Properties
Tools
Help
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

... another orbital,
in combination with two cutting planes



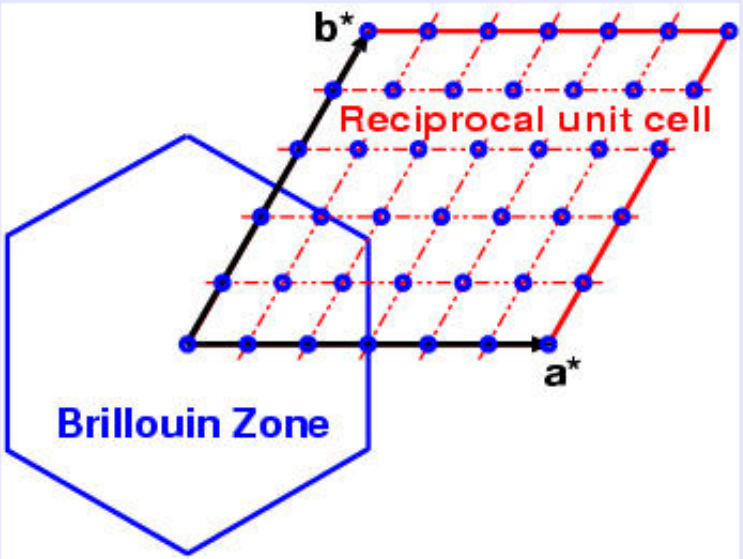
Visualization of Fermi surfaces

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
```

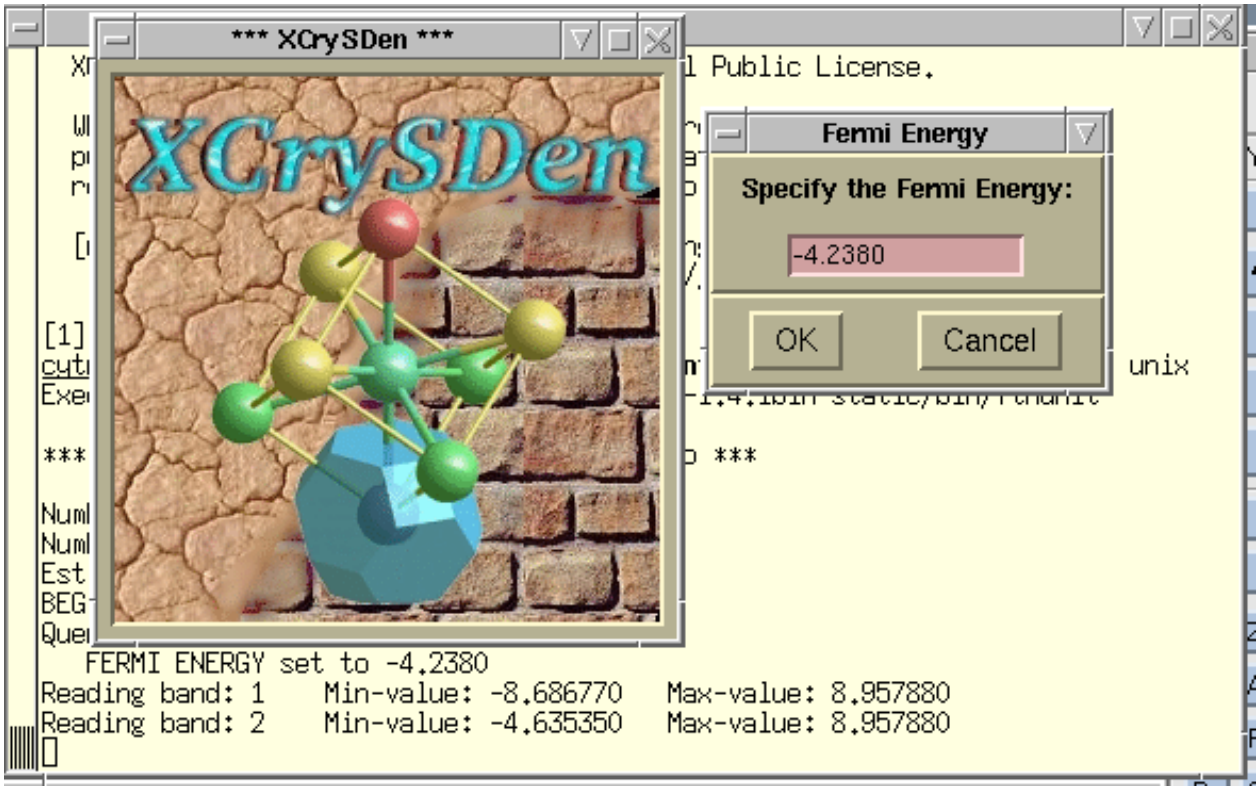
2. get files .XV, .KP, .EIG,
   run eig2bxsf $\longrightarrow$ creates .BXSF
   (or .BXSF_1 and .BXSF_2
   for spin-polarized case).

