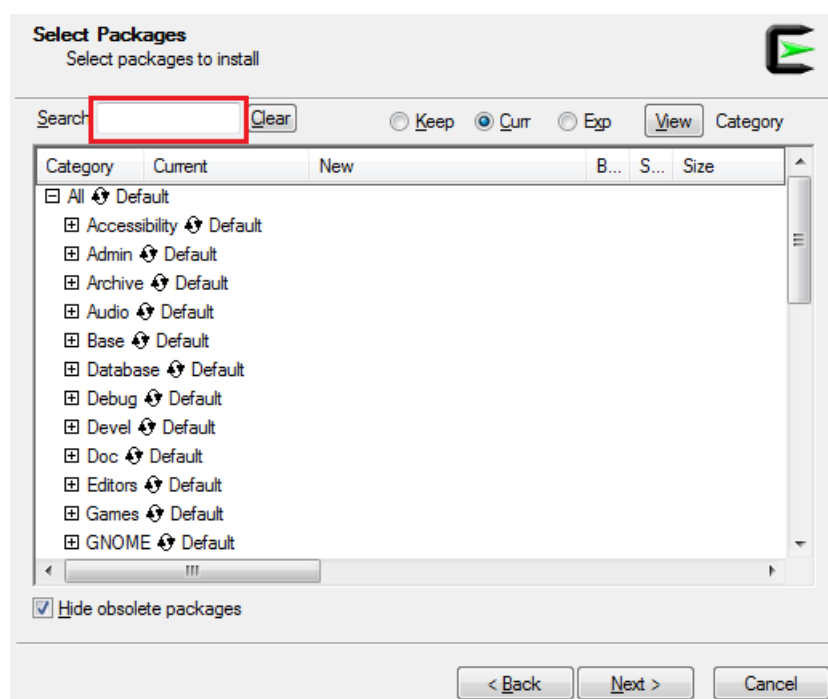


This is a walk-through for windows machines.

1 Initialize

The first thing you need to do is to download crygwin at <http://cygwin.com/install.html>. Download setup.exe. Once you run the setup.exe file hit next and then choose install from internet, next. Select install for all users and choose a root directory for Cygwin (i.e. where you want it installed). Next choose a download location for storing temporary files related to the setup (just go with default folder if you have no other preference). Select next Choose Direct Connection next. Choose a website to download more needed files (specifically outlined below) from. The ftp ones seemed to be quicker than the http. Select next and it should connect to the site and a select packages screen will appear.



There are a number of packages that need to be installed. The four that are absolutely required are

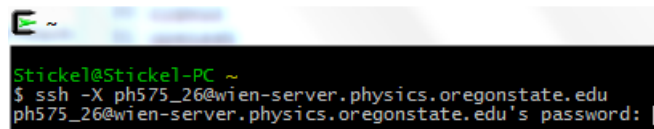
cygwin, openssh, xterm, xinit

Enter each package into the highlighted search bar, as seen above. You will most likely have to run the installer for each package. The above four are required but the packages below are recommended.

bash, bc, coreutils, gawk, grep, gzip, ImageMagick, less, mesa, more, openssl, tcltk, X-start-menu-icons

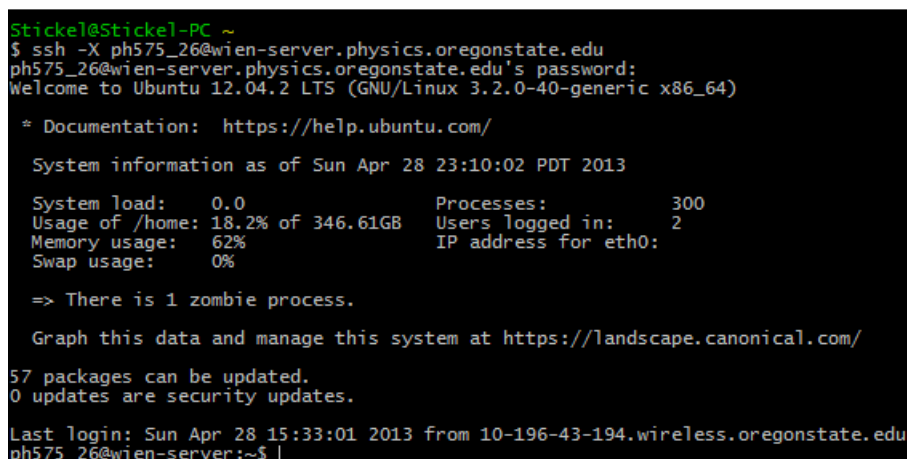
With crygwin set up you can initialize your Wien account. In the start menu you

should see two new folders, one is crygwin and the other is crygwin-X. For now we only need to open the crygwin folder. Open up the crygwin terminal program. type the command “ssh -X ph575_ nn@wien-server.physics.oregonstate.edu” without the quote marks. nn is the number given to you, 26 in the example, as your personal wien id. You should see a screen like below.



```
Stickel@Stickel-PC ~
$ ssh -X ph575_26@wien-server.physics.oregonstate.edu
ph575_26@wien-server.physics.oregonstate.edu's password: |
```

