

# Visualization and post-processing tools for SIESTA

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- 1 What to visualize?
- 2 XCrySDen by Tone Kokalj
- 3 Sies2xsf suite
  - Atomic structure
  - Charge and spin densities
  - Wave functions
  - Fermi surfaces
  - Molecular Dynamics or relaxation
  - Phonons

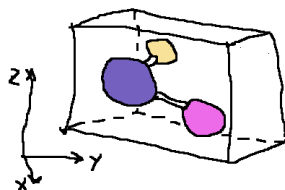
# What to visualize..?

- 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  $\mathbf{k}$ -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”).



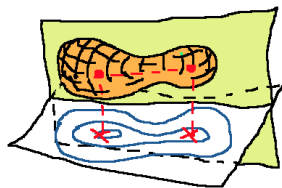
Since the input format is quite flexible (a big advantage!), it is difficult to organize a simple viewer of *input* structure data, without using the *fdf* routines. However, the *.XV* file (created after the completion of electronic structure loop) contains all necessary information, as it was *really*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



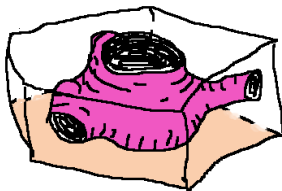
## Kohn-Sham wavefunctions

These are also scalar functions of spatial coordinates, but obtained in SIESTA as 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

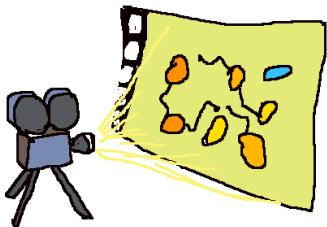
can be calculated using the energy dispersion data  $E(\mathbf{k})$ , available from any band structure code. The difficulty of purely technical character is, how to construct energy isosurfaces and conveniently manipulate them (to choose viewpoint, select different sheets of the Fermi surface, etc.)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

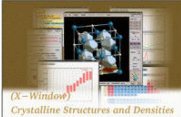
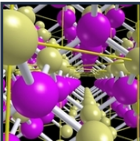
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## XCrySDen ...

X-window CRYstalline Structures and DENsities



### XCrySDen Documentation



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](#)).

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[How to get](#)

[About](#)

[Description](#)  
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## 1.1 What *XCrySDen* can do?

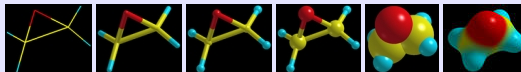
In short: *XCrySDen* is a crystalline and molecular structure render program, with additional capabilities of rendering contours, isosurfaces, Wigner-Seitz cells (also Brillouin zone), Fermi surfaces and so on. Some of its features are the following:

- widget with periodic table of elements:

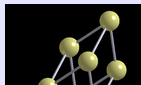


It enables different presentations of atoms and bonds (colors, shadows, ...), measuring distances and angles ...

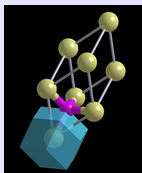
- displaying molecular and crystalline structure in several different display modes:



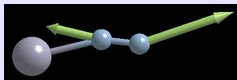
- displaying crystal and Wigner-Seitz cells:



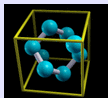
- displaying crystal and Wigner-Seitz cells:



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



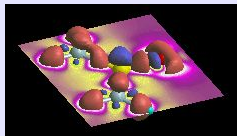
- animations



- displaying contours and colorplanes

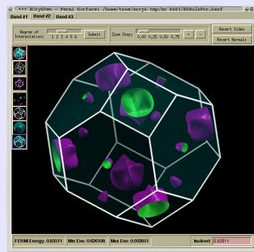
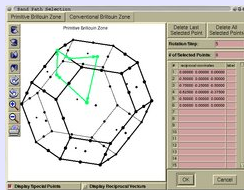
... allows to set arrows on atoms  
(or, on fictitious atoms)  
and make animations ...

- 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

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## 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...

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
```

... including forces (or, velocities)

Done

# 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
  0.000000  2.710000  2.710000
  2.710000  0.000000  2.710000
  2.710000  2.710000  0.000000
PRIMCOORD 1
  2 1
  16  0.000000  0.000000  0.000000
  30  1.355000  -1.355000  -1.355000
PRIMCOORD 2
  2 1
  16  0.000000  0.000000  0.000000
  30  1.255000  -1.255000  -1.255000
```

... and animations for molecular and periodic structures

Where to find them:

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

What do they make out of what:

- **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).

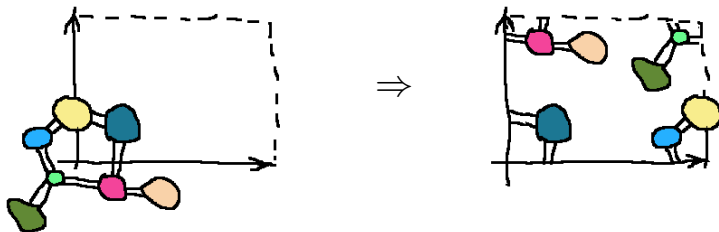
# Visualization of atomic positions

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

I know my structure already, why visualize it? → 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 ...

