

HANDS-ON · QUANTY WORKSHOP 2026

FPLO: Getting Started

fcc aluminum — SCF, DOS, band structure and equilibrium lattice constant



Based on the FPLO22.02-66 "Getting Started" primer by M. Richter, K. Koepernik, O. Janson & H. Rosner

What we do today

1

Self-consistent run

Input editor fedit, run fplo, check populations, convergence and total energy

2

DOS & band structure

Bandplot menu, total and partial DOS, band plot in xfbp

3

Lattice constant

Total energy for $a_0 = 7.50 / 7.55 / 7.60$ Bohr $\rightarrow$ equilibrium

<CR> = press Enter. Hot-keys in fedit are not case sensitive. Use only the main keyboard, not the numeric keypad.

1

SETUP

Create a tidy directory tree

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Key sequence	Explanation
<code>mkdir A1 <CR></code>	create directory A1
<code>cd A1 <CR></code>	change into directory A1
<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>fedit22.02-66-x86_64 <CR></code>	call input editor

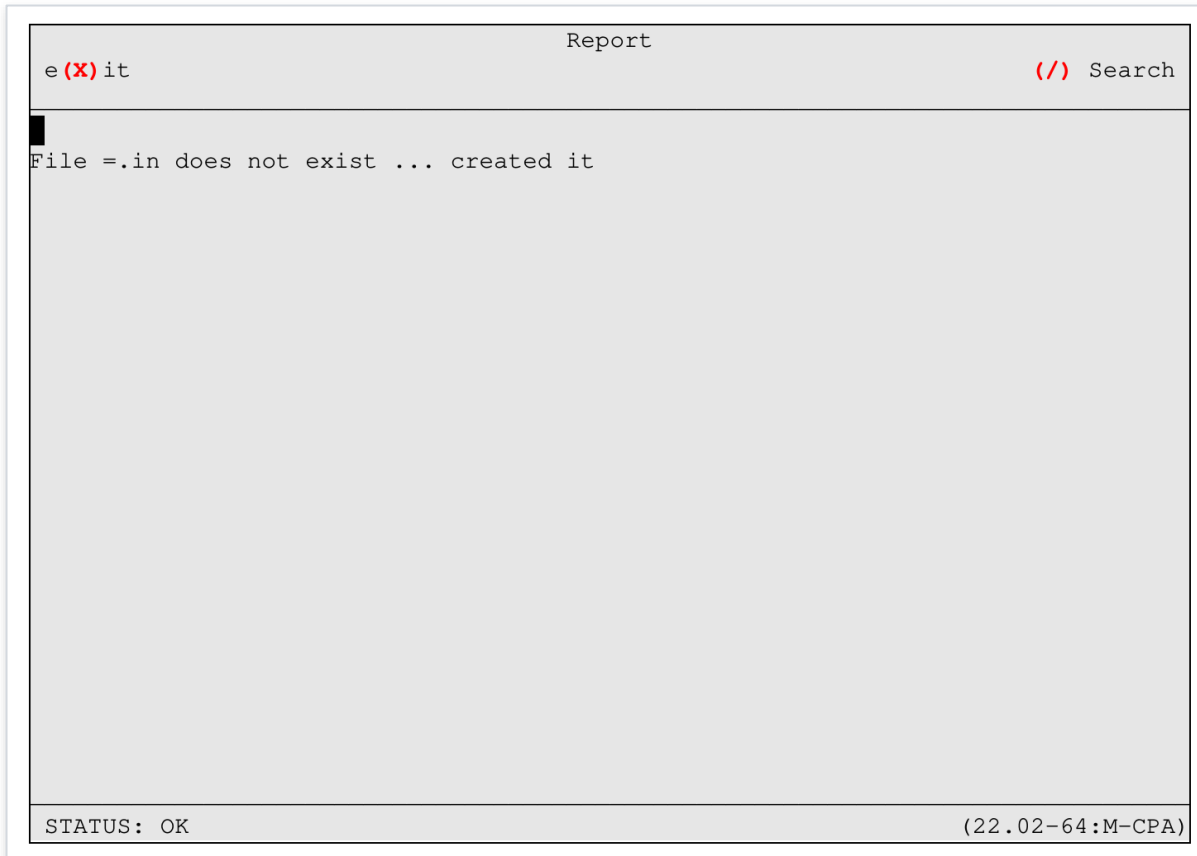
- SC = self-consistent
- Executables carry the full version suffix (no generic fplo / fedit links any more)
- <CR> = press Enter

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INPUT EDITOR

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Start fedit — default input is created



The screenshot shows the fedit input editor interface. At the top, there is a header bar with the text "e (x) it" on the left, "Report" in the center, and "(/) Search" on the right. Below the header, the main area displays the message "File =.in does not exist ... created it". At the bottom, there is a status bar with "STATUS: OK" on the left and "(22.02-64:M-CPA)" on the right.

Key sequence**Explanation****x**

exit initialization information

- fedit calls fplo once and writes the default input file =.in
- Version number is shown in the lower-right corner

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INPUT EDITOR

Main menu

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```
MAIN MENU
[ ] (Q)uit/save (+) Symmetry (/) Search (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
xc-field str(E)ngth : 1.0
(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 (22.02-64:M-CPA)

Key sequence

Explanation

+

select symmetry menu

- Hot-keys, not case sensitive
- Blue keys: entries of this menu
- Red keys: other menus / exit
- h opens help — don't use the numeric keypad

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INPUT EDITOR

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Symmetry menu — fcc Al is predefined

```
SYMMETRY MENU
[ ] e(x)it (+) Update (/) Search (H)elp

(C)ompound : Al example
s(T)ructure type : Crystal
(S)pacegroup/Layergr. : F m -3 m (225)
S(E)tting : F m -3 m (unique)
(U)nit of length : Bohr radii
(L)attice constants : 7.55 7.55 7.55
(A)xis angles : 90. 90. 90.

change gl(O)bal axes : [ ]
new X-ax(I)s : 1 0 0
new (Z)-axis : 0 0 1

Subgroup (G)enerators :

(N)umber of atoms : 1

Wyckoff positions

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

STATUS: OK (22.02-64:M-CPA)
```

Key sequence

Explanation

+

update crystal structure

- Space group 225 (F m -3 m)
- Lattice constant 7.55 Bohr
- One atom: Al at (0, 0, 0)
- After ANY change here: update with +

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INPUT EDITOR

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Update the structure, then go to Options



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

- Update output appears in an info screen (scrollable)

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INPUT EDITOR

Options menu

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```
e (X) it                                OPTIONS                                (/) Search (H)elp

Options
(0) CALC_DOS                : [ ]  (1) NOT_USED                : [ ]
(2) FULLBZ                  : [ ]  (3) CALC_PLASMON_FREQ    : [ ]
(4) EMPTY_LATTICE_TEST     : [ ]  (5) NO_DOS                : [ ]
(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) NOT_USED              : [ ]
(V) NOT_USED               : [ ]

STATUS: OK                                (22.02-64:M-CPA)
```

Key sequence

Explanation

X

exit options menu

- Only NO_SYMMETRYTEST is on by default
- No changes needed — back to the main menu

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INPUT EDITOR

Save the input

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```
MAIN MENU
[ ] (Q)uit/save (+) Symmetry (/) Search (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
xc-field str(E)ngth : 1.0
(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'? (Esc: abort) (y/n):
```

Key sequence	Explanation
q	quit input editor and save input files
y	confirm saving
ls <CR>	list all created files

- Publish every change of the defaults (k-mesh, xc, ...) plus the version number → reproducible calculation

