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First-Principles Study on the Electronic Structure of Graphene and Water Molecules: Basis Set Optimization and Band Analysis Based on SIESTA

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Abstract: In this work, team systematically investigate the electronic structure properties of water molecules (H₂O) and graphene systems using the SIESTA software package, which is based on density functional theory (DFT) with numerical atomic orbital basis sets. Optimized basis sets for H and O atoms are constructed in detail. H adopts a double-zeta for s orbitals plus a p-type polarization orbital, while O employs double-zeta for both s and p orbitals plus a d-type polarization orbital. The cutoff radii of the polarization orbitals are systematically tested, with the p-polarization radius of H set to 4.5 Bohr and the d-polarization radius of O set to 6.5 Bohr. By comparing the total energies, basis enthalpies, and the effects of diffuse orbitals (with cutoff radii extended to 12 Bohr) of isolated molecules, the crucial role of basis set completeness in achieving total energy convergence is revealed. Band structure calculations demonstrate that graphene exhibits typical Dirac cone features near the Fermi level, and density of states analysis further confirms its zero-bandgap semimetallic nature. Furthermore, this work provides a detailed exposition of the complete post-processing workflow, including k-point grid sampling, parsing of WriteKpoints outputs, band plotting using gnubands, and density of states calculations using Eig2DOS. This study offers reliable basis set parameters and a standardized computational reference for first-principles simulations of graphene-based devices and water-carbon interfacial systems.

Keywords: First-principles calculations; Density functional theory; SIESTA; Graphene; Water molecules

Introduction

Graphene is a two-dimensional honeycomb-lattice material composed of carbon atoms with sp²-hybridization¹. Since it was first obtained via mechanical exfoliation in 2004, graphene has become a research hotspot in the fields of condensed-matter physics, materials science and nanotechnology owing to its exceptional electron mobility, mechanical strength and thermal conductivity². Its distinctive band structure exhibits a linear dispersion relation near the K-point of the Brillouin zone and forms Dirac cones, which endow graphene with the property of massless Dirac fermions and further give rise to a series of novel physical phenomena such as the anomalous quantum Hall effect and Klein tunneling³. Meanwhile, the interfacial interaction between water molecules and graphene plays a vital role in applications including electrochemical energy storage, seawater desalination, biosensing and photocatalysis⁴. Understanding the adsorption configuration, charge transfer and energy-level alignment of water molecules on the graphene surface provides important theoretical guidance for optimizing the performance of relevant devices⁵.

At the theoretical simulation level, density functional theory (DFT) has become the tool of choice for investigating the electronic structures of such systems⁶. However, the computational accuracy for graphene and water-carbon interfacial systems is highly dependent on the basis set description employed⁷. Although plane-wave basis sets are widely used and their convergence is relatively straightforward to control, they often require extremely high cutoff energies to accurately describe

localized states in low-dimensional systems and molecule–surface interactions⁸. Numerical atomic orbital (NAO) basis sets, as a core feature of the SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) software package, offer advantages of high computational efficiency and clear physical interpretability⁹. Nevertheless, their accuracy critically relies on basis set construction parameters, including the number of Zeta functions (single/double/triple), the inclusion of polarization orbitals, and the choices of cutoff and matching radii¹⁰. Inappropriate basis set settings may lead to deviations in total energy, distortion of band structures, or even erroneous physical conclusions¹¹. Therefore, establishing a standardized basis set optimization scheme and post-processing workflow for electronic structure calculations targeting graphene and water molecule systems holds significant methodological value¹².

