# REU 2015
# Computational Chemistry Manual

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This manual was created to provide a one-stop-shop for basic computational chemistry procedures for the two-week-long REU computational boot camp during the summer of 2015.

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# Part 1: Remote Computing and Model Building

## Accessing and navigating computer resources

You may want to consider installing some software on your own laptop. Here is a list of software with links to download sites:

- MobaXterm http://mobaxterm.mobatek.net/
- WinSCP (to transfer files) http://winscp.net/eng/download.php

Open MobaXterm, which is found on the desktop or in the list of programs on your computer. You will be prompted to type something.

First, we need to gain admission to the HPC:

>ssh kilin-lab@hpc.usd.edu

You will then be prompted to enter your password.

You now have direct communication with HPC. A few important features:

- Please do not alter folders or files that do not belong to you.
- These folders contain nearly everything you need to complete this research.
- Linux computer language is used.

Using Linux to move through the directory (we will navigate to where we will be saving all of our work):

>cd Folder_name

>cd .. (this command moves you up one level in the folder hierarchy)

Making directories:

>mkdir Folder_name

Everyone should make a directory with his/her name in the following location:

/home/kilin-lab/REU2015/

Moving folders or files:

>mv FILEorFOLDER_name /home/kilin-lab/REU2015/new_location

Copying folders or files:

>cp FILEorFOLDER_name /home/kilin-lab/location

>cp FILEorFOLDER .

Other useful commands:

>ls (lists files and folders in current directory)

>pwd (print working directory, tells you your location within the hierarchy)

## Text editors

>nano optional_file_name

Nano provides on-screen commands so no common commands will be listed.

>vi optional_file_name

Common vi commands:

- i – insert (to begin typing)
- [Esc] – returns to command mode (no typing)
- :wq – exit and save changes
- :q! – exit without saving
- dd – delete current line
- d(number)d – deletes that number of lines

Copying files from HPC to local computer:

Open new MobaXterm window but do NOT log into HPC. Type:

>scp kilin-lab@hpc.usd.edu:/home/kilin-lab/REU2015/my_folder file.txt .

If one uses the above command, the file should be transferred to your computer's MobaXterm folder. Example: C:\MobaXterm\home\MyLaptop. Alternatively, you can use free software such as WinSCP for click-and-drag type transfers.

## Building a model

Several free software packages are available to download, such as Avogadro and JMOL. The major factor in deciding which program to use is being able to convert that file format to a usable format for computations. (Both Avogadro and JMOL meet this criterion.)

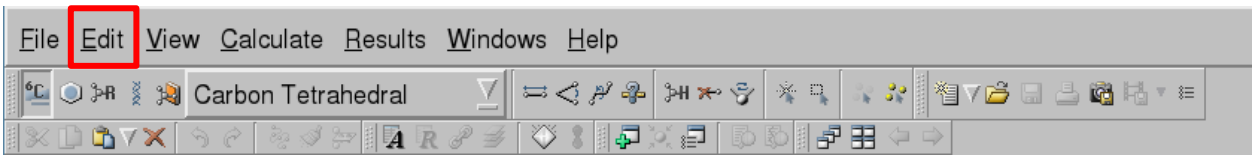
If you use software mentioned above, you must be able to convert between formats. An example if you used Avogadro and saved the file as .xyz and wish to use it as input for Gaussian:

>babel –ixyz filename.xyz –ocom filename.com

Gaussview can be used to build models. This program is available on HPC. To access:

>gv

Once you've built your model, save it and you can use it to submit a job. Click on [$^{6}$C] to choose an atom, then click on the area you'd like to place the atom. Click [Edit], [Clean] to clean the structure.



# Part 2: Gaussian job set-up and analysis

## Intro to Gaussian (building a geometry optimization job)

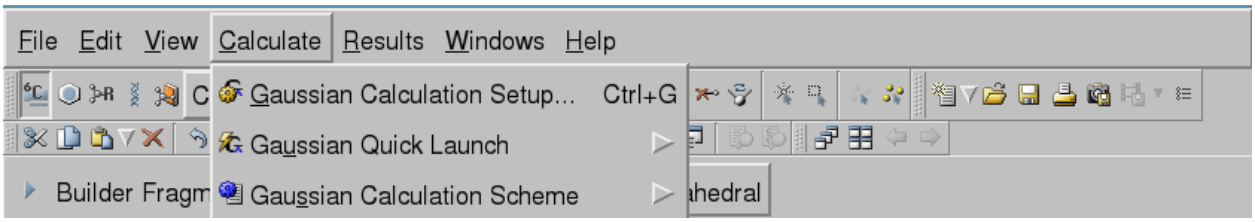
What does "geometry optimization" mean and why is it important?

- An optimized structure occurs at minimized energy which is somewhat synonymous with molecule stability.
    - Example from Wikipedia: when optimizing the geometry of a water molecule, one aims to obtain the hydrogen-oxygen bond lengths and the hydrogen-oxygen-hydrogen bond angle which minimize the forces that would otherwise be pulling atoms together or pushing them apart.
- Global vs local energy minima (saddle points and potential energy surface)

What other kind of jobs can you specify? A few examples:

- **SP**: Single point energy.
- **Opt**: Geometry optimization.
- **Freq**: Frequency and thermochemical analysis.
- **Scan**: Potential energy surface scan.
- **Force**: Compute forces on the nuclei.

Gaussian jobs use one input file, (.com). This file will contain all instructions necessary for the job to complete. First build or load you molecule or system into Gaussview, and when you're ready to set up the job, click on 'Calculate.' A new window pops up in order to select from many options.