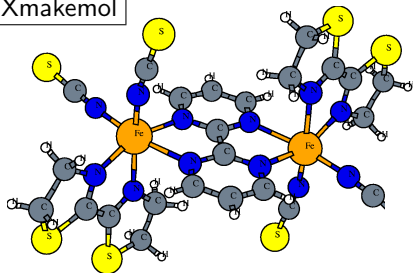




# Visualization of atomic positions

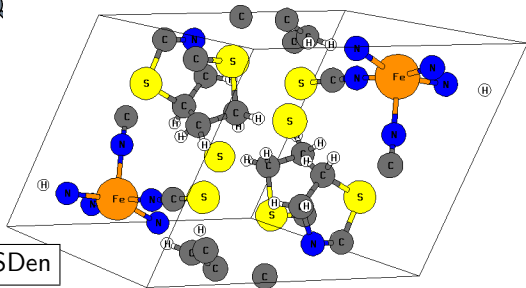
Example of for a crystal of Fe-binuclear units:

Xmakemol



This is “Lighting Off” mode of XCrySDen: no shadows or isosurfaces, but fast manipulations with a structure, and possibility of vectorial PostScript output.

XCrySDen



# 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:

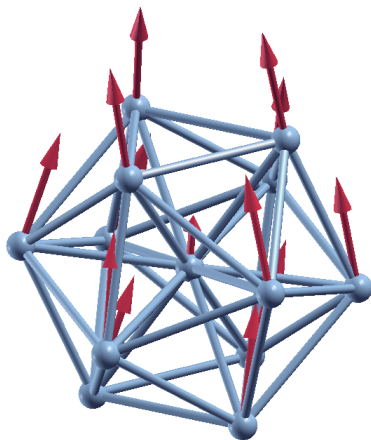
ATOMS

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

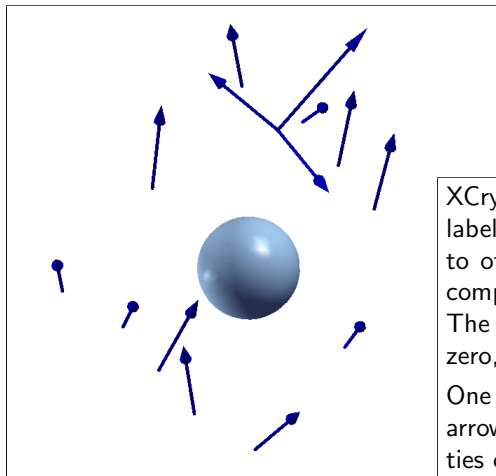


After opening this .XSF file,  
do not forget to activate  
Display → Forces,  
and optionally do  
Modify → Force settings

0.6370	0.7380	1.5400
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  $\text{Co}_{13}$  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 different 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

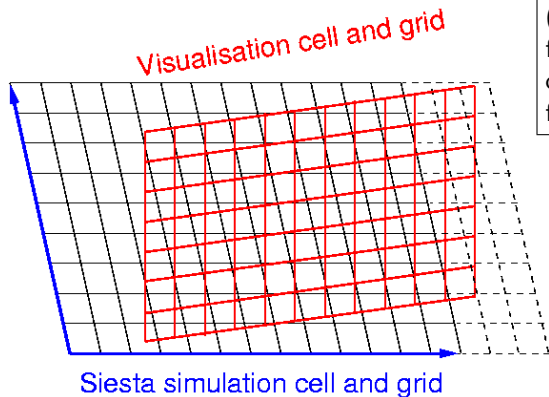
- 1 An input file for XCrySDen is created by **rho2xsf**.
- 2 Accept the same approach as in Denchar: define the output box (by origin point and three spanning vectors, not necessarily orthogonal) and grid size along each grid direction. The values of a Siesta property defined on the internal Siesta 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, or not. XCrySDen can apply translations to the 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 cell, and it needs not to be orthogonal. We'll define it by the origin point and three 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,iyy,iiz= 18 66 75
For is=1: min. grid value = 5.77762E-07 at iix,iyy,iiz= 48 53 50
For is=2: max. grid value = 6.67557E-01 at iix,iyy,iiz= 79 53 32
For is=2: min. grid value = 5.68289E-07 at iix,iyy,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

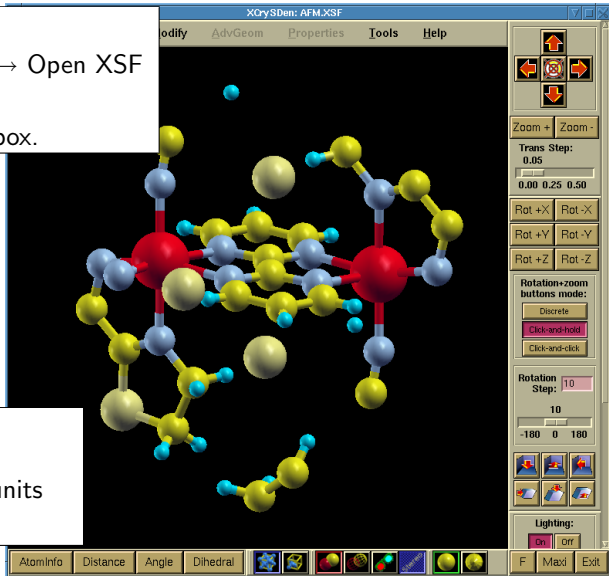
- The fineness of the visualization is limited by the sparciest one of the two grids.
- The cutting planes in XcrySDen may only be those of the visualization grid.