The *bandgrid* for the visualization of Fermi surface



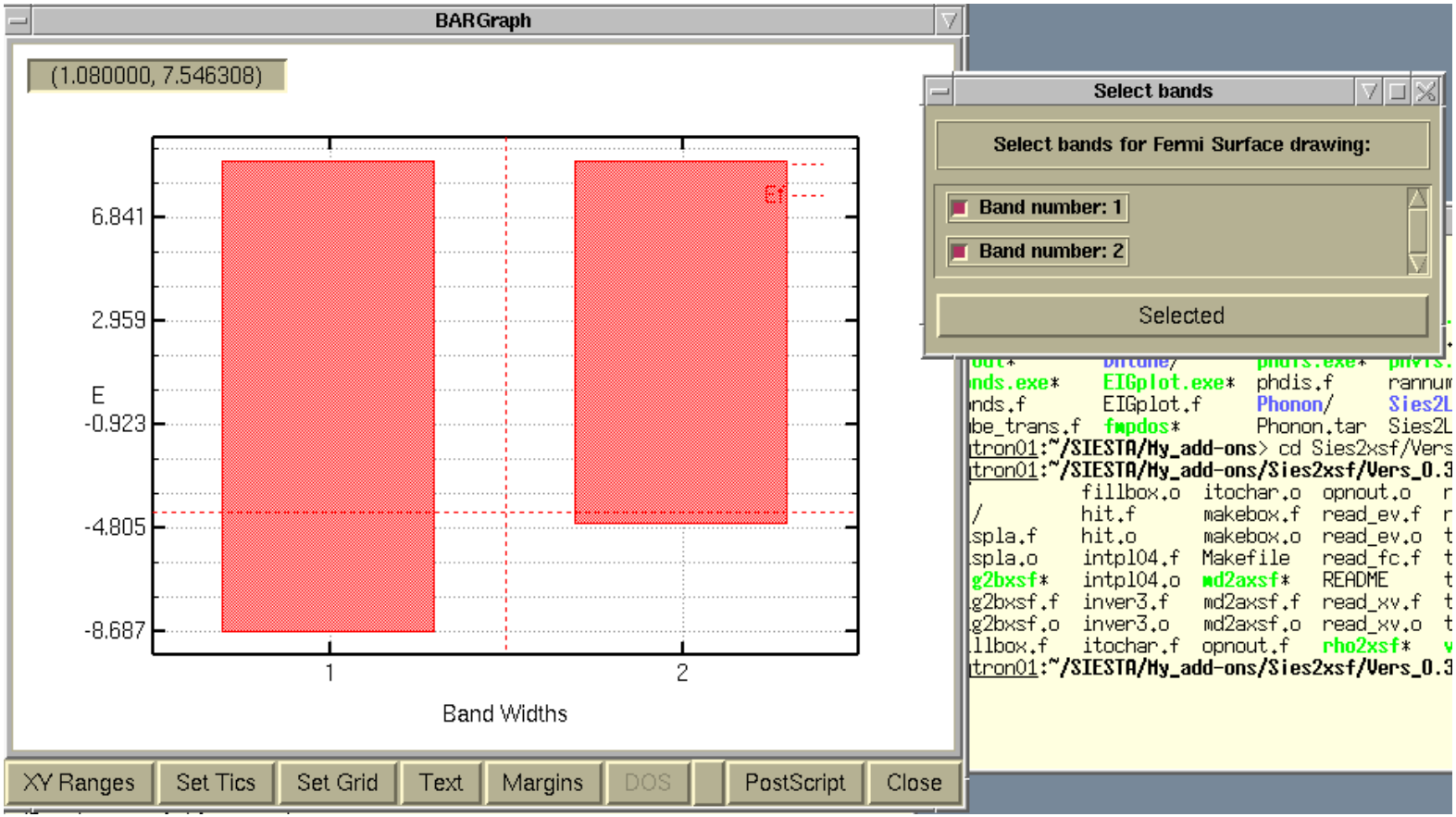
Visualization of Fermi surfaces

in XCrySDen, choose
File → Open Structure → Open BXSF
In the window that pops up,
specify the Fermi energy

