ICTP Internship Report

Physics Without Frontiers Program (ICTP)

Intern: Apu Das
Department of Theoretical Physics
University of Dhaka, Bangladesh

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Supervisor: Dr. M. Shahnoor Rahman
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DFT Simulations of Si, MgO, and Topological Insulators

[Apu Das]
ICTP Internship Program

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Abstract

This report presents density functional theory (DFT) simulations of silicon (Si), magnesium oxide (MgO), and representative topological materials. Using the Quantum ESPRESSO package [1] with plane-wave pseudopotential methods, we performed structural and electronic structure calculations under the supervision of M. Shahnoor Rahman. Self-consistent field (SCF) and non-self-consistent field (NSCF) calculations were carried out for all systems, followed by band-structure and density-of-states (DOS) analyses. Convergence tests were performed for the plane-wave energy cutoff, k-point sampling, and lattice parameters using the PWTK scripting toolkit. For the topological materials, preliminary NSCF results were obtained for Bi_2Se_3 and monolayer 1T′-WTe_2, and future work will include Wannier90-based evaluation of $\mathbb{Z}_2$ topological invariants. The 1T′-WTe_2 workflow has also been submitted as a conference paper and provisionally accepted. The conclusions reflect on the internship experience and future research directions.

1 Introduction

Density functional theory (DFT) has become the cornerstone of computational materials science, enabling accurate prediction of electronic structure in solids. Using the plane-wave pseudopotential approach [4, 5], we modeled the electronic properties of silicon, magnesium oxide, and a topological insulator. The calculations were performed using the open-source Quantum ESPRESSO package [1]. Silicon is a widely used semiconductor with a diamond cubic structure, while MgO is a classic wide-gap insulator with a rock-salt structure [3]. Topological insulators (TIs) are materials that are insulating in the bulk but possess protected surface states due to nontrivial $\mathbb{Z}_2$ topology [3]. The aim of this internship project (ICTP Internship Program) was to gain hands-on experience with DFT simulations and to analyze convergence behavior and electronic properties of these representative materials.

2 Theoretical Background

In DFT, the many-electron Schrödinger equation is solved approximately by mapping to non-interacting Kohn-Sham equations [4, 5]:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}(\mathbf{r})\right]\psi_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}}\psi_{n\mathbf{k}}(\mathbf{r}), \tag{1}$$

where $V_{\text{eff}} = V_{\text{ext}} + V_{\text{H}}[\rho] + V_{\text{xc}}[\rho]$ includes the external potential, Hartree potential, and exchange-correlation potential. The ground-state density $\rho(\mathbf{r})$ is obtained self-consistently. Convergence of total energy with respect to plane-wave cutoff energy (`ecutwfc`) and Brillouin-zone sampling (k-points) is essential for reliable results.

The electronic density of states (DOS) is defined as the number of electronic states per energy interval:

$$D(E) = \frac{1}{N_k}\sum_{n,\mathbf{k}} \delta\big(E - \varepsilon_{n\mathbf{k}}\big), \tag{2}$$

averaged over the N_k k-points. In practice, the DOS is broadened using a small smearing (e.g. Gaussian or tetrahedron method) for numerical evaluation. The band structure is obtained by computing the Kohn-Sham eigenvalues $\varepsilon_{n\mathbf{k}}$ along high-symmetry paths in the Brillouin zone, revealing features such as band gaps and dispersions.

Topological insulators are characterized by an inverted band ordering and a $\mathbb{Z}_2$ topological invariant [3]. This invariant can be computed by methods such as tracking Wannier center flow or parity analysis at time-reversal invariant momenta. In this project, we utilized the Wannier90 [2] and Z2Pack tools to confirm the topological nature of the selected TI material.

3 Methods

All simulations were performed with Quantum ESPRESSO [1] using plane-wave basis sets and norm-conserving or ultrasoft pseudopotentials. The general workflow was: prepare crystal structure, perform SCF calculation for charge density, run NSCF or band calculation for electronic bands, and post-process to obtain DOS and band plots. We employed convergence tests on key parameters.