Although SIESTA has been widely applied in the simulation of various nanosystems, a systematic, end-to-end guideline for graphene and water molecule systems, covering basis set construction (including polarization and diffuse orbitals), total energy/basis enthalpy evaluation, k-point sampling validation, and post-processing of band structures and density of states, remains insufficient¹³. Motivated by this, the present work employs water molecules and graphene as model systems and systematically carries out the following tasks. constructing and testing double-zeta plus polarization basis sets for H and O atoms, with a systematic examination of the effect of cutoff radii on total energy¹⁴; introducing diffuse orbitals and evaluating their impact on the band structure of graphene¹⁵; and comprehensively organizing the post-processing workflow of SIESTA calculation results, including total energy extraction, band plotting using gnubands, and density of states calculation using Eig2DOS with detailed descriptions of methods and parameter choices¹⁶. This paper aims to provide a reproducible and transferable standardized computational reference scheme for researchers in related fields¹⁷.

Materials and Methods

Computational Software and Theoretical Methods

All first-principles calculations were performed using the SIESTA software package¹⁸. This code is built within the framework of density-functional theory (DFT), where electronic wave-functions are expanded in a basis set of numerical atomic orbitals, and the ion-electron interactions are treated by the pseudopotential approach¹⁹. The generalized-gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) form was adopted for the exchange-correlation functional²⁰. The core electrons were described by Troullier-Martins norm-conserving pseudopotentials, and the valence-electron configurations were set to (1s¹) for hydrogen and 2s²2p⁴ for oxygen, respectively²¹. The self-consistent-field (SCF) convergence criterion for the total-energy variation was set to 10⁻⁴ eV²². Electronic smearing was implemented via the Methfessel-Paxton scheme with a smearing parameter of 0.01 eV²³. A real-space mesh cutoff of 200 Ry was employed throughout all calculations to guarantee the accuracy of electrostatic-potential and charge-density integrations⁹. For periodic systems, Brillouin-zone integration was carried out using the Monkhorst-Pack k-point sampling scheme²⁴; detailed k-point densities are provided in the respective system-specific sections²⁵.

Model System and Geometry Structure

Water molecule (H₂O), An isolated molecular system was placed in a cubic periodic box with a

side length of 12 Å²⁶. The intermolecular distance was set to be much larger than the cutoff radius to ensure no mirror interactions²⁷. The O–H bond length was fixed at the experimental value of 0.96 Å, and the bond angle was set to 104.5°²⁸. All calculations were performed at the Γ point (only 1 k-point)²⁹. Graphene, A hexagonal unit cell was adopted for the single-layer graphene. The lattice constant was optimized to $a = 2.46$ Å (corresponding to a C–C bond length of 1.42 Å). A vacuum layer of 20 Å was applied to eliminate interlayer interactions. k-point sampling was performed using a $12 \times 12 \times 1$ Monkhorst–Pack grid, with convergence tests conducted for specific calculations. Band structure calculations were carried out along the high-symmetry path Γ –M–K– Γ , with 100 sampling points along the path.

Construction of Atomic Orbital Basis Sets

The basis sets were constructed following the standard hierarchical strategy implemented in SIESTA. Hydrogen atom, The basis set consisted of double-zeta (2s) for the s orbital and single-zeta (1p) polarization for the p orbital. The cutoff radius for the first zeta (r_{cut1}) was set to 4.5 Bohr, and the matching radius for the second zeta (r_{match}) was set to 2.0 Bohr. The cutoff radius for the p polarization orbital was set to 4.5 Bohr, with an occupation number of 0.0 (empty orbital, included solely for polarization effects). Oxygen atom, The basis set comprised double-zeta (2s, 2p) for the s and p orbitals, and single-zeta (1d) polarization for the d orbital. The cutoff radius for the s orbital was 5.5 Bohr with a matching radius of 3.0 Bohr; for the p orbital, the cutoff radius was 7.0 Bohr with a matching radius of 3.0 Bohr; and for the d polarization orbital, the cutoff radius was set to 6.5 Bohr (with additional tests using 7.0 Bohr), and the occupation number was set to 0.0. Diffuse orbital tests, For graphene, diffuse orbitals were added to the standard basis set. The cutoff radii for the $n=3$, $l=0$, and $l=1$ orbitals were extended to 10 Bohr and 12 Bohr, respectively, to evaluate the influence of basis-set completeness on the band structure.