Enter your password. The unix terminal will not show your password, even as `*****`, though you are still typing it you should see the below.



```
Stickel@Stickel-PC ~
$ ssh -X ph575_26@wien-server.physics.oregonstate.edu
ph575_26@wien-server.physics.oregonstate.edu's password:
Welcome to Ubuntu 12.04.2 LTS (GNU/Linux 3.2.0-40-generic x86_64)

 * Documentation:  https://help.ubuntu.com/

System information as of Sun Apr 28 23:10:02 PDT 2013

System load:  0.0                Processes:    300
Usage of /home: 18.2% of 346.61GB  Users logged in:  2
Memory usage:  62%                IP address for eth0:
Swap usage:    0%

=> There is 1 zombie process.

Graph this data and manage this system at https://landscape.canonical.com/

57 packages can be updated.
0 updates are security updates.

Last login: Sun Apr 28 15:33:01 2013 from 10-196-43-194.wireless.oregonstate.edu
ph575_26@wien-server:~$ |
```

enter w2web and you should be told to direct your browser to `http://wien-server.physics.oregonstate.edu:100nn` (`http://wien-server.physics.oregonstate.edu:10026` for this example). You can now log into Wien via the web.

2 starting your calculations

When you first log in you will get a screen asking for your user name and password. Your screen name is ph575_ nn (ph575_ 26) and the password you used to initialize wien.

The server <http://wien-server.physics.oregonstate.edu:10026> requires a username and password. The server says: w2web.

User Name:

Password:

You should see the main page for Wien. We are going to create a new session that we will title Si_ tutorial.

Welcome to *w2web*
the fully web-enabled interface to WIEN2k

Select stored session:	Create new session:
<input type="text"/> <input type="button" value="show only selection"/>	<input type="text" value="Si_tutorial"/> <input type="button" value="Create"/>
<ul style="list-style-type: none">Si_2Si_realSitest <input type="button" value="Select"/>	<input type="button" value="edit hosts"/>

Click the create button to create the new session. You'll see the below.

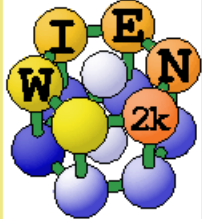
Please **change** into or **create** a new **directory** and "**select**" it
This must not be your home directory!

Current directory: /home/ph575_26/WIEN2k

New directory:

Quick cd:

Click the create/change button to create a new folder. Do not leave the folder as your home folder. After this, select current directory. Then click to restart session. You'll see the home page for calculations, which is pictured below.



Session: [\[Si_tutorial \]](#)
/home/ph575_26/WIEN2k/Si_tutorial

w2web, the fully web-enabled interface to WIEN2

Session Name: Si_tutorial
Session ID: 551719
Directory: /home/ph575_26/WIEN2k/Si_tutorial
Last changed: Sun Apr 28 23:26:27 2013
Comments:

- spin polarized calculation
- AFM calculation
- complex calculation (no inversion)
- parallel calculation

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

The left hand menu is where all of your calculations will take place. Start with the StructGen link. you will be asked for the number of unique atoms. For silicon this is just one; For something like NaCl, this is two. After this you will see the below screen

Title:

Lattice:
 Type: P

[\[Spacegroups from Bilbao Cryst Server \]](#)

Lattice parameters in

a= b= c=
 α = β = γ =

Inequivalent Atoms: 1

Atom 1: Z= RMT= [\[remove atom \]](#)
 Pos 1: x= y= z= [\[remove \]](#) [\[split \]](#)
[\[add position \]](#)

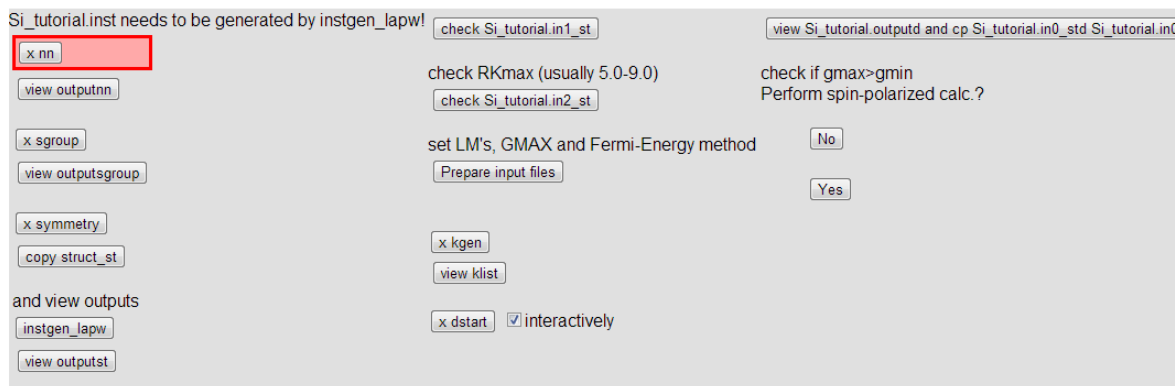
[\[add an atom \]](#)