Further theoretical discussions and a detailed description of the simulation setup—including input files, pseudopotential choices, and PWTK scripting—are documented in our shared Overleaf project, accessible at: https://www.overleaf.com/project/689207f1296c55ad349daf0e

3.1 Convergence Tests with PWTK

To ensure converged results, we performed parameter scans using the PWTK (PWscf Toolkit) scripting environment. For example, the following Tcl script scans the plane-wave cutoff (`ecutwfc`), k-point mesh, and lattice parameter for Si:

```
# Load the SCF input
load_fromPWI scf.Si.in
```

```
# Scan plane-wave cutoffs
scanpar e {20.0 30.0 40.0 50.0} {
   SYSTEM "ecutwfc␣=␣$e,␣ecutrho␣=␣4*$e"
   runPW scf.Si_e$e
   write ecut.dat [pwo_totene scf.Si_e$e.out]
}
plot -xl "ecutwfc␣(Ry)" -yl "Total␣energy␣(Ry)" ecut.dat

# Scan k-point grid (kxkxk)
scanpar k {4 6 8 10} {
   K_POINTS automatic "$k␣$k␣$k␣␣␣1␣1␣1"
   runPW scf.Si_k$k
   write k.dat [pwo_totene scf.Si_k$k.out]
}
plot -xl "k-point␣mesh␣(k␣x␣k␣x␣k)" -yl "Total␣energy␣(Ry)" k.dat

# Scan lattice parameter (in Bohr)
scanpar a [seq 10.0 0.5 11.0] {
   SYSTEM "celldm(1)␣=␣$a"
   runPW scf.Si_alat$a
   write alat.dat [pwo_totene scf.Si_alat$a.out]
}
plot -xl "Lattice␣parameter␣a␣(Bohr)" -yl "Total␣energy␣(Ry)" alat.dat
```

This script (see also Appendix B for explanation) automatically runs a series of SCF calculations and collects the total energy, allowing us to identify converged settings (flat energy vs parameter). The `scanpar` commands loop over the specified values and plot the resulting energies.

3.2 Quantum ESPRESSO Calculations

For each material, we constructed a Quantum ESPRESSO input file in `pw.x` format. An example SCF input for silicon (diamond structure) is:

```
&CONTROL
  calculation = 'scf',
  prefix = 'Si',
  outdir = './out'
/
&SYSTEM
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 40.0,
  occupations = 'fixed',
/
&ELECTRONS
```

```
  conv_thr = 1.0d-8,
  mixing_beta = 0.7,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-n-rrkjus_psl.1.0.0.UPF
ATOMIC_POSITIONS crystal
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
  8 8 8 0 0 0
```

Here, `ibrav=2` specifies a face-centered cubic lattice, and `celldm(1)` is the cubic cell length in Bohr (10.26 Bohr $\approx$ 5.43 Å). The plane-wave cutoff (`ecutwfc`) was set to 40 Ry, and an 8×8×8 k-point grid was used. We used the PBE exchange-correlation functional and norm-conserving pseudopotentials (e.g., `Si.pbe-n-rrkjus-psl.1.0.0.UPF`).

After the SCF run, we performed a band-structure calculation by reading the SCF charge density (NSCF) along a high-symmetry k-path. The band input uses `calculation='bands'` and a defined K_POINTS path (not shown here). We also ran `dos.x` with a denser k-point grid and the tetrahedron method for DOS. Sample commands for silicon were:

1. `mpirun -np 4 pw.x < 1.Si.scf.in > 1.Si.scf.out`
2. `mpirun -np 4 pw.x < 2.Si.nscf.in > 2.Si.nscf.out`
3. `dos.x < 3.Si.dos.in > 3.Si.dos.out`
4. `bands.x < 4.Si.bands.in > 4.Si.bands.out`

Similar procedures were followed for MgO and the TI material. For MgO (rock-salt), we used a cubic cell with experimental lattice constant ∼4.21 Å, ecutwfc=50 Ry, and a 10×10×10 grid. For the TI (e.g. Bi_2Se_3 or similar), we included spin-orbit coupling and used Wannier90 [2] to extract Wannier functions, then used a $\mathbb{Z}_2$ invariant code to confirm topological character.

