

FPLO9.00-33



Getting Started

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In this little primer, you will be explained how to run FPLO9.00-33 on one of the simplest possible systems, *fcc* aluminum.

It is presumed that you have installed FPLO9.00-33 in a UNIX-derived environment. All necessary keystrokes are given, together with a short explanation. Moreover, screenshots are included every now and then. They should give you the doubtlessness that everything is correct when you go through the exercise on your own platform.

In the present example, we will hardly change the default input settings. Even the element and the lattice structure are pre-defined. Nonetheless, you should be reminded of our recommendation to include all changes of the default input settings and the version number in any publication of FPLO results. In many cases, this will only be the chemical composition, the lattice structure and the chosen lattice parameters. Such information is usually given in the publication anyway. You may also choose to work with another **k**-mesh or change the numerics. If you enter such information in your publication, everybody who has FPLO9.00-33 at hand will be able to repeat your calculation and convince himself of the result. This is what one may understand as a **reproducible computer experiment**.

Now, open a terminal at your computer and go ahead! What we learn in this getting started lesson is to run calculations within different **k**-meshes, to calculate the density of states (DOS) and band structure on symmetry lines, and finally the evaluation of the theoretical equilibrium volume.

Remark: `<CR>` stands for carriage return and simply corresponds to pressing the “Enter” key

| Key sequence | Explanation |
|----------------------------------|--------------------------|
| <code>mkdir A1 <CR></code> | create directory A1 |
| <code>cd A1 <CR></code> | change into directory A1 |

Well, everybody who is experienced in computers knows that a tidy organization of the directory tree will keep away (almost) all troubles! We start our course with a very straight calculation. Usually, for a new compound or for the evaluation of sensitive quantities one needs to start with some initial calculations. We run the calculation in a directory called “SC”. Here, “SC” stands for self consistent.

| Key sequence | Explanation |
|---|-------------------------------------|
| <code>mkdir SC <CR></code> | create directory SC |
| <code>cd SC <CR></code> | change into directory SC |
| <code>ls <CR></code> | list all files (directory is empty) |
| <code>fedit9.00-33_64 <CR></code> | call input editor |

Remark: The coexistence of different computer architectures makes it necessary to build individual executables for each architecture. This in turn requires a naming convention to tell the executables apart. The actual executable of FPLO9.00-33 will then have a suffix, which in the version used for this manual results in the executable name `fplo9.00-33-x86_64`. The same holds for other executables like `fedit9.00-33_64` and `bandplot9.00-33_64`¹.

¹In older FPLO versions symbolic links with the generic names `fplo`, `fedit` and `bandplot` were generated. In order to avoid confusion with an increasing number of code updates, this practice has been discontinued. From now on only the full names are used.

```

fpl09.00-33-x86_64 OUTPUT
e(x)it
[...]
```

```

K. Koepernik, B. Velicky, R. Hayn and H. Eschrig,
Phys. Rev. B 55, 5717 (1997)
```

```

main version: 9.00
sub version: M-CPA
release      : 33
```

```

date       : Tue Oct 20 16:05:55 2009
host      : bono
```

```

File =.sym does not exist, will create it!
File =.sym created!
File =.in does not exist, will create it!
TERMINATION: Normal : File =.in created!
-----STDERR:

STATUS: OK (9.00-33:M-CPA)
```

The input editor, `fedit9.00-33_64`, has called, upon invoking, the executable `fpl09.00-33-x86_64`. Several default input files have automatically been created by the code. (To avoid mistakes if various versions are installed, the version number is written in the lower right corner.²)

| Key sequence | Explanation |
|--------------|---------------------------------|
| x | exit initialization information |

This brings us to the main input menu:

```

MAIN MENU
[ ] (Q)uit/save (+) Symmetry (H)elp

GENERAL DATA
(S)pin sorts      : 1 (I)nitial polarization : [ ]
(K)-mesh subdivision : 12 12 12 (O)ccupied bands : -1
(N)umber of iterat. : 30 (A)ccuracy of density : 1.e-6
(T)otal energy calc. : [X] A(C)curacy of Etot : 1.e-8
Conver(G)ence condit : Density (-) Options : ...

(R)elativistic : scalar relativistic
(V)xc-version : Perdew Wang 92 (LSDA)
(F)inite nucleus : Point charge
(W) fixed spin mom. : [ ] (Y) spin moment : 1.0

RELATIVISTIC SETTINGS
Q(U)antization-axis : 0 0 1

OTHERS
(>) verbosity level : more information

STATUS: OK (9.00-33:M-CPA)
```

The input editor is operated by hot-keys (not case sensitive), indicated in red or blue on the screen. The blue keys are used for selecting entries of the present menu. The red keys (in our case the '+') select another menu or exit the input editor. Typing 'h' opens a help screen. Note, that keys of the right-hand (numerical) part of some keyboards do not work. Use only the keys of the central (main) part.

| Key sequence | Explanation |
|--------------|----------------------|
| + | select symmetry menu |

²The version number consists of the main version (9.00 in our case), followed by a minus and the release number (33). The string after the colon is a subversion, which is important for developers only.

```

SYMMEYRY MENU
[ ] e(X)it (+) Update (H)elp

(C)ompound      : Al example
s(T)tructure type : Crystal
(S)pacegroup    : FM3M (225)
(U)nit of length : Bohr radii
(L)attice constants : 7.55 7.55 7.55
(A)xis angles   : 90. 90. 90.

Subgroup (G)enerators :

(N)umber of atoms : 1

Wyckoff positions

(1) -th atom sort : Al      0. 0. 0.

STATUS: OK (9.00-33:M-CPA)

```

The lattice structure and chemical composition have to be defined in every calculation. Looking at the screen, we find that everything is already fine for our example, aluminum. The space group is correctly 225, the lattice parameter is reasonable (7.55 Bohr radii), and the only atom of the elementary cell is in the position (0,0,0).

