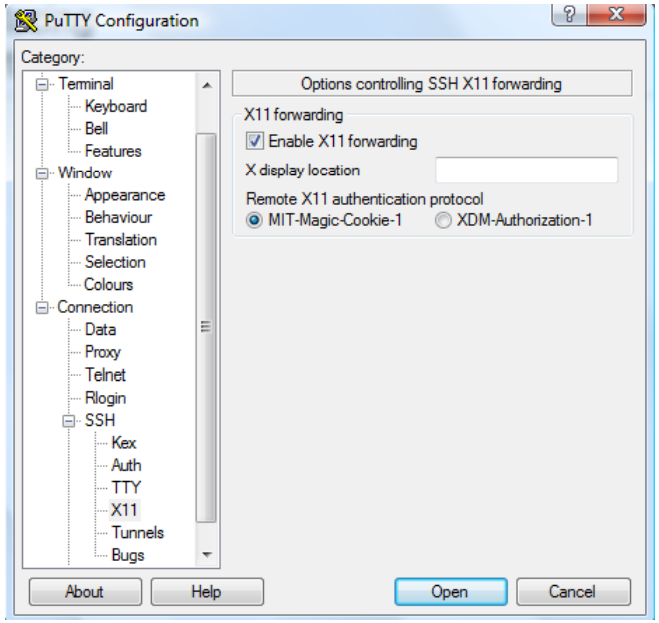
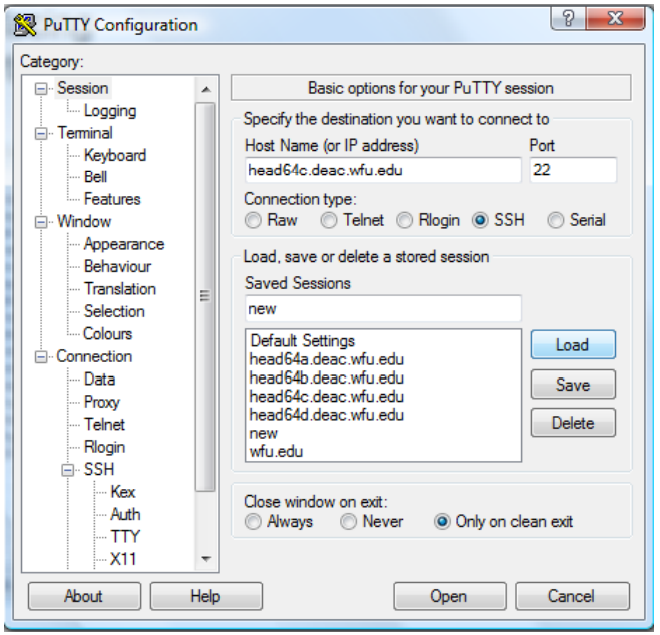
Starting terminal session for interfacing with cluster

•Execute Xming to run in background. (This will allow graphical interfacing
•Start putty





•Set “enable X11 forwarding”
•Save session
•Load session
•Open session

LAPW calculations using WIEN2k code: http://www.wien2k.at/

In order to locating the code on the cluster, it is convenient to add the following to your .tcshrc and/or .cshrc file:

```
# -----------------------------------------------------------
#added by WIEN2k: BEGIN
# -----------------------------------------------------------
alias lsi 'ls -aslp *.in*'
alias lso 'ls -aslp *.ou*'
alias lsd 'ls -aslp *.def'
alias lsc 'ls -aslp *.cl*'
alias lss 'ls -aslp *.sc*'
alias lse 'ls -aslp *.error'
alias matlab '/usr/local/bin/use-faculty-matlab'
alias pslapw 'ps -ef |grep "lapw"'
setenv EDITOR "vim"
setenv SCRATCH $TMPDIR
setenv OMP_NUM_THREADS 1
setenv WIENROOT /home/natalie/EL4/publiccode/wien2k/wien2k_10.1/
setenv PDFREADER /usr/local/bin/acroread

set path = ($WIENROOT $path .)
# -----------------------------------------------------------
# added by WIEN2k: END
# -----------------------------------------------------------
#-----------------------------------------------------------------------------
# this is for XCRYSDEN ; added by XCRYSDEN installation on# Thu Aug  7 18:26:37 EDT 2003
#-----------------------------------------------------------------------------
setenv XCRYSDEN_TOPDIR  /home/natalie/EL4/publiccode/xcrysden/XCRYSDEN
set path = ($XCRYSDEN_TOPDIR $path $XCRYSDEN_TOPDIR/scripts $XCRYSDEN_TOPDIR/uti
l)
#######  Change this line:  natalie ==> your login
setenv XCRYSDEN_SCRATCH /wfurc6/classes/phy752-spr11/natalie/xcrys_tmp
```