# 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

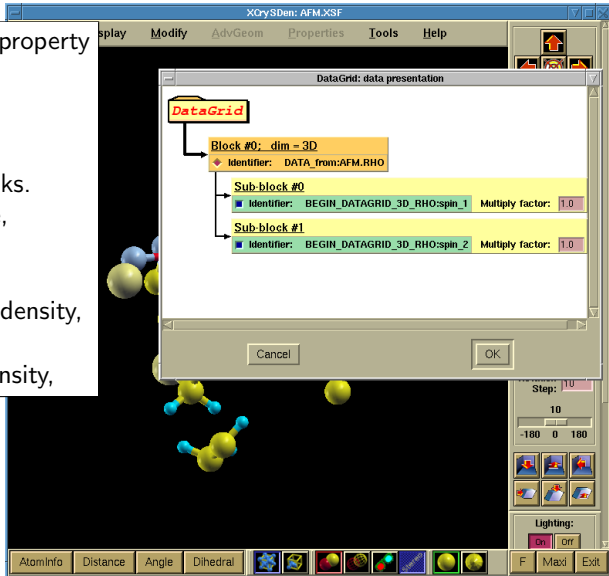
and set the weights of the different subblocks.

In a spin-polarized case, there are two.

Choose 1.0 and 1.0

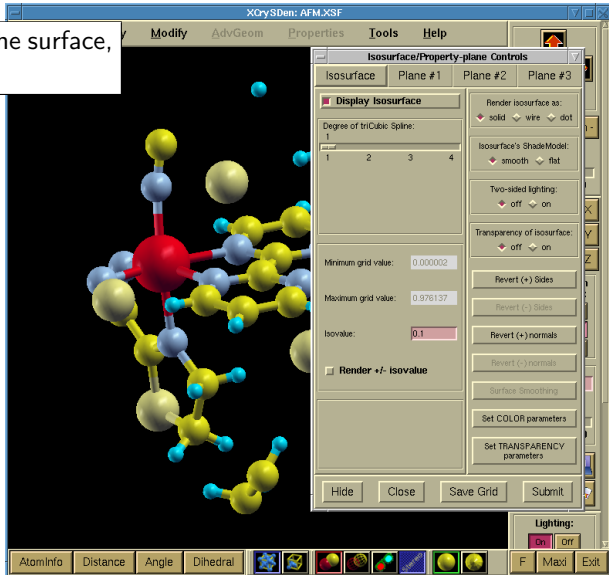
for plotting the charge density, 1.0 and -1.0

