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.
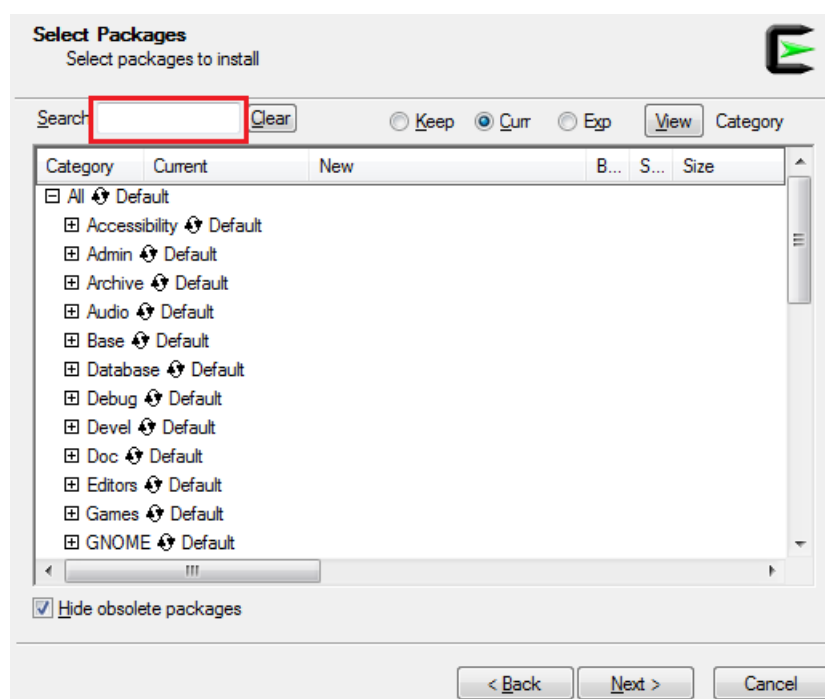
There are a number of packages that need to be installed. The four that are absolutely required are
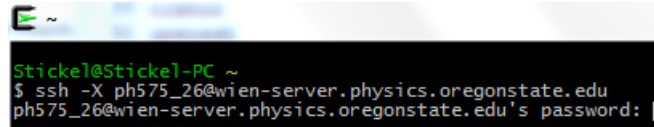
cygwin, openssh, xterm, xinit

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.

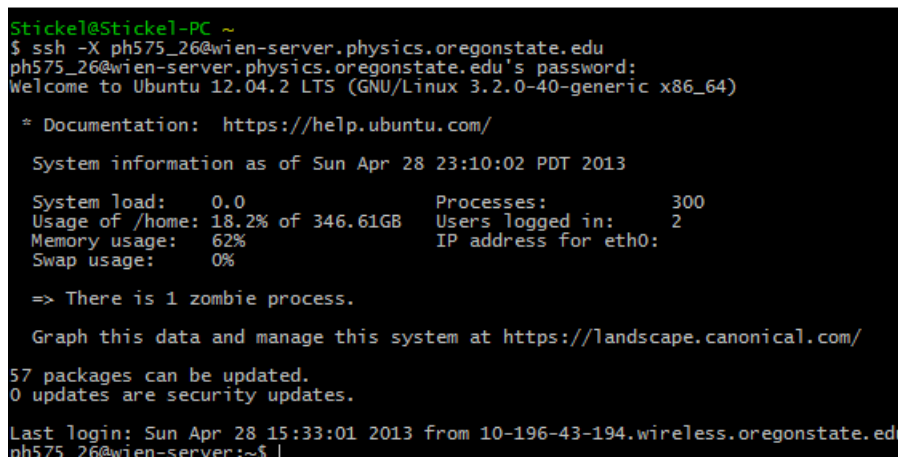bash, bc, coreutils, gawk, grep, gzip, ImageMagick, less, mesa, more, opengl, tcltk, X-start-menu-icons

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.

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

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.

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

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

Select current directory

New directory: Si_tutorial   create/change
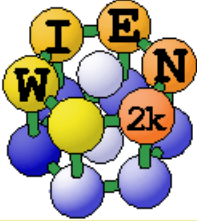
Quick cd: /home/ph575_26/WIEN2k/   cd

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.