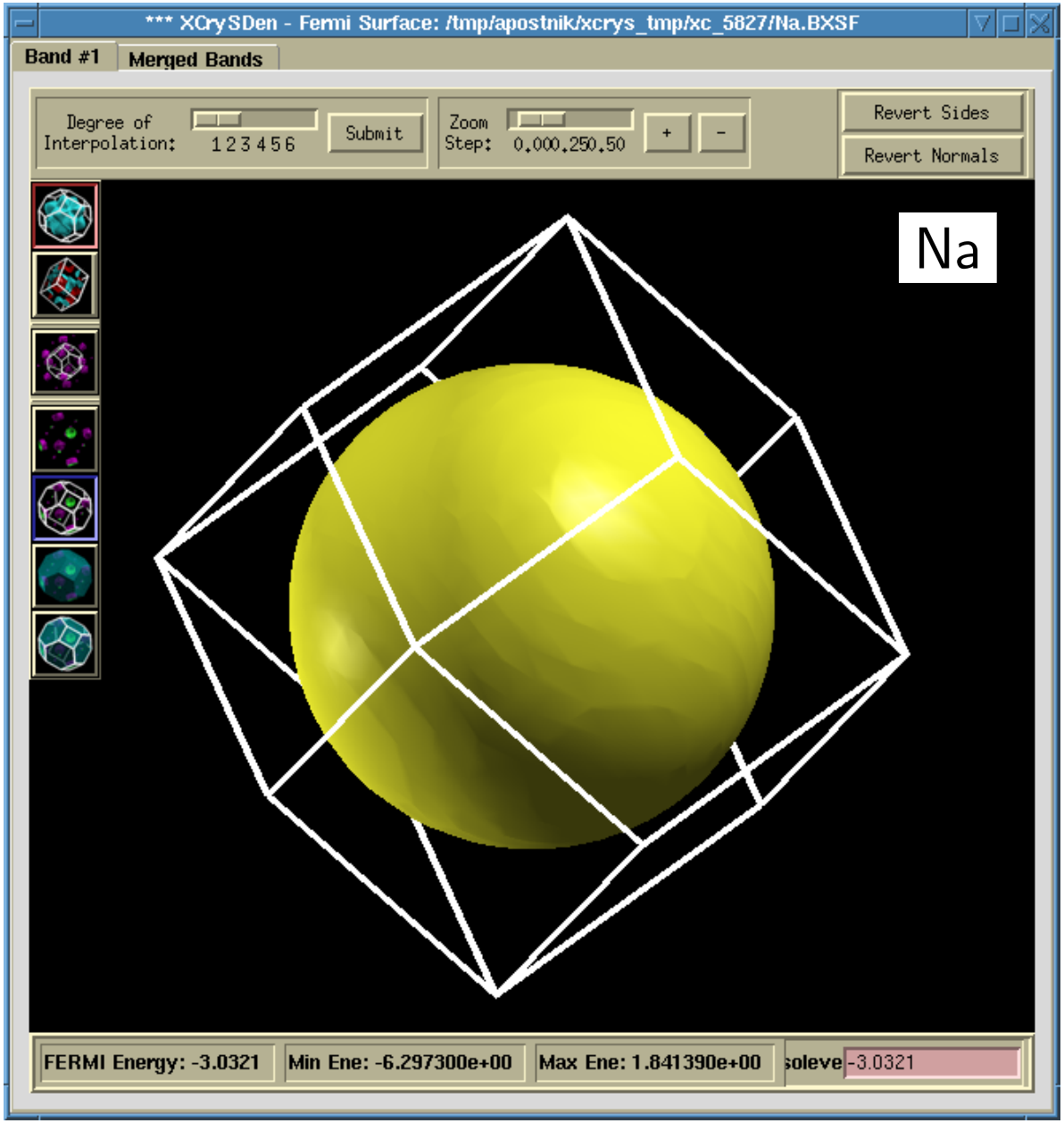


Visualization of Fermi surfaces

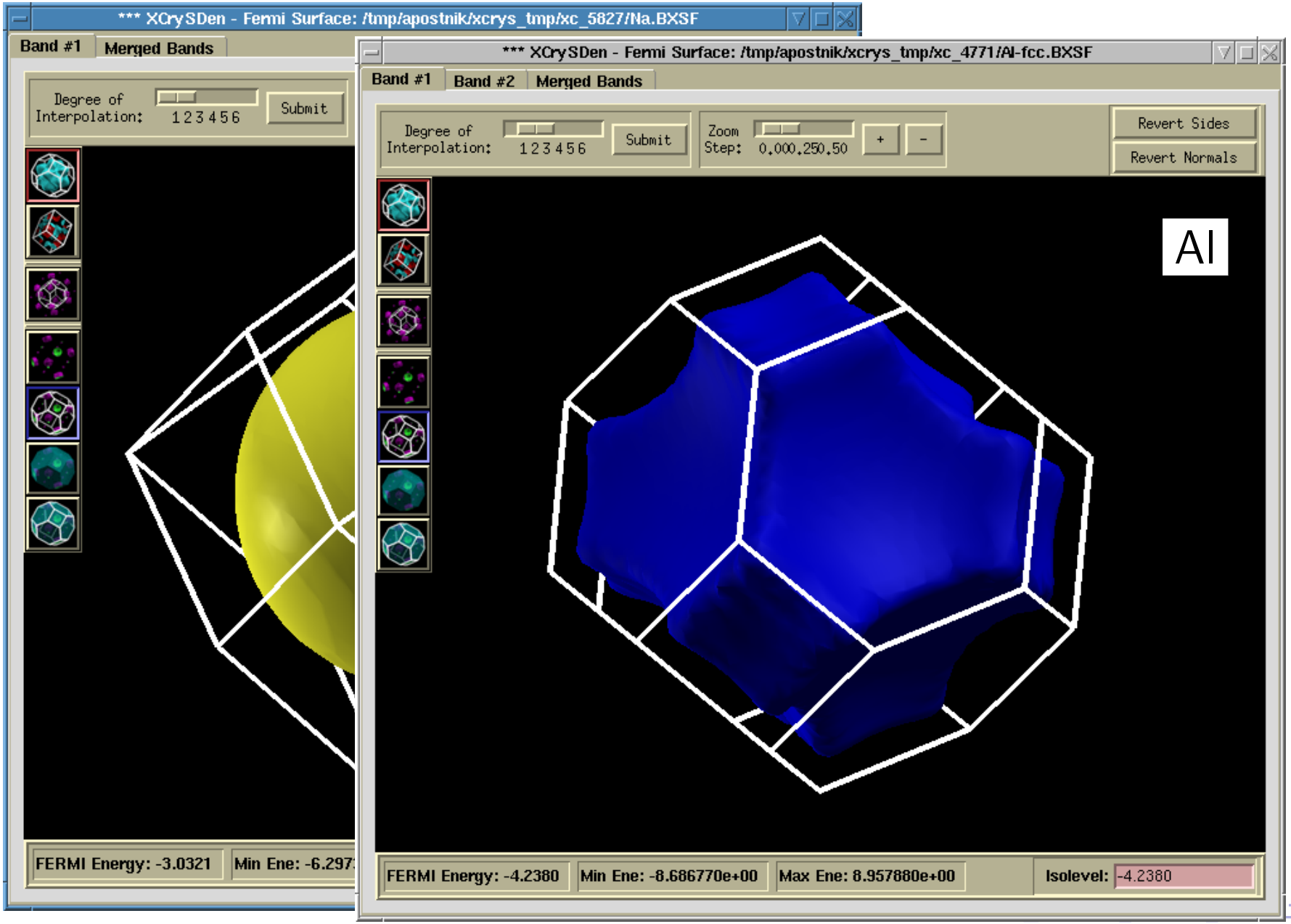
See which bands cross the Fermi energy, and select which of them you want to plot



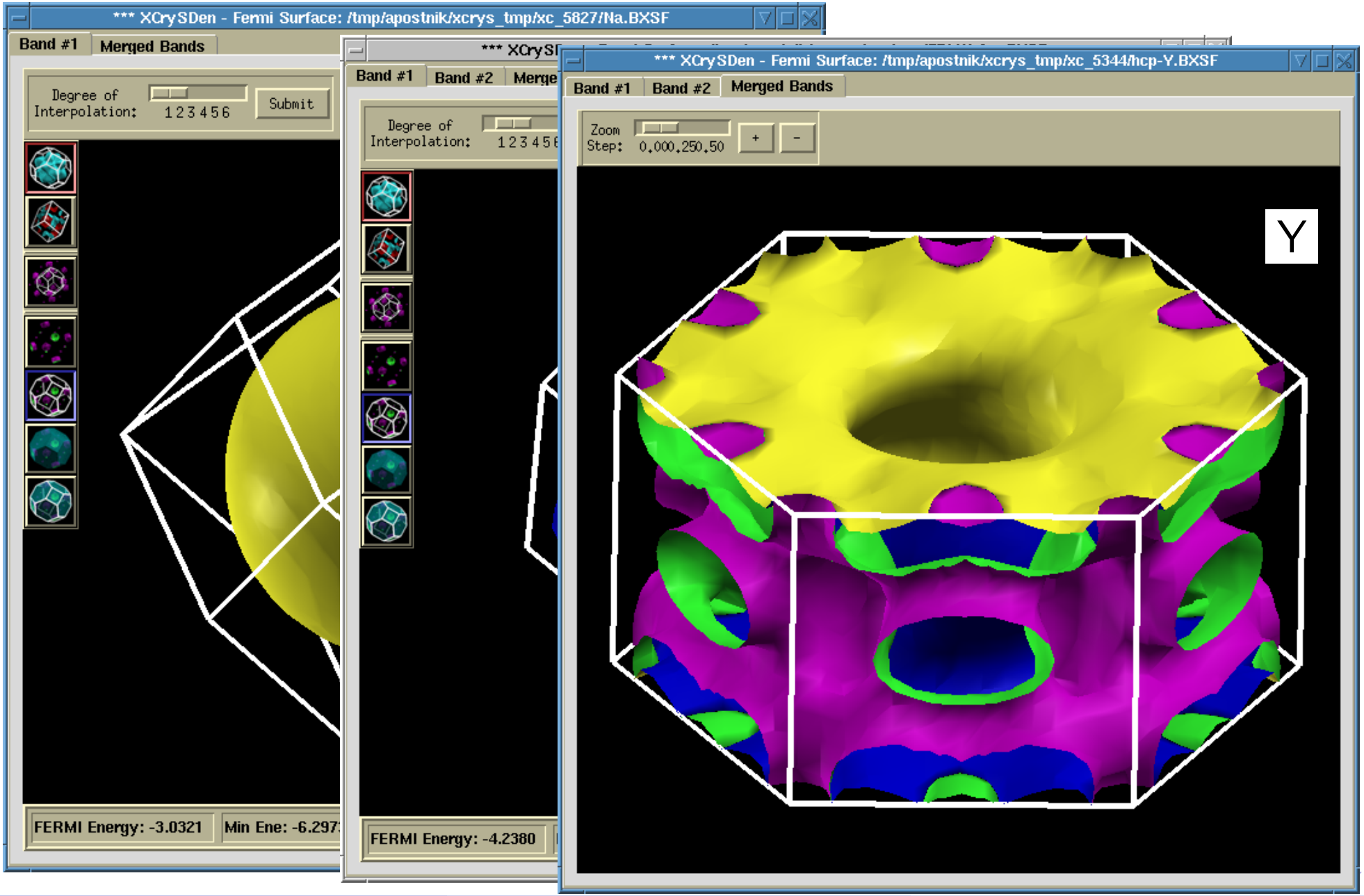
