Plotting of Charge Density Obtained from Siesta run

Dr Mohan L Verma

Computaional Nanoionics Research Lab, Deparment of Applied Physics, FET-SSGI,

Shri Shankaracharya Technical Campus-Junwani Bhilai (Chhattisgarh) INDIA 490020

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In many studies we need to study the charge density analysis if system in different physical conditions. Siesta is quite enough for this study. For this you need to add one more line :

SaveRho .true. in systemlevel.fdf input file.

After successful siesta run we obtained **systemlevel.RHO** file in the directory of siesta run. This is a grid file. Before plotting charge density using xcrysden (http://www.xcrysden.org/), a post-processing tool **rho2xsf** is used to covert into **xsf** file which is compatible in xcrysden**.** This tool is available in form of rho2xsf.f in

~siesta-3.1/Util/Contrib/APostnikov which can be compiled using a simple command

make

You will get a binary file **rho2xsf** in this directory alongwith some more other binary files. Copy this file to the directory where your systemlable.RHO file is present. Now use the command and follow the steps as:

./rho2xsf

You will be asked for system lable of your system. Now open your fdf file of siesta run and give the appropriate systemlable. In my case it is “peorel5-liI-lda”

```
[drmohanlv@localhost peo5-LiI-lda-opt]$ ls
BASIS_ENTHALPY          INPUT_TMP.496033915    peorel5-liI-lda.BONDS_FINAL
BASIS_HARRIS_ENTHALPY   I.psf                  peorel5-liI-lda.CG
BLOCK_INDEXES           Li.ion                 peorel5-liI-lda.DM
C.ion                   Li.ion.xml             peorel5-liI-lda.DOS
C.ion.xml               Li.psf                 peorel5-liI-lda.EIG
CLOCK                   NON_TRIMMED_KP_LIST    peorel5-liI-lda.FA
C.psf                   OCCS                   peorel5-liI-lda.KP
fdf.log                 O.ion                  peorel5-liI-lda.PDOS
field                   O.ion.xml              peorel5-liI-lda.RHO
FORCE_STRESS            O.psf                  peorel5-liI-lda.STRUCT_NEXT_ITER
fort.48                 pdos.xml               peorel5-liI-lda.STRUCT_OUT
H.ion                   peo10-LiI              peorel5-liI-lda.xml
H.ion.xml               peo5-liIm.xyz          peorel5-liI-lda.XSF
H.psf                   peorel5-agi.fdf        peorel5-liI-lda.XV
I.ion                   peorel5-agi.fdf~       peorel5-liI-lda.xyz
I.ion.xml               peorel5-agi.out        rho2xsf
INPUT_TMP.403589736     peorel5-liI-lda.alloc  siesta
INPUT_TMP.403619976     peorel5-liI-lda.ANI    vibra
INPUT_TMP.473340166     peorel5-liI-lda.BONDS
[drmohanlv@localhost peo5-LiI-lda-opt]$ ./rho2xsf
 Specify  SystemLabel (or 'siesta' if none):
```

then you will be asked for scale either in Angstrom or Bohr. I use Angstrom in general

```
[drmohanlv@localhost peo5-LiI-lda-opt]$ ls
BASIS_ENTHALPY          INPUT_TMP.496033915    peorel5-liI-lda.BONDS_FINAL
BASIS_HARRIS_ENTHALPY   I.psf                  peorel5-liI-lda.CG
BLOCK_INDEXES           Li.ion                 peorel5-liI-lda.DM
C.ion                   Li.ion.xml             peorel5-liI-lda.DOS
C.ion.xml               Li.psf                 peorel5-liI-lda.EIG
CLOCK                   NON_TRIMMED_KP_LIST    peorel5-liI-lda.FA
C.psf                   OCCS                   peorel5-liI-lda.KP
fdf.log                 O.ion                  peorel5-liI-lda.PDOS
field                   O.ion.xml              peorel5-liI-lda.RHO
FORCE_STRESS            O.psf                  peorel5-liI-lda.STRUCT_NEXT_ITER
fort.48                 pdos.xml               peorel5-liI-lda.STRUCT_OUT
H.ion                   peo10-LiI              peorel5-liI-lda.xml
H.ion.xml               peo5-liIm.xyz          peorel5-liI-lda.XSF
H.psf                   peorel5-agi.fdf        peorel5-liI-lda.XV
I.ion                   peorel5-agi.fdf~       peorel5-liI-lda.xyz
I.ion.xml               peorel5-agi.out        rho2xsf
INPUT_TMP.403589736     peorel5-liI-lda.alloc  siesta
INPUT_TMP.403619976     peorel5-liI-lda.ANI    vibra
INPUT_TMP.473340166     peorel5-liI-lda.BONDS
[drmohanlv@localhost peo5-LiI-lda-opt]$ ./rho2xsf
 Specify  SystemLabel (or 'siesta' if none): peorel5-liI-lda
 Now define the grid cell for your XCrysDen plot.
 Note that it can be arbitrarily chosen with respect to the Siesta simulation cell, and it needs not to be orthogonal. We'll define it by the origin point and three spa
nning vectors. They can be given in Bohr or Ang.
 Would you use Bohr (B) or Ang (A) ?
```