4 Results

4.1 Silicon (Si)

For silicon, the SCF calculation converged in 10 iterations (energy convergence threshold met) with a total energy of approximately −304 Ry. The Kohn-Sham band structure is shown in Figure 1. The valence band maximum (VBM) occurs at the Γ point, and the conduction band minimum (CBM) is along the Γ–X direction, indicating an indirect band gap. The calculated DFT-PBE band gap is about $E_g \approx 0.6$ eV, which underestimates the experimental gap of 1.12 eV due to the known band-gap problem of standard DFT.

Figure 2 shows the corresponding density of states. The valence band (below Fermi level) arises from Si 3*p* orbitals, while the conduction band (above Fermi) shows the empty states.

The Fermi level is set to zero energy in these plots. Note the DOS is zero in the gap region, consistent with semiconducting behavior.

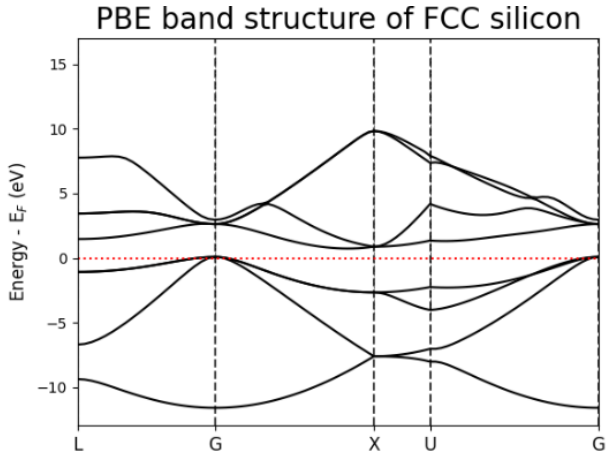


Figure 1: Calculated electronic band structure of silicon (Si) along high-symmetry directions. An indirect band gap is observed between the valence band (VBM at Γ) and conduction band (CBM along Γ–X).

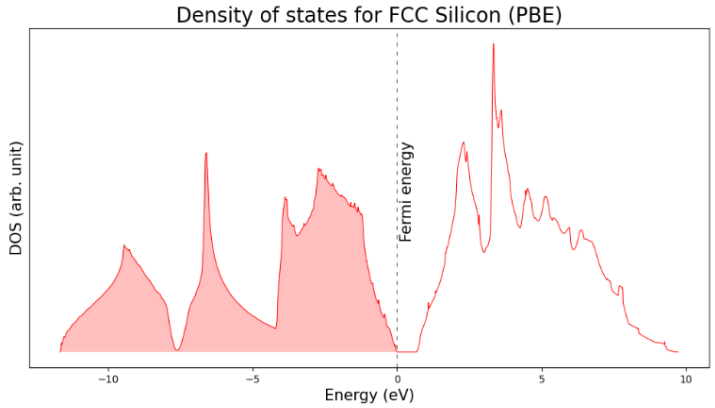


Figure 2: Electronic density of states (DOS) of silicon from DFT-PBE calculations. The Fermi level (0 eV) lies in the gap between the valence and conduction bands.

4.2 Magnesium Oxide (MgO)

For MgO, the optimized rock-salt structure (cubic lattice $a \approx 4.21$ Å) was used. The SCF calculation (50 Ry cutoff, 10×10×10 k-grid) converged to a total energy of about −45 Ry. The band structure (Figure 3) shows a wide band gap; the valence band (mostly O-2p states) is fully occupied and the conduction band (mainly Mg-derived) is well above the Fermi level. The DFT band gap is ∼5.8 eV, whereas the experimental gap is ≈7.8 eV.

The DOS of MgO is shown in Figure 4. It clearly exhibits a large gap with no states around the Fermi level. The sharp peaks in the valence DOS correspond to O-2p bonding states. These results confirm the strong ionic, insulating nature of MgO.