There are several tabs when the new window pops up:


There are many types of jobs and choices to make. We'll go through these together. But briefly, one must specify (and some examples):

- Job type
    - Single point
    - Geometry optimization
- Method
    - Hartree-Fock
    - Density functional theory

- Basis set
    - STO3G
    - 6-31G
    - LANL2DZ

Once complete, click on [Submit] and you'll be prompted to save the file. Choose an appropriate filename and location. Also, it is good practice to view the .com file in a text editor to make sure there are no errors. Also, there must be an empty line at the end of the file.

>nano filename.com

```
%nprocshared=4                          (number of processors requested)
%mem=12GB                               (amount of memory requested)
%chk=ZnTiO3_1x3.chk                     (this generates a .chk file)
#opt hf/lanl2dz                         (job details, type of job and basis set)

ZnTiO3_1x3                              (name of job)

0  1                                    (spin multiplicity)
O       0.00000     0.00000     1.94950     (3D coordinates)
O       0.00000     1.94950     0.00000
O      -0.00000    -1.94950     0.00000
O       0.00000     1.94950     3.89900
O       0.00000    -1.94950     3.89900 (↓)
```

Gaussian output files (.log or .out) contain requested calculations indicated by the input file.

Gaussian checkpoint files (.chk) or formatted checkpoint (.fchk) contain more information about orbitals and electron density that we may want to use later.

## Submitting a geometry optimization job in Gaussian.

If we have completed an input file, we are ready to submit it to the HPC.

>rungaussian filename.com

A prompt will inform you that your job was submitted (assuming there are no errors) and will tell you what your job number is. You can then monitor your job status in a few ways.

To obtain a list of all running jobs within kilin-lab:

>qstat

To obtain only your job's status:

>qstat | grep job_number  (type your job number)

Example: >qstat | grep 254855

# Part 3: Analysis of Gaussian results

- Total energy
- Orbitals and their occupation
- Plotting/visualizing orbitals
- ESP maps
- Density of states

Note: occasionally you run into an error using .chk file. If this happens, you can convert .chk for .fchk by typing:

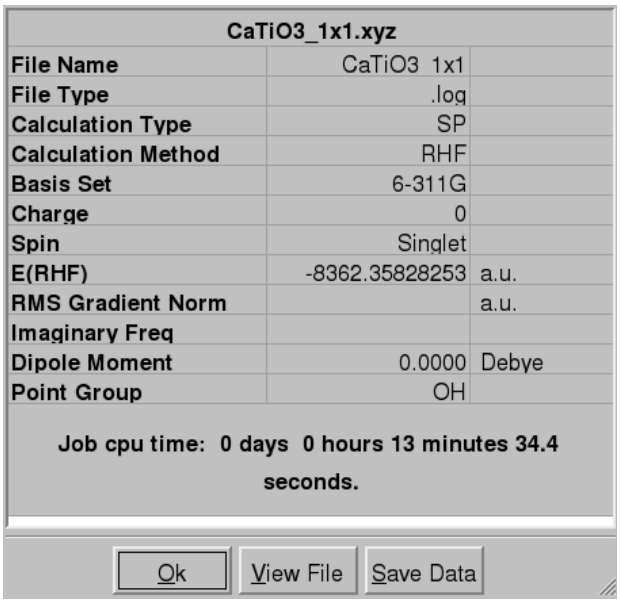
- >formchk filename.chk filename.fchk

## Total Energy

Open Gaussview and load the .chk file for the results you'd like to analyze. The simplest way to do this is to navigate to the folder prior to launching GV. Then you just need to specify which file to open. This can be done in one step.

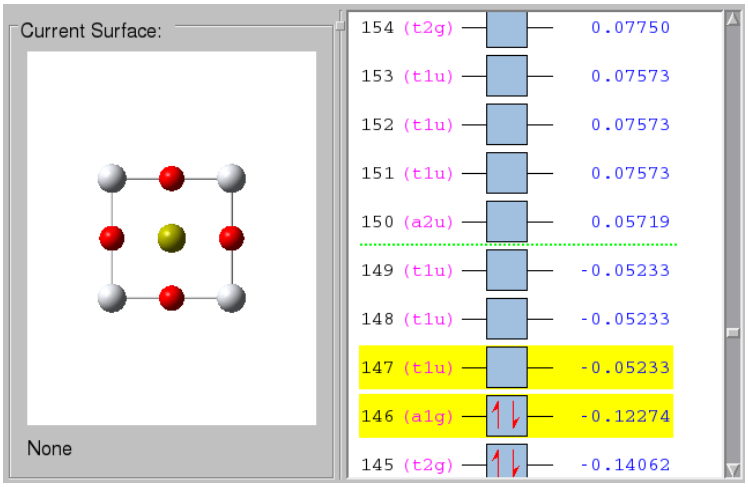
>gv filename.chk

Click on [Results], then [Summary]. Some basic information about your model will be displayed.



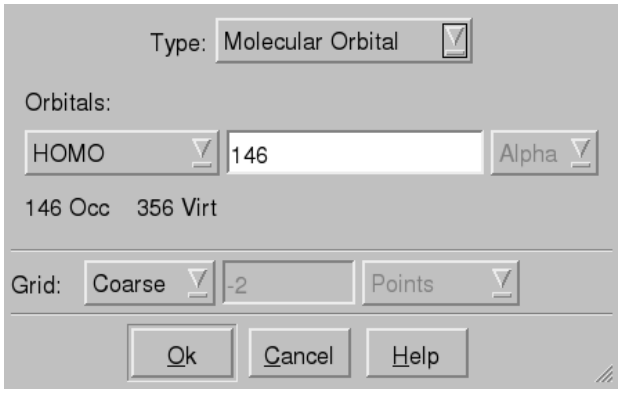

## Orbitals and their occupation

Open the .log/.out file in GV. Click on [edit], then [MOs]. A new window will pop up. This new window shows every orbital in your model and whether or not it is occupied by an electron. It also identifies the location of the band-gap (with a dotted green line) and, depending upon the job type, information about the symmetry of the orbital.