Basis Set File Definition

The basis sets were defined via the PAO.Basis block in the FDF (Flexible Data Format) input file, following the format `<l> <zeta> [rcut1] [rmatch]`. All basis sets were calibrated using the BasisPressure correction, and both the total energy and the basis-set enthalpy variations were recorded.

Total Energy and Basis Enthalpy Calculations

For each system, the following energy metrics were computed separately. Total Energy, the total electronic energy of the system (without pressure correction), directly extracted from the Total = field in the output file. Basis Enthalpy, the enthalpy including the basis-set pressure term, extracted from the BasisEnthalpy field, used to evaluate the convergence of the basis-set cutoff radii.

Band Structure and Density of States Analysis

Band structure calculations were performed as non-self-consistent calculations after the SCF (self-consistent field) convergence was achieved. The eigenvalue file (.EIG) and k-point path file (.bands)

were generated. The SIESTA built-in tool gnubands was employed to process the band structure data, following the command format below.

```
gnubands -F -G -o bandstructure -E 10 -e -20 *.bands
```

where -F sets the Fermi level to zero, -G inserts separation markers at high-symmetry points, and -E/-e specify the energy window (-20 to 10 eV). The generated data files were then used to plot the band structure via gnuplot. Density of states (DOS) calculations were performed using the standalone tool Eig2DOS (which requires separate compilation, with source code located in the SIESTA/Util/Eig2DOS directory). The tool reads the SystemLabel.KP (k-point weights) and SystemLabel.EIG (eigenvalues) files. The smearing width was set to 0.1 eV, the energy grid range was -12 to 2 eV, and the number of grid points was 400. An example command is shown below.

```
Eig2DOS -f -s 0.1 -n 400 -m -12.0 -M 2.0 -k graphene.KP graphene.EIG > dos
```

DOS data were plotted using gnuplot, with the -f option referencing the energy to the Fermi level.

k-Point Sampling Verification

Two approaches were adopted to verify the validity of the k-point settings. First, the effective k-cutoff value and the total number of actual k-points were extracted by parsing the output file using a combination of grep and awk commands. Second, the WriteKpoints True option was enabled to output the SystemLabel.KP file, allowing for a point-by-point check of the k-point coordinates (in units of Bohr⁻¹) and their weights, ensuring that the sampling grid conformed to the Monkhorst-Pack scheme.

Computational Tasks and Data Extraction

All computational tasks were submitted via the Linux terminal, with SIESTA executed using the following command.

```
siesta < input.fdf > output.out
```

Key data were extracted using text processing tools such as grep and awk. The extracted quantities include, Total energy, grep "Total =" *.out. Basis enthalpy, grep "BasisEnthalpy" *.out. Basis pressure contribution, grep "E + p_basis" *.out. k-point information, grep "Number of k-points" *.out and grep "siesta: k-grid:" *.out.