Number of symmetry operations: generate

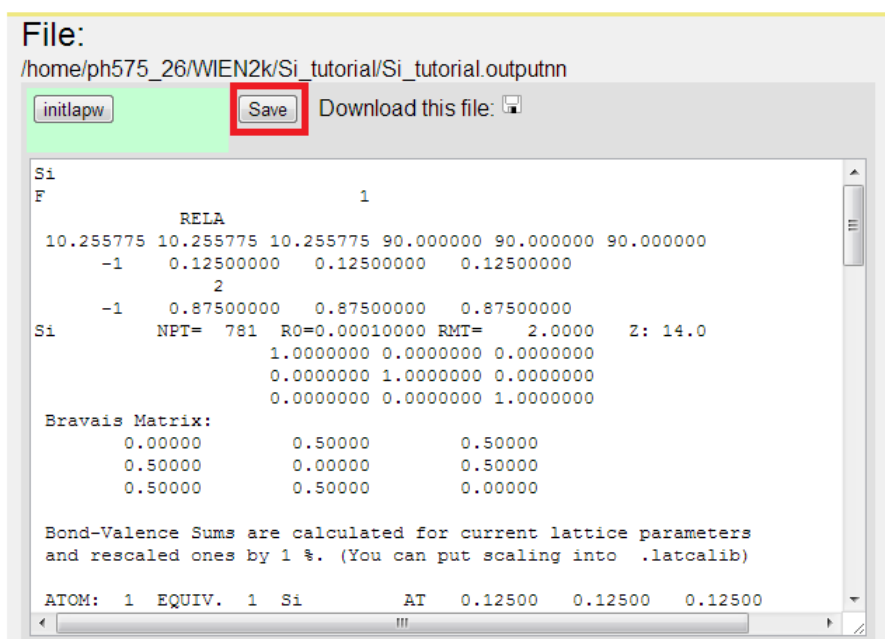
You have to click "Save Structure" for changes to take effect!

Enter the information for silicon including the space group and lattice spacing. When you are done, click save. Make sure to click "set automatically RMT and continue editing" at least once. You may leave the percent at 0% . After you do the optimization once save file and clean up.

After you finish with that click initialize calc. on the left hand menu. You'll see the below.



click though high lighted box. If the option to save a file ever comes up, make sure you click to save

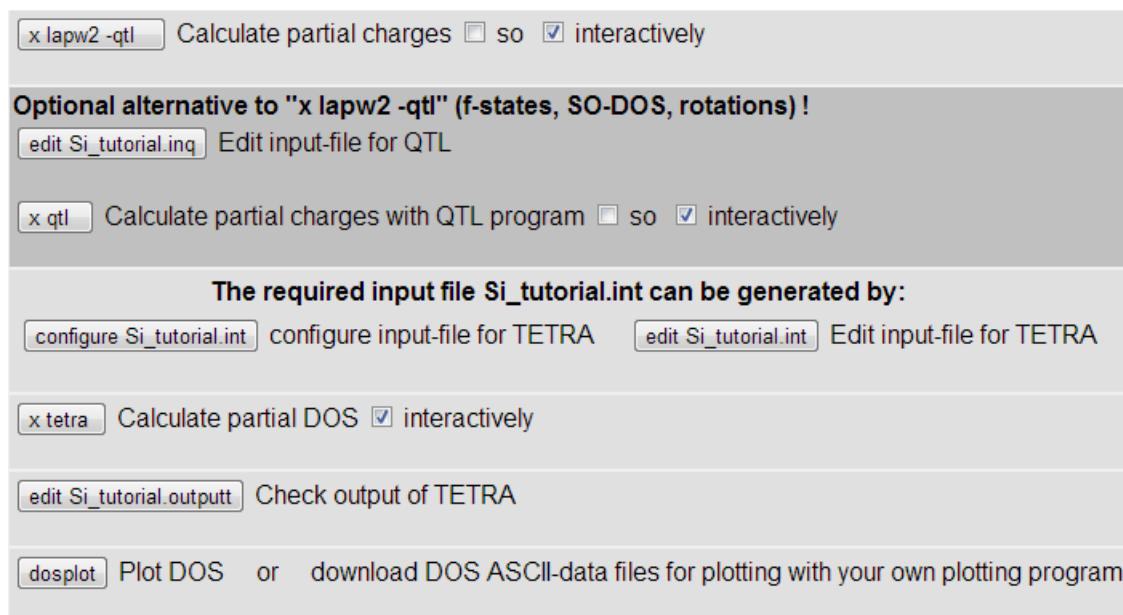


Click through all the the boxes. The one thing to take note of is when you get to x kgen in phase 16 you'll need to enter the number of k points you want to calculate. Around 100 for a semiconductor or a few thousand for metals. After you have clicked though all the steps you will be given the option to "continue with run scf" do this. There are many options here. Ignore all of them and just click the "start scf cycle" button at

the bottom. The screen might go white for a while, just let it load. With this done you can now start doing actual calculations.