Whenever you have changed any detail in the symmetry menu, you need to update the structure (using the '+' sign again). If you forget this action, a warning message will remind you to do it. For training purposes, we will carry out the update now, even if we have not changed anything.

| Key sequence | Explanation |
|--------------|--------------------------|
| + | update crystal structure |

```

fp1o9.00-33-x86_64 OUTPUT
e(X)it
[...].

-----
main version: 9.00
sub version: M-CPA
release      : 33
-----
date        : Tue Oct 20 16:07:00 2009
host        : bono
-----
File =.sym exists!
File =.in exists!
Symmetry changed in =.sym !
Will update file =.in !
File =.in updated!
TERMINATION: Normal : File =.in updated!
-----STDERR:

STATUS: OK (9.00-33:M-CPA)

```

The editor invokes `fp1o9.00-33-x86_64`, and the code updates the input files. The `fp1o9.00-33-x86_64` output is printed on the screen. (You can scroll all screens which are only partially displayed using control and cursor keys as explained in the help screen of the main menu.) We leave this information screen by typing 'x' and proceed further to the main menu. This menu is already known to us (second screen shot).

| Key sequence | Explanation |
|--------------|-------------------------|
| x | exit update information |
| x | exit symmetry menu |
| - | select options menu |

```

e(x)it                                OPTIONS                                (H)elp
Options
(0) CALC_DOS                          : [ ] (1) NOT_USED                    : [ ]
(2) FULLBZ                             : [ ] (3) CALC_PLASMON_FREQ           : [ ]
(4) EMPTY_LATTICE_TEST                 : [ ] (5) NOT_USED                    : [ ]
(6) PLOT_REALFUNC                      : [ ] (7) PLOT_BASIS                  : [ ]
(8) TEST_LOI                           : [ ] (9) TEST_DIAGNO                : [ ]
(A) TEST_SYMMETRIZATION                : [ ] (B) TEST_HS_SYM                  : [ ]
(C) PROT_PRINT_BASIS                  : [ ] (D) PROT_MAKELATTICE            : [ ]
(E) PROT_STRUCTURE_PRNT               : [ ] (F) PROT_TCI                    : [ ]
(G) NOT_USED                           : [ ] (I) NOT_USED                    : [ ]
(J) NOT_USED                           : [ ] (K) NO_SYMMETRYTEST           : [X]
(L) NO_POTENTIAL                      : [ ] (M) NOT_USED                    : [ ]
(N) NO_CORE                            : [ ] (O) NOT_USED                    : [ ]
(P) NO_POPANALYSIS                    : [ ] (Q) NO_LOI                      : [ ]
(R) NO_BASIS                           : [ ] (S) NO_EFCH                     : [ ]
(T) NOT_USED                           : [ ] (U) EXPORT_V3_DENSFILE         : [ ]
(V) NOT_USED                           : [ ]
STATUS: OK                                (9.00-33:M-CPA)

```

There are many options available, and only a few will be used by the routine user. Only one of them is switched on by default, namely the symmetry test is skipped. We do not make any changes and proceed.

| Key sequence | Explanation |
|--------------|--|
| x | exit options menu |
| q | quit input editor and save input files |

```

[ ] (Q)uit/save (+) Symmetry          MAIN MENU                                (H)elp
GENERAL DATA
(S)pin sorts                          : 1 (I)nitial polarization          : [ ]
(K)-mesh subdivision                  : 12 12 12 (O)ccupied bands                : -1
(N)umber of iterat.                  : 30 (A)ccuracy of density           : 1.e-6
(T)otal energy calc.                 : [X] A(C)uracy of Etot          : 1.e-8
Conver(G)ence condit                 : Density (-) Options                  : ...
(R)elativistic                       : scalar relativistic
(V)xc-version                         : Perdew Wang 92 (LSDA)
(F)inite nucleus                     : Point charge
(W) fixed spin mom.                  : [ ] (Y) spin moment              : 1.0
RELATIVISTIC SETTINGS
Q(U)antization-axis                  : 0 0 1
OTHERS
(>) verbosity level                  : more information
CHOOSE: Save now the file '.in' and '.sym'? (Esc: abort) (y/n):

```

Now, we are done with the input preparation. Well, there were no changes of the default settings. In fact, we only had a look at the menus, which contain the data most often altered in practical applications. (Reminder: If you would publish the results of a calculation, you are recommended to tell all essential changes of the default values like **k**-mesh, xc-version, etc.)

| Key sequence | Explanation |
|--------------|------------------------|
| y | confirm saving |
| ls (CR) | list all created files |

