Hands on Session 5: Converging Absorption Spectra and Plotting Exciton Wavefunctions

BerkeleyGW Workshop
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Converging Absorption

General Parameters:

- K-grid sampling (WFN_fi, WFNq_fi)
  - Generally need to be finer when excitons are localized in k-space
- Number of valence bands and conduction bands (eqp.dat)
  - Needs to capture all the transitions in the energy range of interest

Parameters Particular to BGW:

- Coarse k-grid (WFN_co, same as for epsilon)
  - Need to be fine enough to capture correct screening
- Number of coarse grid bands used in interpolation (eqp_co.dat)
  - Interpolation quality reported in dcc_mat.dat and dvv_mat.dat files

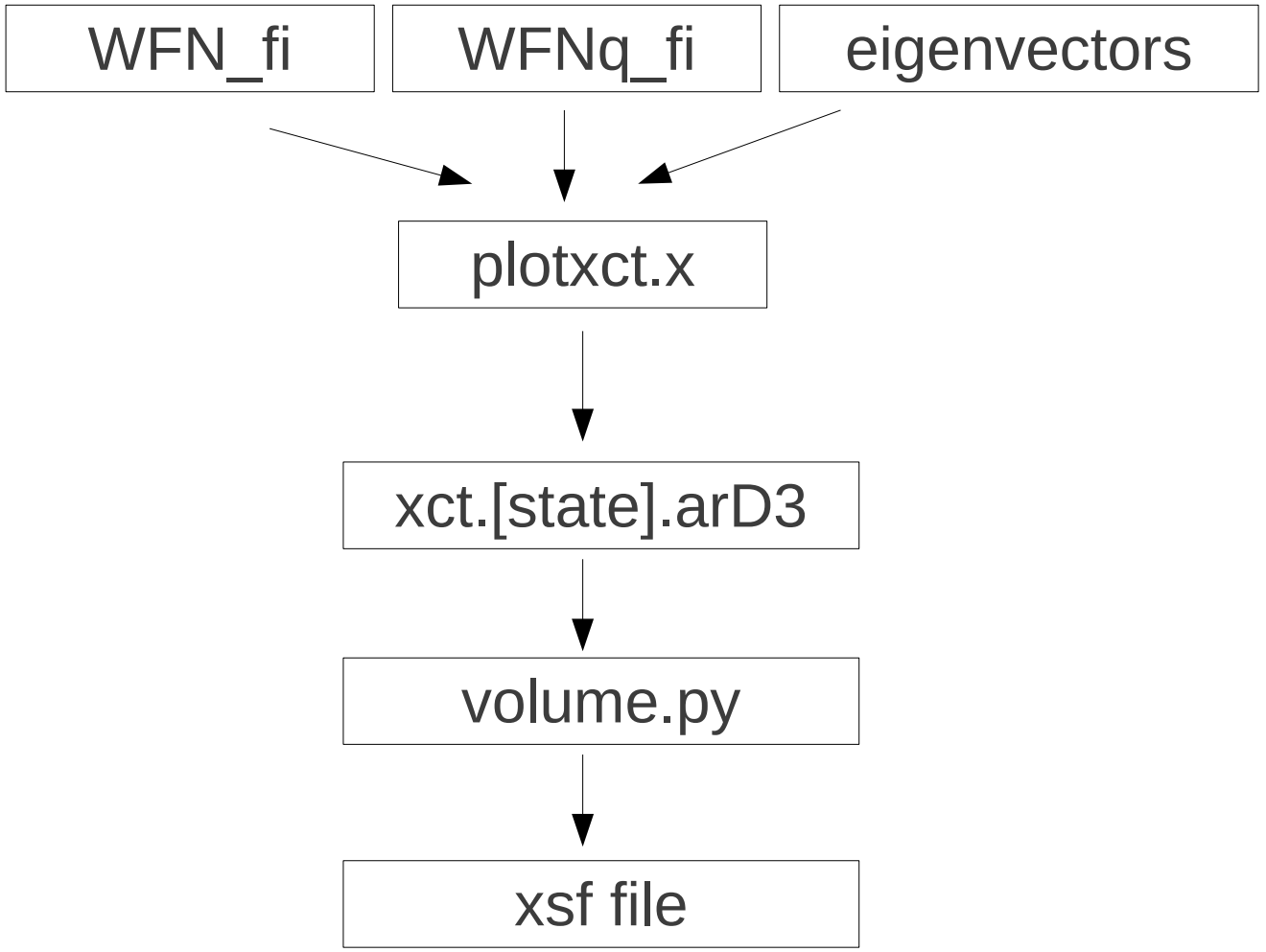
Plotting Exciton Wavefunctions

- Plotxct.x calculates the exciton wavefunction in real-space with the position of the hole ($\mathbf{x}_h$) fixed at one point:

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = \sum_{\mathbf{k},c,v} A^S_{vc\mathbf{k}} \psi_{\mathbf{k},c}(\mathbf{r}_e) \psi^*_{\mathbf{k},v}(\mathbf{r}_h)$$

- You need the following information in plotxct.inp:
  - **plot_state**: the number of the exciton state you wish to plot
  - **q_shift**: the q_shift in your WFNq_fi file
  - **supercell_size**: the size of the real-space supercell
    - This is limited by the smallest k-vector in WFN_fi
  - **hole_position**: position of the hole in real-space