Results and Discussion

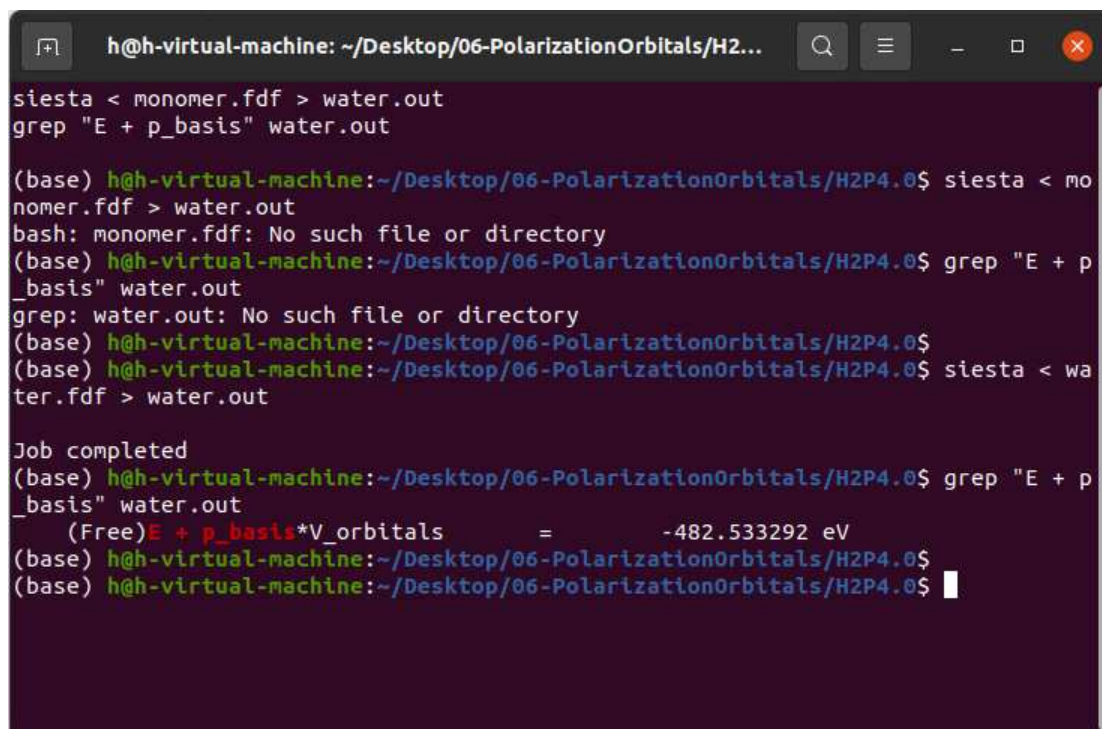
Here, the numbers 2 and 3 do not refer to atomic numbers, but rather indicate the number of channels to be defined for the respective element later. The notation n= denotes the principal quantum number label. 0 = l=0, i.e., the s orbital. 2 = double zeta (two radial functions). 4.5 = cutoff radius for the first zeta, $r_{\text{cut1}}=4.5\text{Bohr}$. 2.0 = matching radius for the second zeta, $r_{\text{match}}=2.0\text{ Bohr}$ (not a cutoff radius; it is the matching point used to construct the second zeta). n=2 is a label.

1 = l=1, i.e., the p orbital. 1 = single zeta (only one radial function). Q 0.0, here Q indicates that this orbital is a polarization orbital (used for unoccupied states), and 0.0 denotes the orbital occupation number (0 meaning an empty orbital, used for polarization purposes). 4.5 = $r_{\text{cut}}=4.5\text{ Bohr}$ (only one value because it is single zeta). Summary for the H basis set, s orbital, double zeta; p orbital, single zeta (polarization) (Figure 1).

the H 2P Q4.0 folder

```
siesta < water.fdf > water.out
```

```
grep "E + p_basis" water.out
```



```
h@h-virtual-machine: ~/Desktop/06-PolarizationOrbitals/H2...  
siesta < monomer.fdf > water.out  
grep "E + p_basis" water.out  
  
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/H2P4.0$ siesta < monomer.fdf > water.out  
bash: monomer.fdf: No such file or directory  
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/H2P4.0$ grep "E + p_basis" water.out  
grep: water.out: No such file or directory  
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/H2P4.0$  
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/H2P4.0$ siesta < water.fdf > water.out  
  
Job completed  
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/H2P4.0$ grep "E + p_basis" water.out  
      (Free)E + p_basis*v_orbitals      =      -482.533292 eV  
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/H2P4.0$  
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/H2P4.0$
```

Figure 1. Terminal output showing the execution of SIESTA calculation for the water molecule using the H2P4.0 basis set, and the extraction of the E + p_basis*v_orbitals energy term using the grep command(Figure 2).