Then choose the origin as (0 0 0). Now you have to define your system size using spaning vectors along x y and z directions. You can follow the lattice vector block of fdf file for help . In this example I used the block as :

%block LatticeVectors

5.0000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 12.0000000000

%endblock LatticeVectors

This will define the size of cell under consideration. You can try different size and see the effect on the final plot.

Finally choose the grid points along the directions under consideration i.e. For 3d one can use :

100 100 100

```
[drmohanlv@localhost peo5-LiI-lda-opt]$ ./rho2xsf
 Specify  SystemLabel (or 'siesta' if none): peorel5-liI-lda
 Now define the grid cell for your XCrysDen plot.
 Note that it can be arbitrarily chosen with respect to the Siesta simulation cell, and it needs not to be orthogonal. We'll define it by the origin point and three spa
nning vectors. They can be given in Bohr or Ang.
 Would you use Bohr (B) or Ang (A) ? A
 Enter origin point in Ang  : 0 0 0
 Enter 1st spanning vector in Ang  : 5 0 0
 Enter 2nd spanning vector in Ang  : 0 10 0
 Enter 3rd spanning vector in Ang  : 0 0 12
  File peorel5-liI-lda.XSF exists. Overwrite? (Y/N)
Y
  The box contains          38  atoms.
 Now define the grid. If you want it two-dimensional,
 give 1 as number of grid points along one spanning vector.
 Enter number of grid points along three vectors: 100 100 100
 Add grid property (LDOS, RHO, ...; or BYE if none):
```