  - **lattice_vectors**: real-space lattice vectors for your supercell

PlotXct Workflow



Exciton eigenvectors are only printed when you include **write_eigenvectors** in absorption.inp

Volume.py takes the real part, imaginary part, modulus, or modulus squared of the wavefunction printed by plotxct.x and writes it in a format readable by XCrysden

Example Outline

Session 5.1: Converging Absorption for Si calculations

- Goals:
  - Look at convergence of absorption with respect to **k-point sampling** and the **number of bands**
  - We will look at absorption on two k-grids in addition to the k-grid used in the last example.

Session 5.2: Plot exciton wavefunctions for LiCl

- Goals:
  - Learn how to use BGW visualization tools to plot the exciton wavefunction

Session 5.1: Converging Absorption

- Please do the following

  ``cp -rP /project/projectdirs/m1649/BGW-2013/5.1-Si_convergence/ $SCRATCH``

  and follow the directions in the README file.

- For the sake of time, we will not generate the mean field wavefunctions during this example. Instead, the WFN and output files are provided in each subdirectory. Take a look at the PARATEC input files, and make sure you understand what's going on.

- When you feel comfortable with the mean field input files go to the directory ``5.1-Si_convergence/2-bgw/`` and follow the directions in the README file.

This section should take ~30 minutes.

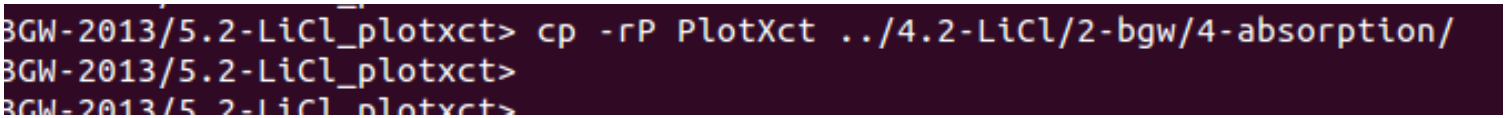
Session 5.2: Plotting Exciton Wavefunctions