Fermi surfaces of some elemental metals



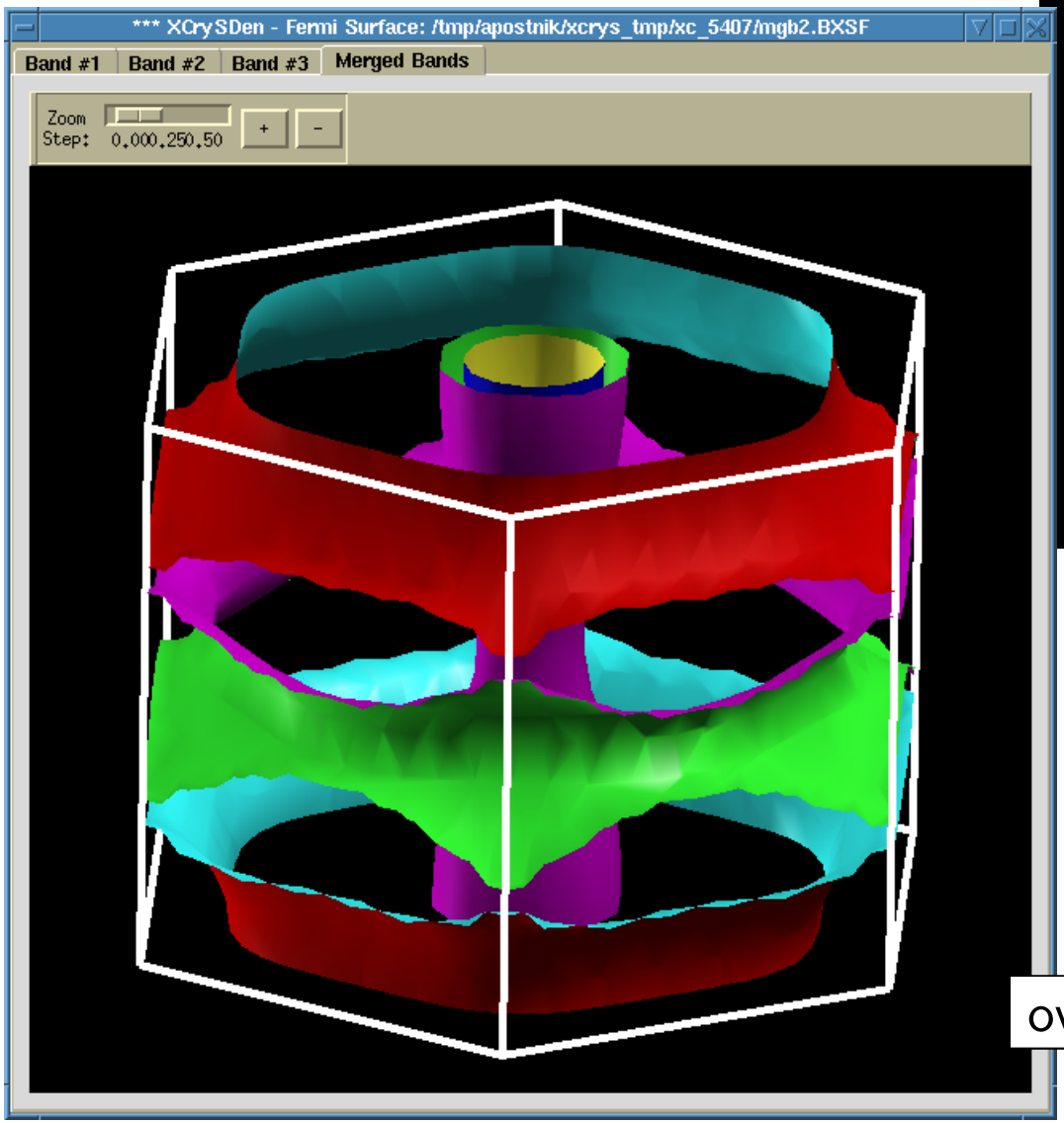
Fermi surfaces of some elemental metals



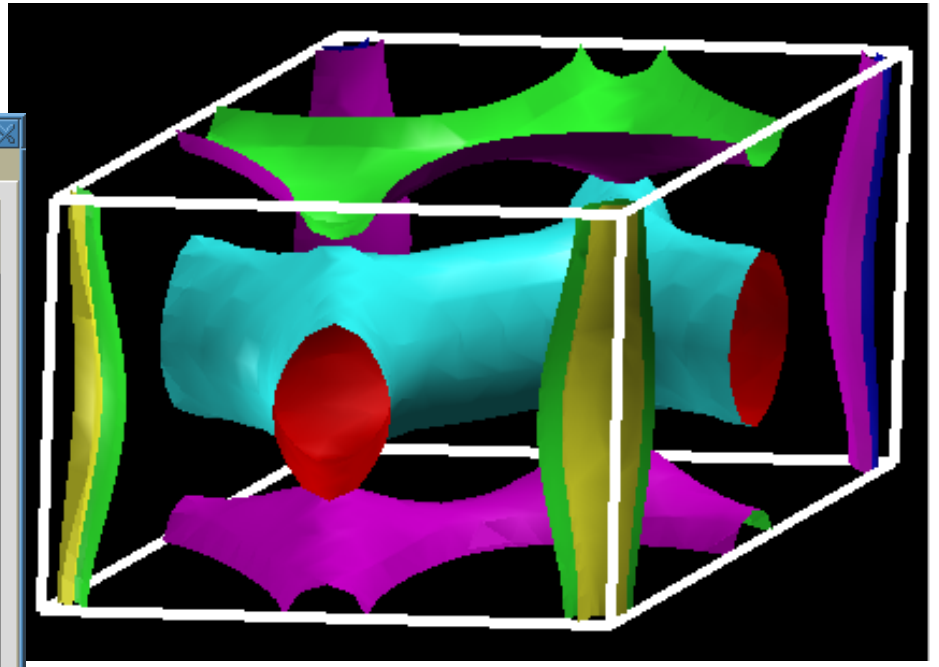
Fermi surfaces of some elemental metals



Fermi surface of MgB_2



