Signature

Alexandre Dufresne-Nappert

20948586

Nov 18 2025

https://github.com/MrDNAlex/NE-451-Simulation-Methods/tree/main/Labs/Lab3-Assignment

---

1. Overview

In this assignment, you will perform a first-principles electronic structure calculation for the semiconductor GaAs using Quantum ESPRESSO. You will:

- Run a self-consistent field (SCF) calculation
- Run a non-self-consistent (NSCF) band calculation
- Perform post-processing with bands.x
- Generate a band structure diagram with python
- Understand the input files, pseudopotentials, and k-point sampling

The exercise strengthens your understanding of plane-wave DFT workflows and band-structure analysis.

2. Files Provided

You can download the following files from LEARN Lab003_Assigment.

Input Files

- GaAs.scf.in
- GaAs.nscf.in (to be edited with the number of band)
- GaAs.band.in

Pseudopotentials

- Ga.pbe-dn-kjpaw_psl.1.0.0.UPF
- As.pbe-n-kjpaw_psl.1.0.0.UPF

plots

- plot.py (to be edited with the fermi energy)

3. Task Instructions

Download and extract the prepared script directory:

4. Understanding the Input Files

4.1 SCF Input (GaAs.scf.in)

- &control — calculation type, prefix, file paths
- &system — lattice, atomic types, cutoff energies
- &electrons — convergence settings
- ATOMIC_SPECIES — elements + pseudopotentials
- ATOMIC_POSITIONS — internal coordinates
- K_POINTS {automatic} — 8×8×8 grid

Key physics concepts:

- GaAs uses zinc-blende structure (fcc-based).
- Cutoff energies (ecutwfc=60, ecutrho=244) follow pseudopotential recommendations.
- SCF uses a coarse k-point grid because only electron density is required.

4.2 NSCF Input (GaAs.nscf.in)

Changes from SCF:

- calculation = 'bands'
- Added nbnd = xxx
- K_POINTS {crystal_b} — piecewise-defined high-symmetry path:
- L → Γ → X → K/U → Γ

Purpose: Use the SCF density to compute eigenvalues along the band path.

Changes Needed for a Band-Structure (NSCF) Calculation

To compute a band structure, we start from the converged SCF density and run a non-self-consistent (NSCF) calculation along a high-symmetry k-path. This requires several key changes to the SCF input.

`calculation = 'bands'` Tells the code to:

- Use the SCF charge density
- Compute eigenvalues only
- Follow a manually defined k-path instead of a uniform k-grid

`nbnd = xxx` Specifies the number of electronic bands to compute.

- SCF only requires enough occupied bands
- Band plots need extra conduction bands
- Choosing ~2–3× the number of occupied bands is typical

2. How to Determine nbnd

Quantum ESPRESSO automatically determines the number of occupied bands from the valence electrons.

Number of electrons Ne=sum of pseudopotential valence electrons

Then the number of occupied bands is: Nocc=⌈Ne/2⌉ (for spin-unpolarized systems)

Example

If your system has 20 valence electrons per primitive cell: Nocc=202=10occupied bands

For a band structure calculation, you also need extra empty (conduction) bands.

Rule of Thumb

Insulators: $nbnd$=Nocc+4–8

Metals: $nbnd$=Nocc+8–16

Complex systems: $nbnd$=2Nocc

How to Check Automatically

After the SCF run completes, QE prints:

```
number of Kohn-Sham states = XX
```

This value is the minimum nbnd. Add the recommended number of conduction bands on top.

K_POINTS {crystal_b} This block defines the high-symmetry k-path used in band-structure plots.

Example path for GaAs: L → Γ → X → K/U → Γ

5 . Post-Processing

GaAs.band.in (for bands.x) contains:

```
&amp;bands
prefix = 'GaAs'
lsym = .true.
/
```

This generates bands.out.gnu, which is plotted by plot.gp or by plot.py

6. Task Instructions Running the Calculations (HPC / SLURM)

This section explains how to run the SCF, NSCF, and band-structure post-processing steps for GaAs using Quantum ESPRESSO on an HPC cluster with SLURM. All commands below assume you are inside the directory containing:

- GaAs.scf.in (to be edited)
- GaAs.nscf.in (to be edited with the number of band)
- GaAs.band.in
- plot.py (to be edited with the fermi energy)
- Pseudopotentials (Ga.UPF, As.UPF)
- Any job scripts you prepare (run_scf.slurm, run_nscf.slurm, etc.)