## Plotting orbitals

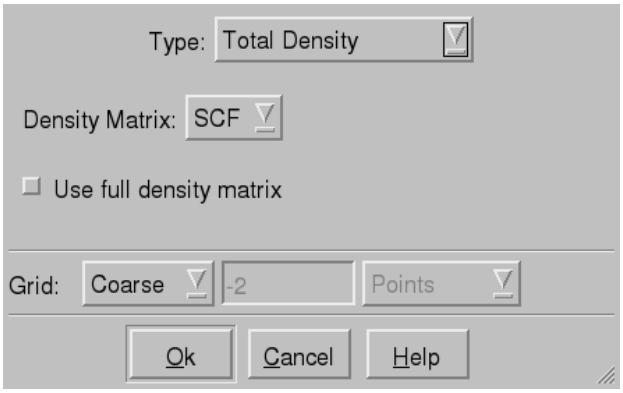
Open Gaussview and load the .chk file for the results you'd like to analyze. Once open, click on [Results], then select [Surfaces and Contours]. Now we must generate a cube. Click on [Cube Actions], then [New Cube]. Select details as desired. (This takes time, be patient.)



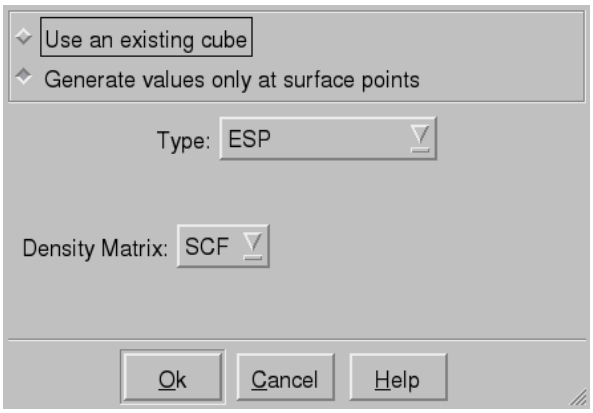

Once the cube has been generated, select [Surface Actions], [New Surface]. The orbital is now being displayed. If you wish, you can save cubes for future use so you do not have to wait for them to be generated.

## ESP (electrostatic potential) maps

Follow the same steps above for plotting orbitals. But when you open the "New Cube" screen, select "Total Density" from the drop-down list. (This takes time, be patient.)



Once the cube has been generated, select [Surface Actions], [New Mapped Surface]. In the new window, select "Generate values only at surface points" and click [OK]. The total electron density is now being displayed (this also takes time.). If you wish, you can save cubes for future use so you do not have to wait for them to be generated.




## Density of states plots for Gaussian

1. Find and inspect .log/.out file for orbital energies
    a. >grep –n "Alpha" Ener.log

    464: Alpha occ. eigenvalues -- -20.60108 -20.59632 -20.59506 -20.59485 -3.17962
    465: Alpha occ. eigenvalues -- -2.10721 -2.10605 -2.10483 -1.33897 -1.33170
    466: Alpha occ. eigenvalues -- -1.32871 -1.32729 -0.68195 -0.67199 -0.66767
    467: Alpha occ. eigenvalues -- -0.65977 -0.55827 -0.55563 -0.55053 -0.54777
2. Automatic parsing
    a. >perl ~/bin/gaus_gap_en_dos_v2.pl filename.log 1000 .01 5 5
        i. Steps = 1000
        ii. Band width = 0.1 eV
        iii. Down from HO = 5 eV
        iv. Up from LU = 5 eV
    b. >cp DOS_w_0.1_filename.log DOS.log
3. Generating the plot
    a. >gnuplot ~/bin/gnuprog_DOS_gauss
4. Converting the plot to pdf
    a. >ps2pdfwr DOS_g09.ps
5. Move the file to local for use
    a. >scp kilin-lab@hpc.usd.edu:/home/kilin-lab/REU2015/myfolder/*.pdf .
6. Note that the "E_Ener.log" file that was generated during this process may be of use to you later.

## Basis sets

Each job must have a basis set specified, but how do we know which to choose? The Gaussian website has all the information, but briefly, what you need to know is that each basis set has pros

and cons. Some may be simple (yet inaccurate) and therefore your job may complete quickly. But if you're preparing something for a publication you may need something more accurate which would take longer. Some are specific to groups of elements or contain specific corrections.