3 DOS and partial DOS

Click the tasks menu on the left. Then click DOS.



x lapw2 -qtl Calculate partial charges so interactively

Optional alternative to "x lapw2 -qtl" (f-states, SO-DOS, rotations) !

edit Si_tutorial.inq Edit input-file for QTL

x qtl Calculate partial charges with QTL program so interactively

The required input file Si_tutorial.int can be generated by:

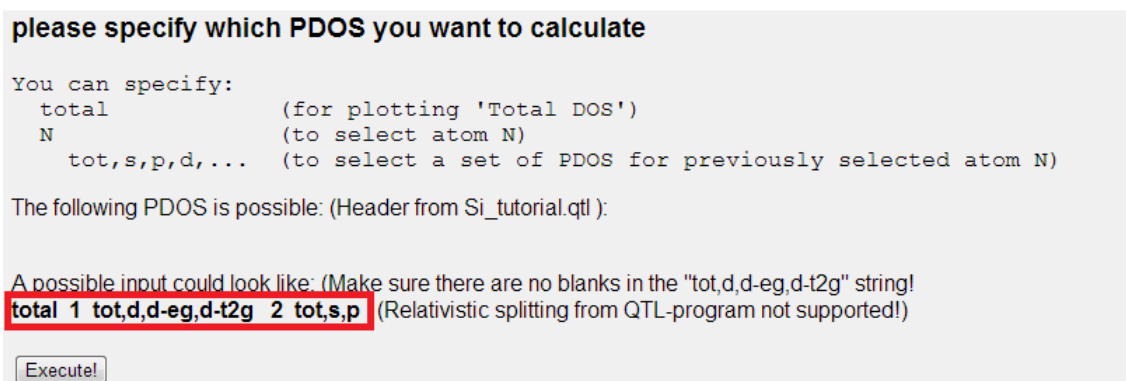
configure Si_tutorial.int configure input-file for TETRA edit Si_tutorial.int Edit input-file for TETRA

x tetra Calculate partial DOS interactively

edit Si_tutorial.outputt Check output of TETRA

dosplot Plot DOS or download DOS ASCII-data files for plotting with your own plotting program

Click through this like you did with the initialize calc. above. You do not need to click on the buttons in the dark gray boxes however. When you click configure Si_tutorial make sure it says "total 1 tot,d,d-eg,d-t2g 2 tot,s,p" as below.



please specify which PDOS you want to calculate

You can specify:

- total (for plotting 'Total DOS')
- N (to select atom N)
- tot,s,p,d,... (to select a set of PDOS for previously selected atom N)

The following PDOS is possible: (Header from Si_tutorial.qtl):

A possible input could look like: (Make sure there are no blanks in the "tot,d,d-eg,d-t2g" string!
total 1 tot,d,d-eg,d-t2g 2 tot,s,p (Relativistic splitting from QTL-program not supported!)

Execute!

The next step is were we can calculate the partial density of states. If you only want the total you can skip this. Click the edit Si_tutorial and you will see the below.

File:
/home/ph575_26/WIEN2k/Si_tutorial/Si_tutorial.int

Download this file:


Header from Si_tutorial.qtl:

	ATOM	COLUMN	
Title			
-0.50	0.002	1.500	0.003 # EMIN, DE, EMAX, Gauss-broadening(>de)
1	N	0.000	# NUMBER OF DOS-CASES specified below, G/L/B bro
0	1	total	# atom, case=column in qtl-header, label
1	1	Atom1	tot
1	2	Atom1	s
1	3	Atom1	p
2	1	Atom2	tot

You see three columns. The first starts with 1, the second with N, and the third 0.000. The first row sets the number of partial density of states that are to be calculated. Set the 1 that is to the left of the N to how ever many PDOS that you want to calculate, for this we will use 6. Below the first row are the most important rows. Each is its own PDOS. The first column in each row is the atom in the crystal. For Si, there is only one atom, but for something like NaCl 0 is both put together, 1 would be the first atom you put into structGen, and 2 is the second and so forth. The second column tells Wien which orbital you want to calculate. 1 is total, 2 is s, 3 is p, 4 is d and so on. The interstitial states can be calculated by setting the number in the first column to 1 higher than total number of atoms in the unit cell, i.e. 2 for Si and 3 for NaCl. We will calculate all of these. The third column is just a title for you to put to remember what each row is for. The image below is the edited file. You can also see above the edited file there is something that says "ATOM Si: 1 tot,s,p,d,D-eg,D-t2g,f" This is must be present for the partial density of states to work. If it is missing go back to the start of the DOS page and click through all the buttons again.