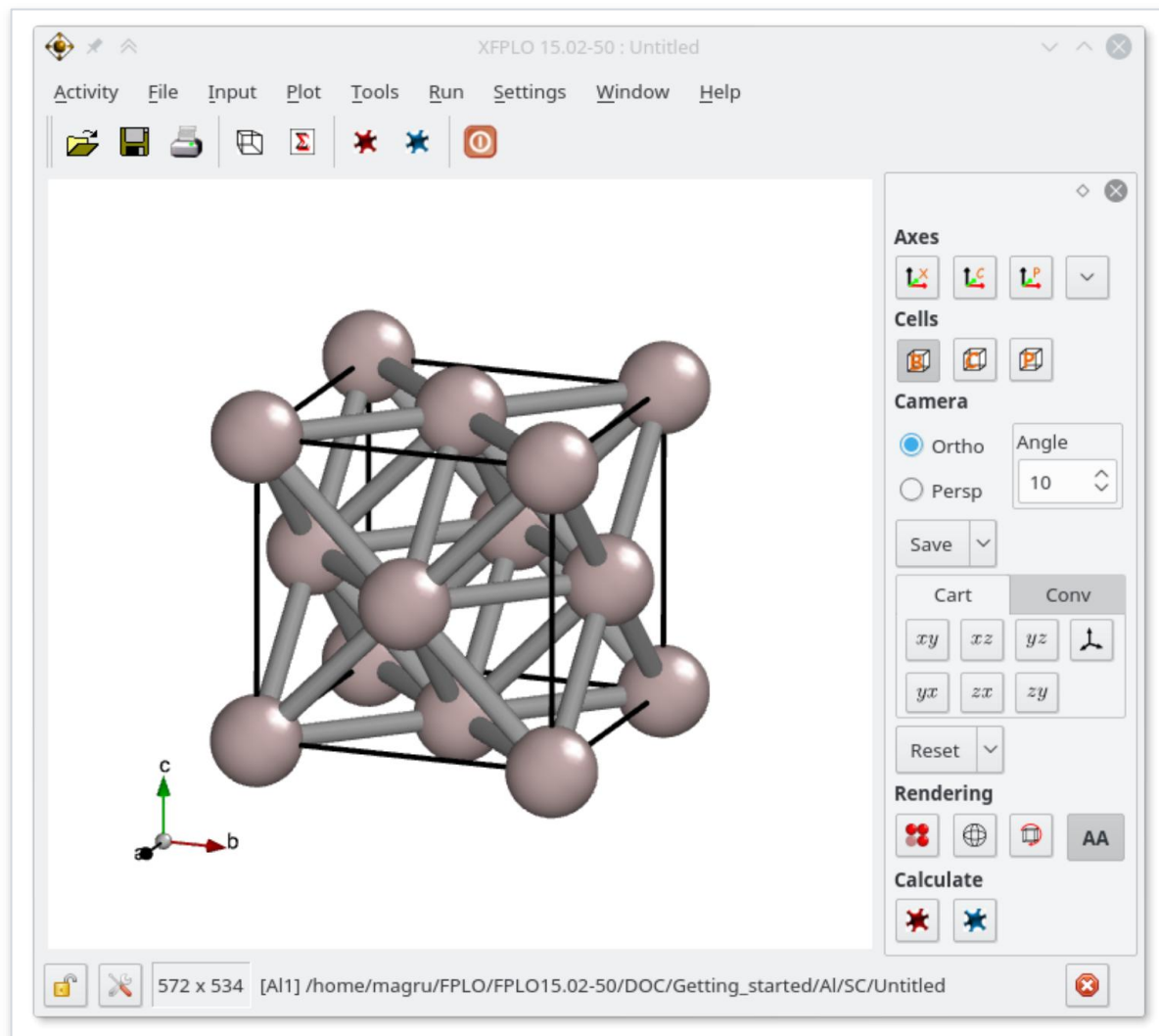


Your terminal now

```
unas:fplo/A1/SC> mkdir A1
unas:fplo/A1/SC> cd A1
unas:fplo/A1/SC> mkdir SC
unas:fplo/A1/SC> cd SC
unas:fplo/A1/SC> fedit22.02-66-x86_64
Will delete directory '/home/magru/fplo/A1/SC/+tmp'.
Directory '/home/magru/fplo/A1/SC/+tmp' removed.
unas:fplo/A1/SC> ls
+fedit =.in =.in.bak
unas:fplo/A1/SC>
```

- New files: +fedit, =.in, =.in.bak

Run FPLO and look at the structure



Key sequence

Explanation

```
fplo22.02-66-x86_64 |  
tee out <CR>
```

run fplo and save
output — a few
seconds

```
ls <CR>
```

list all created files

```
xfplo =.in <CR>
```

look at the crystal
structure

```
Ctrl + w
```

quit xfplo (on the
xfplo screen)

Check the population analysis

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

Key sequence

Explanation

`less out <CR>`

inspect output file

`G`

go to the end of file

`?Population <CR>`

search last population analysis
(backwards)

`:q`

quit less

- 3d: almost pure overlap population → polarization states
- Rule of thumb: gross $\gtrsim$ net, net never negative
- Semi-core 2s, 2p: full occupation within a few 0.01 e

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SCF RUN

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Check SCF convergence

```
unas:fplo/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= 0.11E+00
SCF: iteration 2 dimension 1 last deviation u= 0.10E+00
SCF: iteration 3 dimension 2 last deviation u= 0.14E-01
SCF: iteration 4 dimension 1 last deviation u= 0.99E-02
SCF: iteration 5 dimension 2 last deviation u= 0.19E-03
SCF: iteration 6 dimension 1 last deviation u= 0.11E-03
SCF: iteration 7 dimension 2 last deviation u= 0.12E-04
SCF: iteration 8 dimension 3 last deviation u= 0.78E-05
SCF: iteration 9 dimension 1 last deviation u= 0.15E-05
SCF: iteration 10 dimension 1 last deviation u= 0.46E-08 CONVERGED

unas:fplo/Al/SC>
```

Key sequence

Explanation

```
grep "last deviation" out  
<CR>
```

check iteration

```
grep "st de" out <CR>
```

... or shorter

- u = convergence measure of each SCF cycle
- Default criterion: $u < 10^{-6}$

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SCF RUN

Total energy

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```
unas:fplo/Al/SC> grEE
```

```
-241.9194604174 242.17167366 -466.38219031 -17.70894377
```

```
unas:fplo/Al/SC>
```

Key sequence

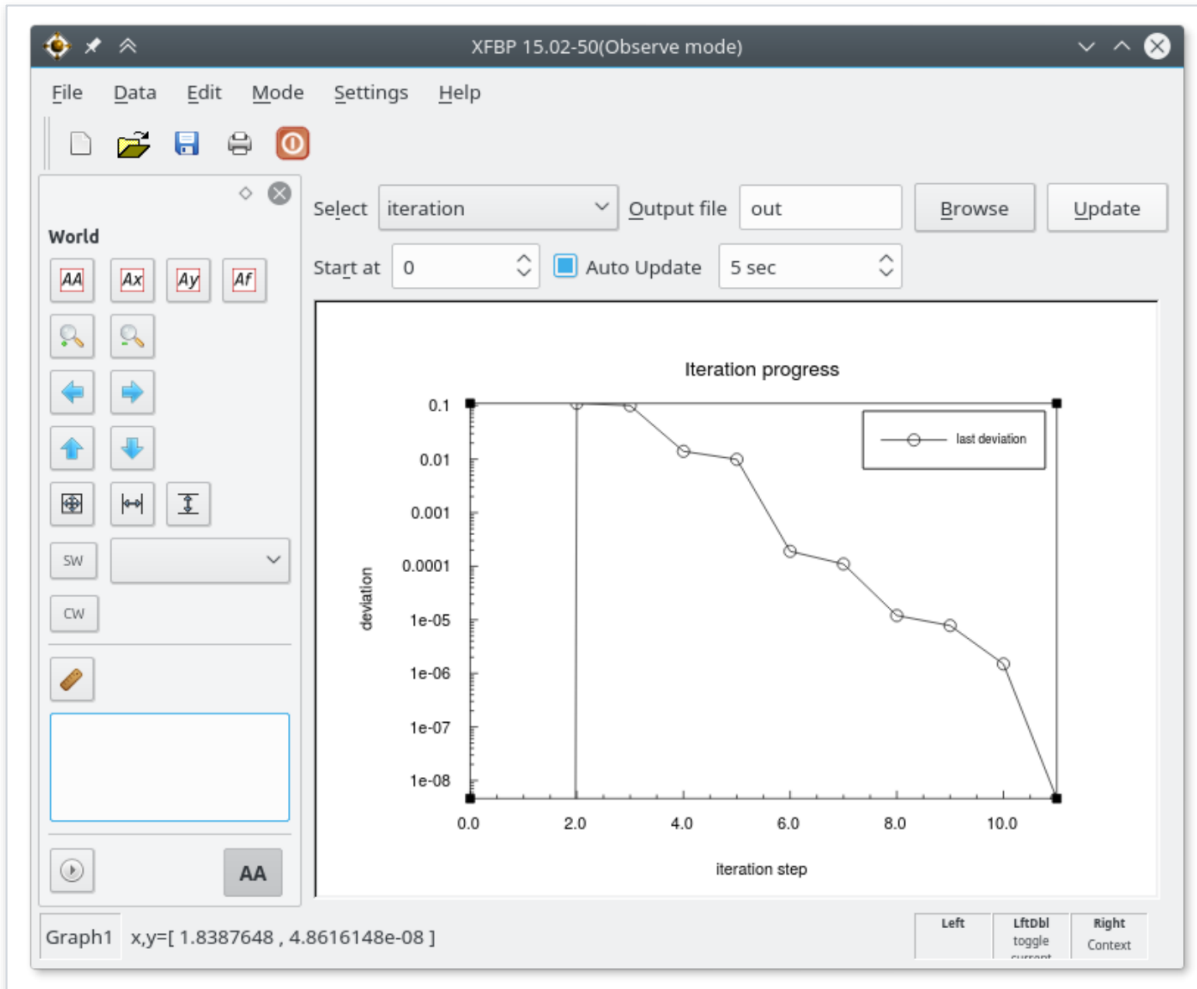
Explanation

grEE <CR>

print total energy values

- Columns: E_tot, E_kin, E_Coulomb, E_xc (Hartree)
- With DFT+U: extra column at the end
- More powerful grepper: grepfplo

Iteration progress in xfbp



Key sequence

Explanation

`xfbp -oi <CR>`

start xfbp, show iteration progress

`Ctrl + q`

quit xfbp

- Same as menu Mode → Observe → Iteration progress

Open the bandplot menu