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

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.
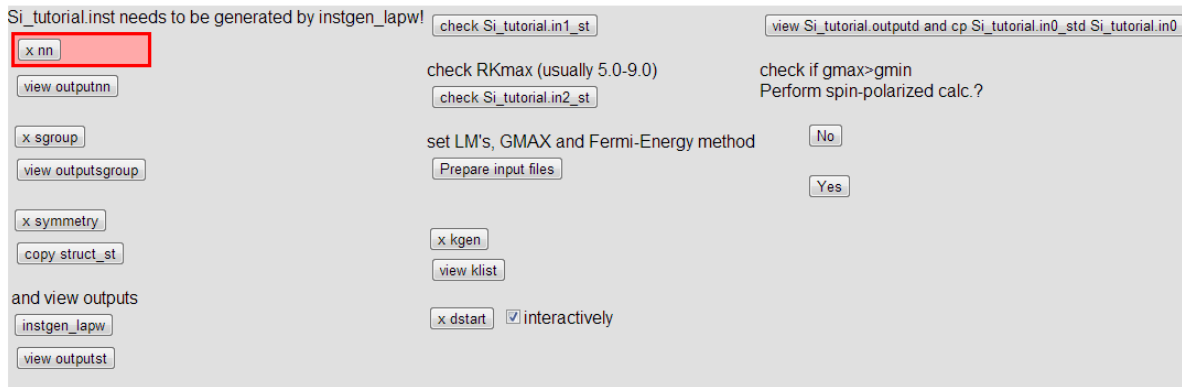
click though high lighted box. If the option to save a file ever comes up, make sure you click to save
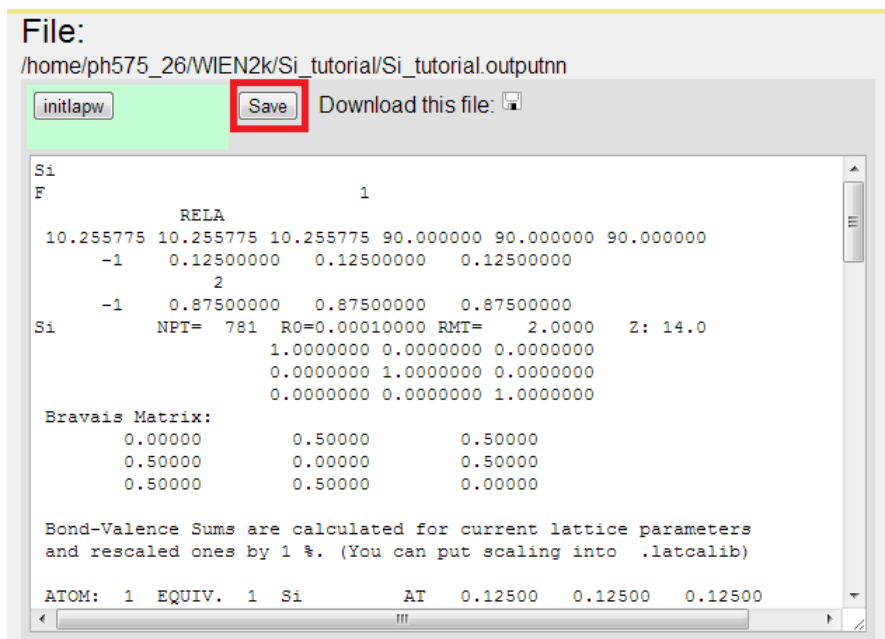
Click through all the the boxes. The one thing to take note of is when you get to x kgen in phase 16 you'll need to enter the number of k points you want to calculate. Around 100 for a semiconductor or a few thousand for metals. After you have clicked though all the steps you will be given the option 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.

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.

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

[ continue with DOS ]          [ Save ]  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 0.0000. 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. 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. The third column is just a title for you to put to remember what each row is for. You can see above the edited file there is something that says "ATOM Si: 1 tot". 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. When you click plot you'll see something that looks like the image below

Set ranges (optional):
xmin=[ ]   xmax=[ ]   ymin=[ ]   ymax=[ ]   [PLOT]

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

no line   ○ ◉ ◉ ◉
line:1 (total DOS) of Si_tutorial   ◉ ○ ○ ○
line:2 (tot) of atom Si   ○ ○ ○ ○
line:3 (s) of atom Si   ○ ○ ○ ○
line:4 (p) of atom Si   ○ ○ ○ ○
line:5 (d) of atom Si   ○ ○ ○ ○
line:6 (d-eg) of atom Si   ○ ○ ○ ○
line:7 (d-t2g) of atom Si   ○ ○ ○ ○