Step 1 — SCF Calculation

modify the GaAs.scf.in : add `verbosity = 'high' in the &control and

Submit the self-consistent calculation to SLURM:

```
sbatch run_scf.slurm
```

Where your run_scf.slurm job script should contain something like:

```
#!/bin/bash
#SBATCH --job-name=GaAs_scf
#SBATCH --nodes=1
```

```
#SBATCH --ntasks=4
#SBATCH --time=00:10:00

module load quantum-espresso

mpirun pw.x < GaAs.scf.in > GaAs.scf.out
```

Step 2 — NSCF Band Calculation

After the SCF job finishes and produces a converged charge density (GaAs.save/),

Look in GaAs.scf.out

Search for:

```
the Fermi energy is
```

or

```
highest occupied level (ev):
```

Also search for

```
number of Kohn-Sham states = XX
```

then edit

`GaAs.nscf.in`

```
nbnd = XX + Nextra
```

submit:

```
sbatch run_nscf.slurm
```

Example NSCF job script:

```
#!/bin/bash
#SBATCH --job-name=GaAs_nscf
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --time=00:10:00

module load quantum-espresso

mpirun pw.x < GaAs.nscf.in > GaAs.nscf.out
```

Step 3 — Band Post-Processing

Once NSCF completes:

```
sbatch run_bands.slurm
```

Example:

```
#!/bin/bash
#SBATCH --job-name=GaAs_bands
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --time=00:05:00

module load quantum-espresso

mpirun bands.x < GaAs.band.in > GaAs.band.out
```

This generates the file GaAs.band.gnu for plotting.

Step 4 — Plotting the Band Structure

python plot.gp This will produce a band-structure figure (e.g., band.png or band.eps depending on your plot.gp settings).

Running the Simulations

Step 1

The first step is to run the SCF Calculation, so I used the following files :

`GaAs.scf.in`

```
in
&control
    calculation = 'scf'
    prefix = 'GaAs'
    pseudo_dir = './'
    wf_collect = .true.
    verbosity = 'high'
    outdir = './tmp/'
/
```

```
&system
    ibrav = 2
    celldm(1) = 10.6867
    nat = 2
    ntyp = 2
    ecutwfc = 60
    ecutrho = 244
/
&electrons
    mixing_mode = 'plain'
    mixing_beta = 0.7
    conv_thr = 1.0d-8
/
ATOMIC_SPECIES
    Ga 69.723 Ga.pbe-dn-kjpaw_psl.1.0.0.UPF
    As 74.921595 As.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS
    Ga 0.00 0.00 0.00
    As 0.25 0.25 0.25
K_POINTS {automatic}
    8 8 8 0 0 0
```

`run-scf .sh`

```
#!/bin/bash
#SBATCH --job-name=GaAs_scf
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=01:00:00
#SBATCH --mem-per-cpu=4000M
#SBATCH --cpus-per-task=2  # 1 thread per rank

module load class-simulations

mpirun -np $SLURM_NTASKS pw.x < GaAs.scf.in > GaAs.scf.out
```

Calculation Results

Once the calculation finished I extracted the following Values from the Output File :

- `Highest Occupied Level` : 6.7106 eV
- `Number of Kohn-Sham States` : 9

This means that for `nbnd` in the `NSCF` calculation I need to run it with $9 + N_{extra}$ bands. In my case I will add 7 bands since the range of a Semiconductor is 4-8. So the value I will use is :

- `nbnd` : 16

Now I'll run the second step...

Step 2

Now for the second step, using the $nbnd = 16$ established from the previous section I use the following files to run the `NSCF` calculation

GaAs.nscf.in

```
in
&control
    calculation = 'bands'
    prefix = 'GaAs'
    pseudo_dir = './'
    wf_collect = .true.
    verbosity = 'high'
    outdir = './tmp/'
/
&system
    ibrav = 2
    celldm(1) = 10.6867
    nat = 2
    ntyp = 2
    ecutwfc = 60
    ecutrho = 244
    nbnd =  16
/
&electrons
    mixing_mode = 'plain'
    mixing_beta = 0.7
    conv_thr = 1.0d-8
    diago_david_ndim = 4
/
ATOMIC_SPECIES
    Ga 69.723 Ga.pbe-dn-kjpaw_psl.1.0.0.UPF
    As 74.921595 As.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS
    Ga 0.00 0.00 0.00
    As 0.25 0.25 0.25
K_POINTS {crystal_b}
    5
    0.00  0.50  0.00  20 !L
    0.00  0.00  0.00  30 !G
    -0.50  0.00 -0.50  10 !X
    -0.375 0.00 -0.675 30 !K,U
    0.00  0.00 -1.00  20 !G
```

run-nscf.sh

```
#!/bin/bash
#SBATCH --job-name=GaAs_nscf
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=01:00:00
#SBATCH --mem-per-cpu=4000M
#SBATCH --cpus-per-task=2  # 1 thread per rank

module load class-simulations

mpirun -np $SLURM_NTASKS pw.x < GaAs.nscf.in > GaAs.nscf.out
```