for plotting the spin density,



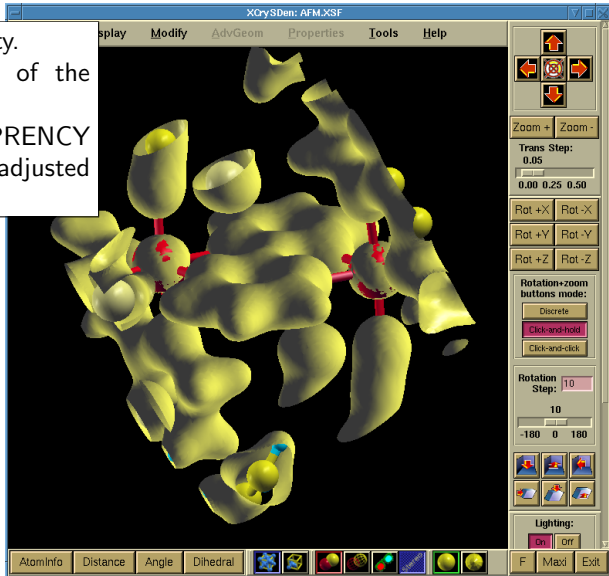
# Plotting of grid properties

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



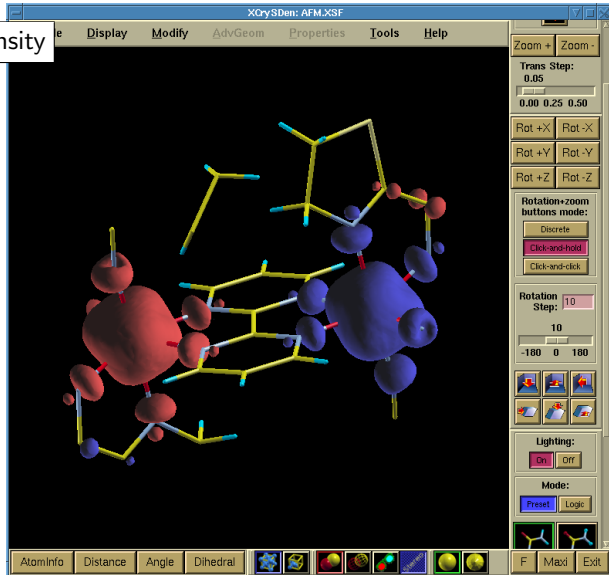
# Plotting of grid properties

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



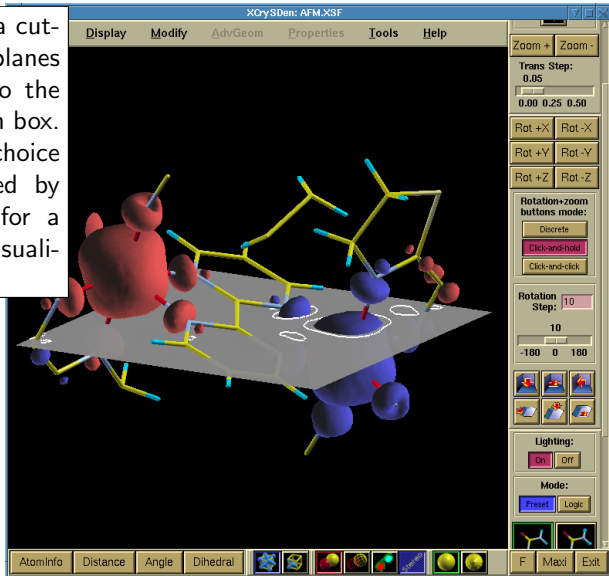
# Plotting of grid properties

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.

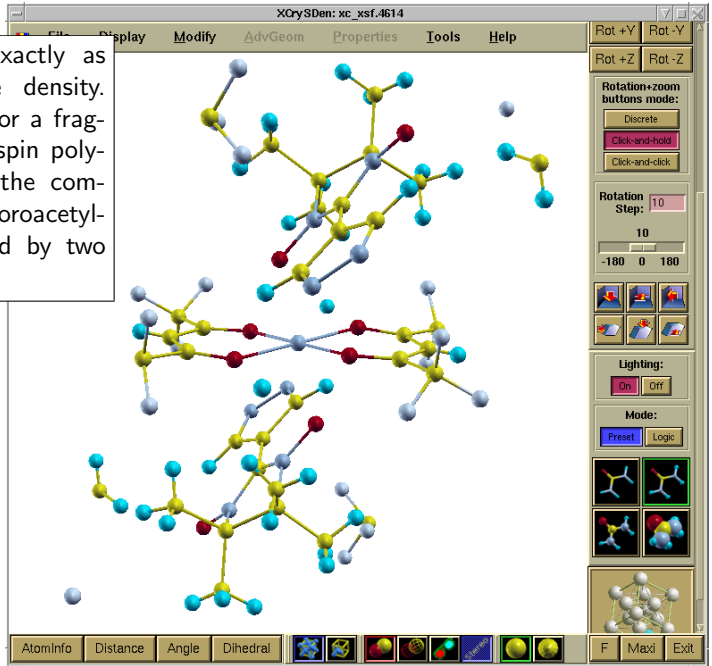


# Visualization of Wave Functions

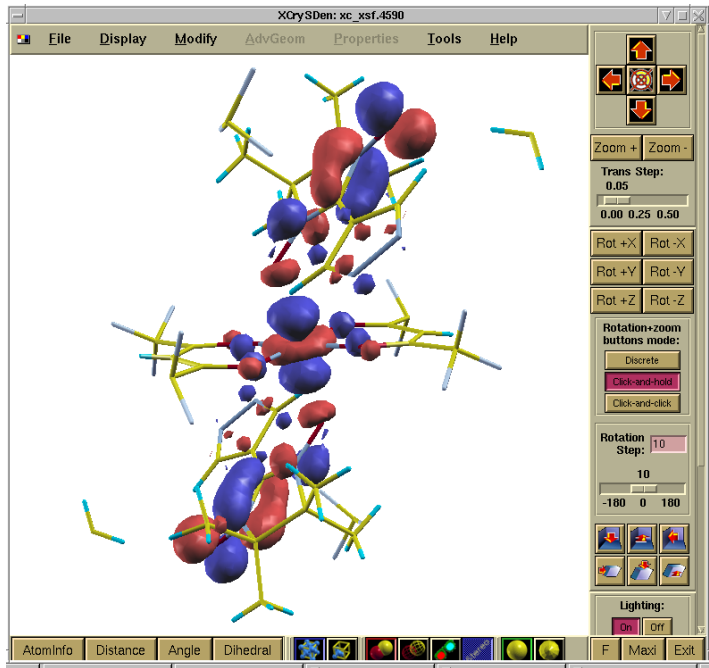
In principle, **Denchar** does this job quite fine. However, we'd like to have an interface to XCrySDen. To this end:

- 1 Use Denchar, define output box there, save result as Gaussian98 Cube file.
- 2 Read this Gaussian98 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 Gaussian 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).