Define for first line: Label=[ ]   Linetype(0-9)=[1]   Linewidth=[1]
Define for second line: Label=[ ]   Linetype(0-9)=[2]   Linewidth=[2]
Define for third line: Label=[ ]   Linetype(0-9)=[3]   Linewidth=[2]
Define for fourth line: Label=[ ]   Linetype(0-9)=[4]   Linewidth=[2]

Plot DOS in [eV ▼]   [Color ▼]   Labelsize=[24]   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

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

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.
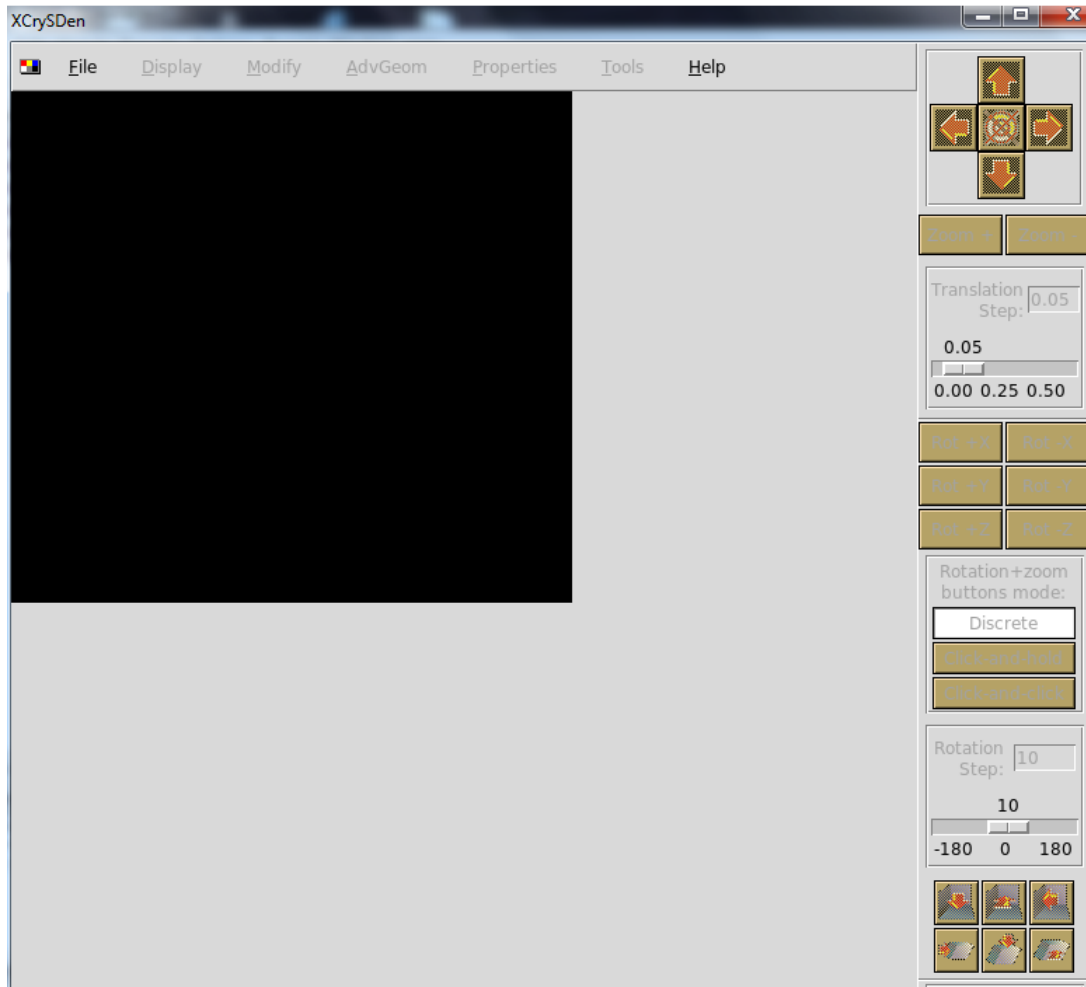
If this opens successfully head back to the web interface and your band structurer calculation. Click the generate k-mesh with xcrysden button. If you just get the message "Requires X-Windows system ..." go to the xterm window and enter the command "ps -u ph575_ 26". kill any process that says w2web 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-meh with xcrysden button again. Two windows should (eventually) open. One is just a pink text document, close it.

```
Automatic labeling of k-points                                         □ ▣ ✕

        NEW FEATURE: automatic labeling of the k-points
        -----------------------------------------------

        1. For a few "supported" Bravais lattices several k-points will be
           labeled automatically
           (Ref: http://www.cryst.ehu.es/cryst/get_kvec.html)

        2. The information within the XSF file are sometimes insufficient
           to determine the Bravais lattice type. The labelling of the k-points
           will be hopefully correct only if correct Bravais lattice type was
           determined

        *** CHECK THIS DATA:

        - the guessed BRAVAIS LATTICE TYPE : F-cubic
          ((the XSF's group number is 5))



                               [ Close ]
```

