NE451
Simulation Methods

Band Structure

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Band Structure Calculations

- Band structure calculations are essential for understanding the electronic properties of materials, such as their electrical conductivity, band gap, and optical behavior.
- The process involves two main steps:
  - Self-Consistent Field (SCF) Calculation – Determines the ground-state electron density, Hartree potential, and exchange-correlation potential for the system.
  - Non-Self-Consistent Field (NSCF) or Bands Calculation – Uses the SCF results to compute Kohn–Sham eigenvalues along specific high-symmetry points in the Brillouin zone without updating the Hamiltonian.
- In Quantum ESPRESSO, we:
  - Prepare an SCF input file with structural, pseudopotential, and computational parameters.
  - Run the SCF calculation to obtain the ground-state data.
  - Define a k-point path (via tools like SeeK-path) for the bands calculation, including both occupied and relevant unoccupied states.
  - Perform bands.x post-processing to convert raw output into a usable band dispersion plot.

The way to run a Band Structure calculation

- 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 Band structure Calculations

```
$ mkdir BStruct-calculations
```

- Step 3: Inside the Band structure Calculations folder create the 3 “Quantum espresso in” files – One for SCF, one for bands calculation and one for post-processing. You may download the in files along with the shell script from the github repo.

The way to run a Band Structure calculation

- First we perform an SCF calculation on the Quantum Espresso in file(pw.scf.silicon_bands.in) using the pw.x command.
- In the next step, we use the ground-state charge density from the SCF step to compute eigenvalues along a chosen k-path without updating the density. Specify k-points and increase nbnd if unoccupied bands above the Fermi level are needed. The number of occupied bands is given in the SCF output. In this step too, we use the pw.x command to the pw.bands.silicon.in file.
- After the bands calculation is performed, we need some postprocessing using bands.x utility in order to obtain the data in a more accessible format. For this we perform the bands.x Quantum Espresso processing on the pp.bands.silicon.in post-processing file.

The way to run a Band Structure calculation

- Step 3:

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

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

- Step 4: Run the batch job using the command

```
$ cd Files/bands
$ sbatch BAND-STRUCTURE.sh
```

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

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

The way to run a Band Structure calculation

- 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
```

to see the output file

The way to plot Band Structures

- Step 7: Copy the .out files from the remote system onto your local computer and run the python script bands_plot.py 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/BandStructure-C1 .
```