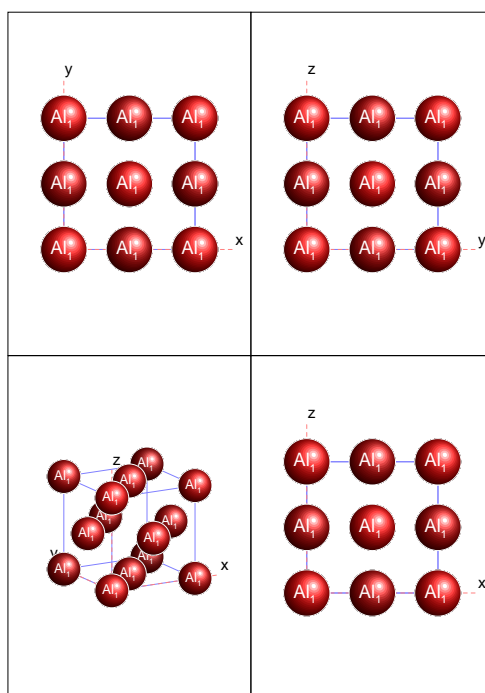
This is how your terminal may look like now:

```

bono:/home/magru>mkdir Al
bono:/home/magru>cd Al
bono:Al>mkdir SC
bono:Al>cd SC
bono:Al/SC>fedit9.00-33-x86_64
FEDIT Version 9.00:M-CPA Release 33 Platform -x86_64
Program      fplo9.00-33-x86_64
Will create temporary directory '/home/magru/Al/SC/+tmp'.
Temporary directory '/home/magru/Al/SC/+tmp' created.
bono:Al/SC>ls
+fedit      +symmetry  =.in       =.str_template =.sym.bak
+fedithelp  +tmp       =.in.bak  =.sym
bono:Al/SC>

```

| Key sequence | Explanation |
|-------------------------------|--|
| fplo9.00-33-x86_64 > out <CR> | run fplo9.00-33-x86_64 and save output wait till finished (on modern machines a few seconds) |
| ls <CR> | list all created files |
| gv bravais.ps <CR> | look at the bravais lattice |



| Key sequence | Explanation |
|-------------------------|----------------------------|
| q (on ghostview screen) | quit ghostview |
| gv primitive.ps <CR> | look at the primitive cell |
| q (on ghostview screen) | quit ghostview |

| Key sequence | Explanation |
|------------------|---|
| view out <CR> | inspect output file |
| ?Population <CR> | search last population analysis (What we really do here is to search for the population analysis from the end of the output. Another viewer will have a different hotkey for this) |

```

-----
                        Population Analysis
                        (valence electron numbers)
-----
El Site      2s      2p      3s      4s      3p      4p      3d      SUM      Excess electrons
N_net Al 1    2.00299  6.01070  1.00634  0.00200  0.67697  0.00309  0.04126  9.74335
N_gros Al 1    1.99994  6.00076  1.21254  -0.01842  1.55011  -0.04580  0.30087  11.00000

total net electron number:          9.74335
total gross electron number:        11.00000  0.00000
-----

```

This is the final population analysis. The 3d orbitals contribute almost exclusively to the overlap population (difference between gross and net). This behavior is typical for polarization states. To check the validity of a calculation, one should always look at the population analysis. As a rule of thumb, the gross population should be larger or not much smaller than the net population. Furthermore, the net population should not be negative. For semi core states (i.e. filled shells that are included in the valence basis) the full electron number (s: 2, p: 6, d: 10, f: 14) should come out within a range of a few hundreds of electrons for both gross and net population. (For very heavy atoms the deviation from the integer occupation can be of the order of a few tens of electrons.) In spin polarized calculations there will be four lines per atom. The first two (marked N_) are the populations and the second two (marked M_) are the magnetic moments of the orbitals.

| Key sequence | Explanation |
|-----------------------------------|--------------------------------|
| :q <CR> | quit inspection of output file |
| grep "last deviation" out <CR> | check iteration |
| or shorter: grep "st de" out <CR> | |

```

bono:Al/SC>grep "st de" out
SCF: iteration 0 dimension 0 last deviation u= 0.00E+00
SCF: iteration 1 dimension 1 last deviation u= 0.16E+00
SCF: iteration 2 dimension 1 last deviation u= 0.92E-01
SCF: iteration 3 dimension 2 last deviation u= 0.68E-02
SCF: iteration 4 dimension 1 last deviation u= 0.33E-02
SCF: iteration 5 dimension 2 last deviation u= 0.26E-03
SCF: iteration 6 dimension 1 last deviation u= 0.20E-03
SCF: iteration 7 dimension 2 last deviation u= 0.76E-05
SCF: iteration 8 dimension 1 last deviation u= 0.57E-05
SCF: iteration 9 dimension 1 last deviation u= 0.36E-06 CONVERGED
bono:Al/SC>

```

Each line shows the information about the iteration progress of one SCF cycle. The real number u to the right is a measure for the convergence of the calculation. The standard criterion to consider a calculation to be converged is if u falls below a certain threshold (default 10^{-6}). However, there are further things to be checked. The values of total energy (of the last step!) can be plotted by a script grEE:

| Key sequence | Explanation |
|--------------|---------------------------|
| grEE <CR> | print total energy values |

```

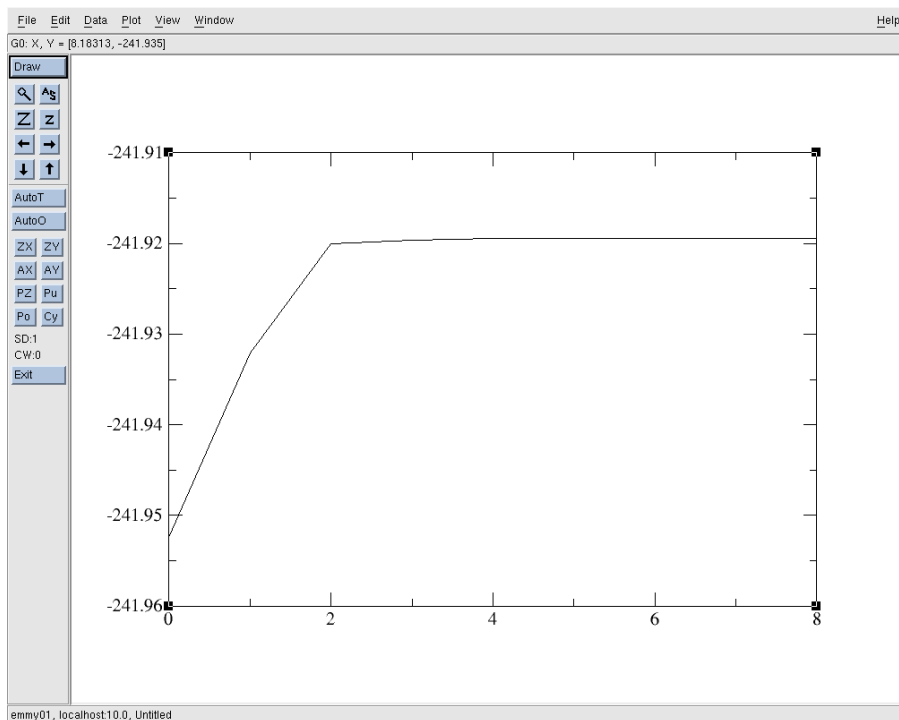
bono:Al/SC>grEE
-241.9194604082 242.17169725 -466.38221207 -17.70894558
bono:Al/SC>

```

The first value is the total energy followed by the kinetic energy, the Coulomb energy and the xc-energy. If LSDA+U is used a column with the additional LSDA+U energy contribution is added at the end.


You can visualize the data by calling the `xmgrace` program.

| Key sequence | Explanation |
|--|---|
| <code>grep "EE" out awk '{print \$1, \$2}' xmgrace -pipe <CR></code> | plot total energy values using <code>xmgrace</code> |

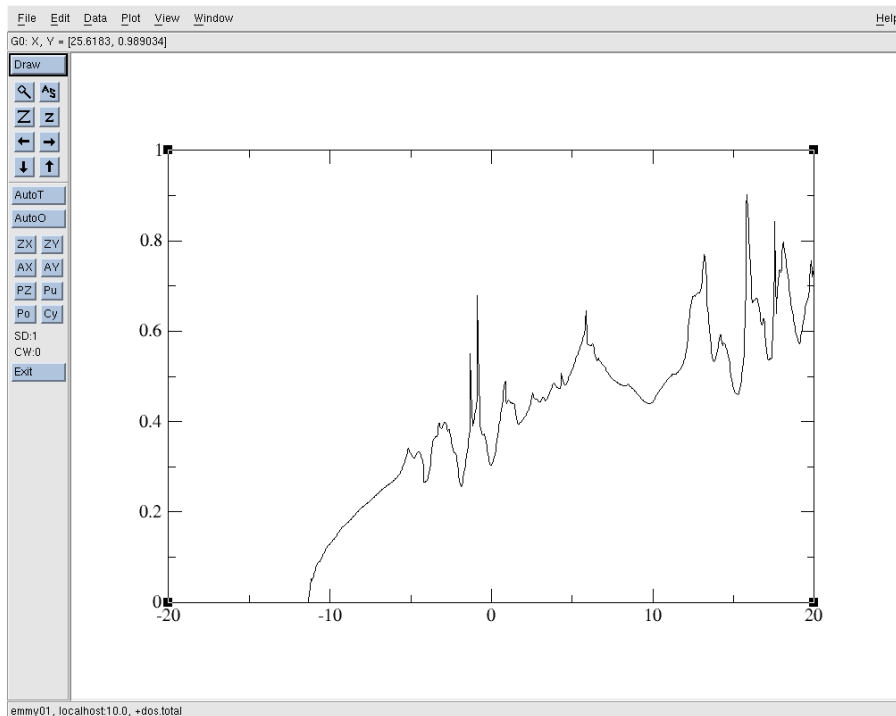


The evolution of the total energy values with the number of iterations is displayed.

| Key sequence | Explanation |
|---------------------------|----------------------------|
| <code><exit></code> | leave <code>xmgrace</code> |

| Key sequence | Explanation |
|---|---|
| <code>fedit9.00-33_64 <CR></code> | call input editor |
| <code><SPACE></code> | select more menus (if the (red) symbol  is shown in the upper menu, then there are further submenus accessible in this way) |
| <code>b</code> | select bandplot menu |

The bandplot menu allows you to define a band structure calculation on symmetry lines. The DOS is provided as well. The latter can also be obtained by switching on the appropriate option in the option menu.



| Key sequence | Explanation |
|--------------|--------------|
| <exit> | exit xmgrace |