Now give the grid file which has to be converted. Here **RHO**

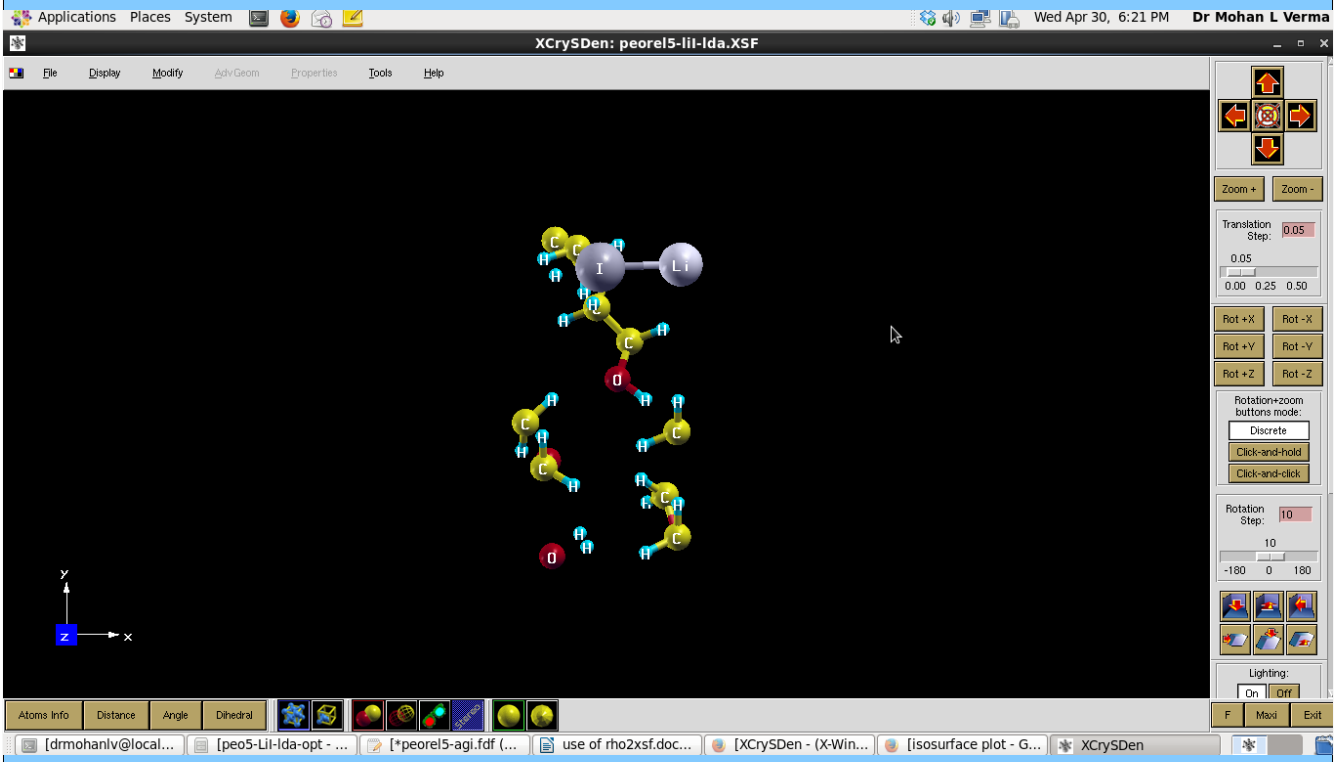
Then finally say **BYE** to the utility rho2xsf. Now search the working dir whether systemlable.XSF file is present or not. If yes then start xcrysden for further plot.

```
[drmohanlv@localhost peo5-LiI-lda-opt]$ ./rho2xsf
 Specify  SystemLabel (or 'siesta' if none): peorel5-liI-lda
 Now define the grid cell for your XCrysDen plot.
 Note that it can be arbitrarily chosen with respect to the Siesta simulation cell, and it needs not to be orthogonal. We'll define it by the origin point and three spa
nning vectors. They can be given in Bohr or Ang.
 Would you use Bohr (B) or Ang (A) ? A
 Enter origin point in Ang  : 0 0 0
 Enter 1st spanning vector in Ang  : 5 0 0
 Enter 2nd spanning vector in Ang  : 0 10 0
 Enter 3rd spanning vector in Ang  : 0 0 12
  File peorel5-liI-lda.XSF exists. Overwrite? (Y/N)
Y
  The box contains          38  atoms.
 Now define the grid. If you want it two-dimensional,
 give 1 as number of grid points along one spanning vector.
 Enter number of grid points along three vectors: 100 100 100
 Add grid property (LDOS, RHO, ...; or BYE if none): RHO
 Found and opened: peorel5-liI-lda.RHO
 mesh0 = (          54         108         128 ),   nspin=           1
 For is=1: max. grid value = 1.09868E+00 at iix,iiy,iiz=   3   8  83
 For is=1: min. grid value =-1.33490E-09 at iix,iiy,iiz=  44  39  12
 Add grid property (LDOS, RHO, ...; or BYE if none): BYE
  A wild guess! There is no file peorel5-liI-lda.BYE; close XSF and quit.
```

Now lets use **xcrysden** for plot using the command :

xcrysden - - xsf systemlevel.XSF

we will get one interactive xcrysden windows with the complete system under study . Make some display modifications and get :