```
BANDPLOT
e (X)it (/) Search (H)elp

(B)andstructure plot : [ ]
(R)ead sym-points : [X]
(S)teps between sym-points : 50

DOS/AKBL/BANDS

Number of e(-)pts (non-CPA) : 1000 (P)lot IDOS : [ ]
plot n(B)t DOS : [ ]

(L)ower energy bound [eV] relative to E_f : -20.0
(U)pper energy bound [eV] relative to E_f : 20.0

Restr(I)ct bands to window : [ ]

Local (D)OS sites :
Output + (C)oeff file : [ ]

BAND WEIGHTS/FAT BANDS

Weights def (F)ile :
(W)eights : [ ]
(T)ransform quant. axis : [ ]
X-(A)xis : 1.0 0.0 0.0
(Z)-axis : 0.0 0.0 1.0

(N)umber of sym-points : 13

No. Label k-point
(1) : $~G : 0 0 0
(2) : X : 0 1 0
(3) : W : 1/2 1 0
(4) : K : 3/4 3/4 0
(5) : $~G : 0 0 0
(6) : L : 1/2 1/2 1/2
(7) : U : 1/4 1 1/4
(8) : W : 1/2 1 0
(9) : L : 1/2 1/2 1/2
(10) : K : 3/4 3/4 0
(11) : <BREAK> : 0 0 0
(12) : U : 1/4 1 1/4
[...]
STATUS: OK (22.02-64:M-CPA)
```

Key sequence

Explanation

`fedit22.02-66-x86_64`
`<CR>`

call input editor

`<SPACE>`

select more menus

`b`

select bandplot
menu

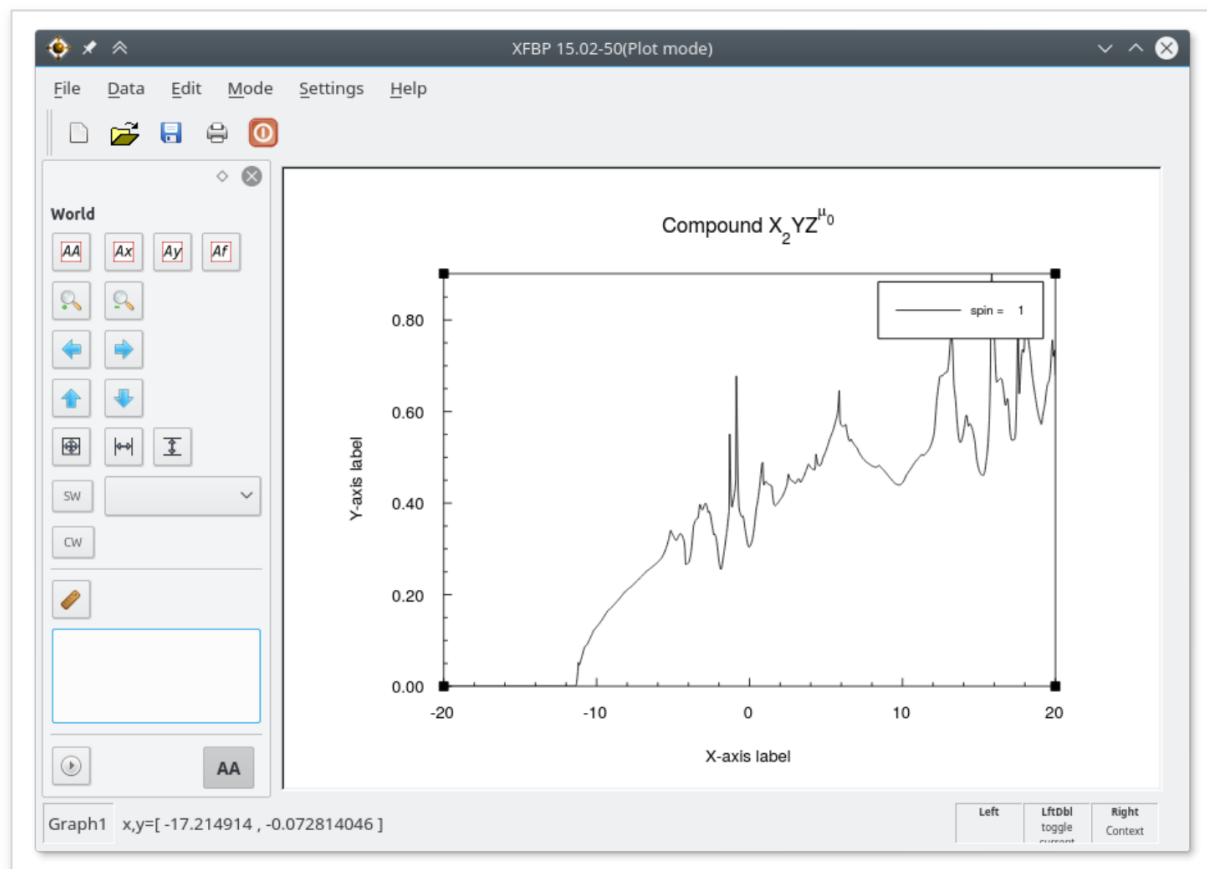
- Red [] in the menu bar → more sub-menus via `<SPACE>`
- Band structure along symmetry lines; DOS comes with it

Switch on the band structure and run

```
unas:fplo/Al/SC> fplo22.02-64-x86_64 >out.bs &
[1] 8987
unas:fplo/Al/SC>
[1]+  Done                  fplo22.02-64-x86_64 > out.bs
unas:fplo/Al/SC> ls
+band                +dos.sort001.n1004  +dos.total.1002  =.in.bak          +symmetry
=.dens               +dos.sort001.n1005  +dos.total.1003  out
+dos.sort001         +dos.sort001.n1006  +dos.total.1004  out.bs
+dos.sort001.n1001   +dos.sort001.n1007  +dos.total.1005  +points
+dos.sort001.n1002   +dos.total          +fedit           +run
+dos.sort001.n1003   +dos.total.1001     =.in             =.str_template
```

Key sequence	Explanation
b	select band structure plot
x	exit bandplot menu
q	quit input editor, save input
y	confirm saving
fplo22.02-66-x86_64 > out.bs & <CR>	run fplo in background (few seconds)
ls <CR>	list all files

- DOS split by sort (Wyckoff position) and basis state (nl)



Key sequence

Explanation

`xfbp +dos.total <CR>`

display total DOS

`Ctrl + q`

quit xfbp

Which file is which orbital?