over the Brillouin zone



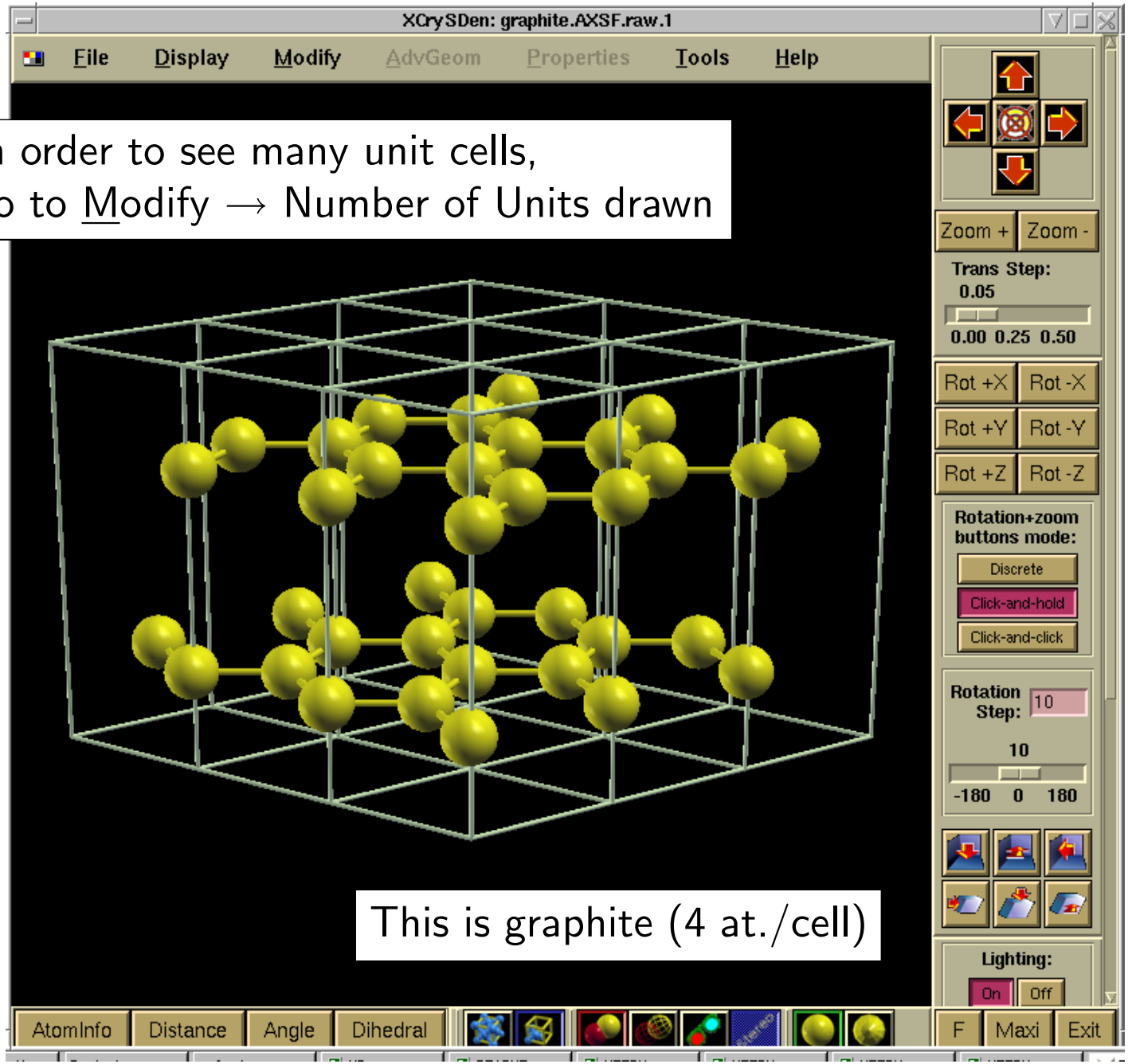
over the reciprocal cell

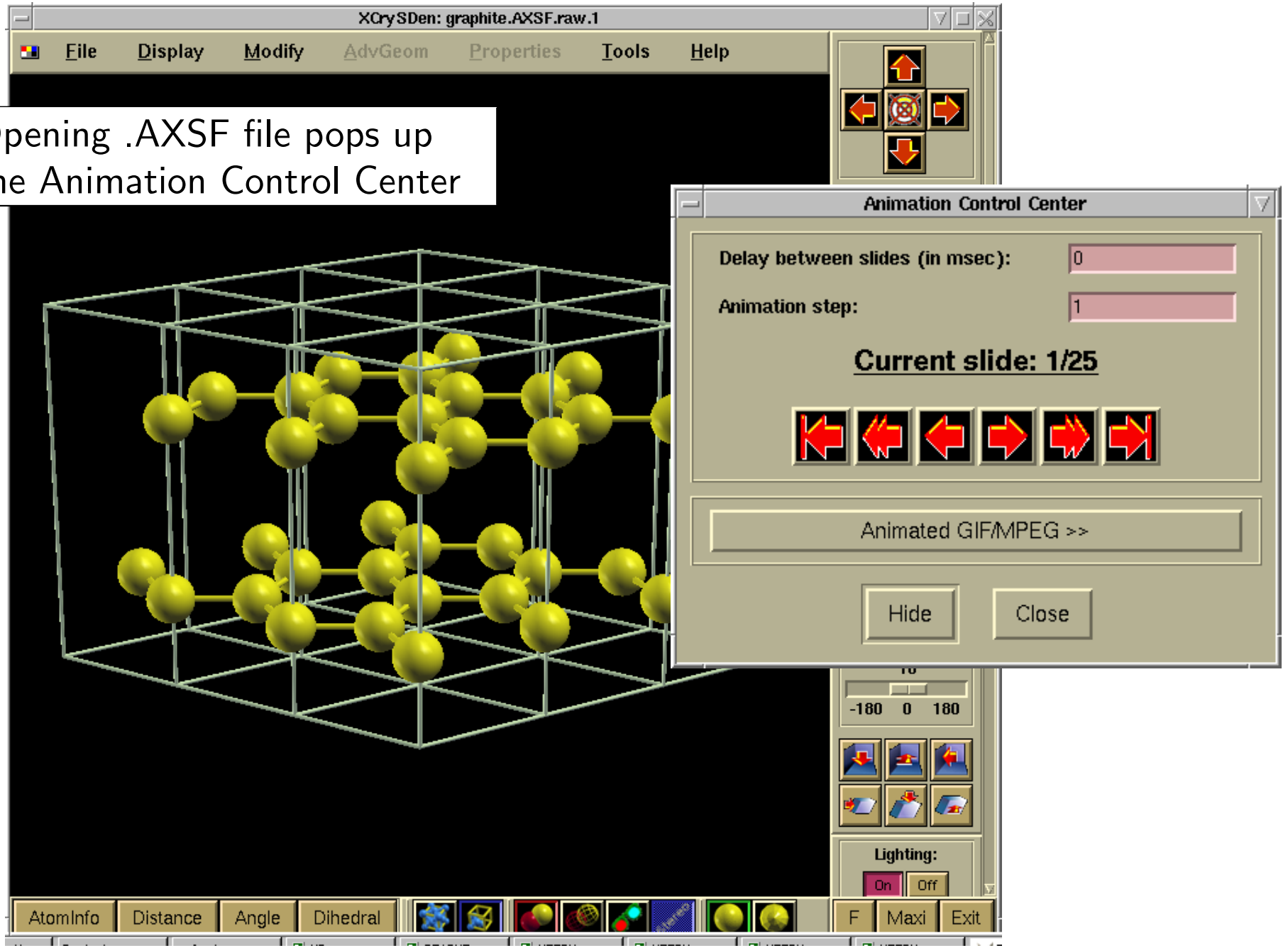
Molecular Dynamics or Relaxation

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).