File:

/home/ph575_26/VIEN2k/Si_2/Si_2.int

Download this file: 

Header from Si_2.qtl:

```
      ATOM      COLUMN
ATOM  Si:  1  tot,s,p,d,D-eg,D-t2g,f
```

```
Title
-0.50 0.002 1.500 0.003 # EMIN, DE, EMAX, Gauss-broadening(>de)
  6   N   0.000         # NUMBER OF DOS-CASES specified below, G/L/B bro
  0   1   total         # atom, case=column in qtl-header, label
  1   1   Atom1 tot
  1   2   Atom1 s
  1   3   Atom1 p
  1   4   Atom1 d
  2   1   interstitial 1
```

Once you get something that looks like the above keep clicking through the rest of the DOS calculations. When you click plot you'll see something that looks like the image below

Set ranges (optional):
xmin= xmax= ymin= ymax=

**You can select from 7 DOS in Si_tutorial.int .
Please select up to 4 lines to plot.**

no line	<input type="radio"/>	<input checked="" type="radio"/>	<input checked="" type="radio"/>	<input checked="" type="radio"/>
line:1 (total DOS) of Si_tutorial	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:2 (tot) of atom Si	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:3 (s) of atom Si	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:4 (p) of atom Si	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:5 (d) of atom Si	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:6 (d-eg) of atom Si	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:7 (d-t2g) of atom Si	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>

Define for first line: Label= Linetype(0-9)= Linewidth=

Define for second line: Label= Linetype(0-9)= Linewidth=

Define for third line: Label= Linetype(0-9)= Linewidth=

Define for fourth line: Label= Linetype(0-9)= Linewidth=

Plot DOS in Labelsiz= pt

Select the PDOS that you want to plot. You can chose your limits as well, though if they are left blank the program fits the plots. Click plot and you should see a DOS plot.

4 band structure and/or spaghetti plot

Now that the PDOS is plotted the band structure can be plotted. Click on bandstructure on the left menu. The band structurer window looks like

Band structure

Generate k-mesh using XCrysden (save klist as xcrysden.klist)

fcc [\[Brillouinzones from Bilbao Cryst Server \]](#)

x lapw1 -band Calculate Eigenvalues orb interactively

needed only for continuous lines in the plot (not for non-symmorphic spacegroups)!

x irrep Calculate irreducible representations so interactively

for band character plots only!

x lapw2 -band -qtl Calculate partial charges ("qtl"-file) so interactively

edit Si_tutorial.insp Insert correct EF

x spaghetti Calculate bandstructure so interactively

plot bandstructure Plot bandstructure or download Xmgrace files for plotting with xmgrace