Please do the following

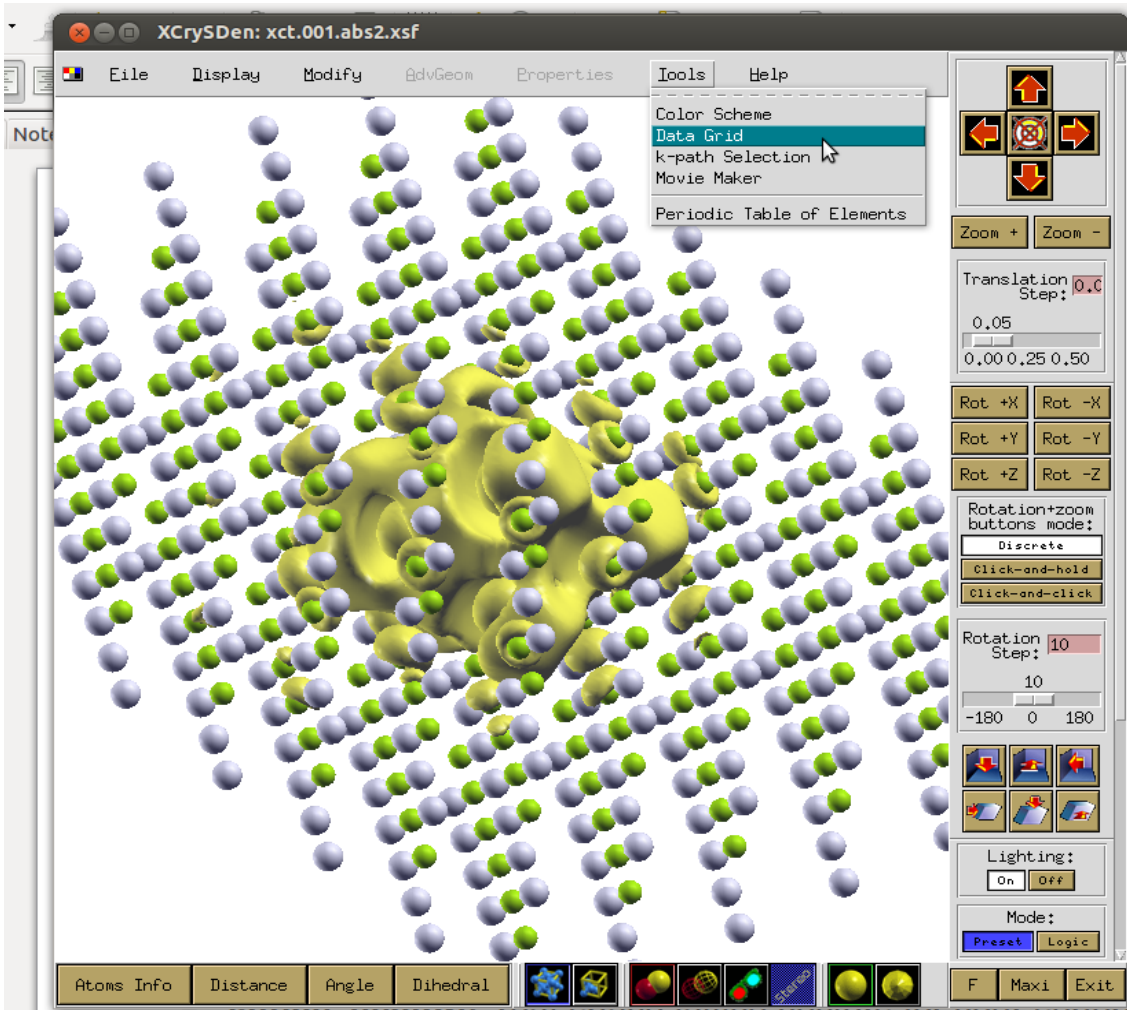
``cp -rP /project/projectdirs/m1694/BGW-2013/5.2-LiCl/PlotXct/ $SCRATCH``

and follow the instructions in the README files.

- You will need to copy the PlotXct directory to the absorption directory for the previous LiCl example:



This section should take ~30 minutes.