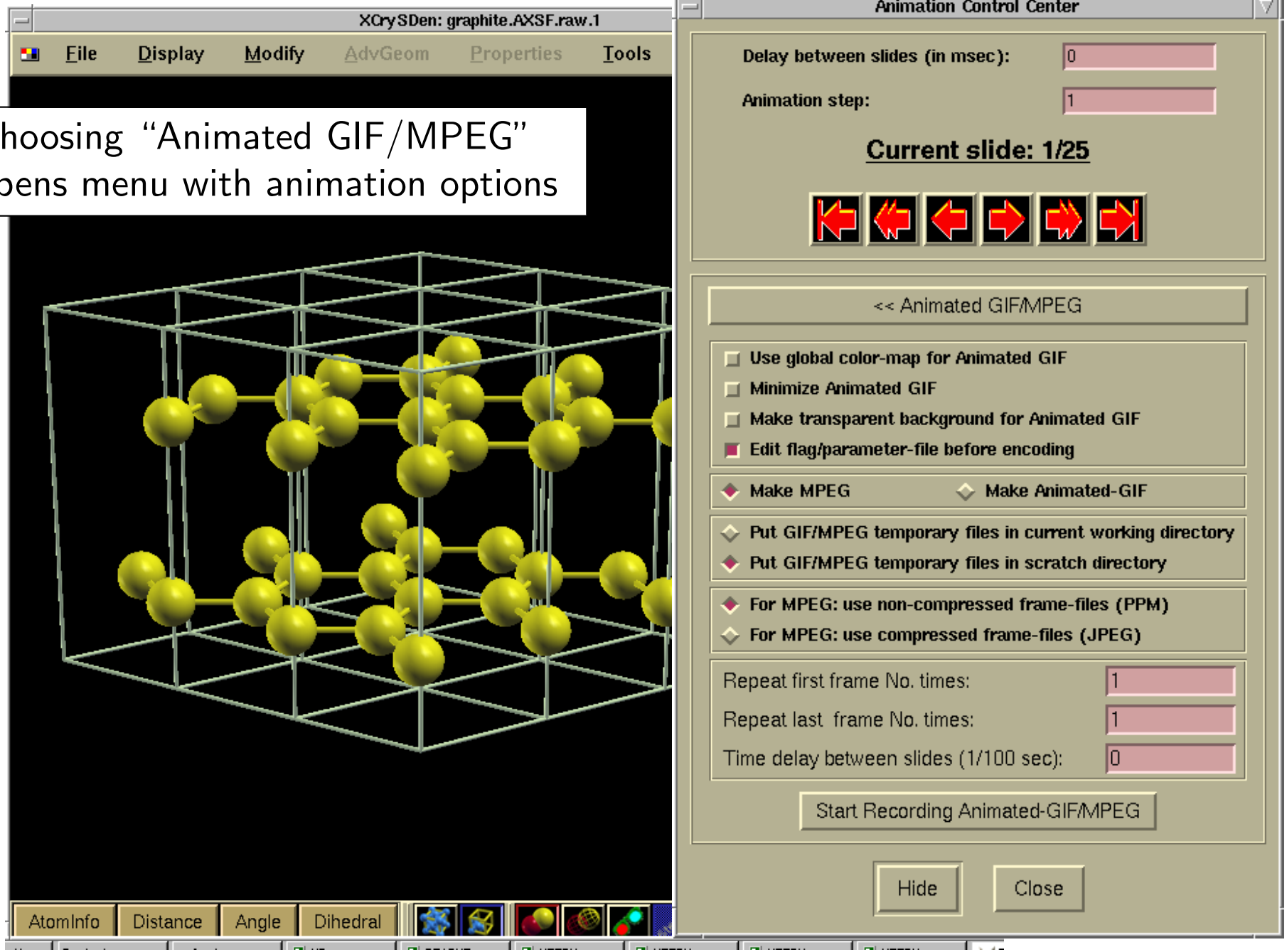
2. Having .XV, and either .MD, or .ANI
   run md2axsf, answering questions about the (optional) choice of output box
   and the MD steps to visualize (first #; last #; keep only each #'s)
   $\longrightarrow$ creates .AXSF.

   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).

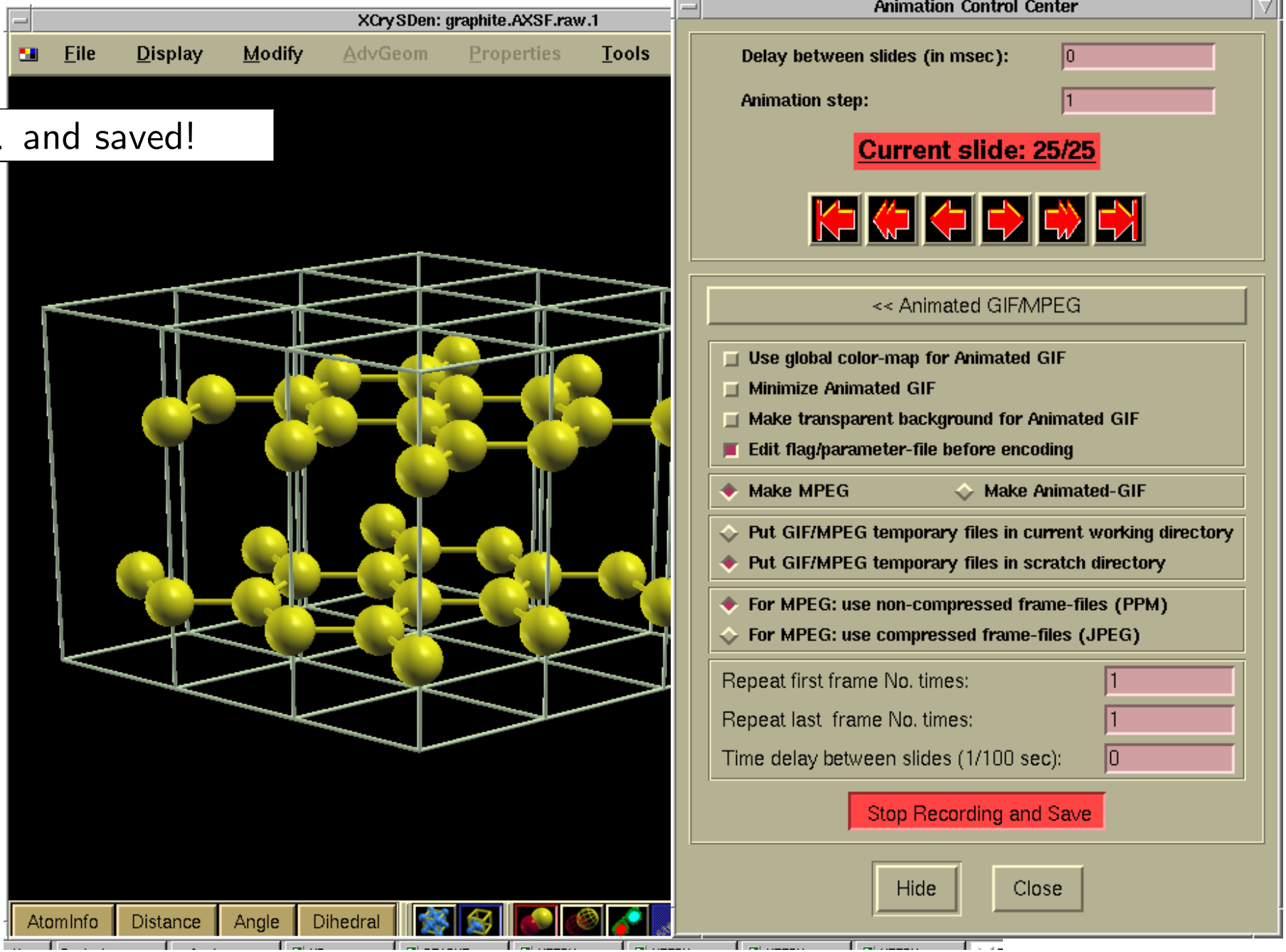

XCrySDen: graphite.AXSF.raw.1
File
Display
Modify
AdvGeom
Properties