Calculation Results

No specific data was requested as a result, I just transferred the results `/tmp` folder to the `Band` calculation folder and started running the Step 3 calculations

Step 3

For the third step I ran the following input file

GaAs.band.in

```
    in
    &bands
       outdir = './tmp/',
       prefix='GaAs',
       filband='GaAs.band',
       lsym=.true.
    /
```

run-bands.sh

```
#!/bin/bash
#SBATCH --job-name=GaAs_bands
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=01:00:00
#SBATCH --mem-per-cpu=4000M
#SBATCH --cpus-per-task=2  # 1 thread per rank

module load class-simulations
```

```
mpirun -np $SLURM_NTASKS bands.x < GaAs.band.in > GaAs.band.out
```

Calculation Results

After running this calculation I received the following files :

- GaAs.band.gnu
- GaAs.band.rap

The file `GaAs.band.gnu` will be used to plot the Band Gaps using the plotting functionality in the next section

Step 4

In this step we need to plot the resulting data from the `GaAs.band.gnu` file. This can be done using the Python in the Next Jupyter Cell

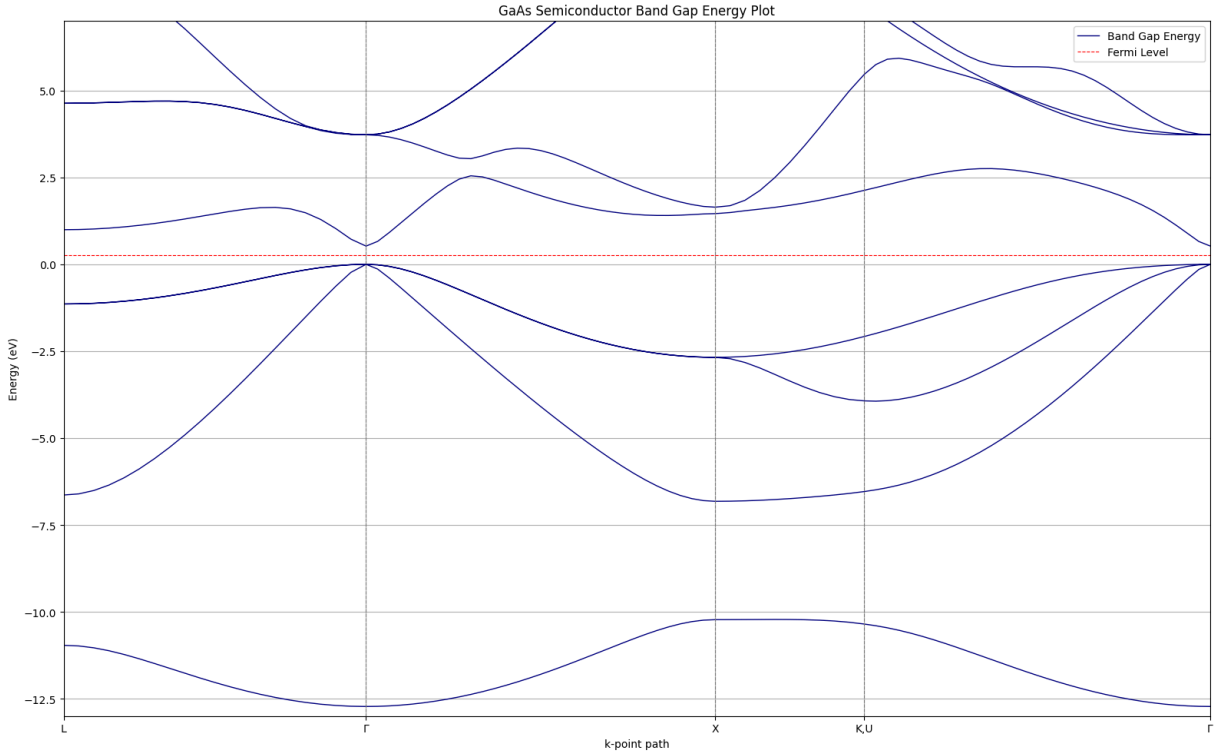
In [ ]:
```python
# Calculating the Fermi Energy Level
import numpy as np
import matplotlib.pyplot as plt

# Create Empty Lists
k_list = []
E_list = []

# Read the File and remove the empty lines causing smearing
with open("Band/GaAs.band.gnu", "r") as f:
    for line in f:
        line = line.strip()
        if line == "":
            # Append NAN to indicate we shouldn't wrap around
            k_list.append(np.nan)
            E_list.append(np.nan)
        else:
            vals = line.split()
            k_list.append(float(vals[0]))
            E_list.append(float(vals[1]))

# Cast it to a Numpy Array
k = np.array(k_list)
E = np.array(E_list)

# Define the Fermi Energy Shift
ef = 6.7106

# Define the Gamma, X, K,U points
x1 = 0.8660
x2 = 1.8660
x3 = 2.2932
```

```
xs = [x1, x2, x3]

# Get the Shifted energy
E_shift = E - ef

# Get the Fermi Energy and Print it
CBMin = np.min(E_shift[E_shift > 0.01])
VBMax = np.max(E_shift[E_shift < 0.01])

fermiEnergy = (CBMin + VBMax)/2

print(f"Fermi Energy is : {fermiEnergy}")
print(f"Global Fermi Energy : {fermiEnergy + ef}")
```

```
Fermi Energy is : 0.26214999999999966
Global Fermi Energy : 6.97275
```