You should see an image like the below appear.
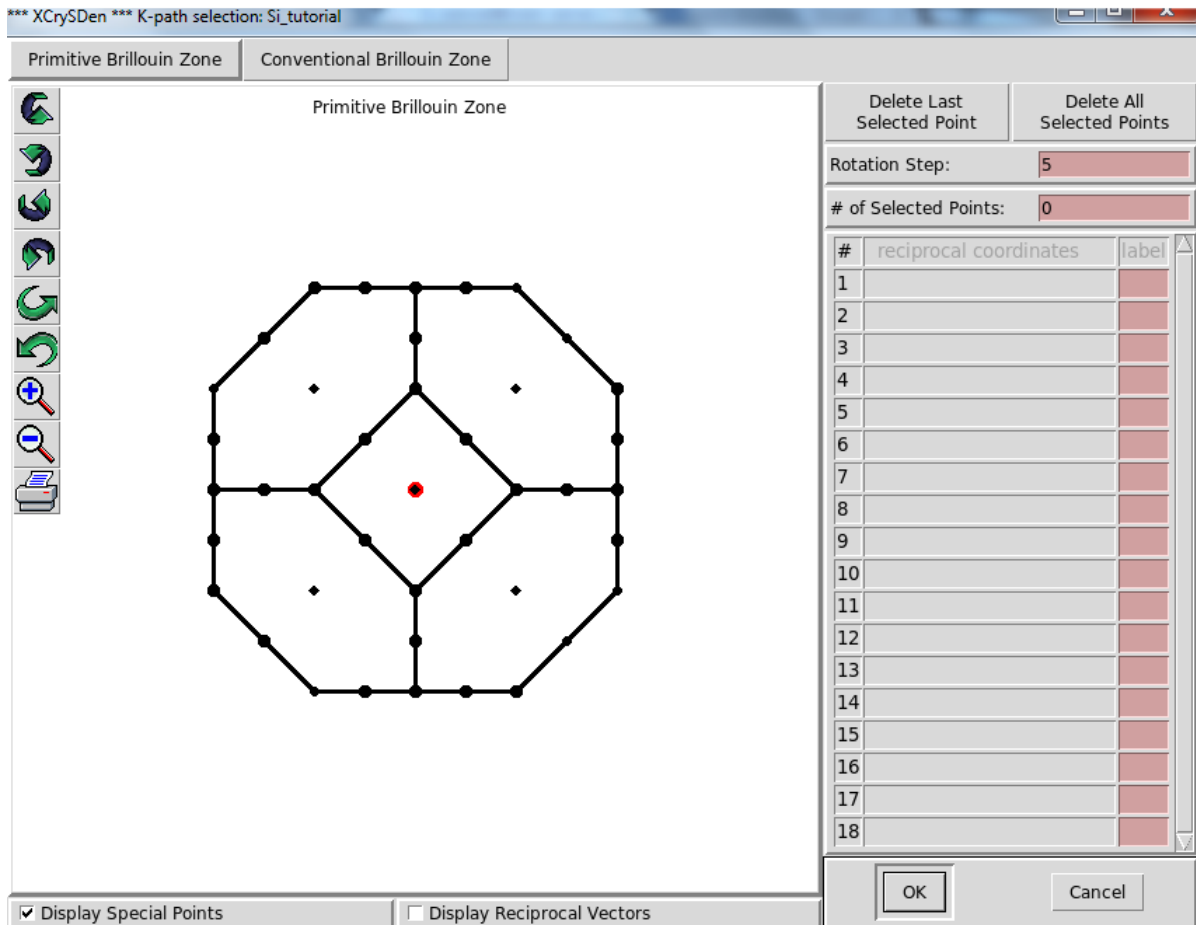
Each point corisponds to a high symmetry point in k-space such as the Γ point or the X point. After you have a path click ok.