Tools
Help
In order to see many unit cells,
go to Modify → Number of Units drawn
Zoom +
Zoom -
Trans Step:
0.05
0.00 0.25 0.50
Rot +X
Rot -X
Rot +Y
Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
10
10
-180 0 180
Lighting:
On
Off
This is graphite (4 at./cell)
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



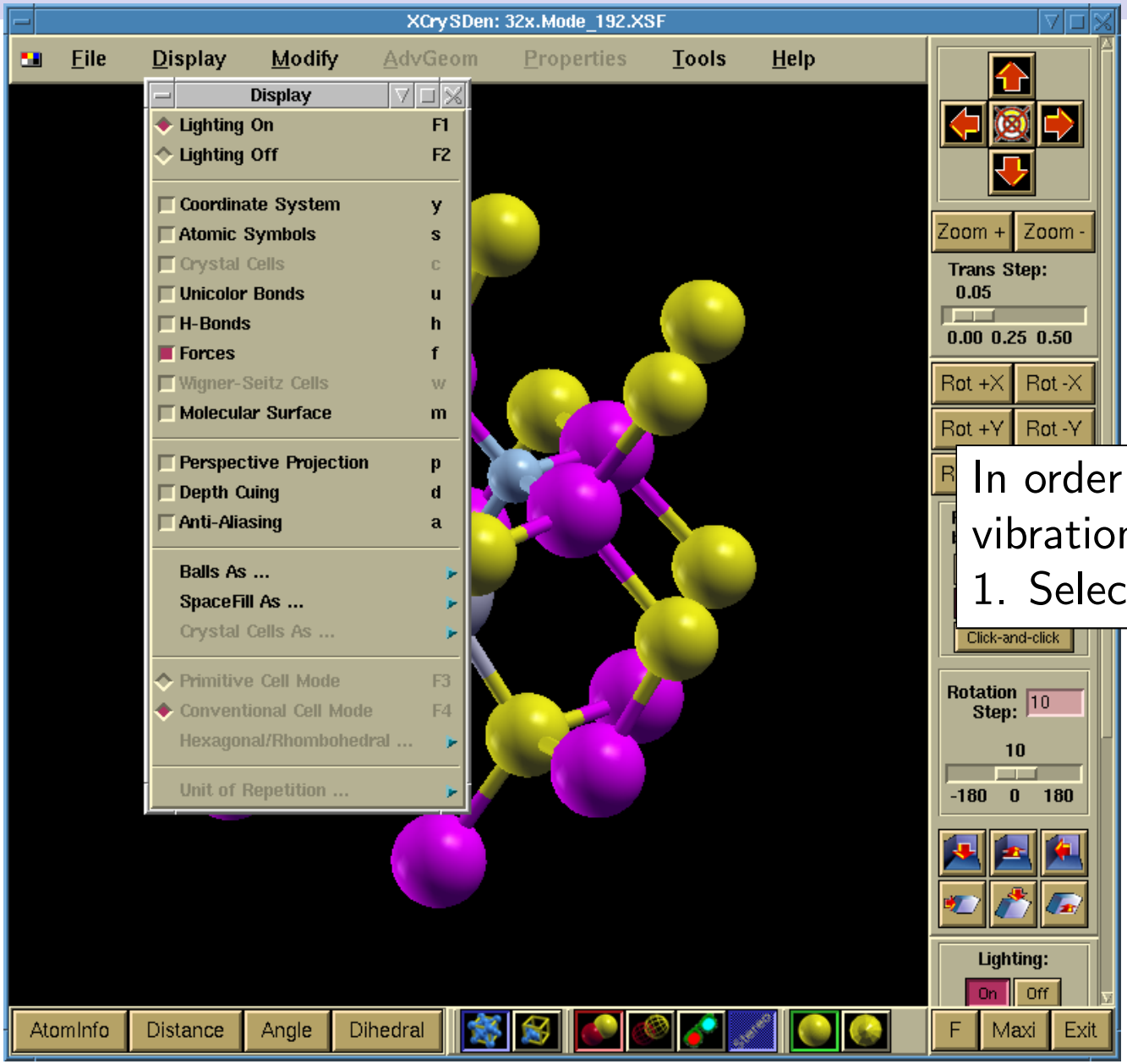
... and saved!


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.