In many cases, the partial density of states is a subject of interest: one can see which states contribute to the total density of states at a certain energy. The partial (Wyckoff/sort averaged) DOS is stored in the `+dos.sort00...n100...` files. The first line of each file contains the information about the basis state:

| Key sequence | Explanation |
|--|--|
| <code>head -n 1 +dos.sort001.n100[1-7] <CR></code> | print the first lines of the partial DOS files |

```

bono:Al/SC>head -n 1 +dos.sort001.n100[1-7]
==> +dos.sort001.n1001 <==
# sort = 1 nl = 2s spin = 1

==> +dos.sort001.n1002 <==
# sort = 1 nl = 2p spin = 1

==> +dos.sort001.n1003 <==
# sort = 1 nl = 3s spin = 1

==> +dos.sort001.n1004 <==
# sort = 1 nl = 4s spin = 1

==> +dos.sort001.n1005 <==
# sort = 1 nl = 3p spin = 1

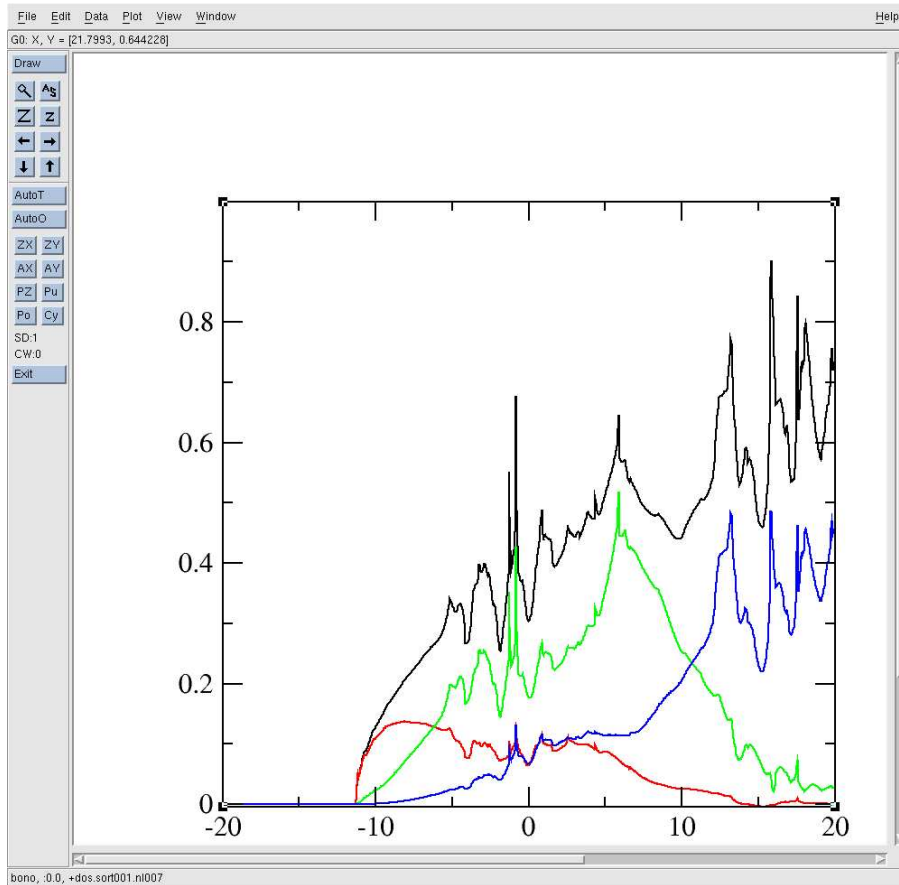
==> +dos.sort001.n1006 <==
# sort = 1 nl = 4p spin = 1

==> +dos.sort001.n1007 <==
# sort = 1 nl = 3d spin = 1
bono:Al/SC>

```

Let's print the partial DOS for 3s, 3p and 3d orbitals together with the total DOS:

| Key sequence | Explanation |
|--|--|
| <code>xmgrace -legend load +dos.total +dos.sort001.n100[3,5,7] <CR></code> | display total and partial DOS (maximize the xmgrace window in order to see the legend) |



The 3s states are lowest in energy, and at Fermi level 3p states dominate, while 3s and 3d have almost the same contribution to the total DOS.

| Key sequence | Explanation |
|--------------------------------|--|
| <exit> | exit xmgrace |
| fedit9.00-33_64 -bandplot <CR> | call input editor for bandplot9.00-33_64 |

```

bandplot9.00-33-x86_64 OUTPUT
e(x)it
---STDOUT:
File '=bp' created!
-----STDERR:

STATUS: OK (9.00-33:M-CPA)

```

The input editor does not only serve fplo9.00-33-x86_64 but also the code producing a postscript file with the band structure, bandplot9.00-33_64.