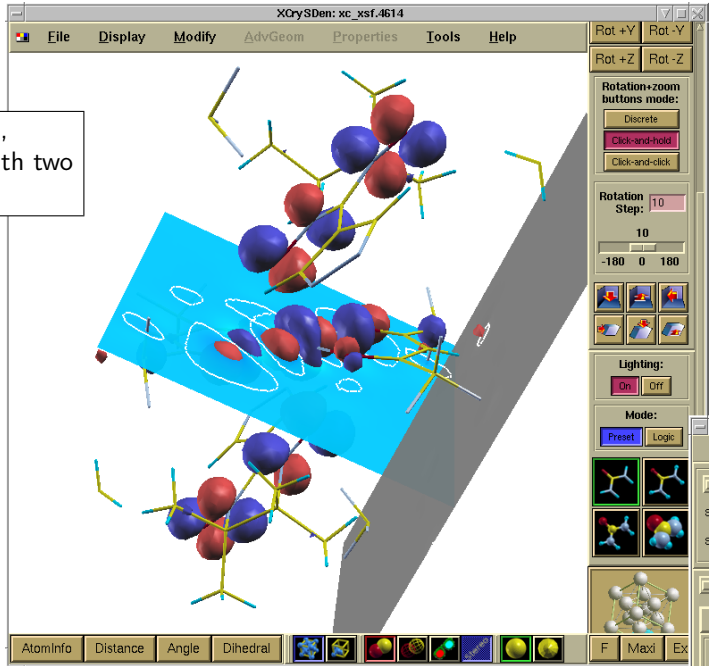


one orbital...