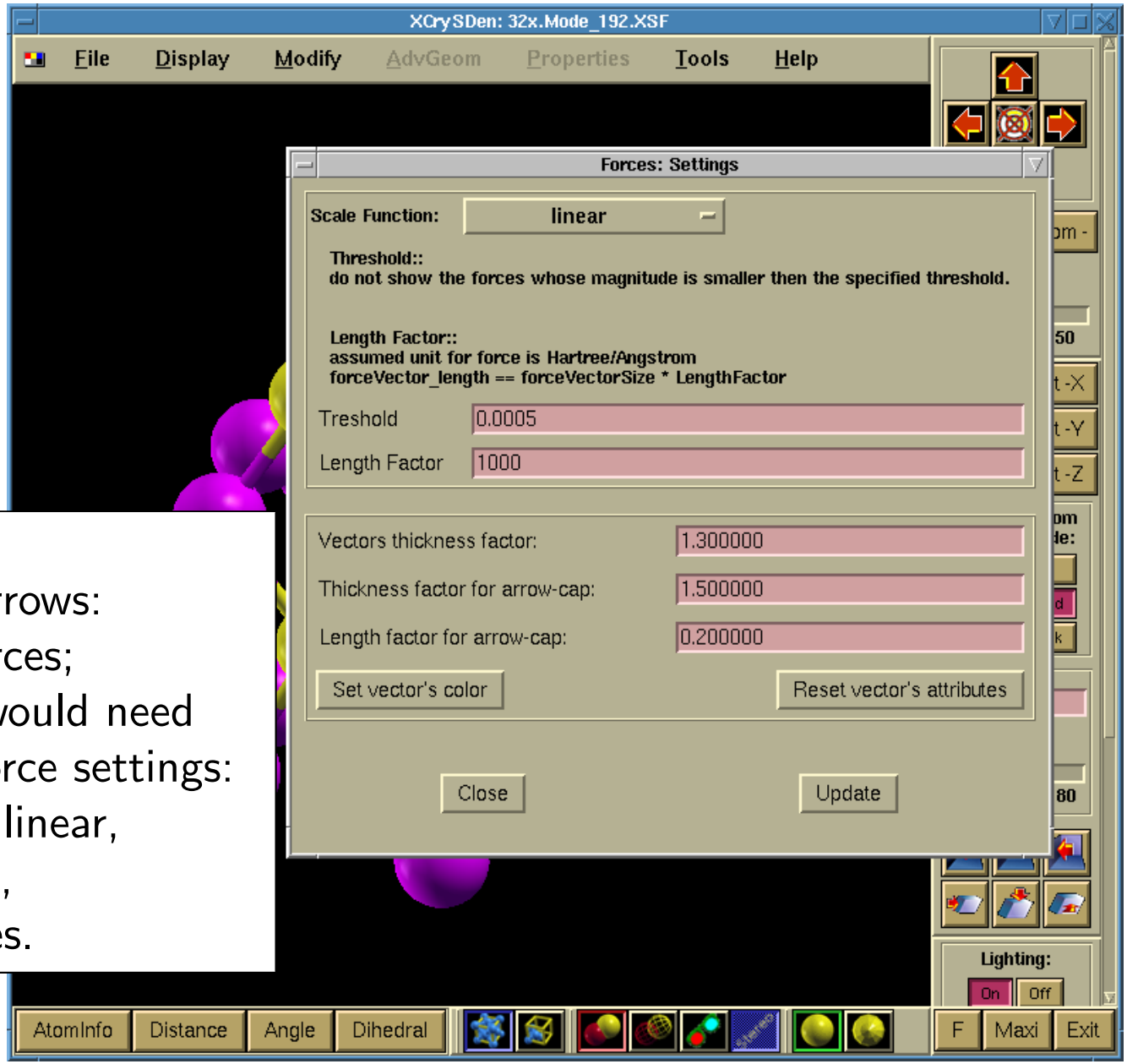
An example of phonons in In- and N-doped GaAs



In order to show vibrations patterns as arrows:

1. Select Display → Forces;

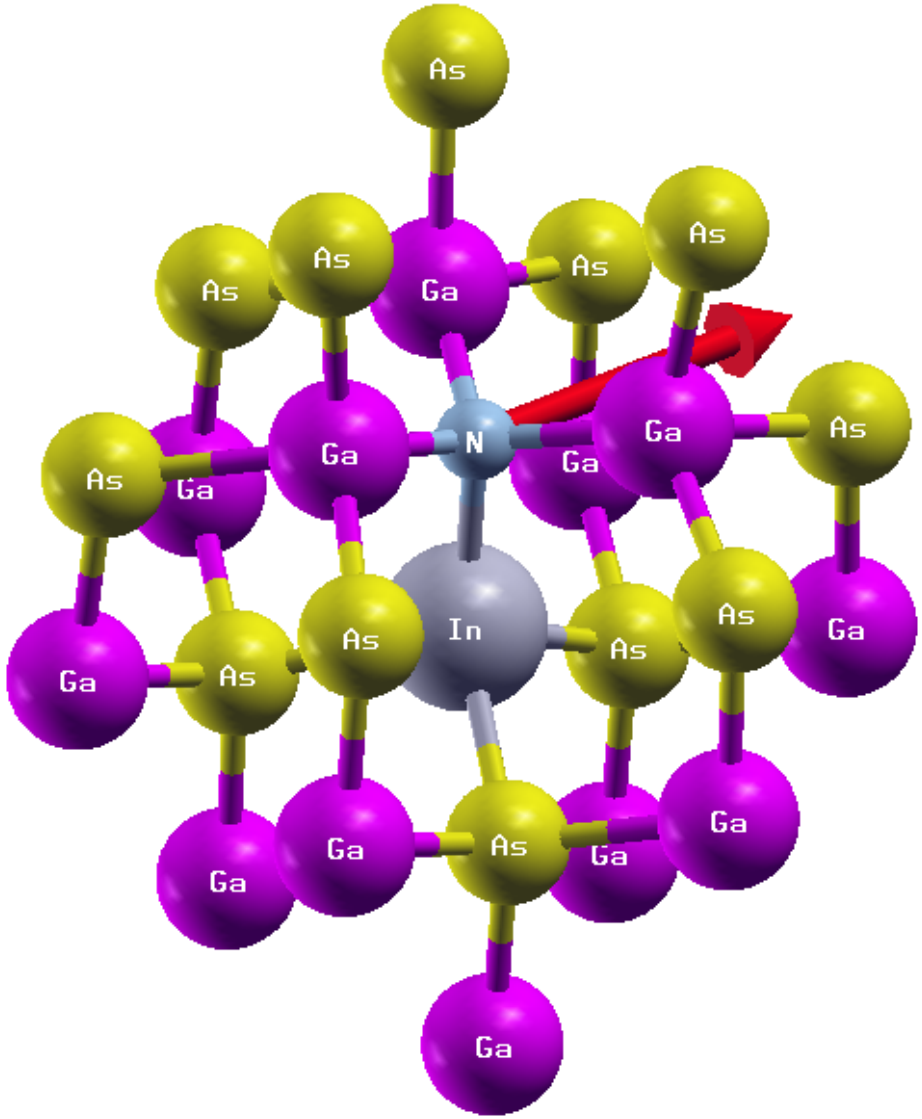
An example of phonons in In- and N-doped GaAs



In order to show
vibrations patterns as arrows:
1. Select Display → Forces;
2. Most probably, you would need to change Modify → Force settings: change Scale Function: linear, (increase) Length factor, change vectors attributes.

An example of phonons in In- and N-doped GaAs

One of N-related modes.
The atoms shown are cut from much bigger supercell by selecting the "visualization box" in **vib2xsf**, and then some more atoms have been removed by hand.



Concluding remarks and known limitations

- XCrySDen allows to manage (almost) all structure-related results from a SIESTA calcultion I can think about... do you have any other suggestions? It is a great software (both, I mean).
- The final results are bitmap (or, other format) damps of the contents of the simulation window (in the full-screen mode if needed), that would normally suffice for publication/presentation purposes. Atomic structure (atoms, bonds and cells, but not grid properties) can also be stored in [Display → Lighting off] mode as a postscript vector graphics.

Concluding remarks and known limitations

- What is missing in XCrySDen is an option *to paint* an isosurface / Fermi surface *with a property* (e.g., Fermi velocity).
- Fermi-surface part of XCrySDen is not as flexible as real-space-grids part in what regards choosing view frame, colours, light sources etc.
- Making 2-dim. cuts of the Fermi surface is not implemented. However, this can be easily done by exporting the $E(\mathbf{k})$ data ordered by the **eig2bxsf** script to other plotting routine.
- A possible extension: representing a vector field – e.g., the magnetization $\mathbf{m}(\mathbf{r})$ from a non-collinear spin calculation. XCrySDen allows to draw a forest of arrors ("forces") stuck to ghost atoms of chemical label 'X', which atoms won't be visible if their radii set to almost zero, but arrors well visible is thick enough.