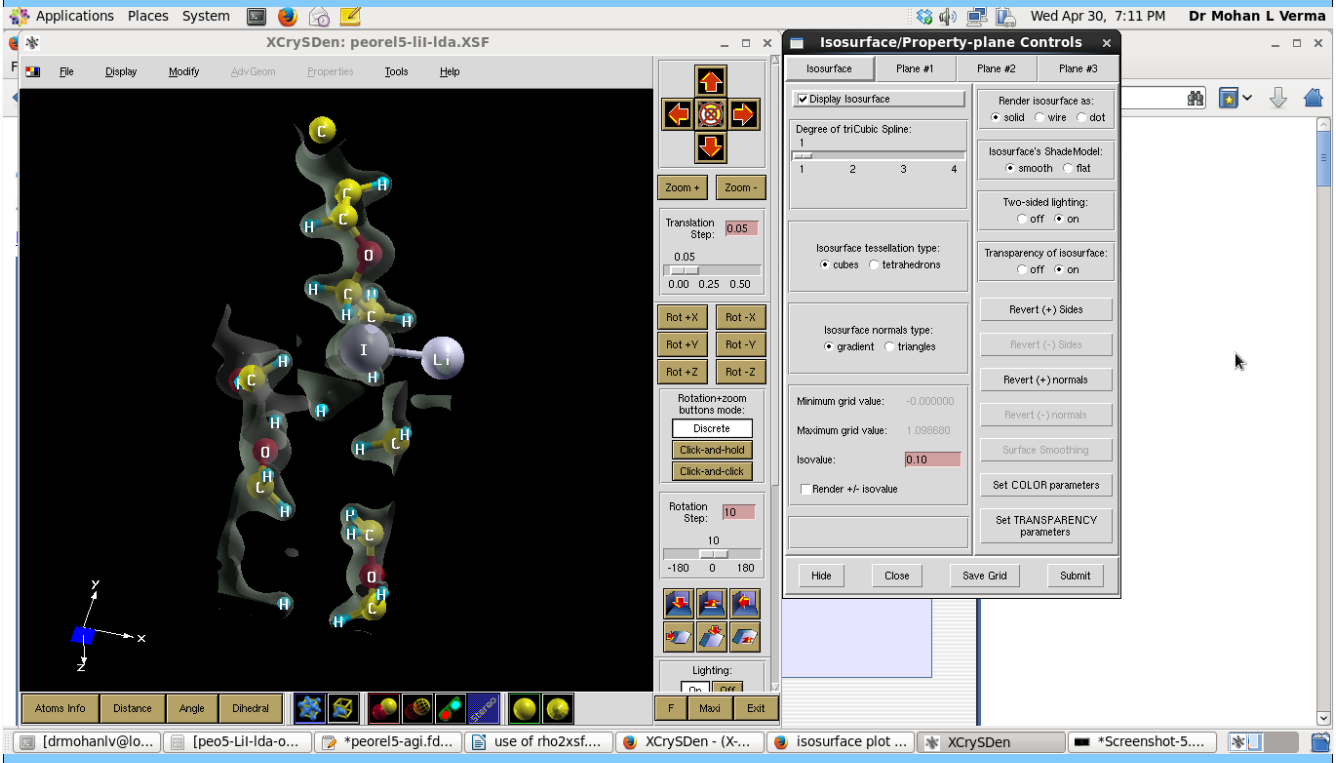


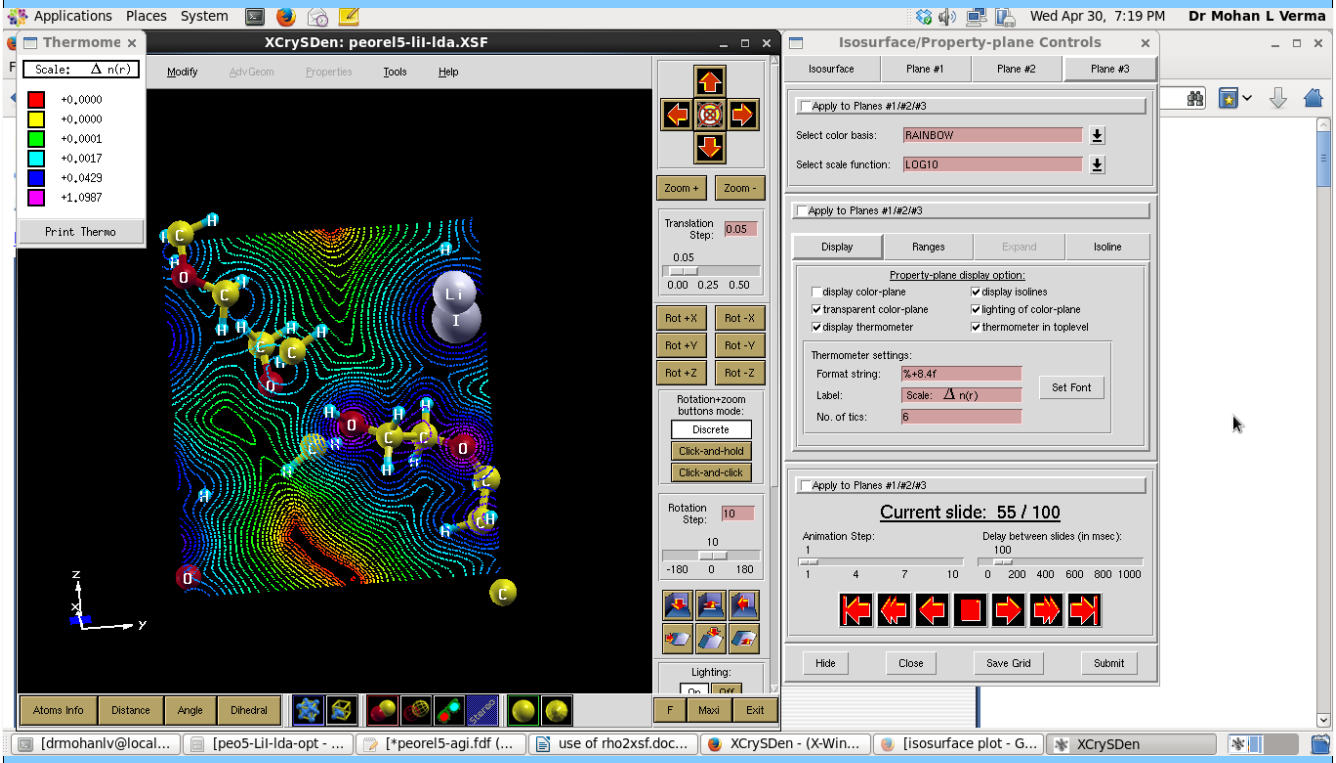
Now follow some steps to make charge density plot. Click on the tool of xcrysden window and use multiply factor =1.0 data grid. Now Use xcrysden manual :