# Part 4: VASP job set up

## VASP Intro

File types and preparation of each:

- POSCAR – this must contain coordinates of the molecule and dimensions of system
    - Copy .out/.log file to new directory (or you start with .xyz and can skip these steps)
    - >babel -ilog filename.log -oxyz POSCAR.xyz
    - Make sure the .xyz file is named POSCAR.xyz
        - >cp filename.xyz POSCAR.xyz
    - >mv POSCAR.xyz SORT.xyz
    - >sort SORT.xyz > POSCAR.xyz
    - Check that POSCAR.xyz has been sorted. The file should have the number of elements at the top, one blank row, and then the coordinates follow.
    - >rotate_XYZ (this command prompts you for input)
    - 0 [Enter] 0 [Enter] 0 [Enter] (unless you're actually rotating)
    - >tink2vasp_wat.pl POSCAR_ROT_tinkXYZ POSCAR X Y Z
        - X Y Z are the distances between the molecule and the end of the cell. Entering values such as 8 8 8 will create an 8 Angstrom distance of vacuum in each direction. Choose numbers between 6 and 20, 8-10 is recommended for most models. If periodic boundary conditions are required, see section on Periodicity.
- INCAR – this tells VASP which type of job to run and with what specifications
    - >cp ~/bin/INCAR/INCAR-(job type) ./INCAR
    - (job type) is chosen from the files in the directory. Don't forget to rename the file to INCAR.
- POTCAR – contains potentials for each atom, in the correct order
    - >cat /home/kilin-lab/POTENTIALS/X/POTCAR /home/kilin-lab /POTENTIALS/Y/POTCAR > POTCAR
    - Perform for every element in the system (represented by X/Y), in the order in which they are listed in the sorted POSCAR.
    - Check yourself:
        - >grep PAW POTCAR
- KPOINTS
    - >cp ~/bin/KPOINTS .

## Periodicity

For periodic structures, use the above procedure, but when you get to the "tink2vasp" step run the code with 0 0 0. Inspect POSCAR for unit cell dimensions. Inspect POSCAR.xyz in Jmol and measure the unit cell in the X Y Z directions after modifying the model accordingly. Then run command again but for the X Y Z input, insert measurement(Jmol) minus dimension(POSCAR) for each of the X Y Z. Check POSCAR for new coordinate matrix.

## Job submission

>runvasp

Job status is monitored in the same way as Gaussian jobs.

- >qstat | grep job#  (type your job #)

## Partial charge density

- Move POSCAR, POTCAR, KPOINTS, and WAVECAR to new directory.
- Copy INCAR-pc to the directory and rename to INCAR.
    - >cp ~/bin/INCAR/INCAR -pc ./INCAR
- In related OUTCAR:
- >grep NBANDS OUTCAR
- Modify INCAR:
    - NBANDS=#of orbitals/states
    - Example: NBANDS=52
    - NSW=0
- Modify INCAR (use the same orbital energy range as DOS, or whichever orbitals you want to plot, choosing a smaller range will decrease amount of time needed for calculation)
    - EINT= -6 -2
- Submit the job.
- If the job is healthy, you should start seeing files called PARCHG000.ALLK appear.

## Pseudo-excited state

- Create a new directory.
- >cp ~/bin/INCAR/INCAR-geometry-optimization ./INCAR
- Modify INCAR:
    - NSW=0
    - ISMEAR=-2
- Add to the end of INCAR:
    - FERWE=(#Occupied-1)*1 0 1 (#Unoccupied-1)*0
    - Example: FERWE=32*1 0 1 13*0

    - This means there are 32 occupied orbitals, followed by a hole and one more occupied orbital, followed by 13 unoccupied orbitals.
- Run the job after you've compiled the rest of the input files.

## Heating

- Create new directory.
- >cp ~/bin/INCAR/INCAR-heat ./INCAR
- Modify INCAR
    - NSW=100 (Choose a number based on model size, accuracy, and time, we'll choose 50-100)
    - TBEG=300 (Temperature in Kelvin)
    - TEND=300 (Temperature in Kelvin)
- Compile other files and submit job.

## Molecular dynamics

- INCAR-md, rename to INCAR
- >cp ~/bin/INCAR/INCAR-md ./INCAR
- Modify INCAR:
    - TBEG=(same as heating)
    - TEND=(same as heating)
    - NSW=(same as heating)
- Move POTCAR, KPOINTS, and WAVECAR (from heating) to the new directory.
- >cp /home/kilin-lab/REU2015/myfolder/WAVECAR .

## Spin-polarized job

- Modify the INCAR (geometry optimization):
    - NSW=0
    - ISPIN=2
- Run the job after compiling other input files.

## Singlet/doublet/triplet excited states (spin-polarized excited)

- Obtain information from related OUTCAR:
    - >grep NUPDOWN OUTCAR
- Modify the INCAR (geometry optimization):

    - NSW=0
    - ISPIN=2
- Add to the end of INCAR: (whatever 'grep NUPDOWN' gave you, add 1 for singlet, 2 for doublet, and 3 for triplet. Example:
    - NUPDOWN=2
- Run the job after compiling other input files.

# Part 5: VASP analysis tools

## Density of States Preparation

- *Extract orbitals from OUTCAR*
- >tail -n 250 OUTCAR > STATES
- *The number may need to be increased in order to find the information. Then edit the STATES file so that only the orbitals are present, including one space at the end of the file.*
- *Gather information for input into DOS command.*
- >grep NELE OUTCAR
- >grep fermi OUTCAR
- >~/bin/DRESS_DOS_NORM
- This command will ask for:
    - Number of states
    - Min energy and max energy and E_fermi, alpha+beta (for min choose HOMO-3, max choose LUMO+3)
    - Enter width of each line eg 0.01eV
    - Magnitude (enter 1)
    - Number of atoms
    - Number of electrons
    - Gap of bulk phase (enter 3)
- >gnuplot ~/bin/gnuprog_DOS
- >ps2pdfwr DOS.ps
- *Copy DOS.pdf to local.*

## Spin-polarized density of states

- After running the Manual Spin-Polarized job.
- >tail -n 350 OUTCAR > STATESup
- >tail -n 350 OUTCAR > STATESdown
- STATESup and STATESdown should contain spin component 1 and 2, respectively. Edit and delete accordingly.
- >~/bin/DRESS_DOS_UP

- >~/bin/DRESS_DOS_DOWN
- >gnuplot ~/bin/gnuprog_DOSup_down
- >ps2pdfwr DOSupdown.ps
- Copy DOSup_down.pdf to local.