NOTES:

    1. Please check if k-point coordinates looks OK. These k-points have integer coordinates, calculated as (kx*M, ky*M, kz*M), where M is an integer multiplier. Actual k-point coordinates are then obtained as: 1/M * (kx*M, ky*M, kz*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: 8

Total number of k-points along the path:

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

OK

Cancel

Ignore the line that starts with M multiple.... The second line is important. The total number of K-points along the path are the number of points that wien plots between the k-points you selected in the above step. (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,ysize [cm]
 1.0   4                         # major ticks, minor ticks
 1.0   1                         # character height, font switch
 1.1   2    4                    # line width, line switch, color swit
### Data configuration
-14.0  8.0  2                    # energy range, energy switch (1:Ry,
1     0.xxxx                     # Fermi switch,  Fermi-level (in Ry u
1    999                         # number of bands for heavier plottin
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.
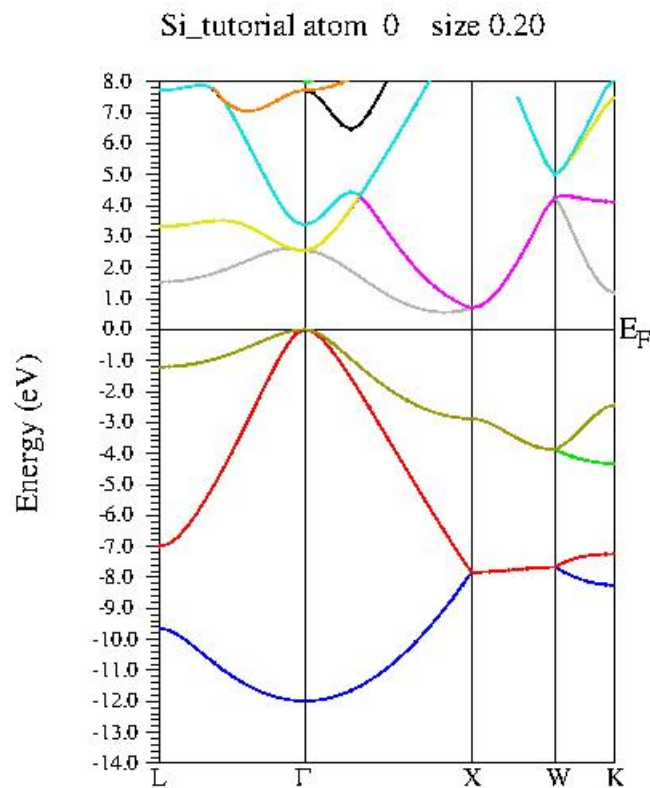
It is also possible to use the standard k-mesh that wien provides. Go back to the band plot menu and instead of using the 'from xcrysden' option in the drop down menu leave it as fcc and click the generate button to the right. You'll be asked to copy the file

click 'copy it' and then go through all of the buttons like you did for the xcrysden 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).
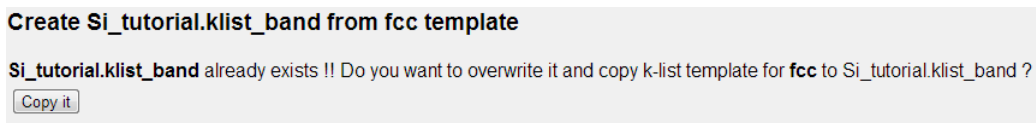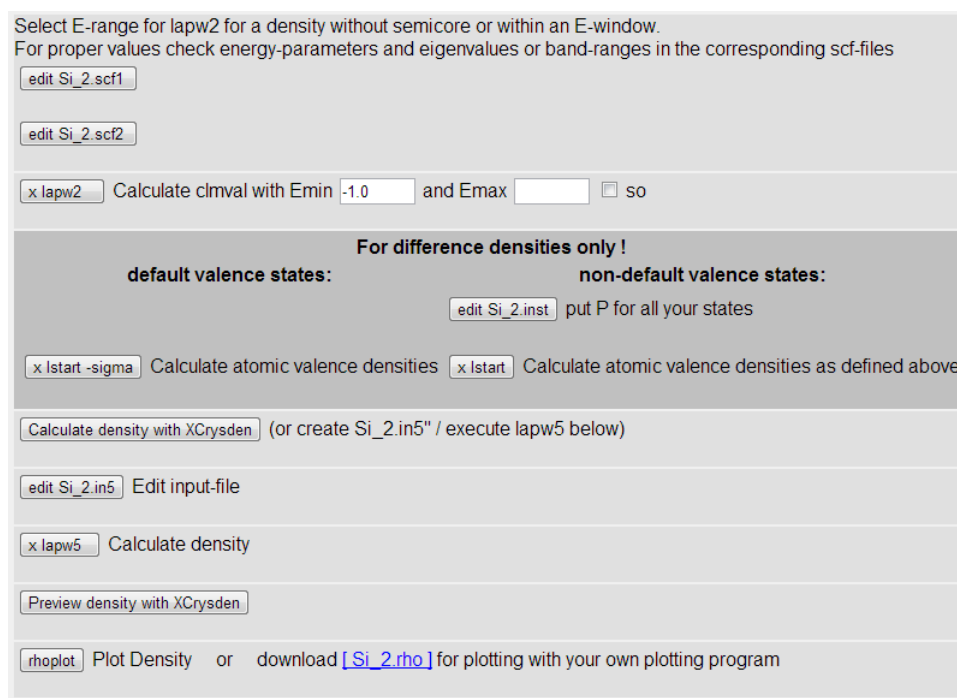
5   electron density