```
unas:fplo/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
unas:fplo/Al/SC>
```

Key sequence

Explanation

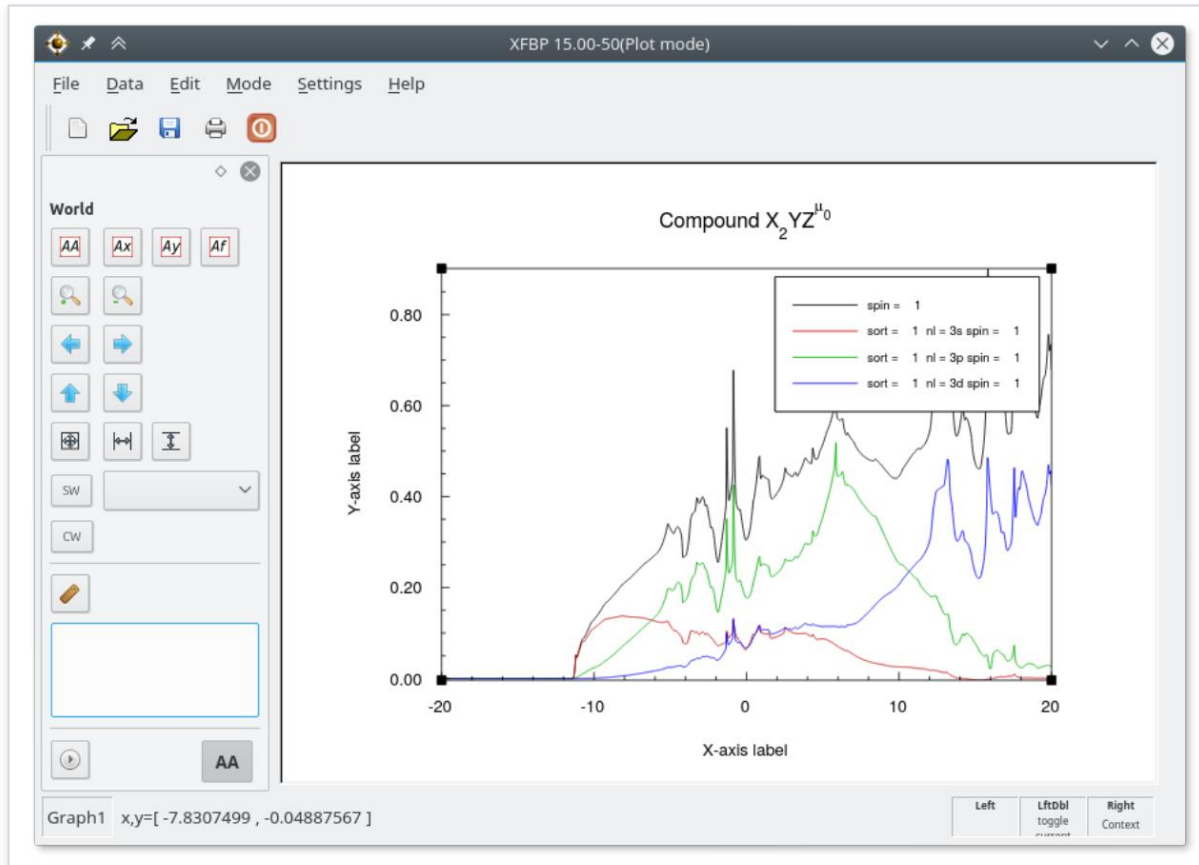
head -n 1

+dos.sort001.n100[1-7] <CR>

print first lines of
the partial DOS files

- First line of each +dos.sort001.n100x names the basis state

Total + partial DOS (3s, 3p, 3d)



Key sequence

Explanation

```
xfbp +dos.total
+dos.sort001.n100[3,5
,7] <CR>
```

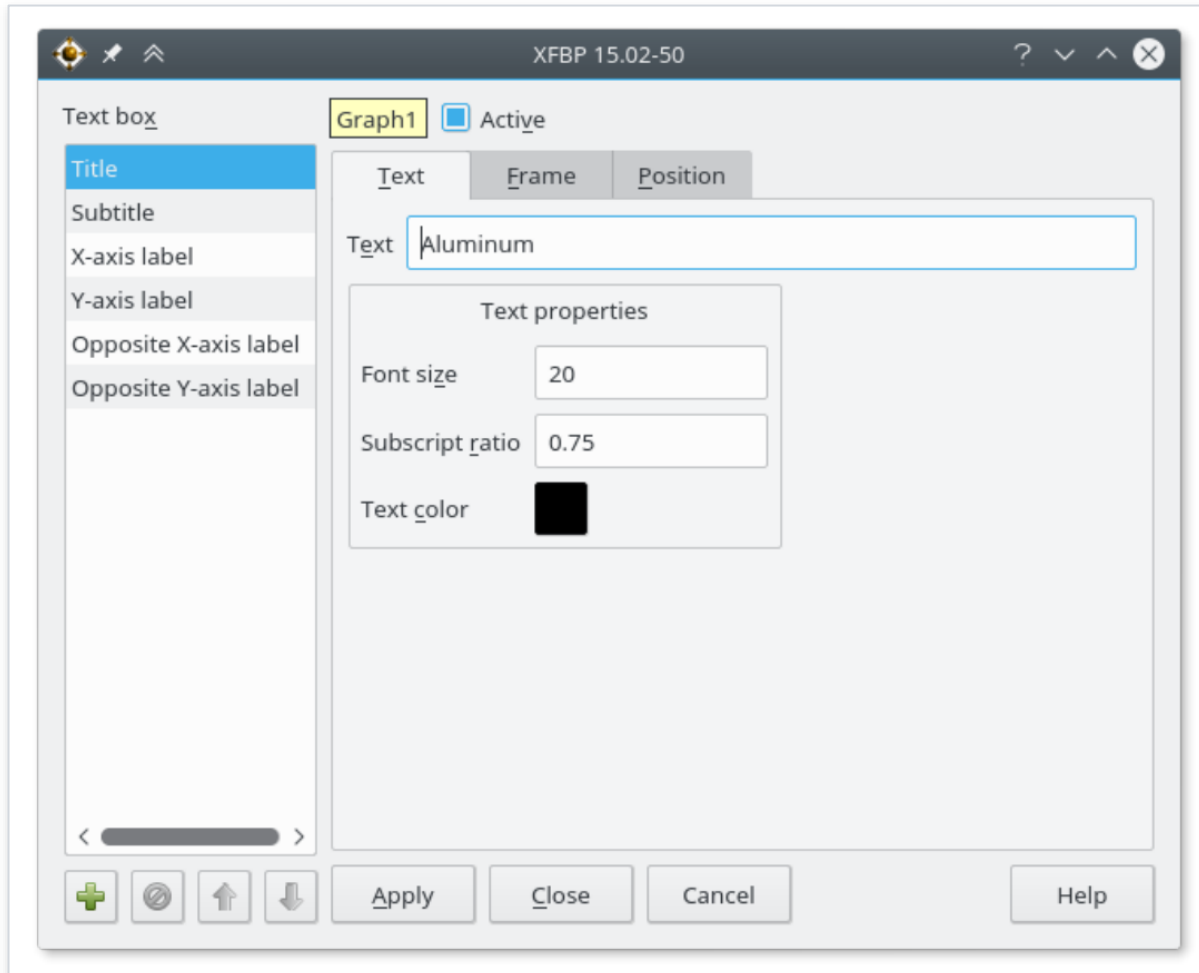
display total and partial DOS

Ctrl + q

quit xfbp

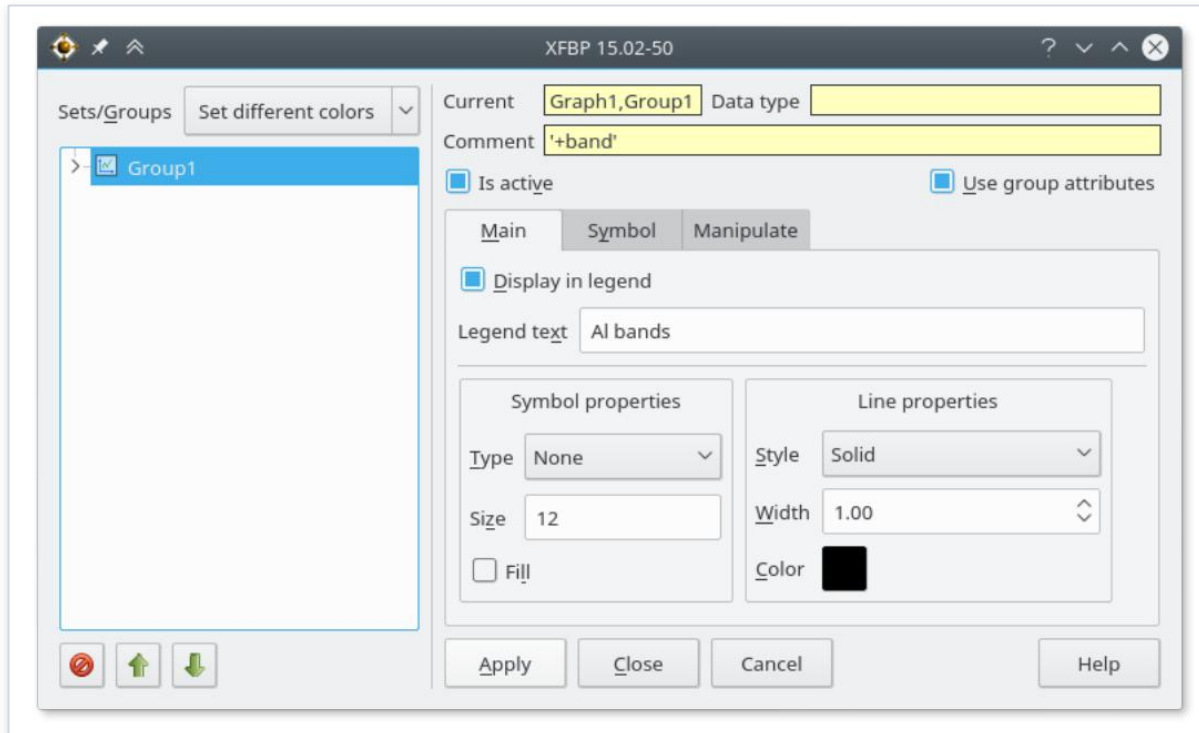
- 3s lowest in energy
- 3p dominates at E_F
- 3s and 3d contribute about equally

Band structure — edit the title



Key sequence	Explanation
<code>xfbp +band <CR></code>	open the band structure file
<code>right-click title</code> → <code>properties</code>	show title properties
<code>Text field</code> → <code>Aluminum</code>	modify the title
<code>Apply, then Close</code>	apply changes, close dialog

Band structure — edit the legend



Key sequence

Explanation

right-click a band → group

open group properties

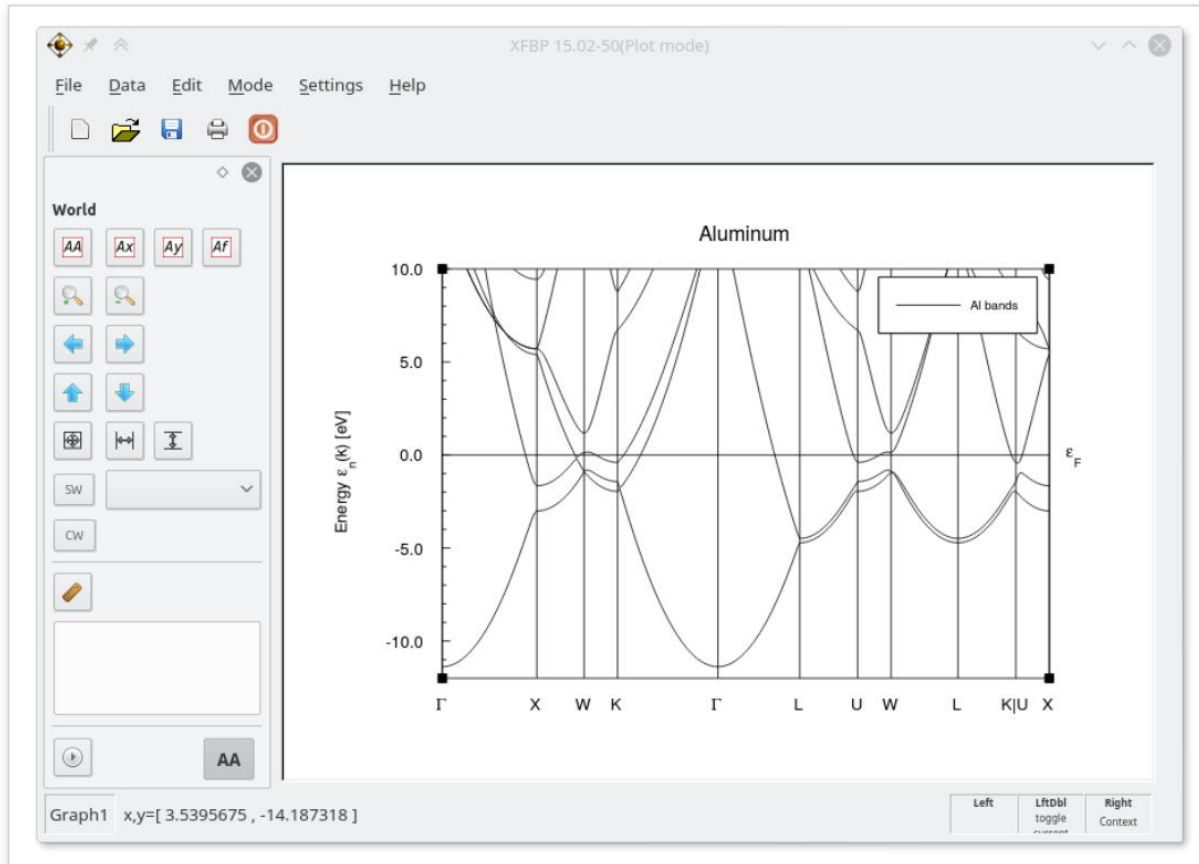
Legend text → All bands

modify the legend text

Apply, then Close

apply changes, close dialog

Valence bands of Al



Key sequence

Explanation

File → **Save**

save the plot with title & legend as “al.bands.xfp” for later use

Ctrl + **q**

quit xfbp

- Change the energy window: Edit → World → Properties (Min / Max)
- *filename.xfp* keeps all plot settings — reopen with *xfbfp filename.xfp*

E(a): prepare three lattice constants

Key sequence	Explanation
<code>cd .. <CR></code>	go to parent directory AI
<code>mkdir a0=7.55 <CR></code>	directory for present a_0
<code>cp SC/* a0=7.55 <CR></code>	copy all files into a0=7.55
<code>mkdir a0=7.50 <CR></code>	directory for another a_0
<code>mkdir a0=7.60 <CR></code>	directory for another a_0
<code>ls <CR></code>	just to look
<code>cp a0=7.55/=* a0=7.50 <CR></code>	copy input files
<code>cp a0=7.55/=* a0=7.60 <CR></code>	copy input files

- $a_0 = 7.50, 7.55, 7.60$ Bohr
- Only the input files (=*) are copied to the new directories

a0 = 7.50: change the lattice constant