## OS_STRENGTH analysis

- Transfer “OS_STRENGTH” and “spectrum” files to local. Open in Excel. Follow steps to create columns (Data→Text to Columns→Fixed Width)
- Graph “spectrum” (first and last columns, this will be in nm).
- Locate interesting peak. Find eV value that corresponds to it.
- Locate that eV value in the “OS_STRENGTH” file (after sorting). Now you know which transition is responsible for the tip of that peak. If that transition seems likely, then you could plot those orbitals.

Also, now that your OS_STRENGTH is sorted, it can be useful to identify which transitions start with HO. Find the transitions originating from HO and plot those orbitals. Interesting characteristics to look for include atom-to-atom transitions, and p-d, d-p, p-p transitions.

## Additional way to identify interesting orbitals to plot

This will display a graph identifying the location of orbital density in space. This method is most useful for models which have discreet areas, such as substrate on the bottom with a ligand attached to the top.

- Navigate to the partial charge directory.
- >perl ~/bin/CENTER.pl 200 300
- The last two numbers specify the orbital range. New file called "wf_center3_angstrom" is generated. It contains the expectation values of the position operator for each orbital as follows:

| #orbital=I | <i\|x\|i> | <i\|y\|i> | <i\|z\|i> |
|---|---|---|---|

- >gnuplot ~/bin/gnuprog_CENTER
- >ps2pdfwr CENTER.ps

## Plotting orbitals

Preferred methods is VMD software.

Basic steps for VMD:

- File→New Molecule→Load POSCAR and choose file type
- Load PARCH.000.ALLK file
- Modify isovalue as desired
- Use ColorID to plot multiple orbitals in one image (useful for describing transitions)

It is recommended to take screenshots of orbitals and place the images in a PowerPoint file so you can have a record of what you've observed.

## Absorption spectrum

Create a file called input_overlap by opening nano. The file should consist of:

1
# of states
1

>cp STATES energy_pop
There should be an empty line at the end of the energy_pop file
>~/bin/OS_dipol_v3
Sometimes the above command only works under 'qlogin.'
>wc OS_STRENGTH
Above: Note number of transitions (lines) using word count: (lines words characters)
>~/bin/SPECTRUM_imp3
This code will ask for:

Number of transitions
MIN-.5 and MAX=3 energy difference (.01-10)
Enter line width eg 0.01eV
Enter # of HOMO (orbital number)

>gnuplot ~/bin/gnuprog_SPE
>ps2pdfwr SPE.ps
Copy SPE.pdf to local.

## For spectrum in nanometers:

Follow above procedure but modify:
>gnuplot ~/bin/gnuprog_SPE_nm
>ps2pdf SPE_nm.ps
Copy SPE_nm.pdf to local.

## Absorption spectrum for spin-polarized models

Preparing absorption spectra for spin-polarized models can be done in six steps

1. vasp computation
2. creating input files
3. running spin-polarized absorption code
4. preparing input files for continuous spectra
5. plotting continuous spectra
6. transferring files to local computer

1. **vasp computation**
2. **creating input files**

launched  spin-polarized calculation

Obtained WAVECAR.

From OUTCAR, one extracts two sets of Kohn-Sham orbital energies:

STATES_UP and STATES_DOWN (see instruction on spin polarized DOS preparation)

Then, one merges these two files into “energy_pop” but, I do it in such way so that UP goes first, DOWN goes second. Current version of the code was tested only is ALL orbitals are stored.

>cat STATES_UP >> energy_pop

>car STATES_DOWN >> energy_pop

Then one creates an input file “input overlap”. This file is changed in such way that it takes into account details of spin polarization. In the earlier version, for spin-restricted calculations such file had only two records: number of first orbital and number of last orbital. Here it is critical, that spin up and spin down components may have different numbers of HO orbital!

Here, in these new modification, this file contains four records:

1. number of lowest orbital corresponding to the file “energy_pop”
2. number of the HOMO orbital for the spin up component.
3. Number of HOMO orbital for spin down components
4. number of the last orbital

> more input_overlap
1
28
27
48

It is interesting that chosen numbers for HO(up)=28 and HO(down)=27.

3. **running spin-polarized absorption code**

Then one runs the new modified code

> ~/bin/SPIN/absorption_xyz_spin_v4

After launching, the code is reading these three input files: WAVECAR, input_overlap, energy_pop

then the code asks some silly questions.

check consistency with "energy_pop" !

nbandmin, has to be ge 1

There is a prompt and we can use this prompt. one answers “1” and hits enter.

1

nbandmax, has to be le 48

There is a prompt and we can use this prompt. one answers “1” and hits enter.

48

Then the code is placing there some service information

After code completes the computation, there appear several new files

OS_STRENGTH

OS_STRRENGTH_UP

OS_STRENGTH_DOWN

Here is the OS_STRENGTH file it contains transitions for both up and down components, as labeled with the first column value s=1 or s=2

The structure of OS_STRENGTH_UP and OS_STRENGTH_DOWN is the same as in the spinless case.

## 4. preparing input files for continuous spectra

In order to plot spectra by older code we commit some renaming of input files.