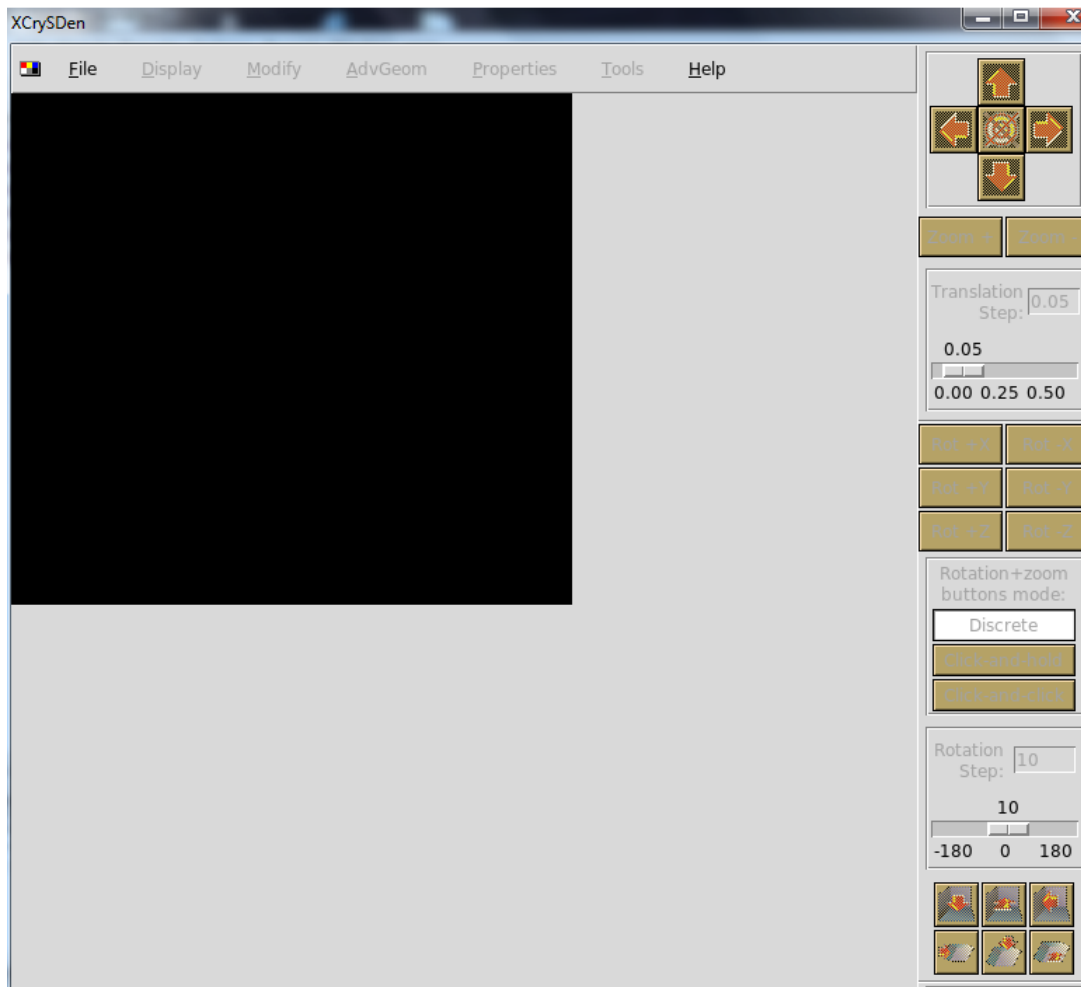
The first option is to create a klist with xcrysden. To run xcrysden you need first open the cygwin-X file in the start menu that was mentioned at the very start of this tutorial. Open XWin server. This can be a bit finicky. I sometimes have to open it a few times. This may or may not open an xterm window. If not, open the xterm from the same cygwin-X file. When the window opens log into your account like you did to initialize using the command `ssh -X ph575_26@wien-server.physics.oregonstate.edu`

```

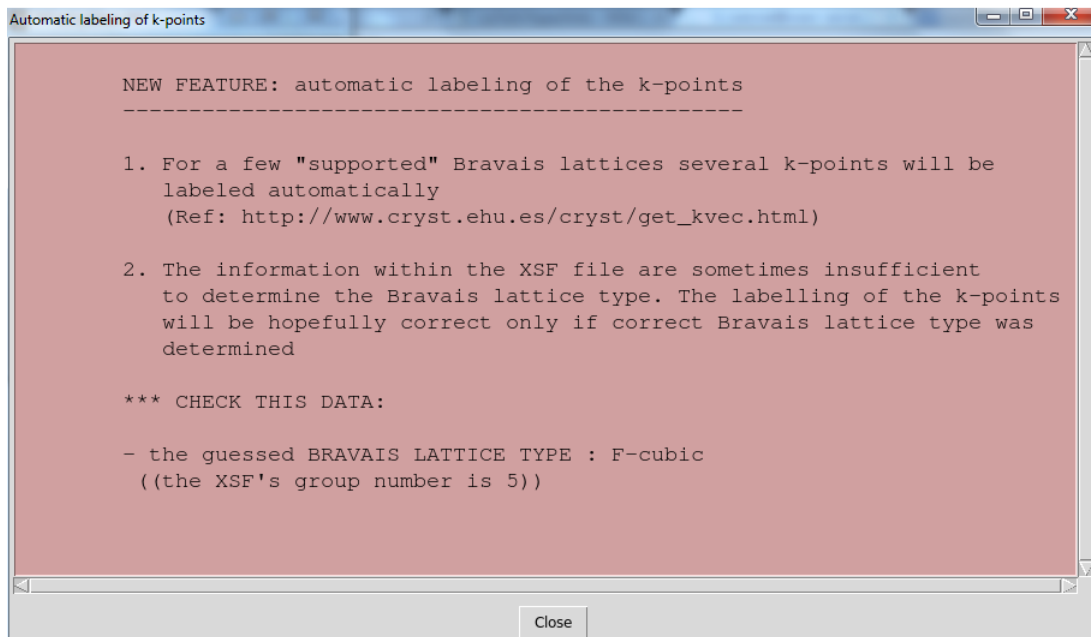
Main Options VT Options VT Fonts
Stickel@Stickel-PC ~
$ ssh -X ph575_26@wien-server.physics.oregonstate.edu
ph575_26@wien-server.physics.oregonstate.edu's password: █