```
Symmetry update
e (x) it (/) Search

WARNING:
Lattice type or lattice constants changed!
Will take default values for bandplot special symmetry points!

STATUS: OK (22.02-64:M-CPA)
```

Key sequence	Explanation
<code>cd a0=7.50 <CR></code>	change into directory a0=7.50
<code>fedit22.02-66-x86_64 <CR></code>	call input editor
<code>+</code>	select symmetry menu
<code>L7.50 , , <CR></code>	change lattice constant
<code>+</code>	update lattice geometry

- Warning: user-defined band-plot symmetry points are reset to defaults

a0 = 7.50: save and run

Key sequence	Explanation
x	exit update information
x	exit symmetry menu
q	quit fedit
y	confirm saving
fplo22.02-66-x86_64 > out & <CR>	run fplo in background

- Runs in the background — continue with $a_0 = 7.60$ meanwhile

a0 = 7.60: same procedure

Key sequence	Explanation
<code>cd ../a0=7.60 <CR></code>	change into directory a0=7.60
<code>fedit22.02-66-x86_64 <CR></code>	call input editor
<code>+</code>	select symmetry menu
<code>L7.60 , , <CR></code>	change lattice constant
<code>+</code>	update lattice geometry
<code>x</code>	exit update information
<code>x</code>	exit symmetry menu
<code>q</code>	quit fedit
<code>y</code>	confirm saving
<code>fplo22.02-66-x86_64 > out & <CR></code>	run fplo in background

Check the running jobs

```
unas:fplo/Al/SC> grit a0=  
  
a0=7.50/out SCF: iteration 5 dimension 1 last deviation u= 0.50E-06 CONVERGED  
a0=7.55/out SCF: iteration 10 dimension 1 last deviation u= 0.46E-08 CONVERGED  
a0=7.60/out SCF: iteration 5 dimension 1 last deviation u= 0.55E-06 CONVERGED  
  
unas:fplo/Al/SC>
```

Key sequence	Explanation
<code>ps <CR></code>	check the running jobs
<code>cd .. <CR></code>	change into parent directory
<code>grit a0= <CR></code>	check convergence

- What you see depends on when you look

Compare total energies