> cp OS_STRENGTH OS_STRENGTH_FULL

**FIRST WE FOCUS ON THE alpha=up spin component**

> cp OS_STRENGTH_UP OS_STRENGTH

Then we need to explore the length of the file

> wc OS_STRENGTH

```
 567  5103 56133 OS_STRENGTH
> ~/bin/SPECTRUM_imp3
 file OS_STRENGTH i  j  OS  Ei-Ej  Pi Pj
 number of transitions ? >wc OS_STRENGTH
567
 MIN=.5 and MAX=3 energy difference
.01
10
 Enter width of each line eg 0.01eV
.01
 Enter # of HOMO (in VASP)
28
 input file OS_STRENGTH has been read
 spectrum - file is written
 S.b-file:
 lamda(nm), dE(eV), Intens, #e(LUMO=1), #h(HOMO=1)
hpc:~/CHEM792_2013/vogel/Six_H2O_Ti>
cp spectrum spectrum_UP
```

**NEXT WE FOCUS ON THE beta=down spin component**

```
> cp OS_STRENGTH_DOWN OS_STRENGTH
> wc OS_STRENGTH
 567  5103 56133 OS_STRENGTH

> ~/bin/SPECTRUM_imp3
 file OS_STRENGTH i  j  OS  Ei-Ej  Pi Pj
 number of transitions ? >wc OS_STRENGTH
567
 MIN=.5 and MAX=3 energy difference
```

.01

10

Enter width of each line eg 0.01eV

.01

Enter # of HOMO (in VASP)

27

input file OS_STRENGTH has been read

spectrum - file is written

S.b-file:

lamda(nm), dE(eV), Intens, #e(LUMO=1), #h(HOMO=1)

> cp spectrum spectrum_DOWN

**NEXT WE FOCUS ON THE COMBINED SPECTRUM**

> rm OS_STRENGTH

> cat OS_STRENGTH_UP >> OS_STRENGTH

> cat OS_STRENGTH_DOWN >> OS_STRENGTH

> wc OS_STRENGTH

1134 10206 112266 OS_STRENGTH

> ~/bin/SPECTRUM_imp3

file OS_STRENGTH i j OS Ei-Ej Pi Pj

number of transitions ? >wc OS_STRENGTH

1134

MIN=.5 and MAX=3 energy difference

.01

10

Enter width of each line eg 0.01eV

.01

Enter # of HOMO (in VASP)

27

input file OS_STRENGTH has been read

spectrum - file is written

S.b-file:

lamda(nm), dE(eV), Intens, #e(LUMO=1), #h(HOMO=1)

> cp spectrum spectrum_COMPLETE

## 5. plotting continuous spectra

> gnuplot ~/bin/gnuprog_SPE_SPIN_eV

> gnuplot ~/bin/gnuprog_SPE_SPIN_nm

> ps2pdfwr SPE_SPIN_nm.ps

> ps2pdfwr SPE_SPIN_eV.ps

## 6. Transferring files to local computer

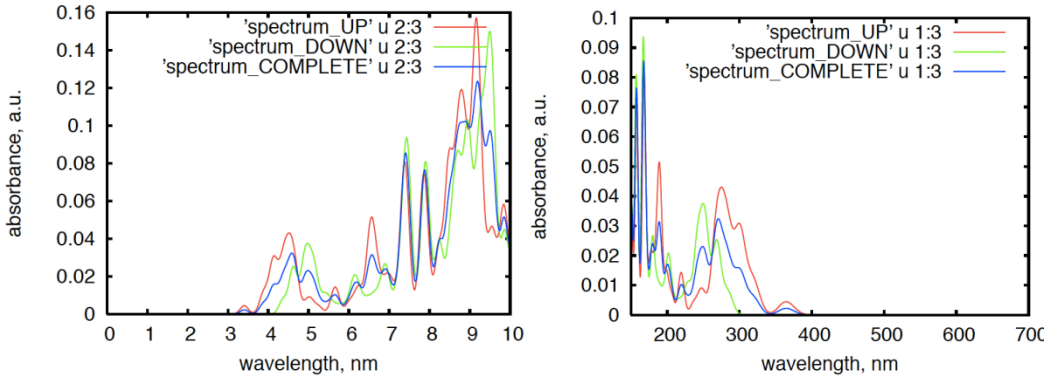
**UPON PREPARING ALL THREE FILES, one TRANSFERS THEM TO the local computer:**

>scp kilin-lab@hpc.usd.edu:/home/kilin-lab/CHEM792_2013/vogel/Six_H2O_Ti/*.pdf .

kilin-lab@hpc.usd.edu's password:

SPE_SPIN_eV.pdf 100% 36KB 36.1KB/s 00:00

SPE_SPIN_nm.pdf 100% 26KB 26.0KB/s 00:00




Here, the blue line is ½ of the sum of red line (majority spin) and green line (minority spin).

Making Movies of Molecular Dynamics

**VMD:**

>mkdir ../Ti4O8_MD_MovieVMD/

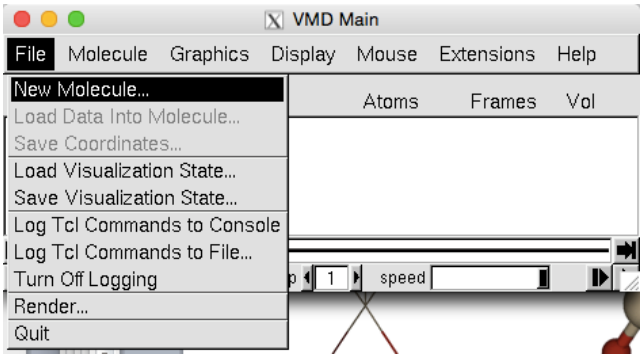
>cd ../Ti4O8_MD_MovieVMD/

>cp ../Ti4O8_MD/OUTCAR .