Now that xcrysden is working we can look at electron density. Choose "El Dens" from the right menu. You should see the fallowing screen

Click though the first two button. The third button had an E_{min} that you can set. This is used to make sure that the core electrons are removed. The two buttons above x lapw2 are supposed to tell you where to set E_{min} but I have yet to figure that out.

Once you have run x lapw2 skip the dark gray sections again. Click "Calculate density with xcrysden". It will open up 2 windows. One xcrysden that looks familiar. The other looks like below (again, if you get the "Requires X-Windows system ... Calc" error fallow the same steps as here.)
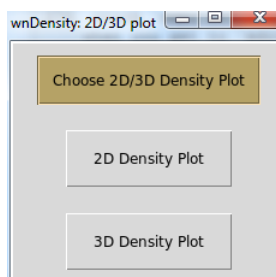
Choose the 2D plot. I haven't played too much at this point, but you'll see a screen that looks like
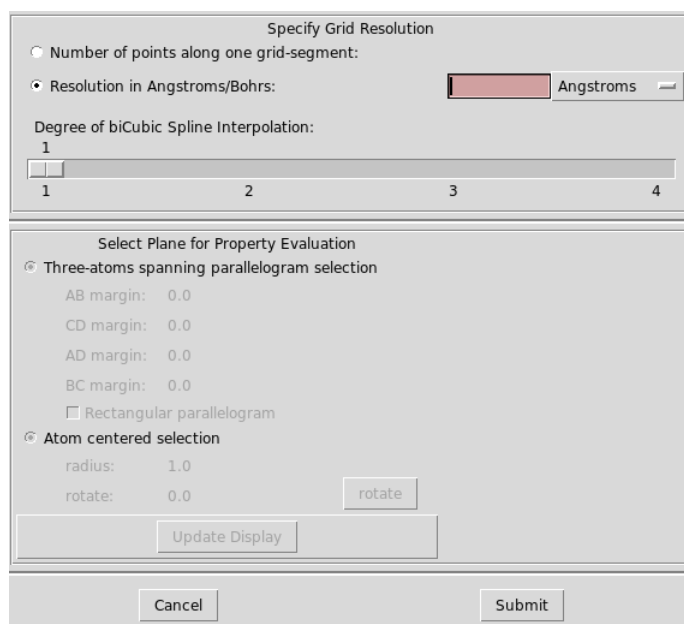
In the top section choose to "set number of points along one grid-segment" and enter a number. The important part is the second section. This is where you pick the three atoms that form what area you look at for your electron density. How wien works is it makes, or is given, three coordinates which it uses to define a plane. This plane is the cross section of the electron density that you will be looking at. What you are doing here are picking 3 atoms that will define this plane.

In the "select plane for property evolution" section select "three atoms spanning parallelogram selection" It looks like it has already been selected but is grayed out, it hasn't. Click it and it will open up a new window

Select a three-atoms spanning parallelogram. Please click on three atoms

```
                    ID Sym Atm.Num  X/Angstrom      Y/Angstrom      Z/Angstrom
---------------------------------------------------------------------------------
Selected Atom No.1:
Selected Atom No.2:
Selected Atom No.3:
---------------------------------------------------------------------------------
```

Display coordinates in units:
⦿ Angstrom   ○ Bohr   ○ Crystal-Convetional   ○ Crystal-Primitive   ○ Alat

[Next]   [Close]   [Selected]

At this point click over to the xcrysden window with the crystal. One atom you pick will be the center of your electron density plot. The other two will define the plane that you will be looking at. Pick any three atoms you want. After you pick three atoms the above will change to