```

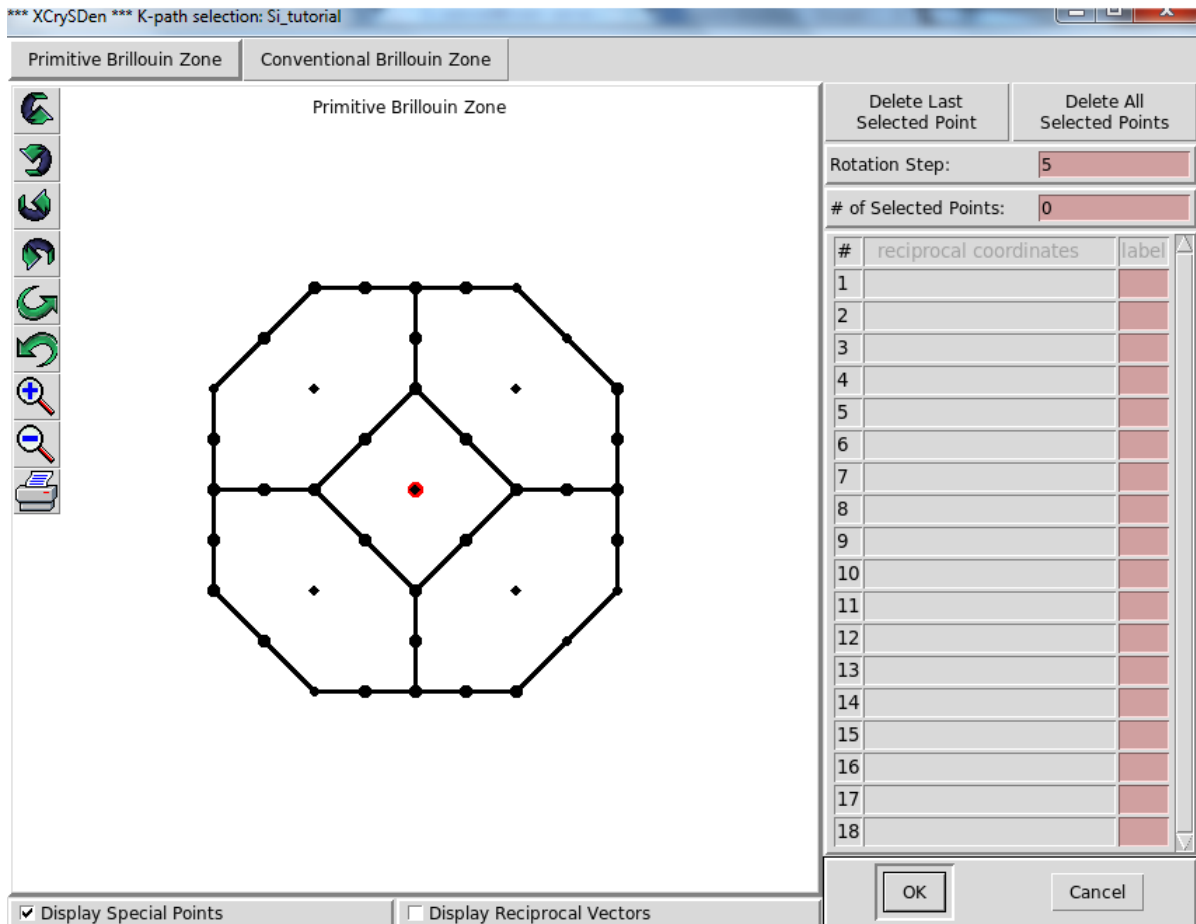
enter your password. At this point I like to test to make sure I can open xcrysden. Working with a few people I found out some computers have issues opening xcrysden, even if all the commands are entered right. To open xcrysden just type `xcrysden` into the xterm window.



If this opens successfully head back to the web interface and your band structure calculation. Click the generate k-mesh with xcrysdn button. If you just get the message “Requires X-Window system ...” go to the xterm window and enter the command “ps -u ph575_26”. kill any process that says w2web with the command “kill # # # #” where # # # # is whatever number is next to the w2web process. Enter the “ps -u ph575_26” command again to make sure that all the w2web process are shut off. Run w2web again in the xterm window. After this, try the generate k-mesh with xcrysdn button again. Two windows should (eventually) open. One is just a pink text document, close it.



You should see an image like the below appear.



Each point corresponds to a high symmetry point in k-space such as the Γ point or the X point. Click along to make a k-path. When you have selected 5-7 points click ok. A new screen will open up.

NOTES:

1. Please check if k-point coordinates looks OK. These k-points have integer coordinates, calculated as $(k_x * M, k_y * M, k_z * M)$, where M is an integer multiplier. Actual k-point coordinates are then obtained as: $1/M * (k_x * M, k_y * M, k_z * M)$!!!
2. You can also specify some new k-points manually.
3. The k-path is obtained by connecting the k-points together.