Otherwise, you can try running: /home/natalie/EL4/publiccode/wien2k/wien2k_10.1/userconfig

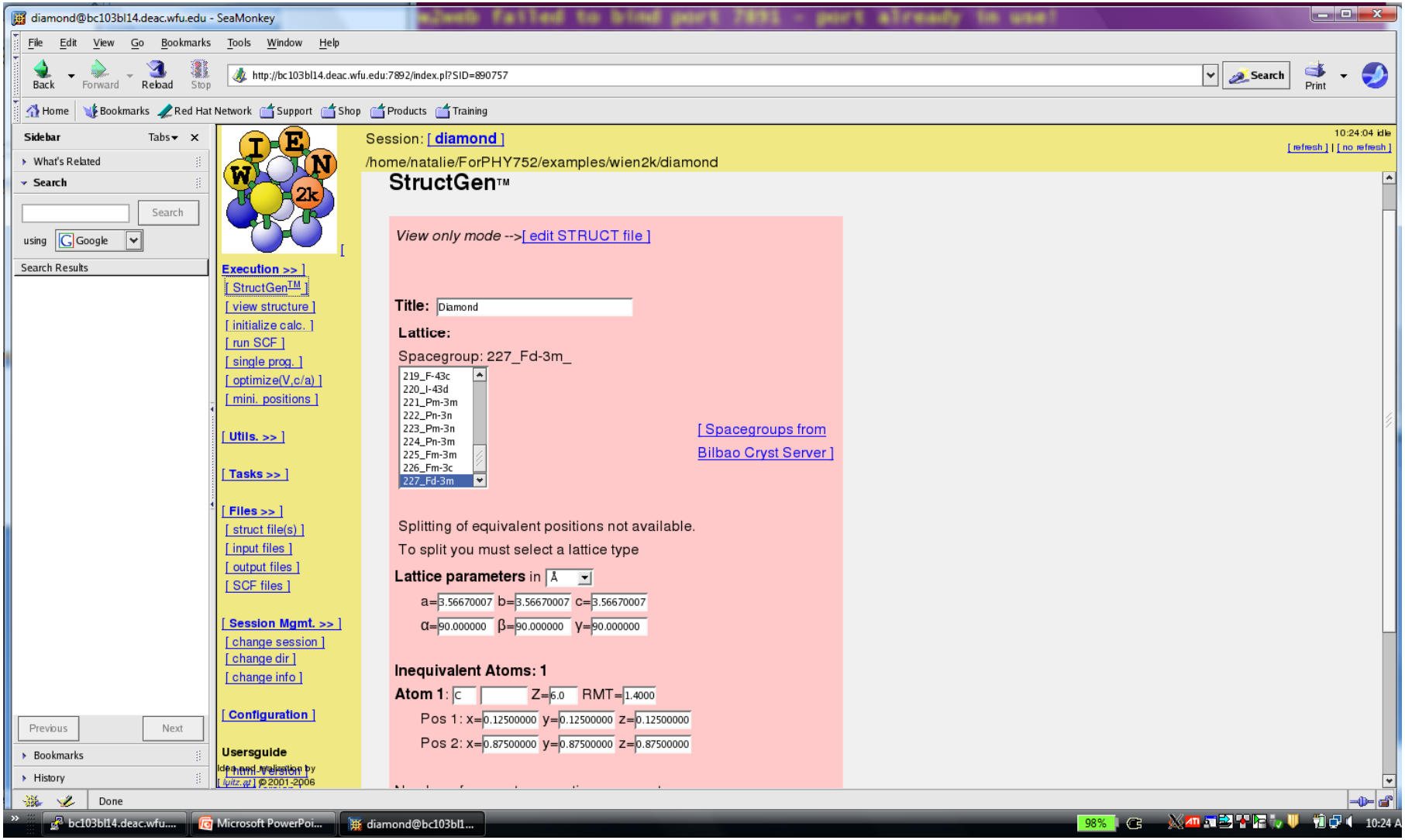
Example case of diamond:

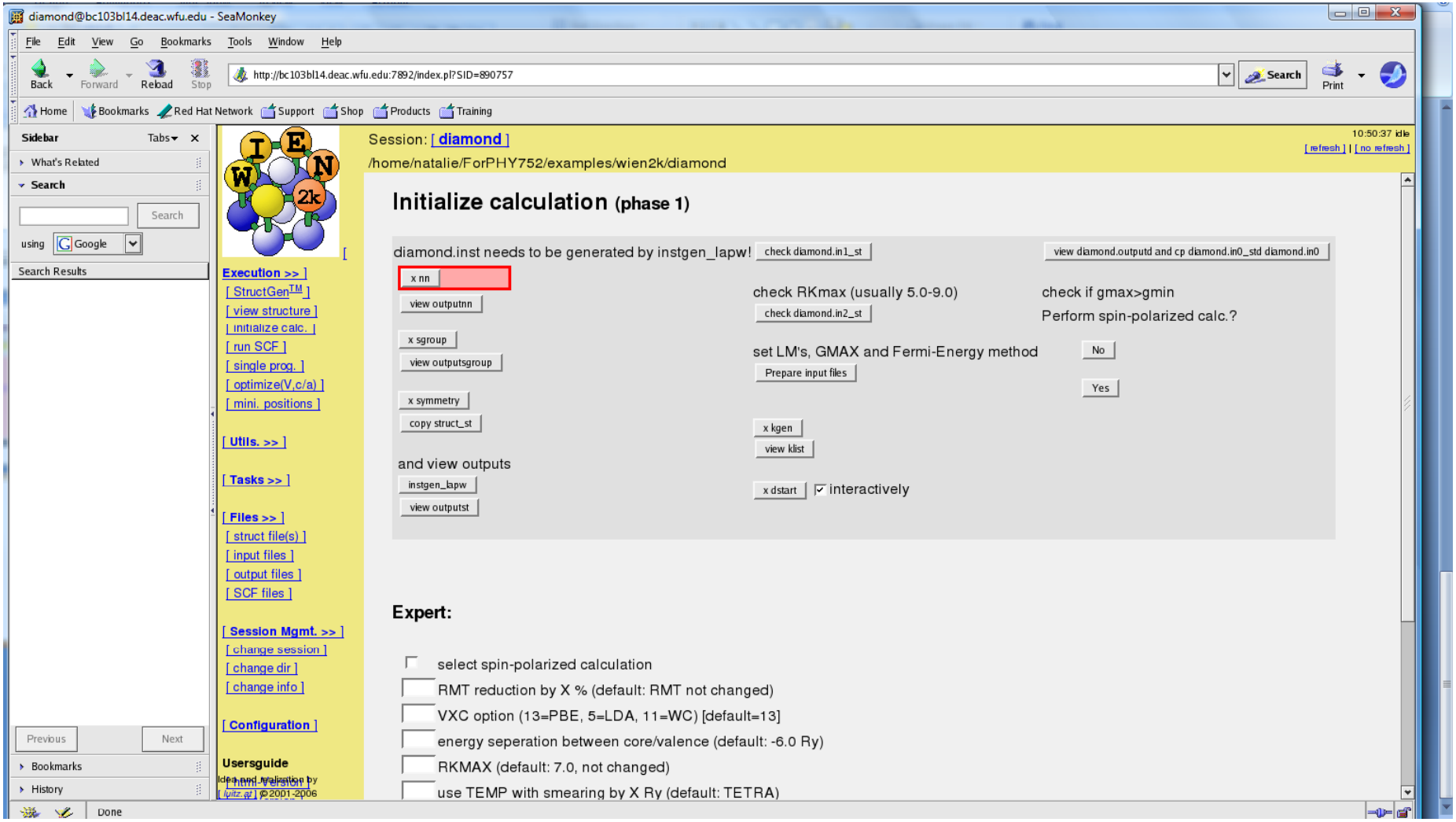
Full example in the cluster directory:
/home/natalie/ForPHY752/examples/wien2k/diamond/diamond1