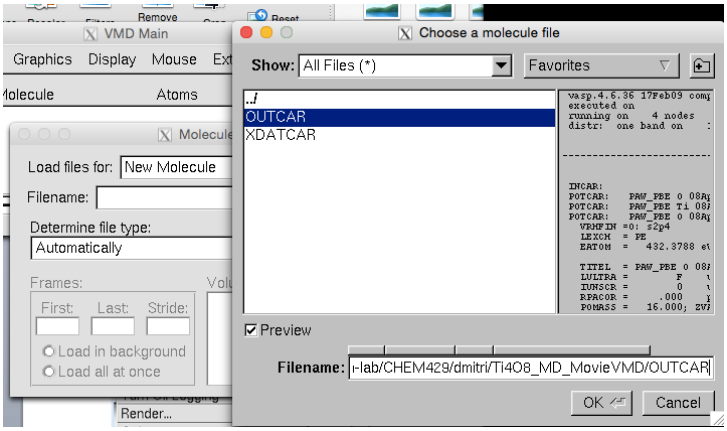
>cp ../Ti4O8_MD/XDATCAR .

>vmd &

[1] 1238




Select file

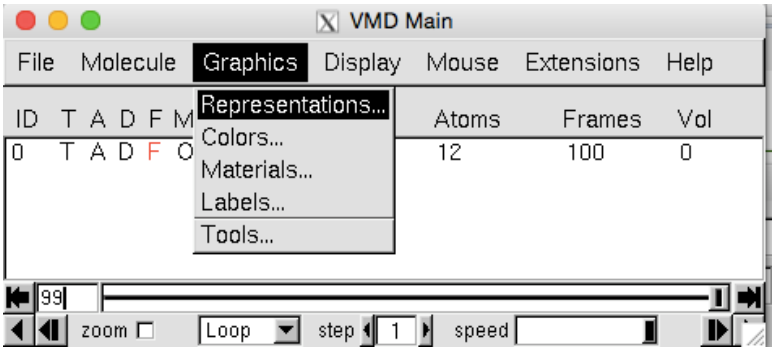



Select file type

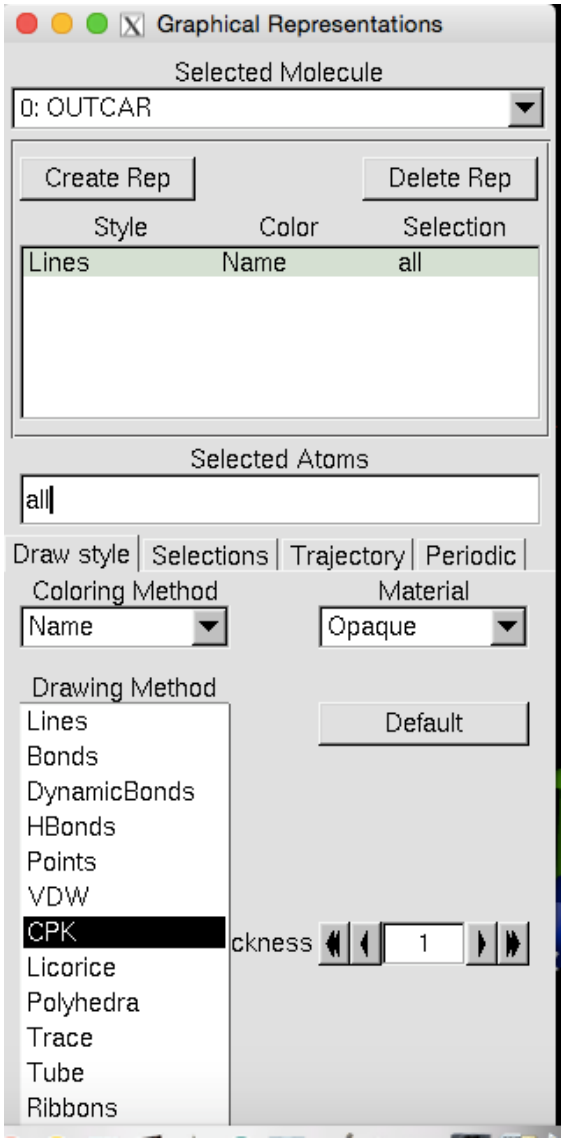
JHBD Grid
VASP_CHGCAR
VASP_OUTCAR
VASP_PARCHG
VASP_POSCAR
VASP_XDATCAR

Load

Graphics, representations



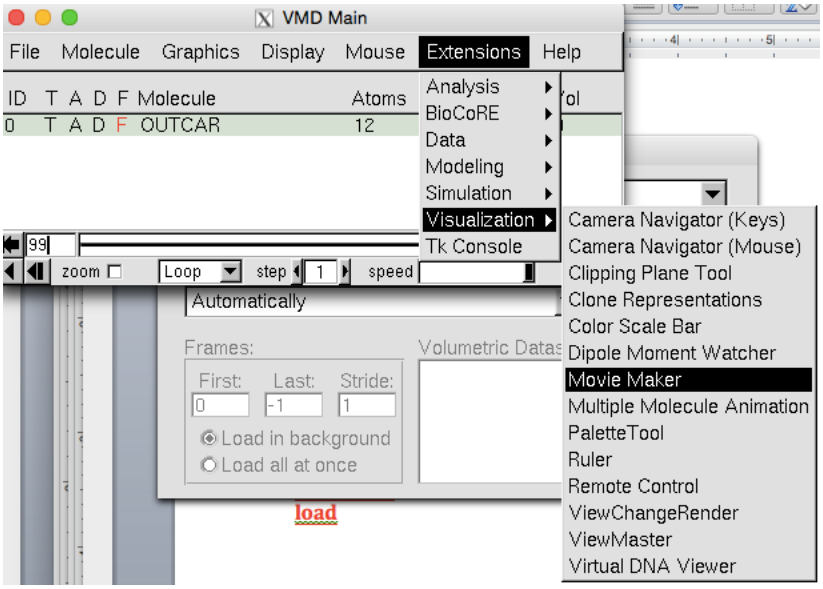

Drawing method: CPK