```
unas:fplo/Al/SC> grEE a0= | tee ea0

7.50 -241.9194426350 242.19211517 -466.39637611 -17.71518170
7.55 -241.9194604174 242.17167366 -466.38219031 -17.70894377
7.60 -241.9193607411 242.15229278 -466.36879406 -17.70285946

unas:fplo/Al/SC>
```

Key sequence

Explanation

grEE a0= | tee ea0 <CR> print energies, save to file ea0

- Columns: a_0 , E_{tot} , E_{kin} , E_{Coulomb} , E_{xc}
- Minimum of E_{tot} close to $a = 7.55$ Bohr

Shortcuts with grepfplo

Key sequence	Explanation
<code>grepfplo -m EE -p a0= tee ea0 <CR></code>	only the total energy, save to ea0
<code>grepfplo -m EE -p a0= -x <CR></code>	show energies directly in xfbp

- Take a rest!

Further reading (FPLO22.02-66/DOC)

In order to get more information visit the `FPLO22.02-66/DOC` directory.

`MANUAL/doc.pdf` a collection of useful information including the xfplo help screens (in case the help screens of xfplo do not show anything on your installation).

`Tutorials` a collection of tutorials from the last workshop(s). Strongly recommended.

`WannierFunctions` Wannier function examples and a documentation. Must read.

`pyfplo` this is the go-to location for every python related issues (except xfbp scripting). It contains a detailed documentation `pyfplo.pdf` and examples. Work through the examples section of `pyfplo.pdf` to learn more. Also have a look at the provided examples.

`Xfbp` the help screens of xfbp (in case the xfbp help screens do not work). This includes the native and python scripting bindings. It also contains examples for scripting. Very useful.

`Getting_started` this beginners tutorial

`Optics_example` examples for optics calculations

`Scripting_example` a simple scripting example base on shell scripts and the pipe-mode of fedit. There are more modern scripting facilities in `pyfplo`.

`Unfolding_example` further examples for band unfolding

`topoins_Z2` examples for Z2 invariant calculations. The `pyfplo` examples on this topic are a better starting point for understanding.



Break

Next: k-point convergence of the DOS — fcc Al with 8^3 , 16^3 and 32^3 meshes

Why converge the k mesh?

512

k points in the full BZ

$8 \times 8 \times 8$

4 096

k points in the full BZ

$16 \times 16 \times 16$

32 768

k points in the full BZ

$32 \times 32 \times 32$

$NBZ = N^3$ — printed in the output: AUTOSUBDIVISION: actual nkxyz = 8 8 8 NBZ= 512

Recipe increase N until the quantity you care about stops changing — fix everything else.

- DOS and E_{tot} are integrals over the Brillouin zone — sampled on an $N \times N \times N$ mesh (tetrahedron method)
- Finite size effects $N \times N \times N$ k-grid $\leftrightarrow$ $N \times N \times N$ supercell with periodic boundary conditions
- Metals: the Fermi surface cuts the bands $\rightarrow$ sharp occupation step $\rightarrow$ slow convergence
- Insulators: filled bands only $\rightarrow$ converge much faster

Set up three k meshes

Key sequence	Explanation
<code>cd .. <CR></code>	go to parent directory AI
<code>mkdir k8 k16 k32 <CR></code>	one directory per mesh
<code>cp SC/=* k8 <CR></code>	copy input files
<code>cp SC/=* k16 <CR></code>	copy input files
<code>cp SC/=* k32 <CR></code>	copy input files
<code>cd k8 <CR></code>	change into directory k8
<code>fedit22.02-66-x86_64 <CR></code>	call input editor
<code>K8 8 8 <CR></code>	change k-mesh subdivision
<code>q</code>	quit fedit
<code>y</code>	confirm saving
<code>fplo22.02-66-x86_64 > out & <CR></code>	run fplo in background

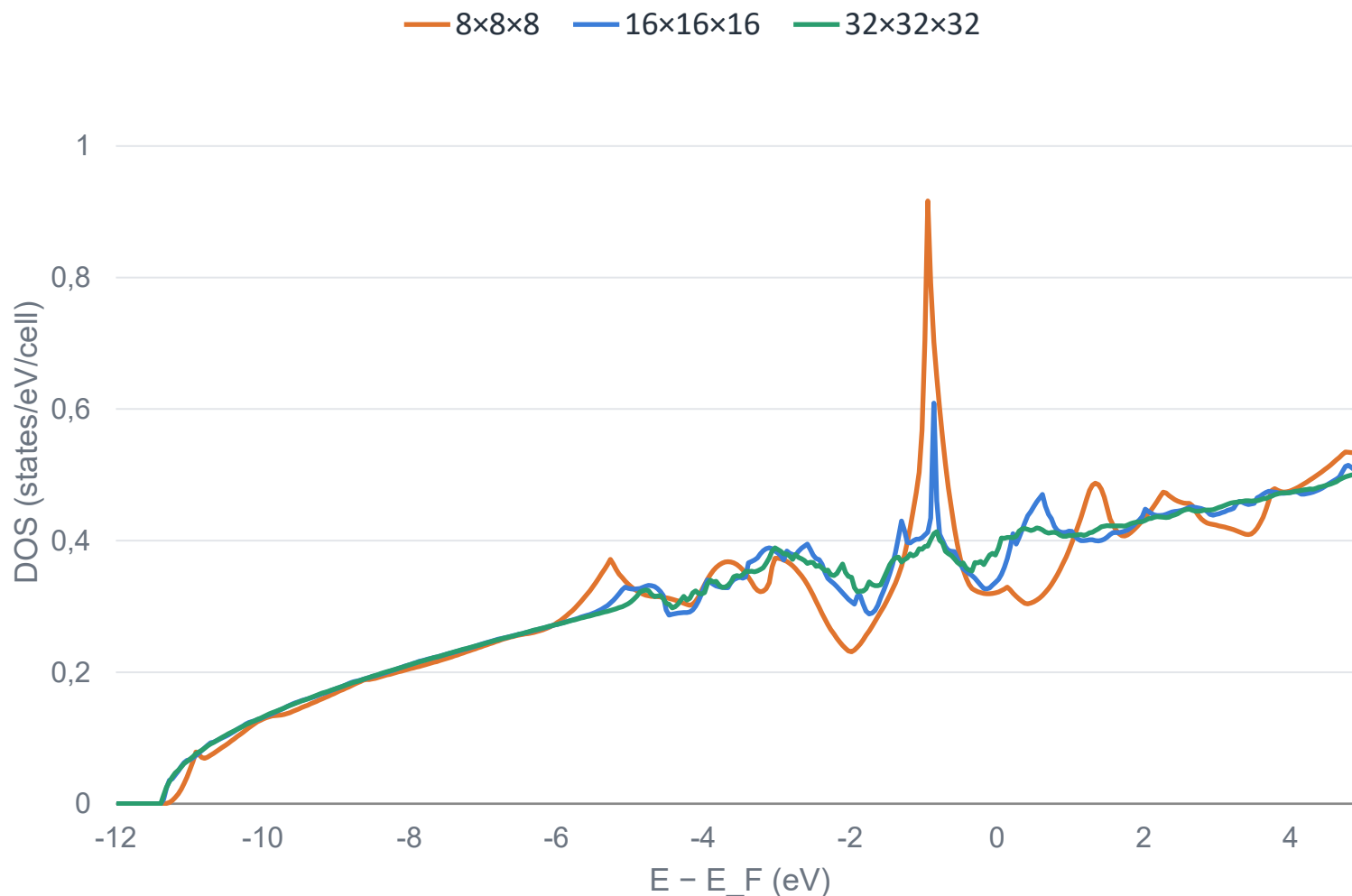
- Bandplot / DOS is still switched on — copied from SC
- Only the k mesh changes; everything else stays fixed

Repeat for $16 \times 16 \times 16$ and $32 \times 32 \times 32$

Key sequence	Explanation
<code>cd ../k16 <CR></code>	change into directory k16
<code>fedit22.02-66-x86_64 <CR></code>	call input editor
<code>K16 16 16 <CR></code>	change k-mesh subdivision
<code>q</code>	quit fedit
<code>y</code>	confirm saving
<code>fplo22.02-66-x86_64 > out & <CR></code>	run fplo in background
<code>cd ../k32 <CR></code>	... same with K32 32 32
<code>cd .. <CR></code>	back to AI
<code>grit k <CR></code>	check convergence of all meshes
<code>grEE k <CR></code>	compare total energies

- 32^3 takes noticeably longer: 8× more k points than 16^3
- Check the k mesh actually used: `grep nkxyz out`

Compare the DOS: 8^3 vs 16^3 vs 32^3

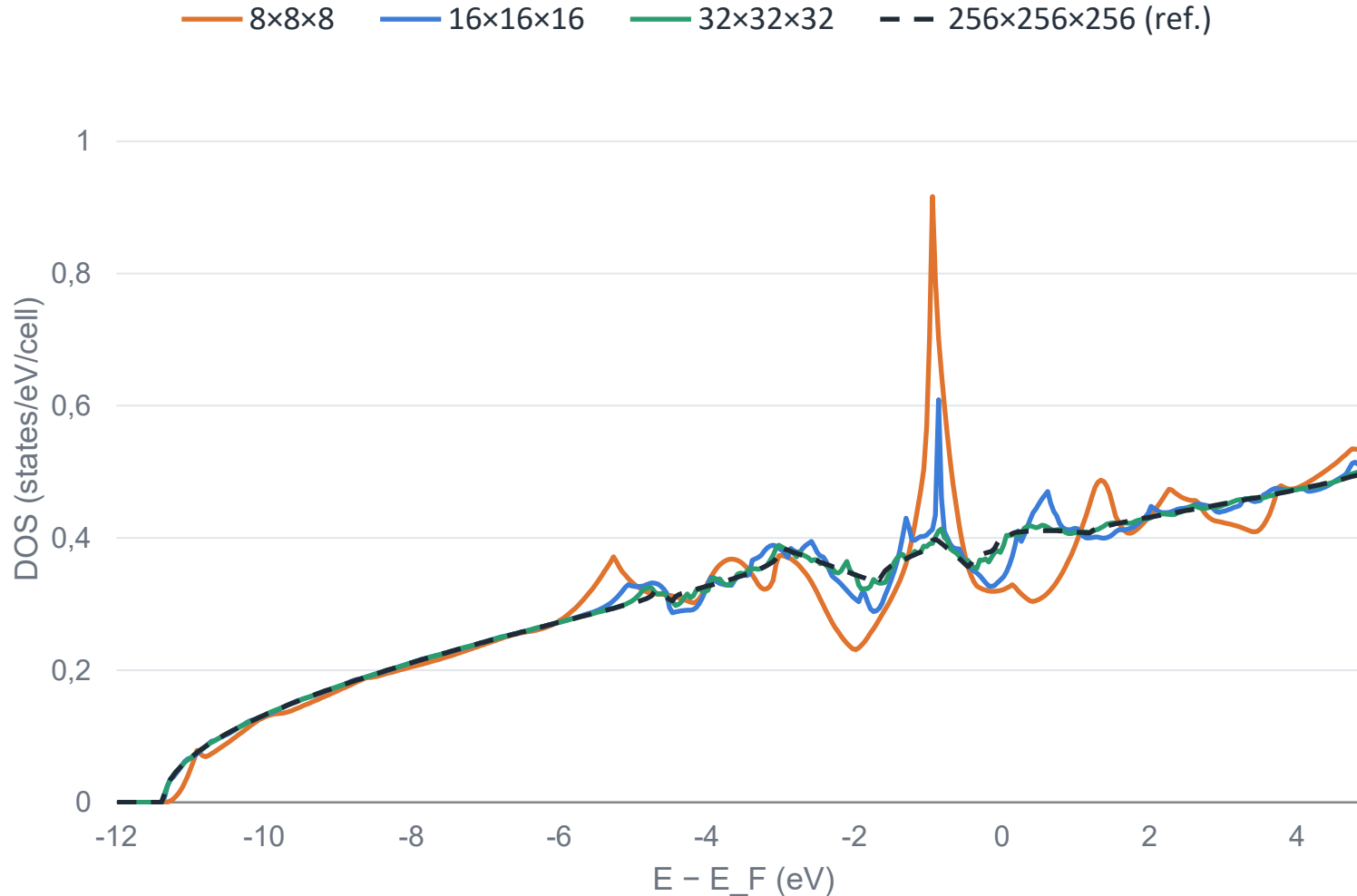


Key sequence