For running your example, you should create your own directory on the data disk:
/wfurc6/classes/phy752-spr11/[your login]/diamond

Additional steps:

- Run w2web (if this is the first time)
- Run mozilla on the cluster
- Type in the address of the w2web server (such as http://bc103bl05.deac.wfu.edu:7892)
- Login to w2web with your own name and password


diamond@bc103bl14.deac.wfu.edu - SeaMonkey
File Edit View Go Bookmarks Tools Window Help
Back Forward Reload Stop
http://bc103bl14.deac.wfu.edu:7892/index.pl?SID=890757
Search Print
Home Bookmarks Red Hat Network Support Shop Products Training
Sidebar Tabs
What's Related
Search
Search
using Google
Search Results
Previous Next
Bookmarks
History
Done
Session: [diamond]
/home/natalie/ForPHY752/examples/wien2k/diamond
10:24:04 idle
[refresh] | [no refresh]
StructGen™
View only mode -->[edit STRUCT file]
Execution >>]
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V,c/a)]
[mini. positions]
[Utils. >>]
[Tasks >>]
[Files >>]
[struct file(s)]
[input files]
[output files]
[SCF files]
[Session Mgmt. >>]
[change session]
[change dir]
[change info]
[Configuration]
Usersguide
Title: Diamond
Lattice:
Spacegroup: 227_Fd-3m_
219_F-43c
220_I-43d
221_Pm-3m
222_Pn-3n
223_Pm-3n
224_Pn-3m
225_Fm-3m
226_Fm-3c
227_Fd-3m
[Spacegroups from Bilbao Cryst Server]
Splitting of equivalent positions not available.
To split you must select a lattice type
Lattice parameters in Å
a=3.56670007 b=3.56670007 c=3.56670007
α=90.000000 β=90.000000 γ=90.000000
Inequivalent Atoms: 1
Atom 1: C Z=6.0 RMT=1.4000
Pos 1: x=0.12500000 y=0.12500000 z=0.12500000
Pos 2: x=0.87500000 y=0.87500000 z=0.87500000
bc103bl14.deac.wfu....
Microsoft PowerPoi...
diamond@bc103bl1...
98%
10:24 A