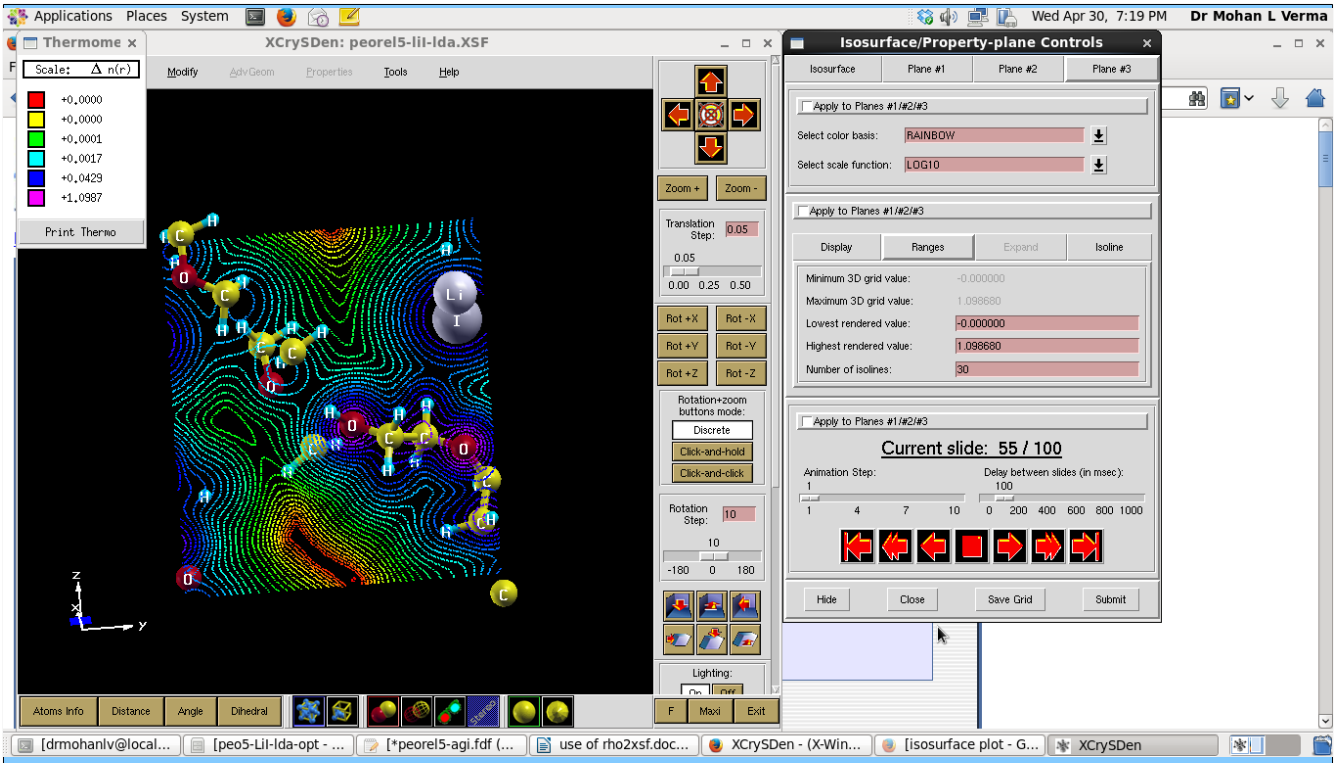
http://www.xcrysden.org/doc/isocontrol.html#__toc__5 and