| Key sequence | Explanation |
|---------------|---------------------------------|
| x | exit initialization information |
| t | change title |
| Aluminum <CR> | |
| 1 <CR> | change legend |
| Al-bands <CR> | |

```

MAIN MENU
[ ] (Q)uit/save (+) plot (G)v (H)elp

GENERAL
(P)lot type : bands
(L)ower energy bound : 1
(U)pper energy bound : -1
(T)itle : Aluminum
(Y)axis title : Energy  $\epsilon_c(k)$  [eV]
(A)uto x-labels : [X]
(DL) display legend : [X] (DS) spin dependend : [X]
(R1) relative x positi : 0.8
(R2) relative y positi : -0.05

POSTSCRIPT
(O)ut file prefix : band
(V)iewer : gv

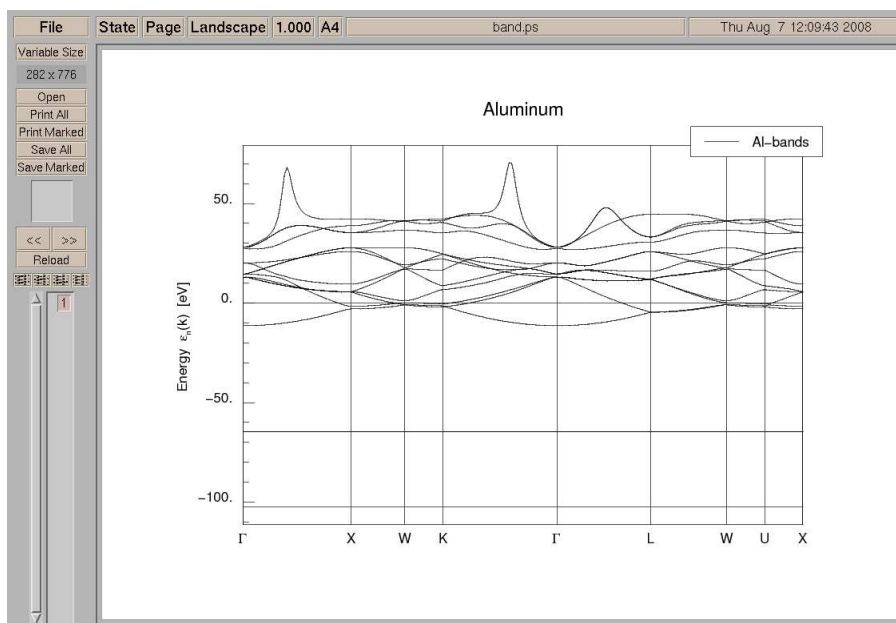
BAND STRUCTURE
(N)umber of files to load : 1
file legend
-----
(1) : +band Al-bands

BANDWEIGHTS
[...]
STATUS: OK (9.00-33:M-CPA)

```

| Key sequence | Explanation |
|--------------|---|
| + | fedit9.00-33_64 calls bandplot9.00-33_64 internally |
| x | exit information screen |
| g | let fedit9.00-33_64 call gv |

bandplot9.00-33_64 creates a postscript file with the band structure on symmetry lines, which is then displayed with gv.



What you see is the bands of Al. At about -100 and -60 eV the semi-core 2s and 2p states are drawn (nearly

dispersionless). You may switch to the window running `fedit9.00-33_64` and use the lower and upper energy bound to set an appropriate energy range for the valence bands, but lets continue for now.

| Key sequence | Explanation |
|--|--|
| (use <code>q</code> to leave <code>gv</code>) | |
| <code>x</code> | exit information screen |
| <code>q</code> | quit input editor and save input files |
| <code>y</code> | confirm saving |

Our next goal is to change the **k**-mesh. In general, all calculations should be done in the thermodynamic limit. This simply means that you should always check if the results of your calculations approximate reasonably well the limit of an infinitesimally dense **k**-mesh. The default **k**-mesh is $12 \times 12 \times 12$. We will examine three further **k**-meshes: $16 \times 16 \times 16$, $20 \times 20 \times 20$ and $24 \times 24 \times 24$.

| Key sequence | Explanation |
|--|---|
| <code>fedit9.00-33_64</code> <code><CR></code> | call input editor |
| <code><SPACE>b</code> | go to bandplot submenu |
| <code>b</code> | switch off band structure plot in order to save time in the subsequent calculations |
| <code>x</code> | exit bandplot menu |
| <code>qy</code> | quite and save changes |
| <code>cd ..</code> | goto parent directory "A1" |
| <code>mkdir k=12</code> <code><CR></code> | create directory for present k -mesh |
| <code>cp SC/* k=12</code> <code><CR></code> | copy all files into k=12 |
| <code>mkdir k=16</code> <code><CR></code> | create directory for another k -mesh |
| <code>mkdir k=20</code> <code><CR></code> | create directory for another k -mesh |
| <code>mkdir k=24</code> <code><CR></code> | create directory for another k -mesh |
| <code>ls</code> <code><CR></code> | just to look |
| <code>cp k=12/=* k=16</code> <code><CR></code> | copy input files into the new directory |
| <code>cp k=12/=* k=20</code> <code><CR></code> | copy input files into the new directory |
| <code>cp k=12/=* k=24</code> <code><CR></code> | copy input files into the new directory |
| <code>cd k=16</code> <code><CR></code> | change into directory k=16 |
| <code>fedit9.00-33_64</code> <code><CR></code> | call <code>fedit9.00-33_64</code> |
| <code>k16 , ,</code> <code><CR></code> | change k -mesh |
| <code>qy</code> | quit and save changes |

The last but one command line from below deserves a short explanation. The double-comma is a short-hand for a two-fold repetition of the previous number (16 in our example).

| Key sequence | Explanation |
|--|---|
| <code>fplo9.00-33-x86_64 > out &</code> <code><CR></code> | run <code>fplo9.00-33-x86_64</code> in background |
| <code>cd ..</code> | goto parent directory "A1" |
| <code>cd k=20</code> <code><CR></code> | change into directory k=20 |
| <code>fedit9.00-33_64</code> <code><CR></code> | call <code>fedit9.00-33_64</code> |
| <code>k20 , ,</code> <code><CR></code> | change k -mesh |
| <code>qy</code> | quit and save changes |
| <code>fplo9.00-33-x86_64 > out &</code> <code><CR></code> | run <code>fplo9.00-33-x86_64</code> in background |
| <code>cd ..</code> | goto parent directory "A1" |
| <code>cd k=24</code> <code><CR></code> | change into directory k=24 |
| <code>fedit9.00-33_64</code> <code><CR></code> | call <code>fedit9.00-33_64</code> |
| <code>k24 , ,</code> <code><CR></code> | change k -mesh |
| <code>qy</code> | quit and save changes |
| <code>fplo9.00-33-x86_64 > out &</code> <code><CR></code> | run <code>fplo9.00-33-x86_64</code> in background |
| <code>cd ..</code> | goto parent directory "A1" |