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



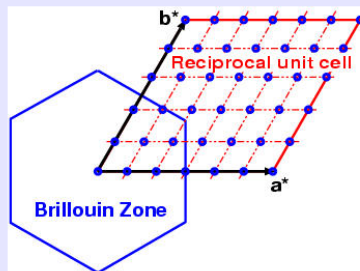
# Visualization of Fermi surfaces

- 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
```

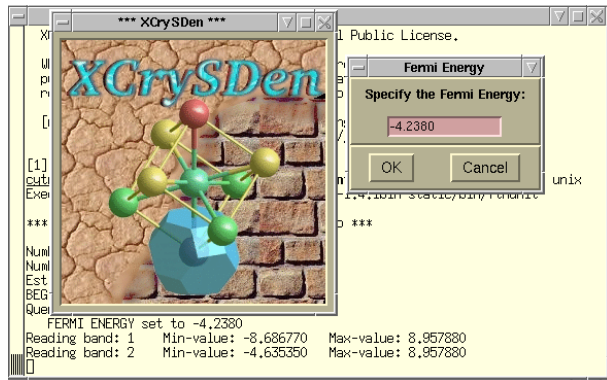
- 2 get files .XV, .KP, .EIG,  
run eig2bxsf → creates .BXSF  
(or .BXSF\_1 and .BXSF\_2  
for spin-polarized case).

The *bandgrid* for the visualization of Fermi surface



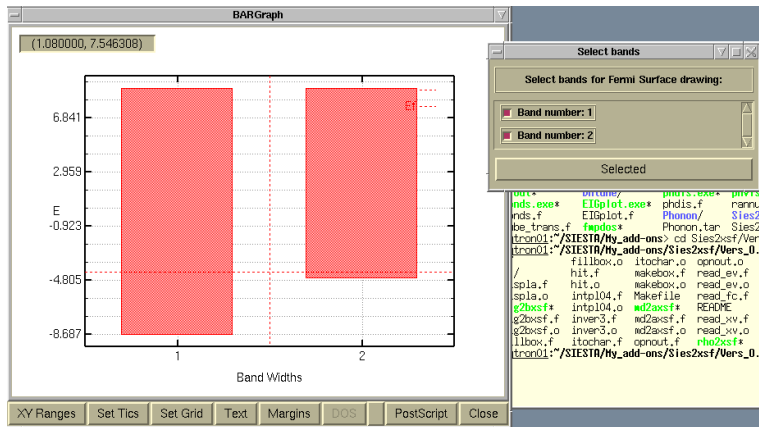
# Visualization of Fermi surfaces

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

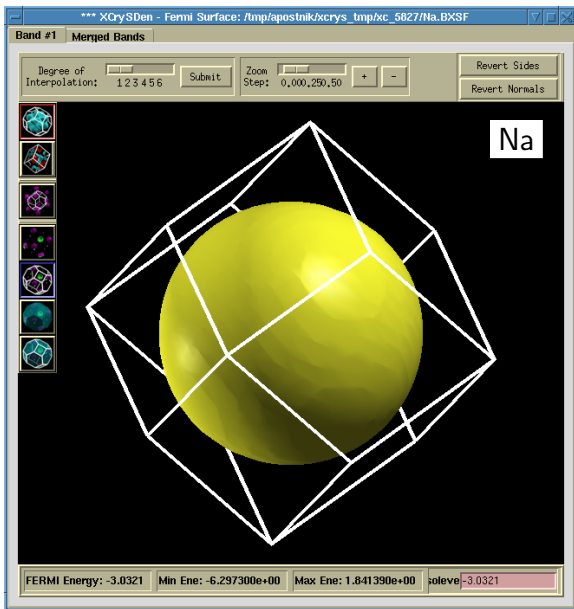


# Visualization of Fermi surfaces

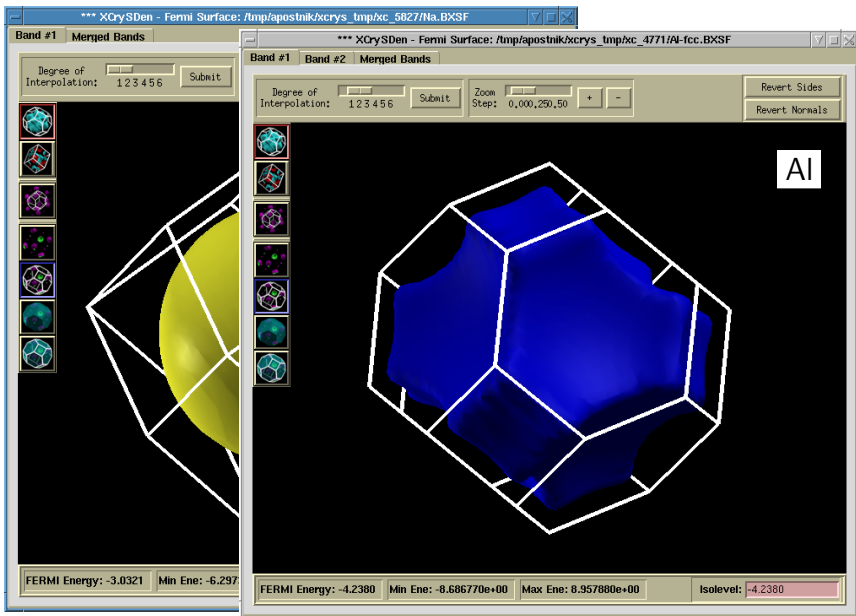
See which bands cross the Fermi energy, and select which of them you want to plot



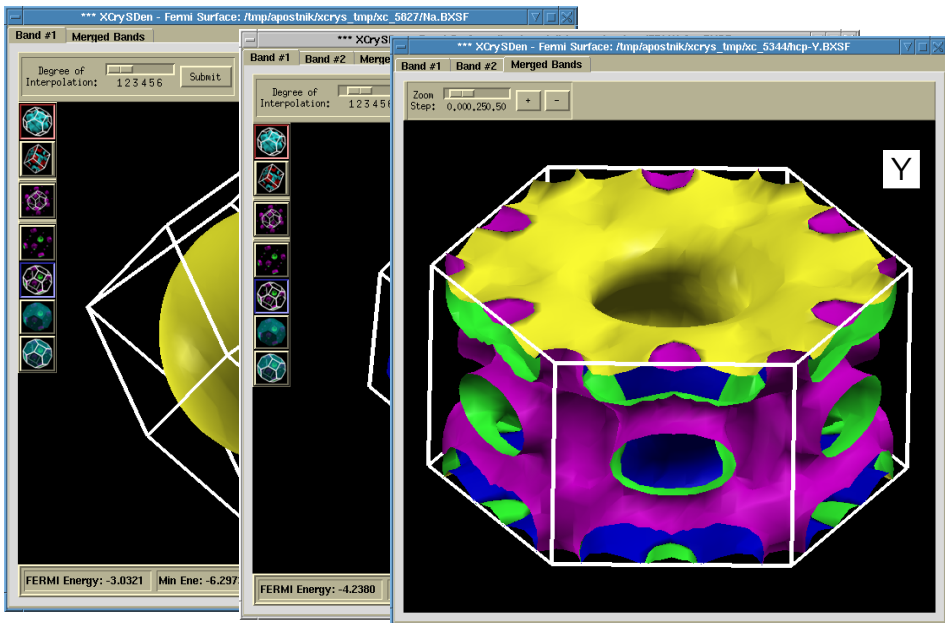
# Fermi surfaces of some elemental metals



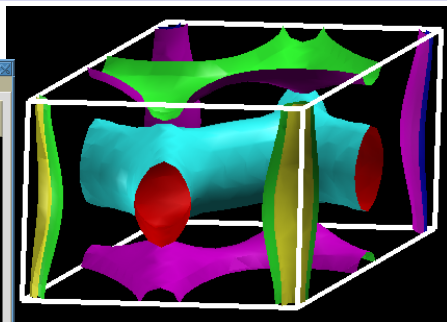
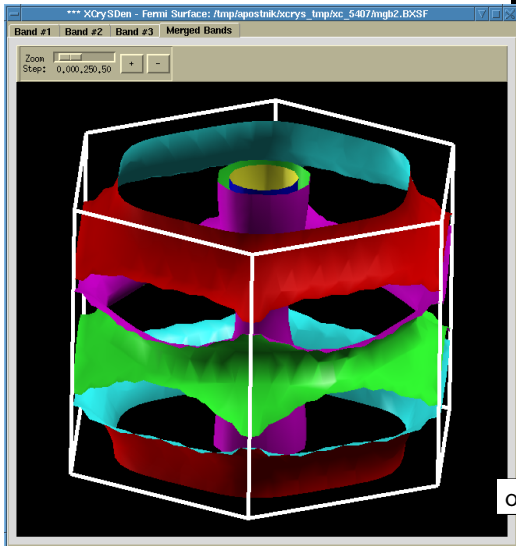
# Fermi surfaces of some elemental metals



# Fermi surfaces of some elemental metals



# Fermi surface of $\text{MgB}_2$



over the reciprocal cell