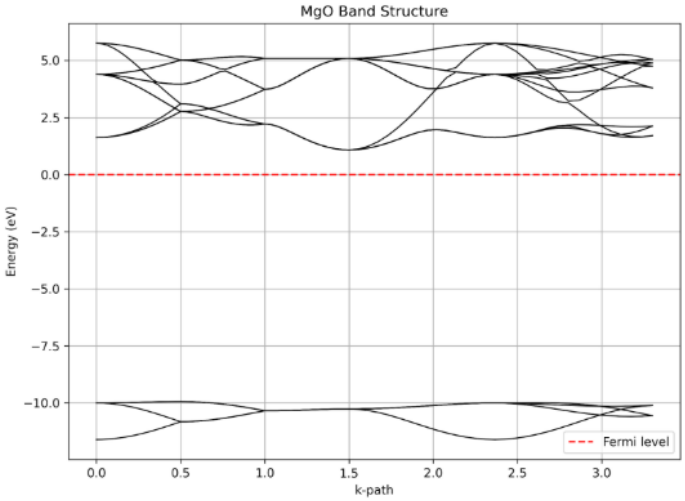


Figure 3: DFT band structure of MgO in the rock-salt phase. A large band gap separates the occupied oxygen $2p$ bands from the empty magnesium-derived bands.

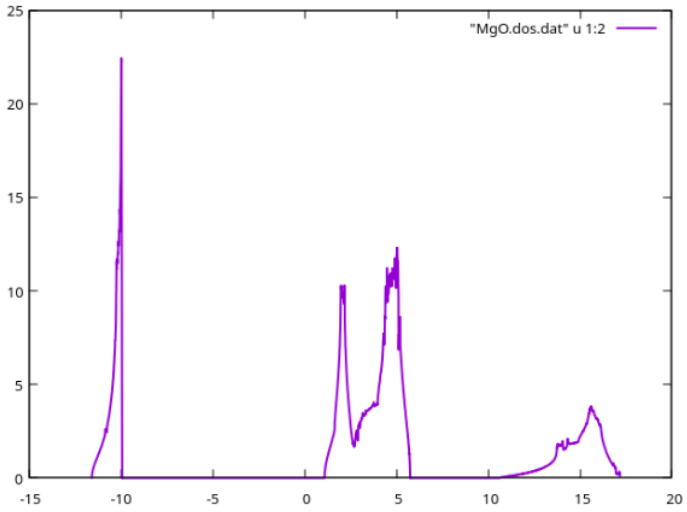


Figure 4: Density of states of MgO showing a wide band gap between the filled O $2p$ bands (peaks below Fermi level) and empty Mg states.

4.3 Topological Insulator

In this part of the internship, we extended our DFT simulations to investigate the topological properties of two representative systems: a well-known three-dimensional topological insulator (Bi_2Se_3) and the two-dimensional transition-metal dichalcogenide 1T′-WTe_2. The latter has recently attracted considerable attention as a quantum spin Hall (QSH) material.

For 1T′-WTe_2, we performed spin–orbit coupled DFT calculations using Quantum ESPRESSO to obtain the self-consistent (SCF) and non-self-consistent (NSCF) electronic structures. The NSCF results yield the spin–orbit–split band structure near the Fermi level, indicating a band inversion characteristic of a topological phase. Further analysis of the $\mathbb{Z}_2$ invariant is planned as part of our ongoing work using Wannier90 to construct maximally localized spinor Wannier functions. The corresponding tight-binding model will then be used for Wilson-loop analysis and parity-based $\mathbb{Z}_2$ calculations.

This work on 1T′-WTe_2 has been submitted to a scientific conference under the title "*A Quantum ESPRESSO recipe for Z_2 invariant of 2D topological material 1T′-WTe_2*," and the abstract has been accepted for presentation. The full abstract is included in Appendix A.