Wait for a half of minute and check the convergence as well as the total energies. This can be done as follows:

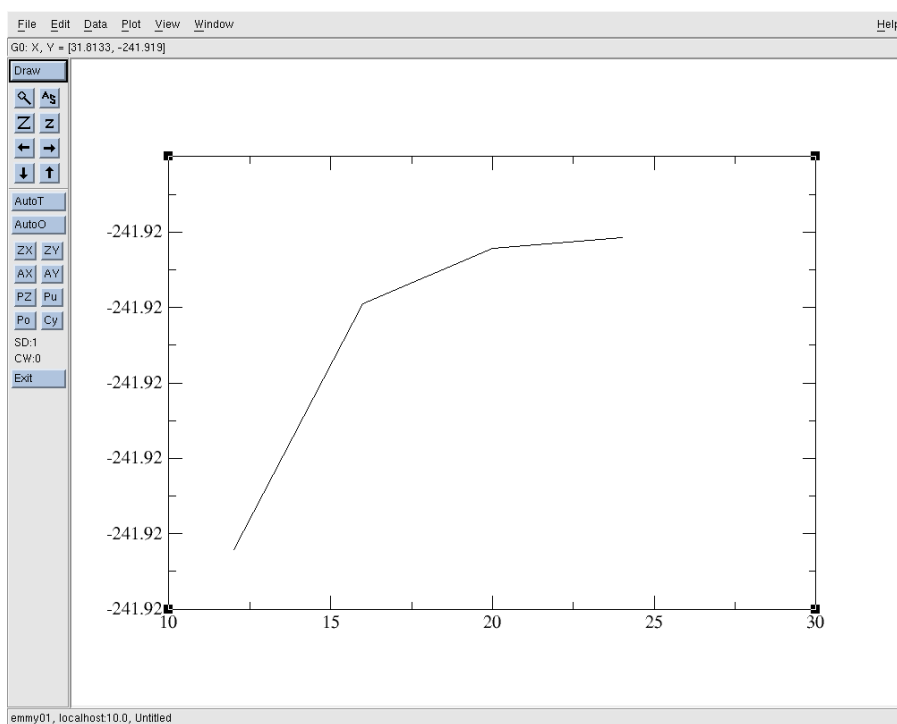
| Key sequence | Explanation |
|--|---|
| <code>grit k= <CR></code> | print last iteration message for all directories named k=... |
| <code>grEE k= tee ek <CR></code> | print the values of total energy for all calculations and simultaneously save output to file 'ek' |

```

bono:Al>grit k=
k=12/out SCF: iteration 9 dimension 1 last deviation u= 0.36E-06 CONVERGED
k=16/out SCF: iteration 5 dimension 1 last deviation u= 0.18E-06 CONVERGED
k=20/out SCF: iteration 5 dimension 1 last deviation u= 0.19E-06 CONVERGED
k=24/out SCF: iteration 5 dimension 1 last deviation u= 0.55E-07 CONVERGED
bono:Al>grEE k= | tee e
12 -241.9194604082 242.17169725 -466.38221207 -17.70894558
16 -241.9192975171 242.17187789 -466.38227794 -17.70889746
20 -241.9192606676 242.17233128 -466.38269696 -17.70889499
24 -241.9192536841 242.17302256 -466.38333384 -17.70894240
bono:Al>

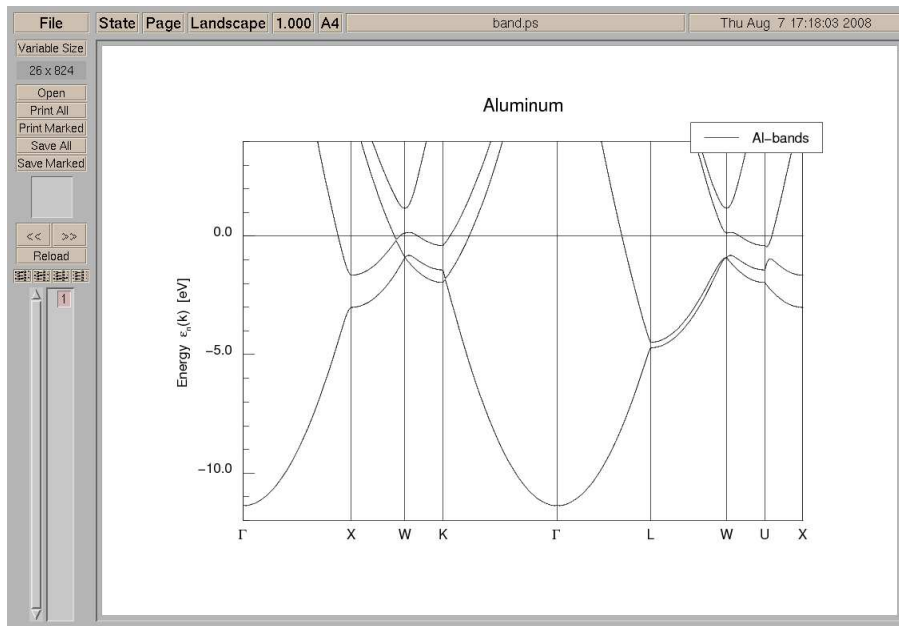
```

| Key sequence | Explanation |
|---|---------------------------------------|
| <code>grEE k= xmgrace -pipe <CR></code> | visualize the total energy dependence |



