

NE451

Simulation Methods

Density of states tutorial

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Introduction to Density of States (DOS) Calculations

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- ▶ The density of states (DOS) describes how many electronic states are available for occupation within a small energy range around a given energy level E . Mathematically, $\rho(E)dE$ represents the number of states in the interval $(E, E+dE)$. DOS provides crucial insights into a material's electronic structure, influencing properties such as conductivity, magnetism, and optical behavior.
- ▶ In plane-wave based density functional theory (DFT), the electronic states are represented by Bloch functions of the form $e^{ik \cdot r}$ with energies $E = \frac{\hbar^2 k^2}{2m}$. To compute the DOS:
 - ▶ Self-Consistent Field (SCF) Calculation – First, perform a fixed-ion SCF calculation to obtain the ground-state charge density.
 - ▶ Non-Self-Consistent Field (NSCF) Calculation – Next, run an NSCF calculation on a much denser k -point grid, since DOS accuracy depends on fine integration in k -space.
 - ▶ DOS Evaluation – Finally, integrate the electronic states over the Brillouin zone to obtain $\rho(E)$.



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- ▶ Step 1: Login to c1cluster using the procedure in the lecture "Introduction to HPC and Linux for Beginners" You can use

```
$ ssh c1cluster
```

and type the password when prompted if you have created the config file and the ssh keys

- ▶ Step 2: Create a folder for your DOS Calculations

```
$ mkdir DOS-calculations
```

- ▶ Step 3: Inside the DOS Calculations folder create the 3 "Quantum espresso in" files – One for SCF, one for NSCF and one for DOS. You may download the in files along with the shell script from the github repo.

```
$ cd DOS-calculations  
$ wget https://github.com/Feugmo-Group/NE451/  
archive/refs/heads/main.zip  
$ unzip main.zip
```



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- ▶ The files folder contains the following three .in files:
 - ▶ pw.scf.silicon_dos.in
 - ▶ pw.nscf.silicon_dos.in
 - ▶ pp.dos.silicon.in
- ▶ The SCF file and NSCF files are used for the SCF and NSCF calculations respectively.
- ▶ They are run using the pw.x command in Quantum Espresso
- ▶ The pp.dos.silicon.in is a post-processing file to compute the Density of states and is operated upon by the dos.x command in Quantum Espresso



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► Step 3:

```
$ cd NE451-main  
$ ls
```

This command shows the two folders "Files" and "Plots"

► Step 4: Run the batch job using the command from the convergence folder.

```
$ cd Files/dos  
$ sbatch DOS.sh
```

► Step 5: Verify if the status of the batch job periodically by using the

```
$ squeue -u <Your_username>
```

► Step 6: Once the batch job is completed check that there are many output (.out) files with one file for each of the input files You may use

```
$ nano your_filename.out
```



Plotting the DOS calculations

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- ▶ Step 7: Copy the .out files from the remote system onto your local computer and run the python script dos_plot.py to see the output file to plot your results. Exit the remote system by typing the command

```
$ exit
```

Then on your local computer type

```
$ scp -r c1cluster:/your/  
file/path/Plots/DOS-C1 .
```

You may use

```
$ python3 dos_plot.py
```

to run the python script on your local linux computer

- ▶ Step 8: You may also use the site <https://xfroggie.com/index.cgi/dosplot> in order to plot your Density of States. Just upload the .dat file which you can find along with your .out files

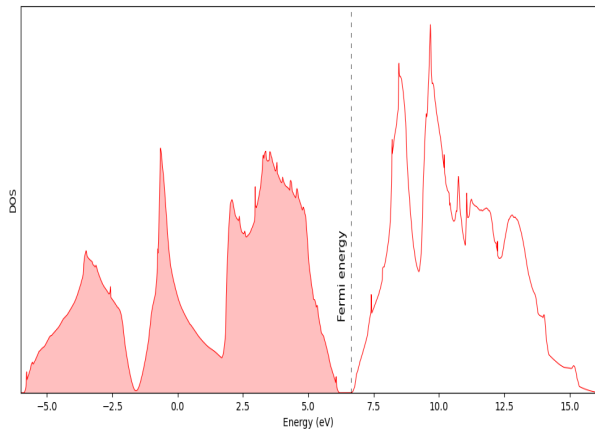


The DOS Plot by using Python

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The DOS Plot by using XFroggie

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