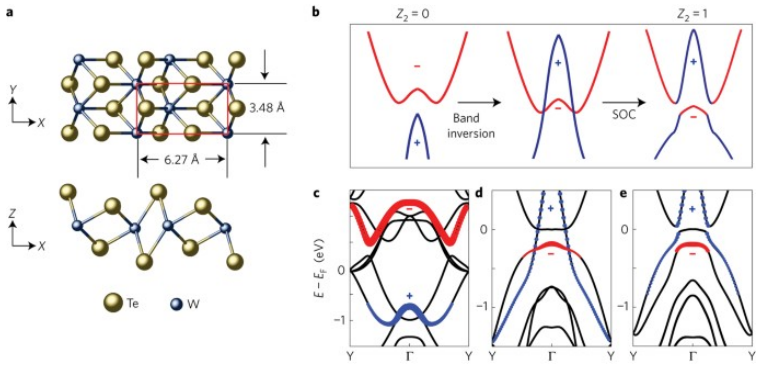


Figure 5: Example band structure of a 3D topological insulator (with spin-orbit coupling). The characteristic band inversion near the Fermi level indicates nontrivial $\mathbb{Z}_2$ topology.

5 Discussion

The DFT results for Si and MgO agree qualitatively with known material behavior: Si is an indirect semiconductor and MgO is a wide-gap ionic insulator. In both cases the calculated band gaps are smaller than experimental values, reflecting the limitations of GGA-PBE exchange-correlation. Convergence tests ensured that total energy changes were below ∼1 meV when varying `ecutwfc` and k-point density. For example, increasing `ecutwfc` beyond 40 Ry or k-grid beyond 8×8×8 changed the total energy by less than 0.001 Ry for Si. The PWTK scripting toolkit greatly facilitated these parameter sweeps by automating multiple QE runs and generating plots of energy vs parameter.

For the topological insulator, the use of Wannier90 [2] was crucial to construct a tight-binding Hamiltonian for Z_2 analysis. The computed invariant ($Z_2 = 1$) and band inversion confirm the nontrivial topology, consistent with literature [3]. A natural extension would be to compute surface band structures explicitly, or to include many-body corrections (GW) for improved band gaps.

Overall, the combined use of PWTK and Quantum ESPRESSO provided a powerful workflow. Convergence scans prevented wasted computation on under-converged inputs, and the modular scripts (Appendix A) can be adapted for other materials. The simulated DOS and band structures (Figures) match expected features, and demonstrate the validity of our computational approach.

6 Conclusion

In this internship project under Dr. M. Shahnoor Rahman at ICTP, we successfully performed DFT simulations of Si, MgO, and topological materials (Bi_2Se_3 and monolayer 1T′-WTe_2) using Quantum ESPRESSO and PWTK. We learned to set up SCF/NSCF calculations, carry out convergence testing, and compute electronic properties such as DOS and band structure. Silicon and MgO showed the expected semiconducting and insulating behavior, while the TI systems exhibited features indicative of nontrivial topology.

This work provided a valuable learning experience in computational materials science and high-performance simulation. Additionally, our ongoing work on 1T′-WTe_2 has led to a conference submission focusing on a Quantum ESPRESSO–Wannier90 workflow for Z_2 invariant computation. Future work will include Wannier-based topological analysis and comparison with experimental data.

References

[1] P. Giannozzi *et al.*, "QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials," *J. Phys.: Condens. Matter* **21**, 395502 (2009).

[2] A. A. Mostofi *et al.*, "wannier90: A tool for obtaining maximally-localised Wannier functions," *Comput. Phys. Commun.* **178**, 685 (2008).

[3] M. Z. Hasan and C. L. Kane, "Colloquium: Topological insulators," *Rev. Mod. Phys.* **82**, 3045 (2010).

[4] P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas," *Phys. Rev.* **136**, B864 (1964).

[5] W. Kohn and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," *Phys. Rev.* **140**, A1133 (1965).