diamond@bc103bl14.deac.wfu.edu - SeaMonkey
File Edit View Go Bookmarks Tools Window Help
Back Forward Reload Stop
http://bc103bl14.deac.wfu.edu:7892/index.pl?SID=890757
Search Print
Home Bookmarks Red Hat Network Support Shop Products Training
Sidebar Tabs
What's Related
Search
Search
using Google
Search Results
Previous Next
Bookmarks
History
Done
Session: [diamond]
/home/natalie/ForPHY752/examples/wien2k/diamond
10:50:37 idle
[refresh] | [no refresh]
Initialize calculation (phase 1)
diamond.inst needs to be generated by instgen_lapw!
check diamond.in1_st
view diamond.outputd and cp diamond.in0_std diamond.in0
x nn
view outputnn
check RKmax (usually 5.0-9.0)
check diamond.in2_st
check if gmax>gmin
Perform spin-polarized calc.?
x sgroup
view outputsgroup
set LM's, GMAX and Fermi-Energy method
Prepare input files
No
Yes
x symmetry
copy struct_st
x kgen
view klist
and view outputs
instgen_lapw
view outputst
x dstart
interactively
Expert:
select spin-polarized calculation
RMT reduction by X % (default: RMT not changed)
VXC option (13=PBE, 5=LDA, 11=WC) [default=13]
energy seperation between core/valence (default: -6.0 Ry)
RKMAX (default: 7.0, not changed)
use TEMP with smearing by X Ry (default: TETRA)
Execution >>]
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V,c/a)]
[mini. positions]
[Utils. >>]
[Tasks >>]
[Files >>]
[struct file(s)]
[input files]
[output files]
[SCF files]
[Session Mgmt. >>]
[change session]
[change dir]
[change info]
[Configuration]
Usersguide
[html-version]
Idea and realization by
[lyitz.at] ©2001-2006

Output for lstart: (for C)

```
E-up(Ry)      E-dn(Ry)   Occupancy   q/sphere  core-state
  1S     -19.895104    -19.895104  1.00  1.00    0.9999  T
  2S      -1.001612     -1.001612  1.00  1.00    0.4608  F
  2P*     -0.398288     -0.398288  0.50  0.50    0.4135  F
  2P      -0.398288     -0.398288  0.50  0.50    0.4135  F
```

Input for lapw1: diamond1.in1

```
WFFIL  EF= 0.50000       (WFFIL, WFPRI, ENFIL, SUPWF)
  9.00       12   6 (R-MT*K-MAX; MAX L IN WF, V-NMT
  0.30    3  0      (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0   -0.70      0.002 CONT 1
 0    0.30      0.000 CONT 1
 1    0.30      0.000 CONT 1
K-VECTORS FROM UNIT:4  -12.9       2.5    21   emin/emax/nband
```

Input for lapw2: diamond1.in2

```
TOT             (TOT,FOR,QTL,EFG,FERMI)
    -15.9       8.0 0.50 0.05               EMIN, NE, ESEPERMIN, ESEPER0
TETRA    0.000          (GAUSS,ROOT,TEMP,TETRA,ALL      eval)
  0 0  4 0  4 4  6 0  6 4 -3 2
 14.00          GMAX
NOFILE        FILE/NOFILE  write recprlist
```

PBS script:

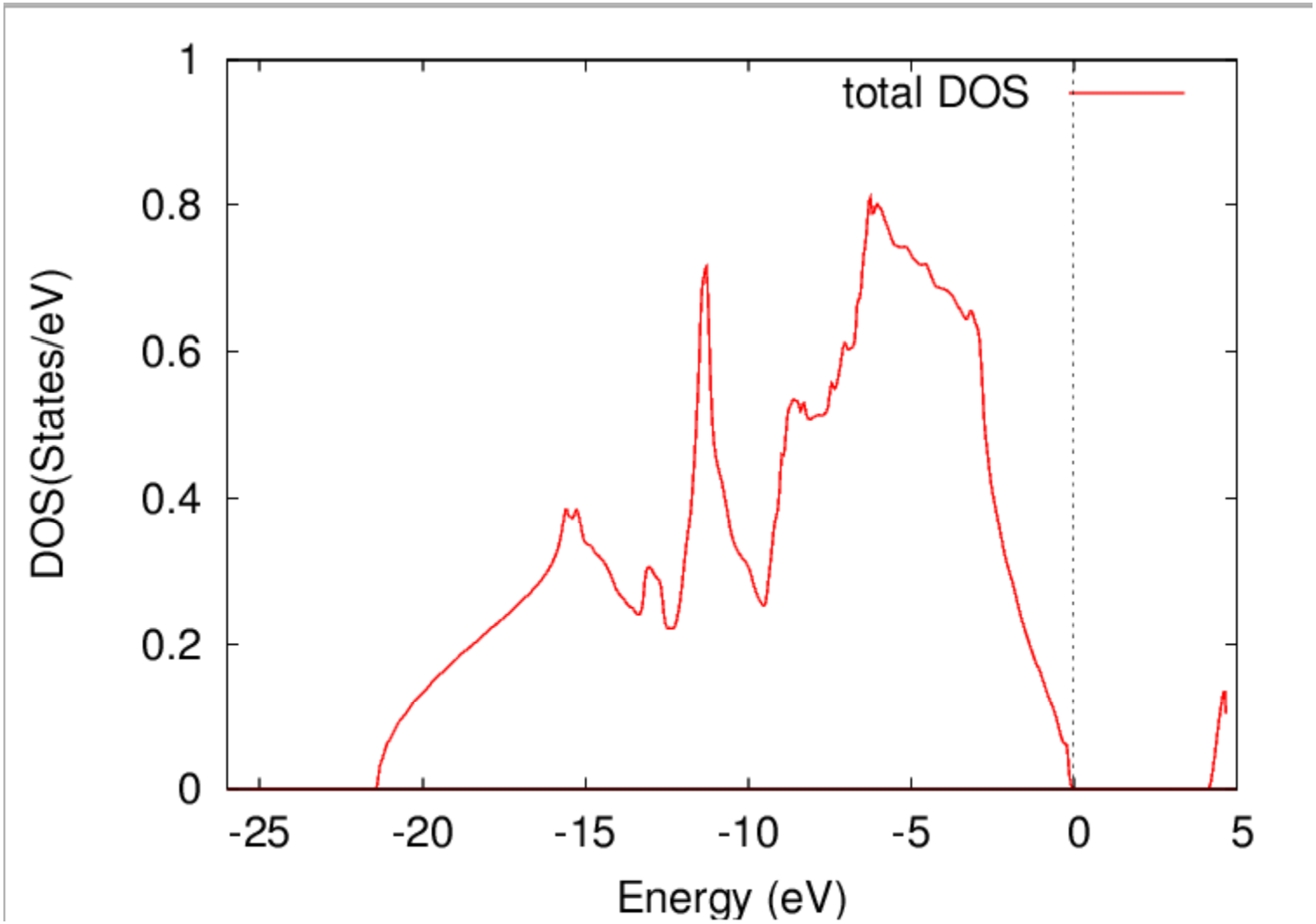
```
#!/bin/tcsh
#
#PBS -l nodes=1:ppn=1:ethernet
#PBS -l ncpus=1
#PBS -W group_list=classes
#PBS -j oe
#PBS -m bea
#PBS -M natalie@wfu.edu
#PBS -l walltime=48:30:30
#PBS -l cput=48:00:00
#PBS -l mem=512mb
#PBS -l pmem=512mb
#PBS -q x86_64
#
echo 'hostname' `/bin/hostname`
echo 'job directory' `pwd`
#
setenv TMPDIR /scratch/$PBS_JOBID
echo 'Reset TMPDIR for this job to ' $TMPDIR
setenv SCRATCH  $TMPDIR
setenv OMP_NUM_THREADS 1
cd ${PBS_O_WORKDIR}

 run_lapw  -ec 0.000001
```

← Change to your ID

Output:

>grep :ENE *scf

```
:ENE  : ********** TOTAL ENERGY IN Ry =        -151.24528576
:ENE  : ********** TOTAL ENERGY IN Ry =        -151.24145573
:ENE  : ********** TOTAL ENERGY IN Ry =        -151.18844930
:ENE  : ********** TOTAL ENERGY IN Ry =        -151.18838311
:ENE  : ********** TOTAL ENERGY IN Ry =        -151.18808528
:ENE  : ********** TOTAL ENERGY IN Ry =        -151.18808616
:ENE  : ********** TOTAL ENERGY IN Ry =        -151.18808495
```


total DOS
DOS(States/eV)
Energy (eV)
1
0.8
0.6
0.4
0.2
0
-25
-20
-15
-10
-5
0
5