over the Brillouin zone



# Molecular Dynamics or Relaxation

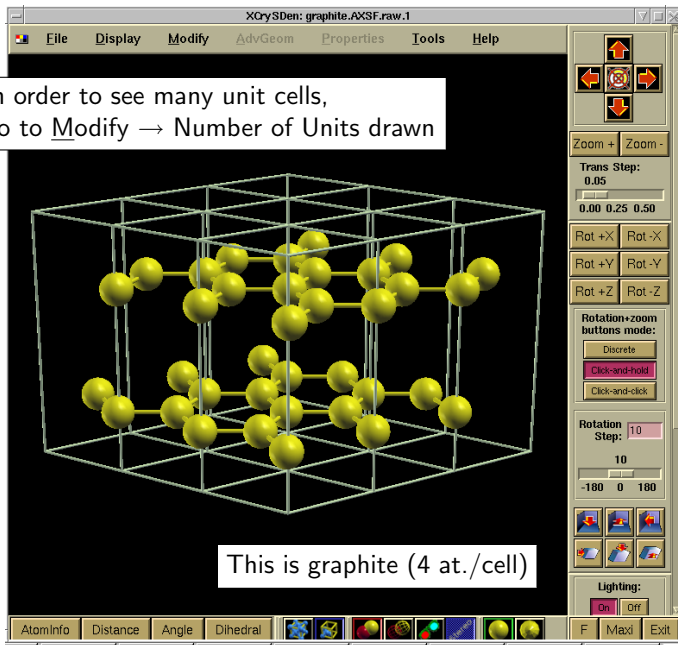
## ① Calculate MD history:

`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).

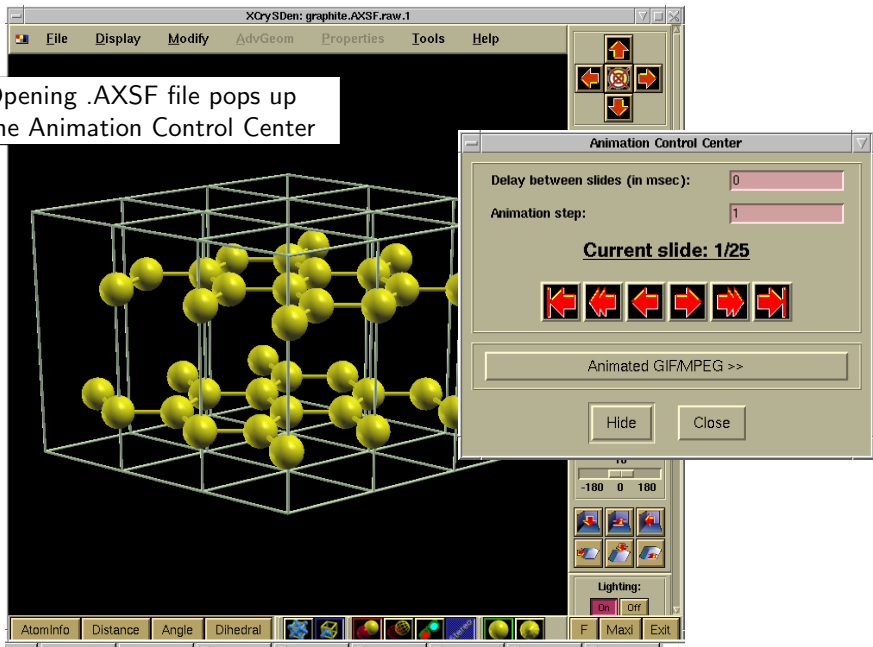
## ② Having .XV, and either .MD, or .ANI run `md2axsf`, answering questions about the (optional) choice of output box and the MD steps to visualize (first #; last #; keep only each #'s) → creates .AXSF.

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).

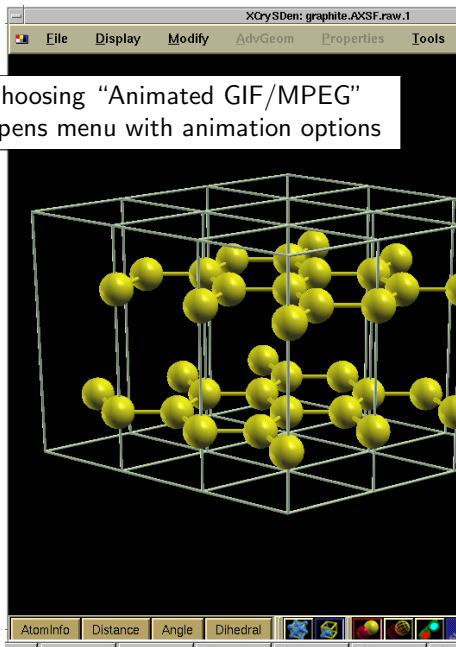
In order to see many unit cells,  
go to Modify → Number of Units drawn



Opening .AXSF file pops up  
the Animation Control Center



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:

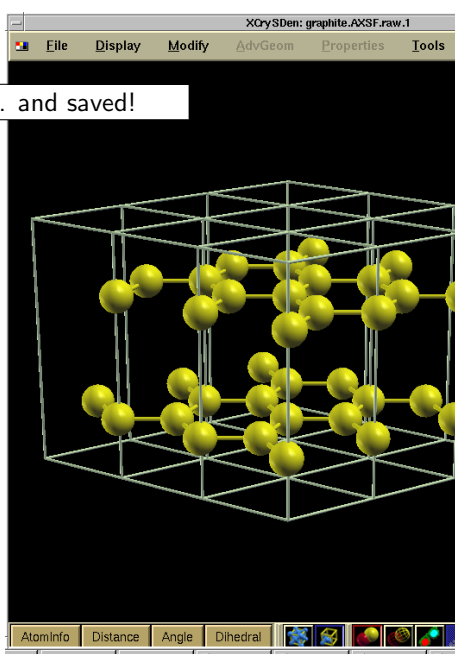
Repeat last frame No. times:

Time delay between slides (1/100 sec):

Start Recording Animated-GIF/MPEG

Hide Close

... and saved!



Animation Control Center

Delay between slides (in msec): 0