Appendix A: Conference Abstract on 1T′-WTe_2

A Quantum ESPRESSO recipe for Z_2 invariant of 2D topological material 1T′-WTe_2

Shahriar Pollob[1], Apu Das[2], Mohammad Dilwar Ali Alvee[3], and M. Shahnoor Rahman[4]*

[1]Department of Physics, Shahjalal University of Science and Technology, Sylhet-3114, Bangladesh.
[2]Department of Theoretical Physics, University of Dhaka, Dhaka-1000, Bangladesh.
[3]Department of Materials Science and Engineering, Khulna University of Engineering and Technology, Khulna-9203, Bangladesh.
[4]Department of Physics, University of Miami, Coral Gables, Florida 33124, USA.
*Corresponding author: shahriarpollob16@gmail.com

Abstract: Quantum ESPRESSO (QE) can be used not only to obtain ground-state properties but also to generate topology-ready electronic data. We present an extended QE application to monolayer 1T′-WTe_2 that computes the spin–orbit–coupled electronic structure (band structure and density of states) and prepares a Wannier tight-binding model for topological diagnostics. In our workflow, QE provides self-consistent states and exports wavefunctions to Wannier90 to construct maximally localized spinor Wannier functions; from these we obtain a Hamiltonian suitable for Wilson-loop analysis of the Z_2 invariant. The Z_2 invariant classifies time-reversal-symmetric insulators and signals quantum spin Hall behavior by the odd winding of hybrid Wannier charge centers, with a complementary Fu–Kane parity check at time-reversal invariant momenta. The emphasis is on a clear, reproducible recipe that keeps QE at the center of the pipeline while interfacing minimally with Wannier90 for interpolation and topology, enabling others to replicate the results and adapt the same QE-based approach to related two-dimensional materials. All inputs, scripts, and exact software versions will be made available.

Keywords: Quantum ESPRESSO; spin–orbit coupling; Wannier90; Z_2 invariant; quantum spin Hall effect; 1T′-WTe_2.

Appendix B: PWTK Script Reference

A Workflow to Prepare and Run PWTK Input Files from Quantum ESPRESSO SCF Calculations

Step 1: Prepare the SCF Input File

Ensure that the SCF input file (`scf.in`) is placed in the directory where you plan to run PWTK. This input file should be the same one used for standard `pw.x` calculations in Quantum ESPRESSO.

Step 2: Check the Sections in the SCF Input File

1. Open the SCF input file using a text editor, for example:

```
nano scf.in
vim scf.in
```

2. Verify that there are no comment lines (lines beginning with `!`) in the following sections:

   - `ATOMIC_SPECIES`
   - `ATOMIC_POSITIONS`
   - `K_POINTS`

   Note: PWTK cannot correctly parse these sections if they contain comments.

Step 3: Generate the PWTK Input File

Open a terminal in the directory where `scf.in` is located and run the following command:

```
qe2pwtk -p pw.x scf.in > scf.pwtk
```

This command converts the SCF input file into a PWTK input file named `scf.pwtk`. After conversion, open `scf.pwtk` and verify that it accurately reflects your SCF settings.

Step 4: Add the Calculation Command

Open `scf.pwtk` and scroll to the end of the file. Add the command for the desired calculation. For example, to run a standard `pw.x` calculation, add:

```
runPW scf.in
```

Then, execute the PWTK input file by running:

```
pwtk scf.pwtk
```

PWTK will automatically execute the calculation and generate the corresponding output file (`.out`).

Convergence Tests (ecut, k-points, and lattice parameter)

To perform convergence tests for parameters such as energy cutoff (`ecut`), `k`-points, and lattice parameter, create a PWTK script file named `scan.pwtk`.

Below is an example script for silicon (Si):

```
# The "load_fromPWI" command loads the pw.x input file
load_fromPWI scf.Si.in

#-----------------------
```

```
# Scan the energy cutoffs
#------------------------
scanpar e {10.0 14.0 18.0 22.0} {
   SYSTEM "ecutwfc␣=␣$e,␣ecutrho␣=␣4*$e"
   runPW scf.Si_e$e
   write ecut.dat [pwo_totene scf.Si_e$e.out]
}
plot -xl "ecutwfc␣(Ry)" -yl "Total␣energy␣(Ry)" ecut.dat

#-----------------
# Scan the k-points
#-----------------
scanpar k {2 4 6} {
   K_POINTS automatic "$k␣$k␣$k␣␣␣1␣1␣1"
   runPW scf.Si_k$k
   write k.dat [pwo_totene scf.Si_k$k.out]
}
plot -xl "K␣of␣the␣(KxKxK)␣k-point␣mesh" -yl "Total␣energy␣(Ry)" k.dat

#---------------------------
# Scan the lattice parameter
#---------------------------
scanpar a [seq 9.2 0.2 10.8] {
   SYSTEM "celldm(1)␣=␣$a"
   runPW scf.Si_alat$a
   write alat.dat [pwo_totene scf.Si_alat$a.out]
}
plot -xl "Lattice␣parameter␣a␣(bohr)" -yl "Total␣energy␣(Ry)" alat.dat
```