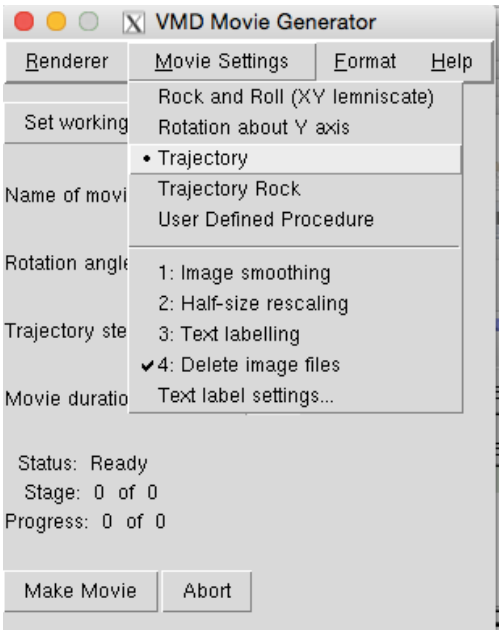

Create rep

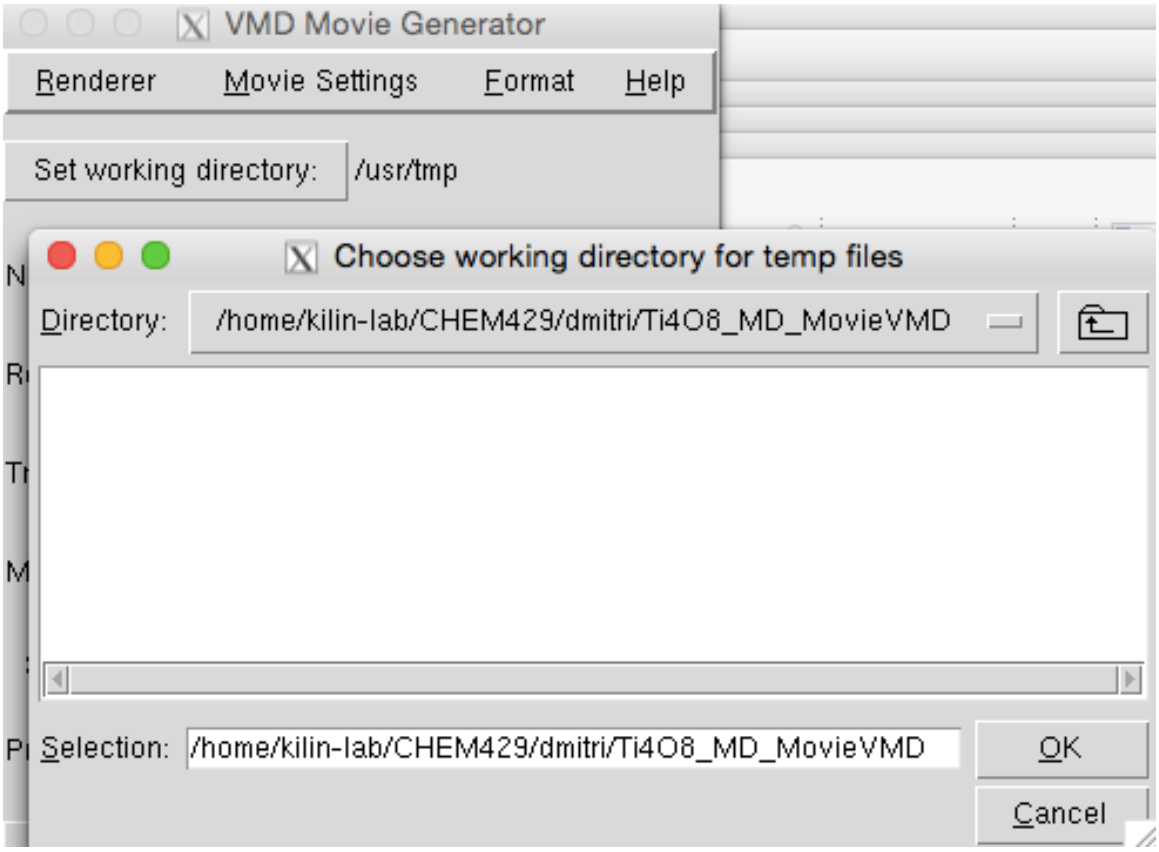
Drawing method: dynamic bonds

Extensions-Visualization-MovieMaker



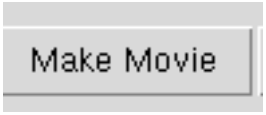

Movie Settings: Trajectory






Set working directory

Make movie




MPEG file created in: /home/kilin-lab/CHEM429/dmitri/Ti4O8_MD_MovieVMD/Ti4O8.mpg