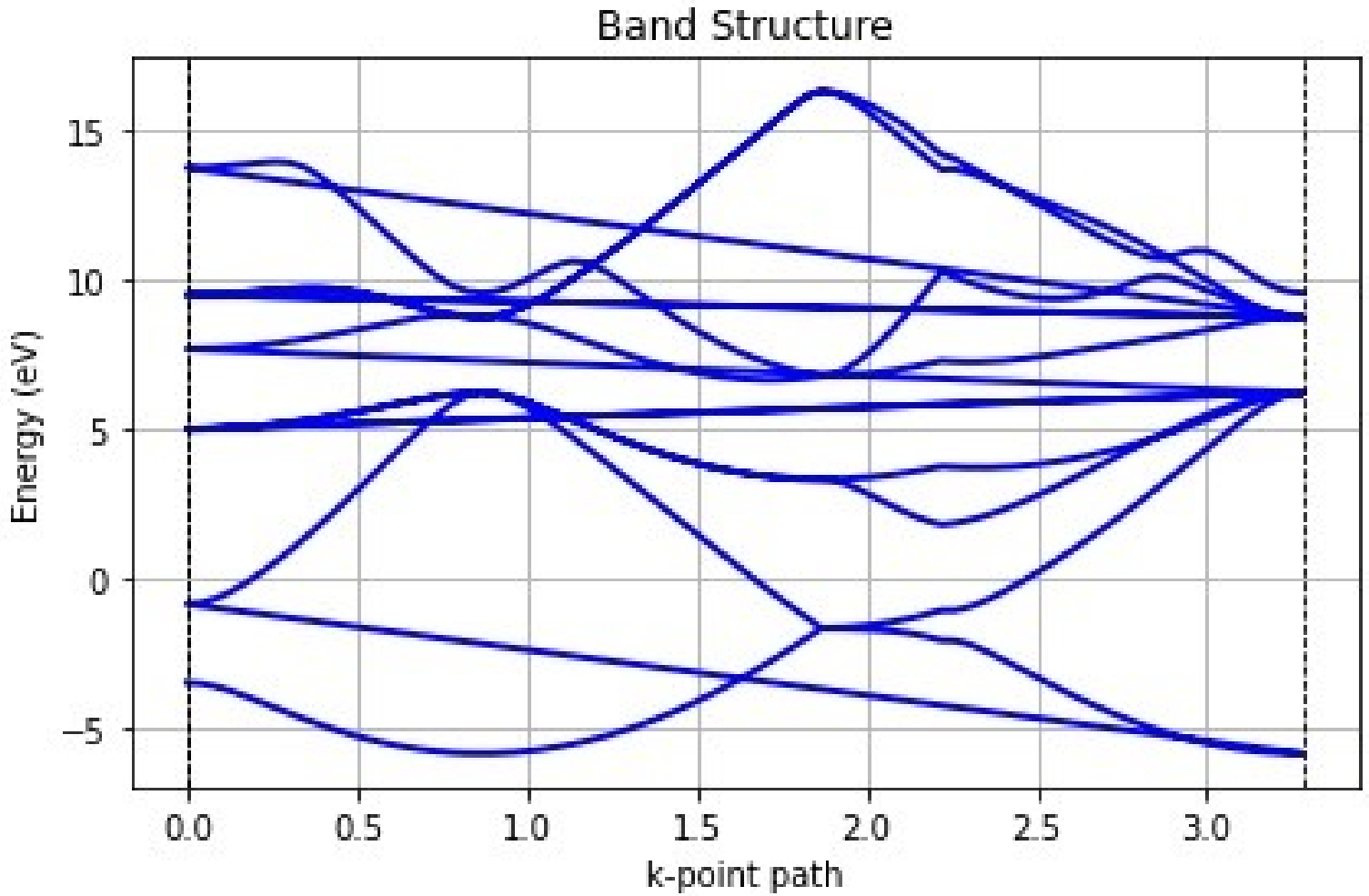
You may use

```
$ python3 bands_plot.py
```

to plot.

- Step 8: You can also plot the Band structure using XFroggie website. Just upload the .dat.gnu ,found along with the .out files.:https://xfroggie.com/bandplot/upload

The Band Structure Plot using Python

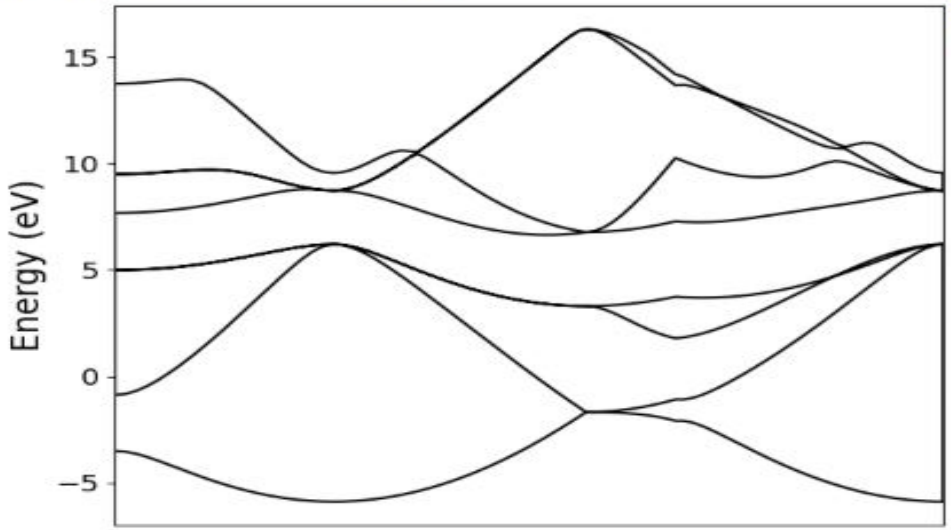


The Band Structure Plot using XFroggie

xfroggie.com/bandplot/upload

Plot band structure obtained by QE

Upload band structure file (.gnu) ?
Choose File No file chosen Upload



High symmetry points
Upload bands.x output
Choose File No file chosen Upload

Fermi energy Update
Read from pw.x output Choose File No file chosen

ymin, ymax Update

Donwload figure as image file
EPS: Encapsulated Postscript Download

xfroggie