M multiplier was set to:

Total number of k-points along the path:

Format: M*kx	M*ky	M*kz	label
-4	0	0	L
0	0	0	GAMMA
0	4	4	X
-2	4	2	W
-3	3	0	K

Ignore the line that starts with M multiple.... The second line is important. The total number of K-points along the path are the physical number of points that wien plots between the k-points you selected in the above step. Around 50-100 should suffice. (too few and the band plot is just straight lines....trust me) Click ok. A third window will pop up and ask for a file name. Enter xcrysden.klist and then save. A final pink text window will appear, close it. Go back to the website and the band plot. In the second line there is a drop down menu that starts with fcc. Open the drop down menu and select 'from xcrysden' and click the create button next to the drop down menu. The menu will revert back to its default fcc, this is fine, don't worry about it. Click the third button x lapw1 -band. skip the two dark gray sections. I found that when you use these, the k-list file from xcrysden does not work. when you get to 'edit Si_ tutorial' you'll see a series of xxxx that I have highlighted below. Replace these xxxx with the number above the text box, on the right that is also highlighted, which is the fermi energy. The highlighted number may change a bit. I've done this a few times and have gotten between .37 and .4 so if its not exactly that number I wouldn't worry.

continue with bandstructure Save Download this file:

Header from Si_tutorial.qtl and possible FERMI energies:

```

ATOM Si: 1 tot,s,p,d,D-eg,D-t2g,f
/home/ph575_26/WIEN2k/Si_tutorial/Si_tutorial.scf: EF (TETRAH.M.)= 0.40237

```

```

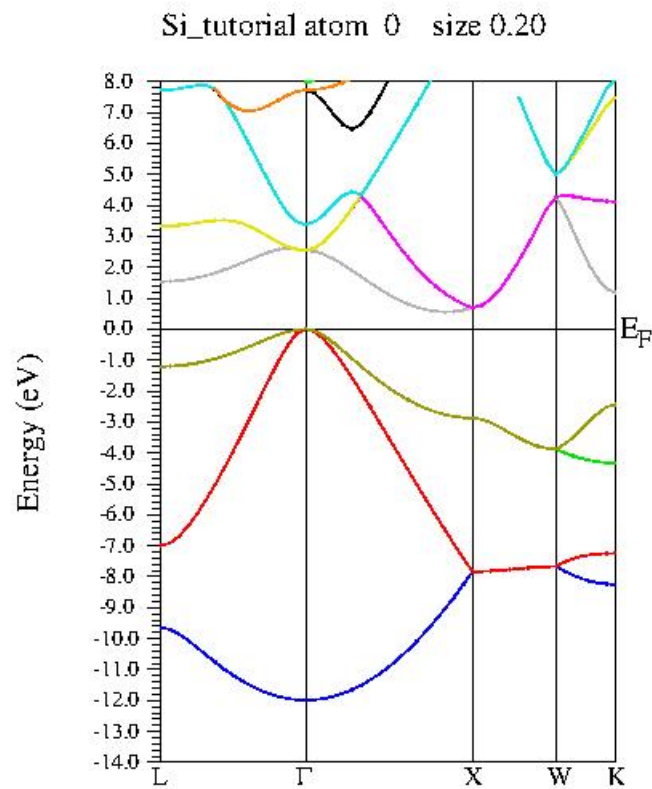
### Figure configuration
5.0 3.0 # paper offset of plot
10.0 15.0 # xsize,y size [cm]
1.0 4 # major ticks, minor ticks
1.0 1 # character height, font switch
1.1 2 4 # line width, line switch, color switch
### Data configuration
-14.0 8.0 2 # energy range, energy switch (1:Ry, 2:eV)
1 0.xxxxx # Fermi switch, Fermi-level (in Ry unit)
1 999 # number of bands for heavier plotting
0 1 0.2 # jatom, jtype, size of heavier plot

```

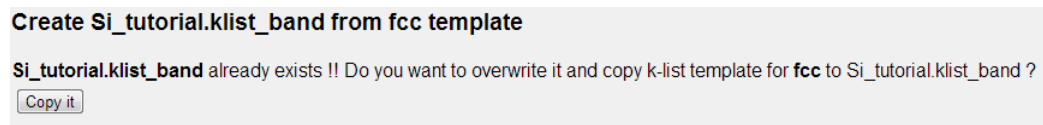
Fermi switch:
0...no line
1...solid line
2...dashed line
3...dotted line

Line switch:

Click save and click through till you get to the band plot. This is the band plot that I get.



It is also possible to use the standard k-mesh that wien provides. Go back to the band plot menu and instead of using the 'from xcrysdn' option in the drop down menu leave it as fcc and click the generate button to the right. You'll be asked to copy the file



click 'copy it' and then go through all of the buttons like you did for the xcrysdn option, again double checking the fermi energy when you get to 'edit Si_tutorial'. You'll get a new band plot (most likely, unless you picked the exact same path as wien).

5 electron density

TBC