XCrySDen: xct.001.abs2.xsf
File
Display
Modify
AdvGeom
Properties
Tools
Help
Color Scheme
Data Grid
k-path Selection
Movie Maker
Periodic Table of Elements
Zoom +
Zoom -
Translation Step:
0.05
0.00 0.25 0.50
Rot +X
Rot -X
Rot +Y
Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
10
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Lighting:
On
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Mode:
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Logic
Atoms Info
Distance
Angle
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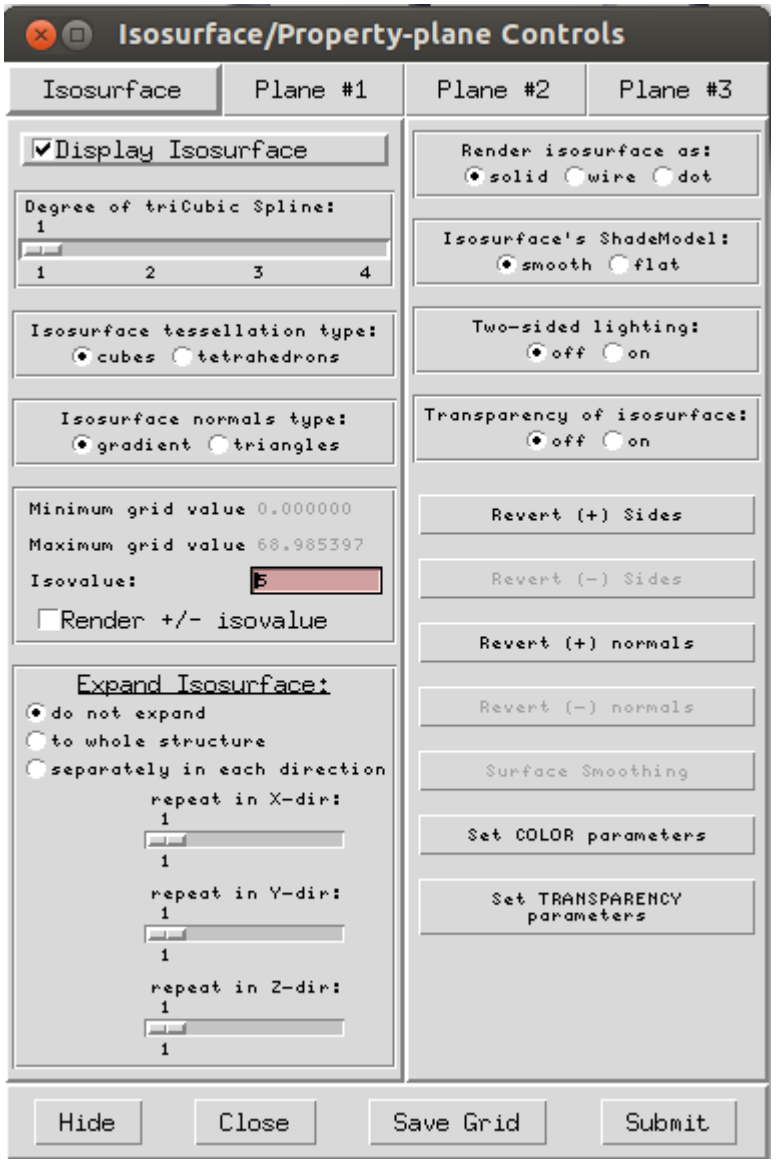
Isosurface/Property-plane Controls
Isosurface
Plane #1
Plane #2
Plane #3
Display Isosurface
Degree of triCubic Spline:
1
1 2 3 4
Isosurface tessellation type:
cubes
tetrahedrons
Isosurface normals type:
gradient
triangles
Minimum grid value 0.000000
Maximum grid value 68.985397
Isovalue:
Render +/- isovalue
Expand Isosurface:
do not expand
to whole structure
separately in each direction
repeat in X-dir:
repeat in Y-dir:
repeat in Z-dir:
Render isosurface as:
solid
wire
dot
Isosurface's ShadeModel:
smooth
flat
Two-sided lighting:
off
on
Transparency of isosurface:
off
on
Revert (+) Sides
Revert (-) Sides
Revert (+) normals
Revert (-) normals
Surface Smoothing
Set COLOR parameters
Set TRANSPARENCY parameters
Hide
Close
Save Grid
Submit