```
xfbp k8/+dos.total  
k16/+dos.total  
k32/+dos.total <CR>
```

- 8^3 : spiky — individual k points show up as artificial peaks
- 16^3 : overall shape right, fine structure still noisy
- 32^3 : smooth; differences to 256^3 below 0.03 states/eV

DOS vs the 256³ reference

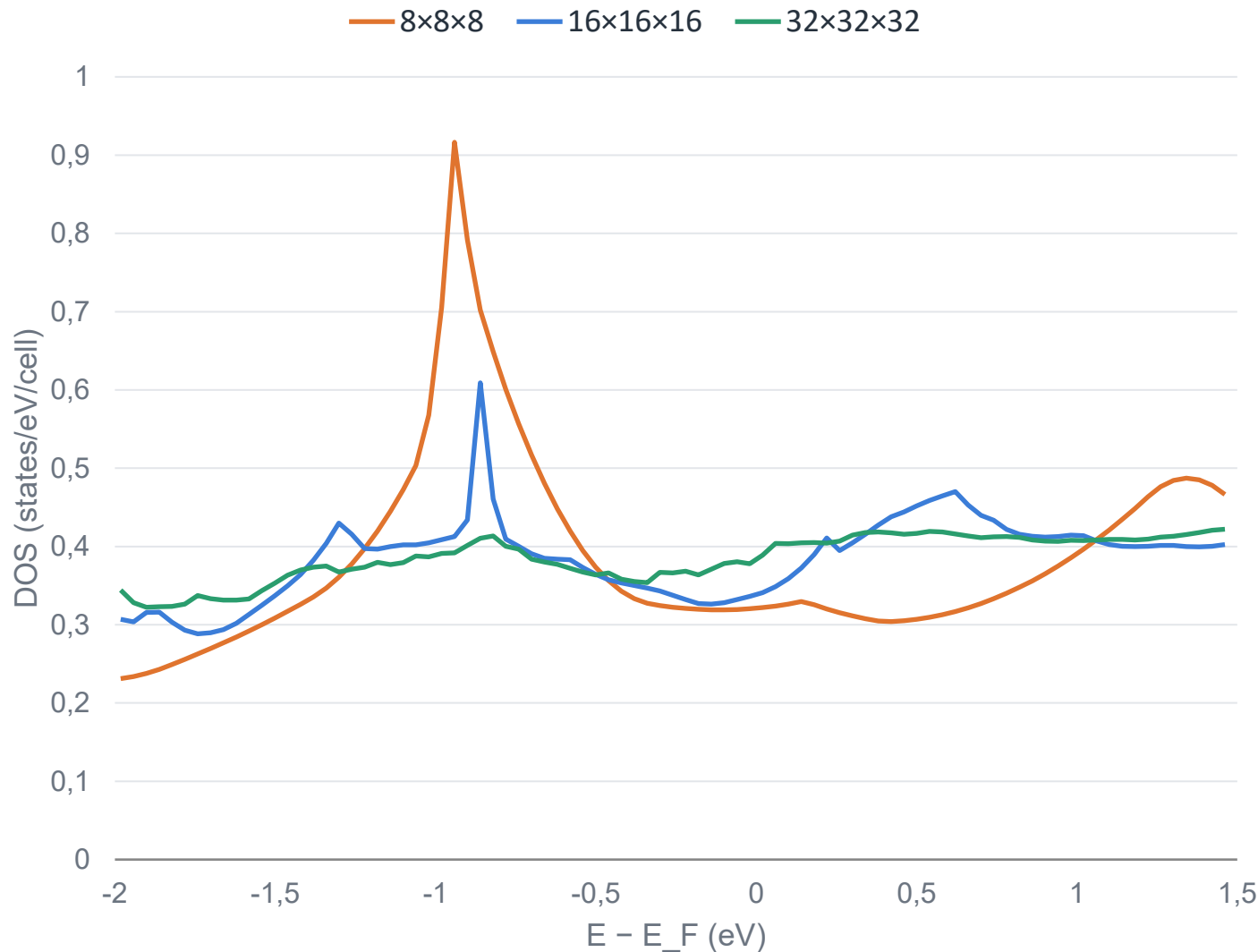


Key sequence