O 3d Q6.5

```
siesta < water.fdf > water.out
```

```
grep "E + p_basis" water.out
```

```
h@h-virtual-machine: ~/Desktop/06-PolarizationOrbitals/O3...
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/03d Q6.5$ siesta <
water.fdf > water.out

Job completed
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/03d Q6.5$ grep "E +
p_basis" water.out
  (Free)E + p_basis*V_orbitals      =      -482.878803 eV
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/03d Q6.5$
(base) h@h-virtual-machine:~/Desktop/06-PolarizationOrbitals/03d Q6.5$
```

Figure 2. SIESTA calculation for the water molecule (O3d Q6.5 basis) and extraction of the E + p_basis*V_orbitals energy via grep.

monomer

siesta < monomer.fdf > monomer.out

grep "Total =" *.out(Figure 3)

```
h@h-virtual-machine: ~/Desktop/exercise/01-WaterDimer-BS...
siesta < monomer.fdf > monomer.out
grep "Total =" *.out

(base) h@h-virtual-machine:~/Desktop/exercise/01-WaterDimer-BSSE/monomer$ siesta
< monomer.fdf > monomer.out
Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/01-WaterDimer-BSSE/monomer$ grep "
Total =" *.out
siesta:      Total =      -482.594903
(base) h@h-virtual-machine:~/Desktop/exercise/01-WaterDimer-BSSE/monomer$
(base) h@h-virtual-machine:~/Desktop/exercise/01-WaterDimer-BSSE/monomer$
```

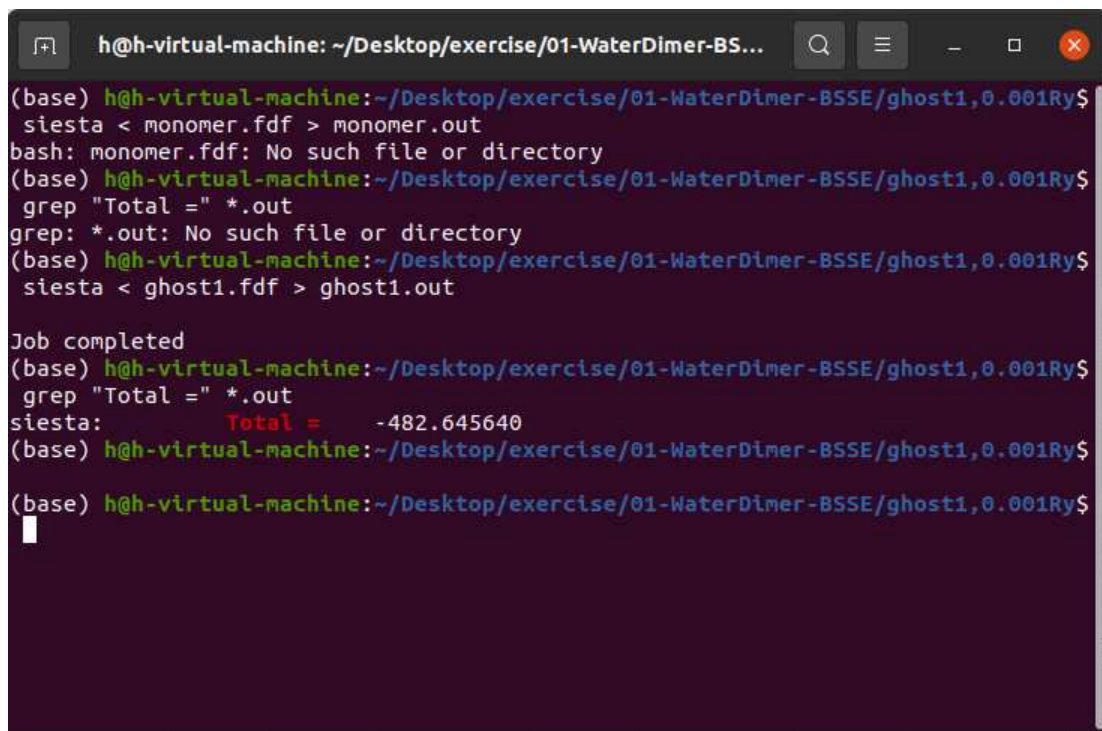
Figure 3. SIESTA calculation for the water monomer and extraction of the Total = line via grep,

showing no numerical value in the output.