Select a three-atoms spanning parallelogram. Please click on three atoms

```
                    ID Sym Atm.Num  X/Angstrom      Y/Angstrom      Z/Angstrom
---------------------------------------------------------------------------------
Selected Atom No.1:  5   Si  14     +2.035170093    +2.035170093    +4.748730216
Selected Atom No.2:  2   Si  14     +0.678390031    +3.391950154    +3.391950154
Selected Atom No.3:  6   Si  14     +2.035170093    +4.748730216    +2.035170093
---------------------------------------------------------------------------------
```

Display coordinates in units:
⦿ Angstrom   ○ Bohr   ○ Crystal-Convetional   ○ Crystal-Primitive   ○ Alat

[Next]   [Close]   [Selected]

hit the selected button. NOT NEXT, if you hit next you have to reselect the atoms. Not really a problem, just annoying if you forget and do it a few times......again, trust me. After you hit submit you'll go back to first window where you set the number of points along a grid segment. Select submit again. A new window will pop up, just hit ok, and then ok once again. A new window will open up, click submit and close. You can go back to your browser and wien at this point. The next button is edit case.in5. This is where you can manually set the which atoms define the plane instead of clicking on them in xcrysden. It should look like

[continue with electron density]   [Save] Download this file: ⬇

```
      1250000        6250000        6250000        10000000
      3750000        8750000        3750000        10000000
      3750000        3750000        8750000        10000000
3 2 3
50 50
RHO ADD
ATU VAL NODEBUG
NONORTHO
```

It will probably not be those exact numbers as they are specific to the atoms I choose and to what the system is but will have that pattern of three rows and four columns with

the 4th column being something like just 2 or 3 or something. Click save and continue. Click x lapw5, continue, and then click phoplot. You can preview it with xcrysden, but all this does it overlay the electron density plot with the atoms. After you hit rhoplot just click plot. You should see something that looks like
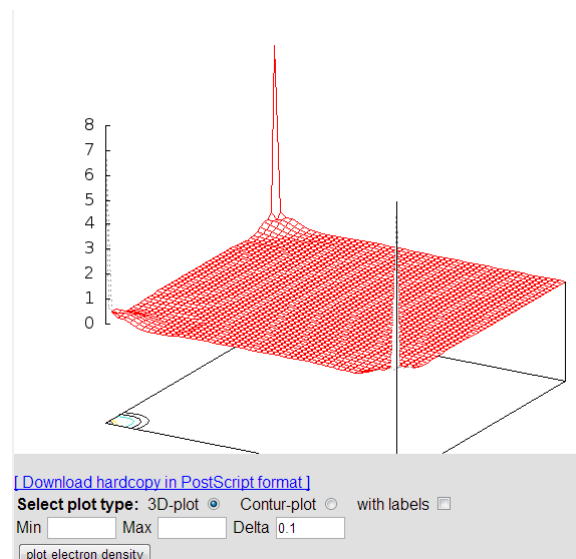
This doesn't look like much. After some playing (an exorcise I'll leave to the reader) you should be able to get a plot that looks something like
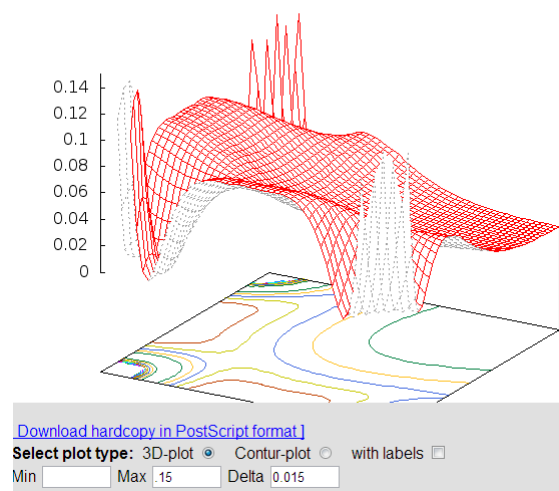
Now, you can go back to xcrysden and select a different set of three atoms for a new plane and a new perspective on your electron density.