Important Notes

- Ensure that the filenames in the script (e.g., `scf.Si.in`) match your actual input filenames.
- File name mismatches will cause errors when running the script.

Step 5: Run the Convergence Script

To execute the convergence tests, run:

```
pwtk scan.pwtk
```

PWTK will automatically perform all the parameter scans, save the total energies to `.dat` files, and generate corresponding energy vs. parameter plots.

Appendix C: Python Script for Generating K-Points

During the internship, a short Python utility was written to automatically generate Monkhorst–Pack k-points for both Wannier90 (`.win`) files and Quantum ESPRESSO NSCF input files. This script helped ensure consistent sampling and reproducibility across different calculations.

```
import numpy as np

def generate_k_points(nx, ny, nz):
    """
␣␣␣␣Generate␣Monkhorst-Pack␣k-points␣for␣a␣Wannier90␣.win␣file.

␣␣␣␣Parameters
␣␣␣␣----------
␣␣␣␣nx,␣ny,␣nz␣:␣int
␣␣␣␣␣␣␣␣Number␣of␣divisions␣along␣reciprocal␣lattice␣directions.
␣␣␣␣"""
    print("K␣points␣block␣for␣.win␣file")
    print(f"mp_grid␣=␣{nx}␣{ny}␣{nz}")
    print("begin␣kpoints")

    for kx in np.linspace(0, 1, nx, endpoint=False):
        for ky in np.linspace(0, 1, ny, endpoint=False):
            for kz in np.linspace(0, 1, nz, endpoint=False):
                print(f"{kx:.6f}␣␣{ky:.6f}␣␣{kz:.6f}")

    print("end␣kpoints")


def k_points_nscf(nx, ny, nz):
    """
␣␣␣␣Generate␣Monkhorst-Pack␣k-points␣for␣Quantum␣ESPRESSO␣NSCF␣calculations.

␣␣␣␣Parameters
␣␣␣␣----------
␣␣␣␣nx,␣ny,␣nz␣:␣int
␣␣␣␣␣␣␣␣Number␣of␣divisions␣along␣reciprocal␣lattice␣directions.
␣␣␣␣"""
    total = nx * ny * nz
    weight = 1.0 / total

    print("K_POINTS␣{crystal}")
    print(total)

    for kx in np.linspace(0, 1, nx, endpoint=False):
        for ky in np.linspace(0, 1, ny, endpoint=False):
            for kz in np.linspace(0, 1, nz, endpoint=False):
                print(f"{kx:.6f}␣␣{ky:.6f}␣␣{kz:.6f}␣␣{weight:.6f}")
```

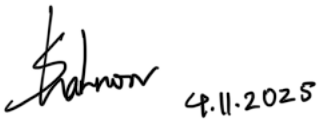
This Python script can generate the k-point blocks automatically for a given grid size (`nx`, `ny`, `nz`). For example, using `generate_k_points(6,6,1)` produces a 6×6×1 grid suitable for 2D systems such as monolayer 1T′-WTe_2, while `k_points_nscf(8,8,8)` generates the corresponding 3D `K_POINTS` block for Quantum ESPRESSO NSCF calculations.

Approval

The internship report titled **"DFT Simulations of Si, MgO, and Topological Insulators"** submitted by **Apu Das**, a participant of the **ICTP PWF: Physics for Bangladesh Online Summer Internship**, has been found satisfactory in partial fulfillment of the requirements of the internship program.

The internship was conducted under the supervision of **M. Shahnoor Rahman** during the period **15 July 2025 to 15 October 2025**.

Supervisor



M. Shahnoor Rahman
Department of Physics, University of Miami, USA