In [26]:

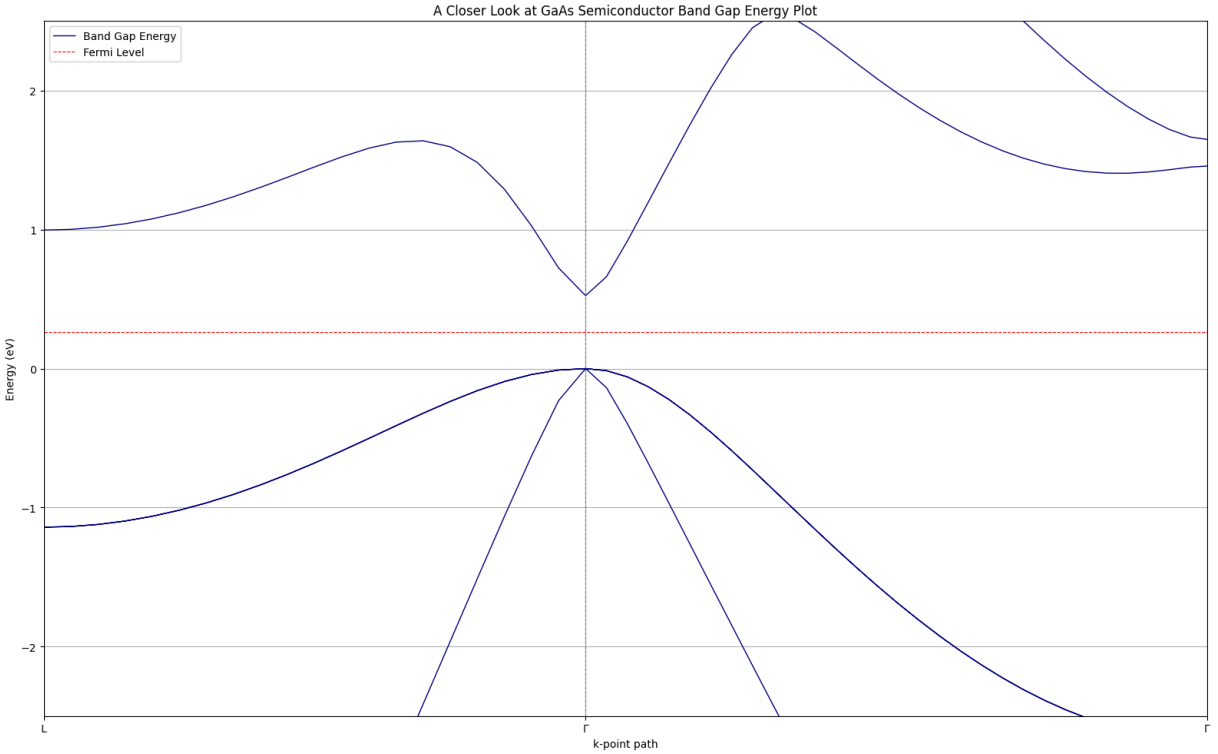
```
# Define Graph Limits
xmax = 3.2844
ymin = -13
ymax = 7

# Plot the graph
plt.figure(figsize=(16, 10))
plt.plot(k, E - ef, linewidth=1, color='navy', label="Band Gap Energy")

# Plot the Variable Lines
for xline in xs:
    plt.axvline(x=xline, color='gray', linestyle='--', linewidth=0.8)

# Add X Ticks
plt.xticks(
    [0, x1, x2, x3, xmax],
    ["L", r"$\Gamma$", "X", "K,U", r"$\Gamma$"]
)

# Plot a Red Line for the Fermi Energy
plt.axhline(y=fermiEnergy, color='red', linestyle='--', linewidth=0.8, label="Fermi

plt.ylabel("Energy (eV)")
plt.xlabel("k-point path")
plt.title("GaAs Semiconductor Band Gap Energy Plot")

plt.ylim(ymin, ymax)
plt.xlim(0, xmax)

plt.tight_layout()
plt.grid()
plt.legend()
plt.show()
```