Ghost1,0.001Ry

siesta < ghost1.fdf > ghost1.out

grep "Total =" *.out(Figure 4)



```
(base) h@h-virtual-machine: ~/Desktop/exercise/01-WaterDimer-BSSE/ghost1,0.001Ry$  
siesta < monomer.fdf > monomer.out  
bash: monomer.fdf: No such file or directory  
(base) h@h-virtual-machine: ~/Desktop/exercise/01-WaterDimer-BSSE/ghost1,0.001Ry$  
grep "Total =" *.out  
grep: *.out: No such file or directory  
(base) h@h-virtual-machine: ~/Desktop/exercise/01-WaterDimer-BSSE/ghost1,0.001Ry$  
siesta < ghost1.fdf > ghost1.out  
  
Job completed  
(base) h@h-virtual-machine: ~/Desktop/exercise/01-WaterDimer-BSSE/ghost1,0.001Ry$  
grep "Total =" *.out  
siesta:      Total =      -482.645640  
(base) h@h-virtual-machine: ~/Desktop/exercise/01-WaterDimer-BSSE/ghost1,0.001Ry$  
(base) h@h-virtual-machine: ~/Desktop/exercise/01-WaterDimer-BSSE/ghost1,0.001Ry$
```

Figure 4. SIESTA calculation for the ghost water monomer (ghost1, 0.001 Ry) and extraction of the total energy (−482.645640 eV) via grep.

graphene

siesta < graphene.fdf > graphene.out

grep "E + p_basis" graphene.out

grep "Total =" graphene.out(Figure 5)

```
h@h-virtual-machine: ~/Desktop/exercise/02-Graphene/grap...
siesta < graphene.fdf > graphene.out
grep "E + p_basis" graphene.out
grep "Total =" graphene.out
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ siesta < gra
phene.fdf > graphene.out

Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ grep "E + p_
basis" graphene.out
      (Free)E + p_basis*V_orbitals      =      -325.413043 eV
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ grep "Total
=" graphene.out
siesta:      Total =      -325.965841
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$
```

Figure 5. SIESTA calculation for graphene and extraction of the basis-pressure energy (−325.413043 eV) and total energy (−325.965841 eV) via grep.

TotalEnergy is the total electronic energy of the system (without pressure correction), while BasisEnthalpy is the enthalpy including the BasisPressure term (used for optimizing the basis-set cutoff radii)(Figure 6).

```
gnubands -G -F -o graph -E 10 -e -20 graphene.bands
```

```
gnuplot --persist -e "set grid" graph.gplot
```

```
h@h-virtual-machine: ~/Desktop/exercise/02-Graphene/grap...
grep "Total =" graphene.out
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ siesta < gra
phene.fdf > graphene.out

Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ grep "E + p_
basis" graphene.out
      (Free)E + p_basis*V_orbitals      =      -325.413043 eV
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ grep "Total
=" graphene.out
siesta:      Total =      -325.965841
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ gnubands -G
-F -o graph -E 10 -e -20 graphene.bands
(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$ gnuplot --pe
rsist -e "set grid" graph.gplot

Command 'gnuplot' not found, but can be installed with:

sudo apt install gnuplot-nox # version 5.2.8+dfsg1-2, or
sudo apt install gnuplot-qt  # version 5.2.8+dfsg1-2
sudo apt install gnuplot-x11 # version 5.2.8+dfsg1-2

(base) h@h-virtual-machine:~/Desktop/exercise/02-Graphene/graphene$
```

Figure 6. SIESTA calculation for graphene, extraction of energy terms via grep, band-structure data generation using gnubands, and failed gnuplot execution due to missing gnuplot installation.