As you can see, the values of total energy are strongly dependent on the number of **k**-points. The reason is the presence of a flat band region close to Fermi level. It can be seen in the valence band near the **W** **k**-point.

| Key sequence | Explanation |
|--------------------------------|--|
| <exit> | exit xmgrace |
| cd SC <CR> | go to the directory SC |
| fedit9.00-33_64 -bandplot <CR> | call input editor for bandplot9.00-33_64 |
| L-12 <CR> | set the lowest energy value to -12 eV |
| u4 <CR> | set the highest energy value to 4 eV |
| + | fedit9.00-33_64 calls |
| | bandplot9.00-33_64 internally |
| x | exit information screen |
| g | let fedit9.00-33_64 call gv |



The feature near the **W** point is clearly visible.

| Key sequence | Explanation |
|---------------------|--|
| (use q to leave gv) | |
| x | exit information screen |
| q | quit input editor and save input files |
| y | confirm saving |
| cd .. | go to the parent directory |

We now proceed to the final goal, the calculation of the total energy in dependence of the lattice parameter.

| Key sequence | Explanation |
|---------------------------|---|
| mkdir a0=7.55 <CR> | create directory for present a ₀ |
| cp SC/* a0=7.55 <CR> | copy all files into a ₀ =7.55 |
| mkdir a0=7.50 <CR> | create directory for another a ₀ |
| mkdir a0=7.60 <CR> | create directory for another a ₀ |
| ls <CR> | just to look |
| cp a0=7.55/* a0=7.50 <CR> | copy input files into the new directory |
| cp a0=7.55/* a0=7.60 <CR> | copy input files into the new directory |
| cd a0=7.50 <CR> | change into directory a ₀ =7.50 |
| fedit9.00-33_64 <CR> | call fedit9.00-33_64 |
| + | select symmetry menu |
| L7.50 , , <CR> | change lattice constant |
| + | update lattice geometry |

```

fplo9.00-33-x86_64 OUTPUT
e(x)it
[...]
```

```

K. Koepernik, B. Velicky, R. Hayn and H. Eschrig,
Phys. Rev. B 55, 5717 (1997)

```

```

main version: 9.00
sub version: M-CPA
release      : 33

```

```

date       : Tue Oct 20 16:13:47 2009
host      : bono

```

```

File =.sym exists!
File =.in exists!
Symmetry changed in =.sym !
Will update file =.in !
WARNING in MODULE IO(fplo_io):
lattice type or lattice constants changed!
Will take default values for special bandplot symmetry points!
File =.in updated!
TERMINATION: Normal : File =.in updated!
-----STDERR:

```

```

STATUS: OK (9.00-33:M-CPA)

```

The warning message refers to possibly user-defined points for the band structure plot, that are overwritten now with the default settings.

| Key sequence | Explanation |
|---------------------------------|---------------------------------------|
| x | exit update information |
| x | exit symmetry menu |
| q | quit fedit9.00-33_64 |
| Y | confirm saving |
| fplo9.00-33-x86_64 > out & <CR> | run fplo9.00-33-x86_64 in back-ground |
| cd ../a0=7.60 <CR> | change into directory a0=7.60 |
| fedit9.00-33_64 <CR> | call fedit9.00-33_64 |
| + | select symmetry menu |
| L7.60 , , <CR> | change lattice constant |
| + | update lattice geometry |
| x | exit update information |
| x | exit symmetry menu |
| q | quit fedit9.00-33_64 |
| Y | confirm saving |
| fplo9.00-33-x86_64 > out & <CR> | run fplo9.00-33-x86_64 in back-ground |
| ps <CR> | check the running jobs |
| cd .. <CR> | change into parent directory |
| grit a0= <CR> | check convergence |

What you see now depends on the moment when you look at the progress...

```

bono:A1>grit a0=
a0=7.50/out SCF: iteration 5 dimension 1 last deviation u= 0.88E-06 CONVERGED
a0=7.55/out SCF: iteration 9 dimension 1 last deviation u= 0.36E-06 CONVERGED
a0=7.60/out SCF: iteration 5 dimension 1 last deviation u= 0.90E-06 CONVERGED
bono:A1>

```

When both calculations are **finished** after a minute, you may compare the total energies and estimate the theoretical lattice constant.

| Key sequence | Explanation |
|-------------------------|---------------------------------------|
| grEE a0= tee ea0 <CR> | print energies and save to file 'ea0' |

```

bono:Al>grEE a0= | tee ea0
7.50 -241.9194426306 242.19209781 -466.39636011 -17.71518033
7.55 -241.9194604082 242.17169725 -466.38221207 -17.70894558
7.60 -241.9193607370 242.15231227 -466.36881200 -17.70286102
bono:Al>

```

In the left column, you see the lattice parameter, the next column gives the related total energies. The minimum of the total energy is close to $a = 7.55$ Bohr radii.

Take a rest !