6 XSPEC

This section will deal with XSPEC. XSPEC is a means of calculating the xray xpectrum for your materials. Before you can run XSPEC you must have partial density of states plotted. See section 3. Click XSPEC on the left and you will see
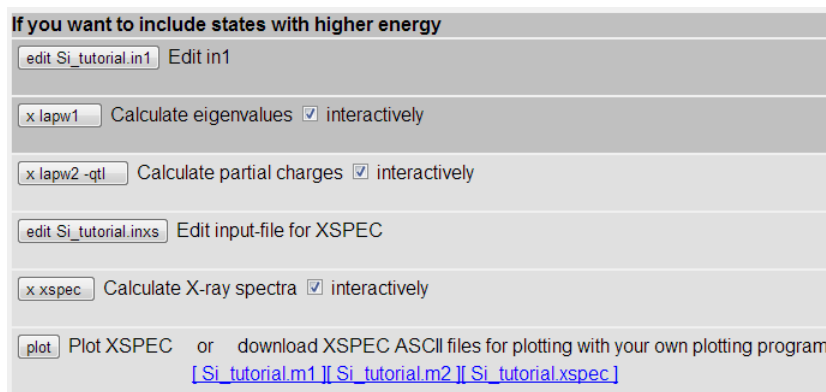
Skip the dark gray entries and start with xlapw2 -qtl. Click the edit next and then save and continue. Click x xspec, and then plot. In the plot you have various options for plots, such as broadened or unbroadened. You must also choose a column. The spectrum I get is
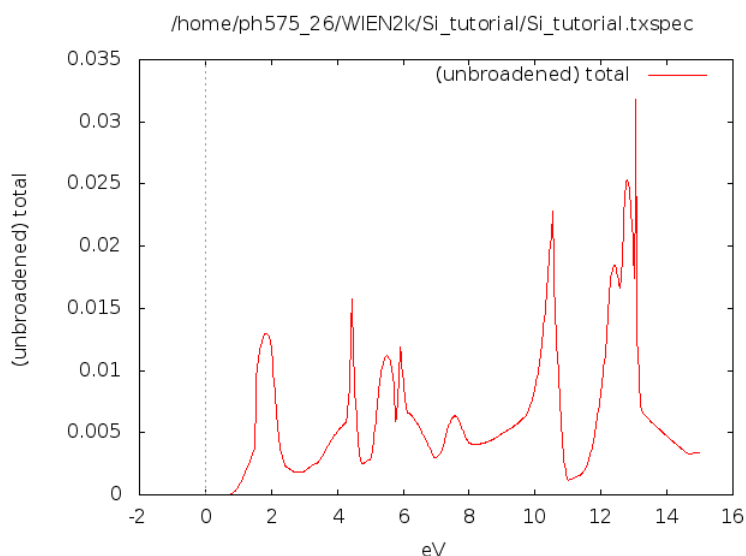
7 Optical properties

The last of the utilities I will look at is the OPTIC which lets us looks at the optical properties of the material. You must also have partial DOS plotted for this (see section 3). Select OPTIC on the left menu and you should get

```
x lapw2 -fermi   Calculate weights ☐ so ☑ interactively

edit Si_tutorial.inop   Edit Si_tutorial.inop

x optic   Calculate optics matrixelements ☐ so ☑ interactively

edit Si_tutorial.injoint   Edit Si_tutorial.injoint

x joint   Calculate epsilon-2 ☑ interactively

edit Si_tutorial.inkram   edit Si_tutorial.inkram

x kram   Calculate optical constants by Kramers-Kronig ☑ interactively

opticplot   Plot optical properties    or    download ASCII files for plotting with your own plotting program
```

Click through the first button. The second opens up the window

```
99999 1        number of k-points, first k-point
-5.0 3.0 9999 Emin, Emax for matrix elements, NBvalMAX
2              number of choices (columns in *outmat): 2: hex or tetrag. ca
1              Re xx
3              Re zz
OFF            ON/OFF   writes MME to unit 4

Choices:
1......Re <;x>;<;x>;
2......Re <;y>;<;y>;
3......Re <;z>;<;z>;
4......Re <;x>;<;y>;
5......Re <;x>;<;z>;
6......Re <;y>;<;z>;
7......Im <;x>;<;y>;
8......Im <;x>;<;z>;
9......Im <;y>;<;z>;
```

This lets you pick what components you want to look at. I.e. do you want to look at xx part or the yz. It also lets your select the real or imaginary part for complex components. The number of points you can chose is the number in the third column. It is currently set to 2. The two rows below it are which components are being selected. they are currently 1 the xx and 3 the zz. This is made clear in the table bellow this labeled choices. Make your choices and save and continue. Do x optic. Next is edit case.injoint You will see

This is where you select what optical property to look at, though, at the end, it seems all are plotable. For now you can just click save and continue. Click through the rest of the buttons. When you get to plot you can see a list off optical properties to plot. I have selected epsilon and got the fallowing plot