In [27]:

```python
# Closer View at the Band Gap
import numpy as np
import matplotlib.pyplot as plt

# Define Graph Limits
xmax = 1.86
ymin = -2.5
ymax = 2.5

# Plot the graph
plt.figure(figsize=(16, 10))
plt.plot(k, E - ef, linewidth=1, color='navy', label="Band Gap Energy")

# Plot the Variable Lines
for xline in xs:
    plt.axvline(x=xline, color='gray', linestyle='--', linewidth=0.8)

# Add X Ticks
plt.xticks(
    [0, x1, x2, x3, xmax],
    ["L", r"$\Gamma$", "X", "K,U", r"$\Gamma$"]
)

# Plot a Red Line for the Fermi Energy
plt.axhline(y=fermiEnergy, color='red', linestyle='--', linewidth=0.8, label="Fermi

plt.ylabel("Energy (eV)")
plt.xlabel("k-point path")
plt.title("A Closer Look at GaAs Semiconductor Band Gap Energy Plot")

plt.ylim(ymin, ymax)
plt.xlim(0, xmax)
```

```
plt.tight_layout()
plt.grid()
plt.legend()
plt.show()
```



7. Assignment Questions

Answer the following in a short report :

1. What Is the fermi energy?
2. Why is the SCF calculation performed on a coarse k-point grid, while the NSCF calculation uses a dense path?
3. Is GaAs a direct or indirect semiconductor based on your calculation?
4. How did you decide on the number of bands?

Answers

---

1. What is the Fermi Energy

The Fermi Energy Level for the following GaAs semiconductor is `6.97275 eV`. This was calculated by getting the `Highest Occupied Level` which was `6.7106 eV`. This value is equivalent to the Maximum Valence Band energy level, and since the Fermi Energy Level is in the center between the `Maximum Valence Band` and the `Minimum Conduction Band`

level where the bandgap is ≈ 0.5, the Fermi level is therefor ≈ 0.25 higher than the Maximum Valence Band value.

2. Why is the SCF calculation performed on a coarse k-point grid, while the NSCF calculation uses a dense path?

The reason we use a coarser k-point grid for the SCF claculation and a Denser Path for the NCSF calculation can be attributed to efficency and saving computations.

In the SCF calculation we are trying to find the ground state Electron Density, Where this structure can vary due to the 3 dimensions each atom can be moved in and is an expensive calculation since it updates the electron density. The goal for this calculation is in reality just to find the approximate region of the ideal solution, so we get a low detailed 3D mesh to find a approximate location of ground state density.

Now, once we have an approximate location / low quality guess from the SCF calculation, we now want to find the eigen values along the path of L -> Gamma -> X -> K, U -> Gamma. Since the NSCF calculation isn't expensive to compute since it doesn't update the electron density we can evaluate a lot more points. This dense line of points will then be used to make the Band Plot and if we want a smooth plot, then we need a high density along the line

3. Is GaAs a direct or indirect semiconductor based on your calculation?

Based off the plot made in the section above, the GaAs is a Direct Semiconductor. This is because the Maximum Valence Band energy and Minimum Conduction Band energy are both aligned on Gamma

4. How did you decide on the number of bands?

I decided on `16` for the number of bands because of the following reasons :

1. I wanted a pair number of bands
2. I wanted a number of bands that would make it an insulator, but would bring it close to the transition of behaving like a Metal, so in this state it truly behaves like a Semiconductor
3. Based off this value, this also makes it close to Complex System, I wanted to examine how it would behave as well when it is close to that state

8. Deliverables

Upload the following:

Your band structure plot (PNG) Short Answer to the questions