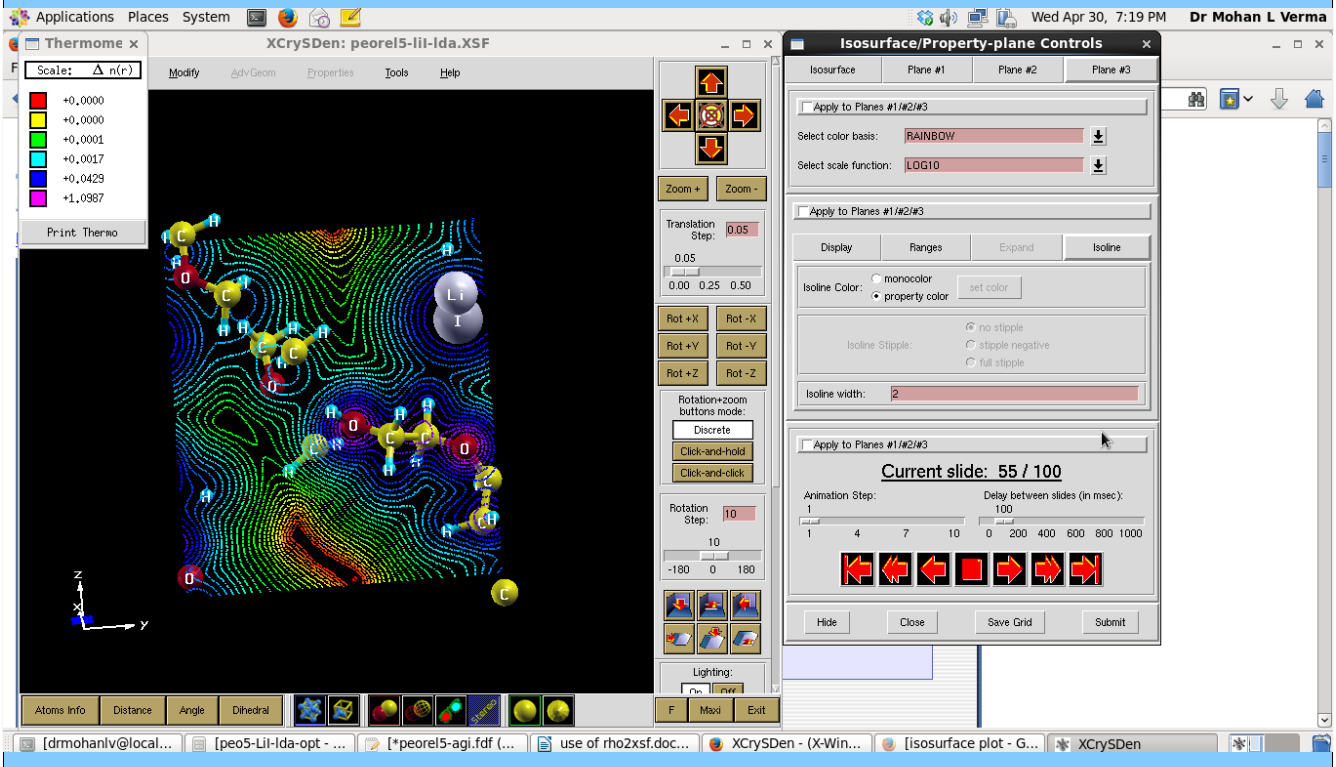
http://www.xcrysden.org/doc/plane1control.html

Some snaps from my system :









For any doubt during the process you can contact in : drmohanlv@gmail.com