```
xfbp k8/+dos.total  
k16/+dos.total  
k32/+dos.total  
k256/+dos.total <CR>
```

- 256³ (black, dashed) = converged reference
- 32³ lies on top of it: max. deviation 0.02 states/eV (128³: 0.003)
- 8³ off by up to 0.5 states/eV, 16³ by 0.2

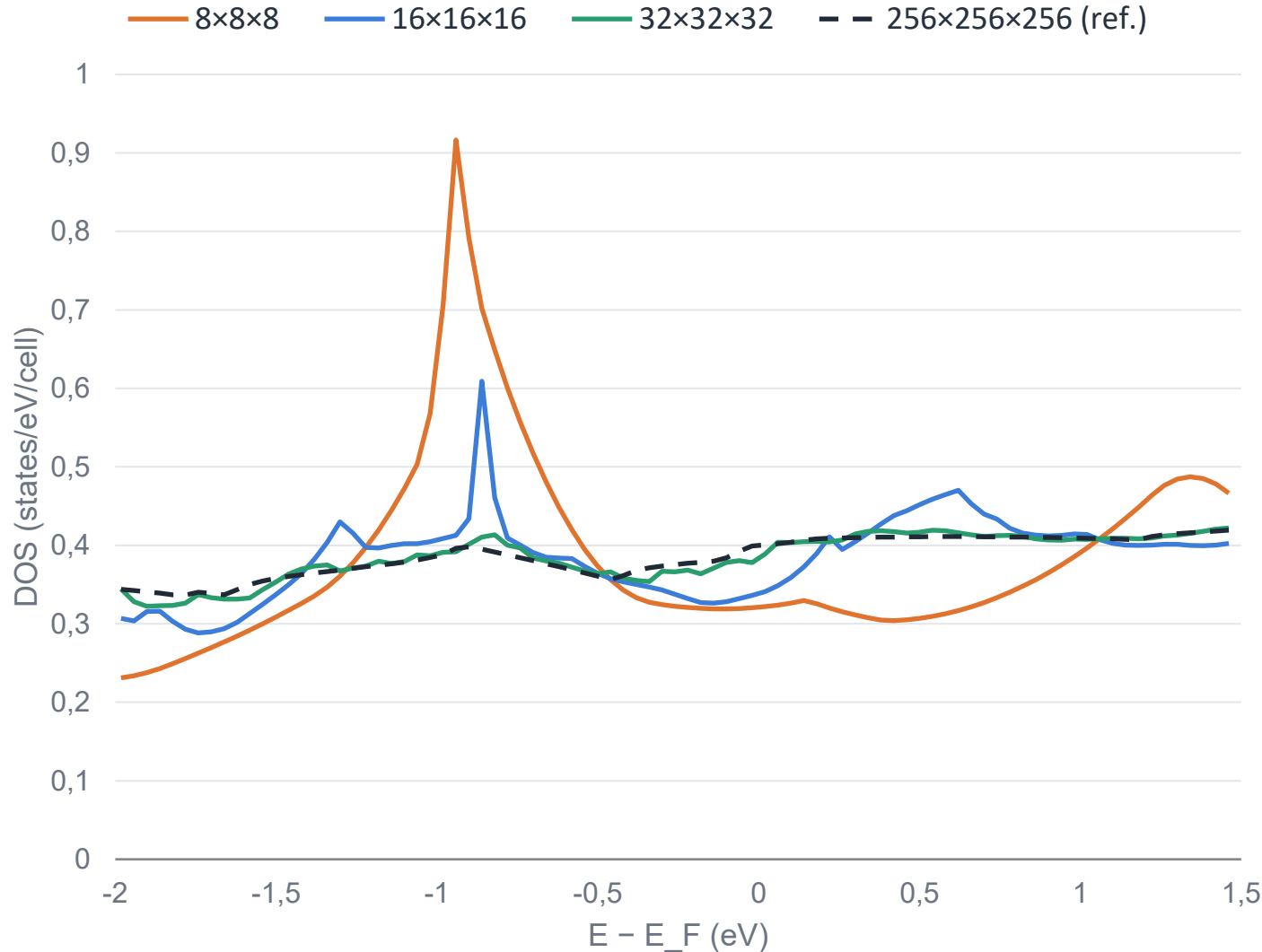
Zoom on the Fermi level



k mesh	N(E _F) (st./eV)
8 ³	0.321
16 ³	0.339
32 ³	0.384
64 ³	0.400
128 ³	0.400
256 ³	0.400

- N(E_F) converges slowest: 32³ still 4 % off
- Matters for γ (specific heat), Pauli χ , Stoner, transport
- Converge the property you need, not just E_{tot}

Zoom on the Fermi level — with 256^3 reference



k mesh	$N(E_F)$ (st./eV)
8^3	0.321
16^3	0.339
32^3	0.384
64^3	0.400
128^3	0.400
256^3	0.400

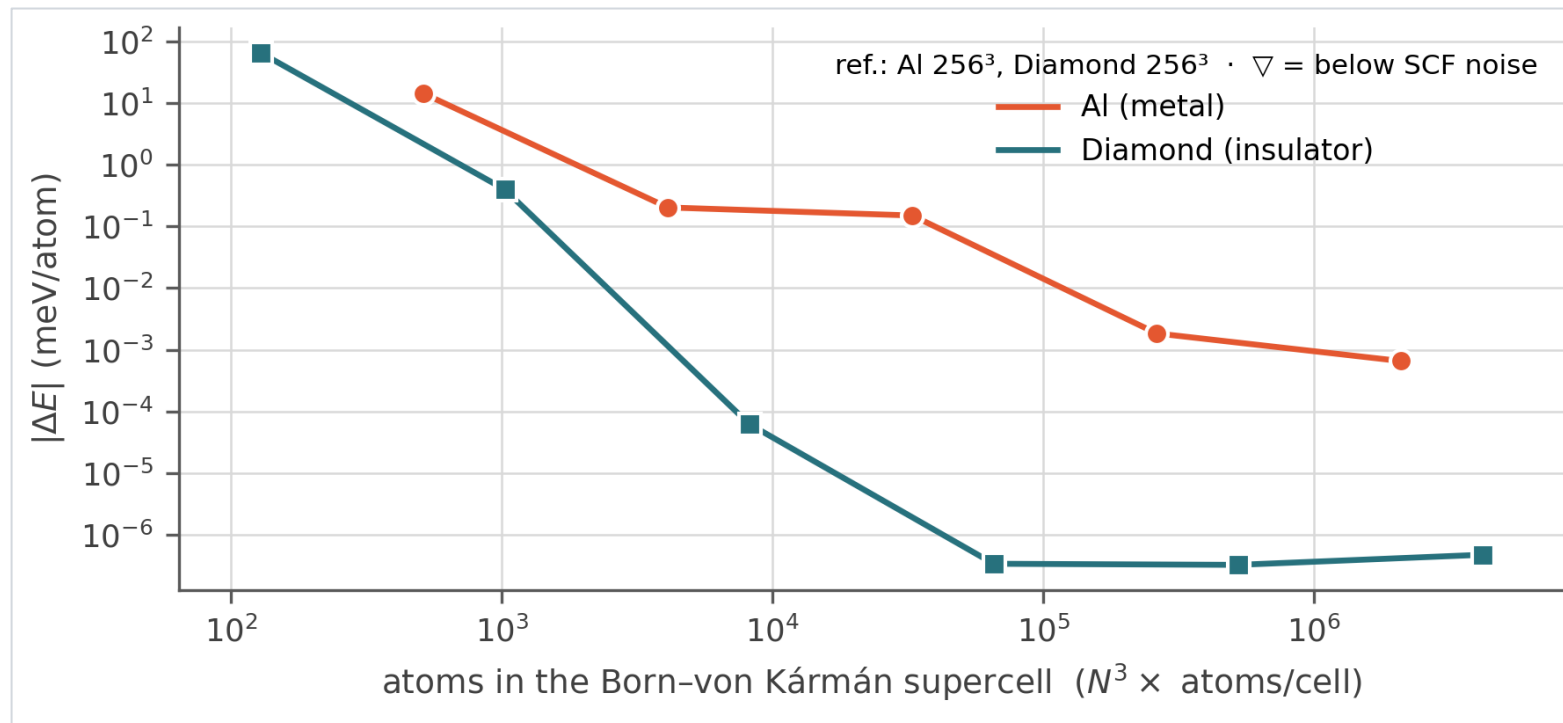
- $N(E_F)$ converges slowest: 32^3 still 4 % off
- Matters for γ (specific heat), Pauli χ , Stoner, transport
- Converge the property you need, not just E_{tot}

What converges how fast? (fcc Al)

k mesh	k points	ΔE_{tot} (meV/atom)	ΔE_{F} (meV)	$N(E_{\text{F}})$ (st./eV)
8^3	512	-14.2	-29	0.321
16^3	4 096	-0.20	+27	0.339
32^3	32 768	-0.15	+8.2	0.384
64^3	262 144	+0.002	+2.1	0.400
128^3	2 097 152	-0.0007	+0.4	0.400
256^3 (ref.)	16 777 216	0	0	0.400

- Total energy: sub-meV already at 16^3 · DOS shape: 32^3 · $N(E_{\text{F}})$ and E_{F} : $\geq 64^3$
- $\Delta = \text{value}(N) - \text{value}(256^3)$; E_{tot} and E_{F} taken from the FPLO output (EE: and TETWTS: Fermi energy)

The full fplo_kconv data set: metal vs insulator



- Diamond: fast convergence — 10^{-4} meV/atom at 16^3
- Al: slow convergence — 0.15 meV/atom off at 32^3 , $\sim 10^{-3}$ meV/atom at 64^3 – 128^3