Animation step: 1

**Current slide: 25/25**

Navigation buttons: Previous, Previous, Previous, Next, Next, Next

<< 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

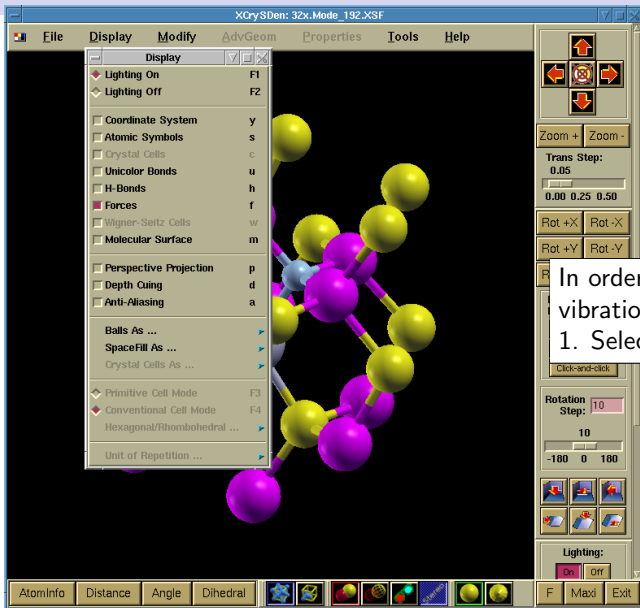
**Stop Recording and Save**

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 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 in In- and N-doped GaAs

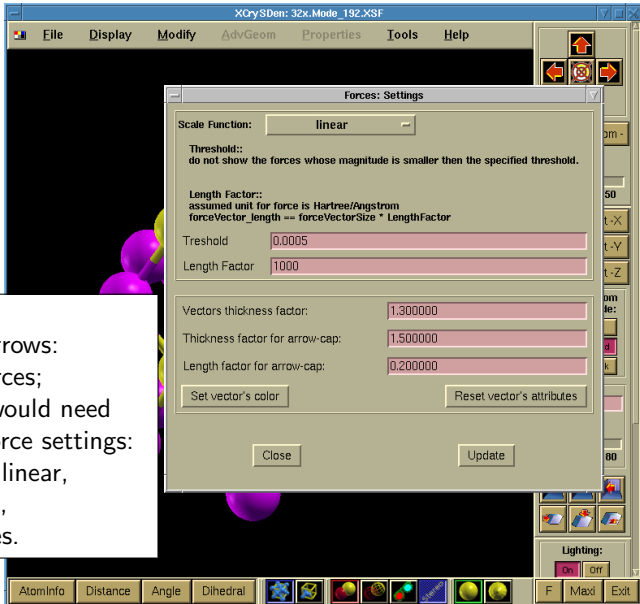


In order to show vibrations patterns as arrows:  
1. Select Display → Forces;

# 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.

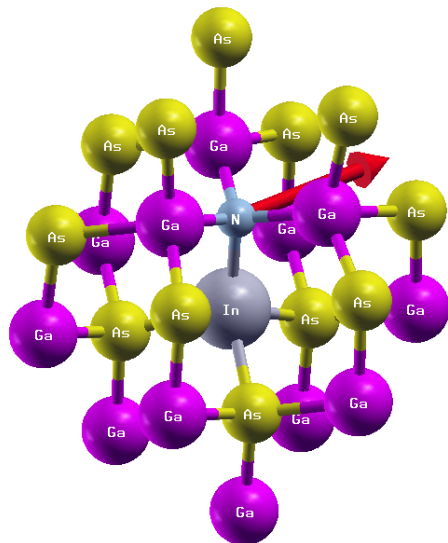




# An example of phonons in In- and N-doped GaAs

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 calculation 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) dumps 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 arrows (“forces”) stuck to ghost atoms of chemical label 'X', which atoms won't be visible if their radii set to almost zero, but arrows well visible is thick enough.