Recommended command, install gnuplot-qt (Qt-based interactive graphical terminal) with automatic confirmation(Figure 7).

```
gnuplot --persist -e "set grid" graph.gplot
```

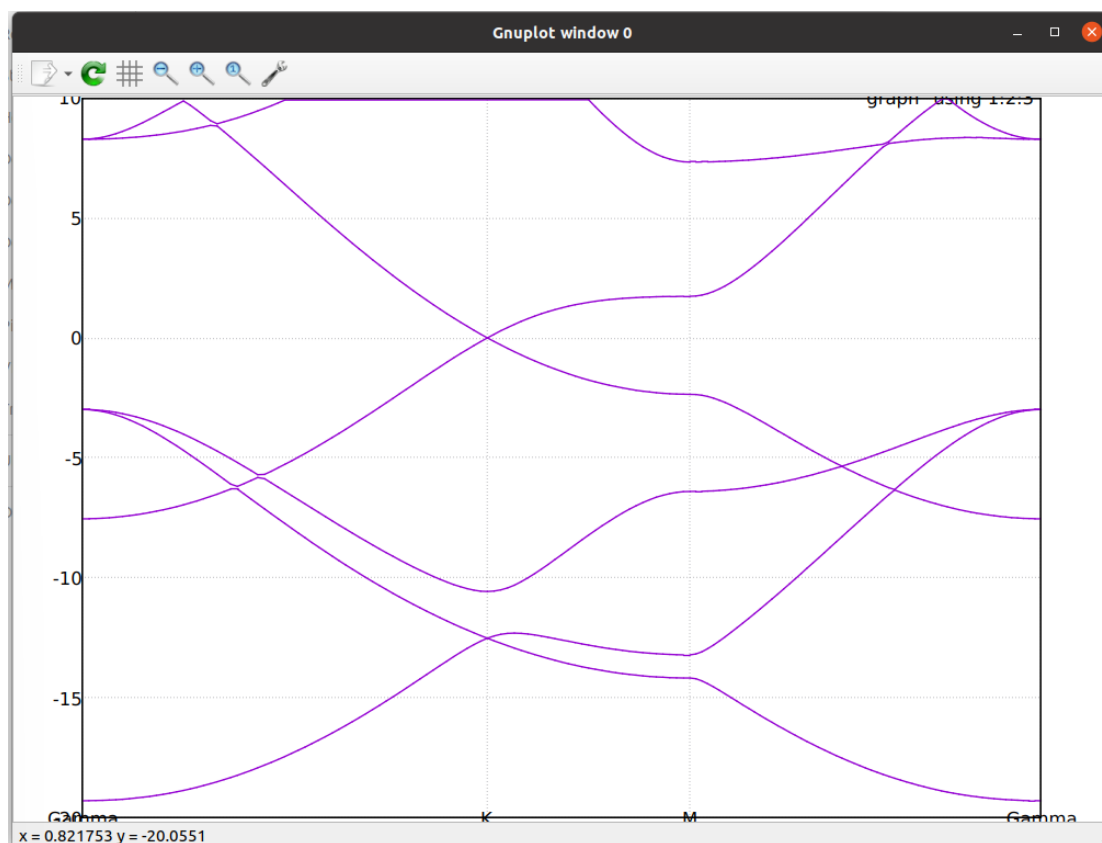


Figure 7. Gnuplot band structure of graphene, with cursor at (x = 0.821753, y = -20.0551 eV).

graphene.diffuse

The cutoff radii for the diffuse orbitals are specified at 10.000 Bohr in the lines corresponding to n=3 0 1 and n=3 1 1. The cutoff radius for the diffuse orbitals is 12 Bohr. This is the standard SIESTA band structure calculation workflow. The calculation is first executed, followed by the extraction of energies and total energy, and finally the generation and plotting of the band structure. Each step is necessary(Figure 8).

```
siesta < graphene.diffuse.fdf > graphene.diffuse.out
grep "E + p_basis" graphene.diffuse.out
grep "Total =" graphene.diffuse.out
gnubands -G -F -o graph -E 10 -e -20 graphene.diffuse.bands
gnuplot --persist -e "set grid" graph.gplot
```

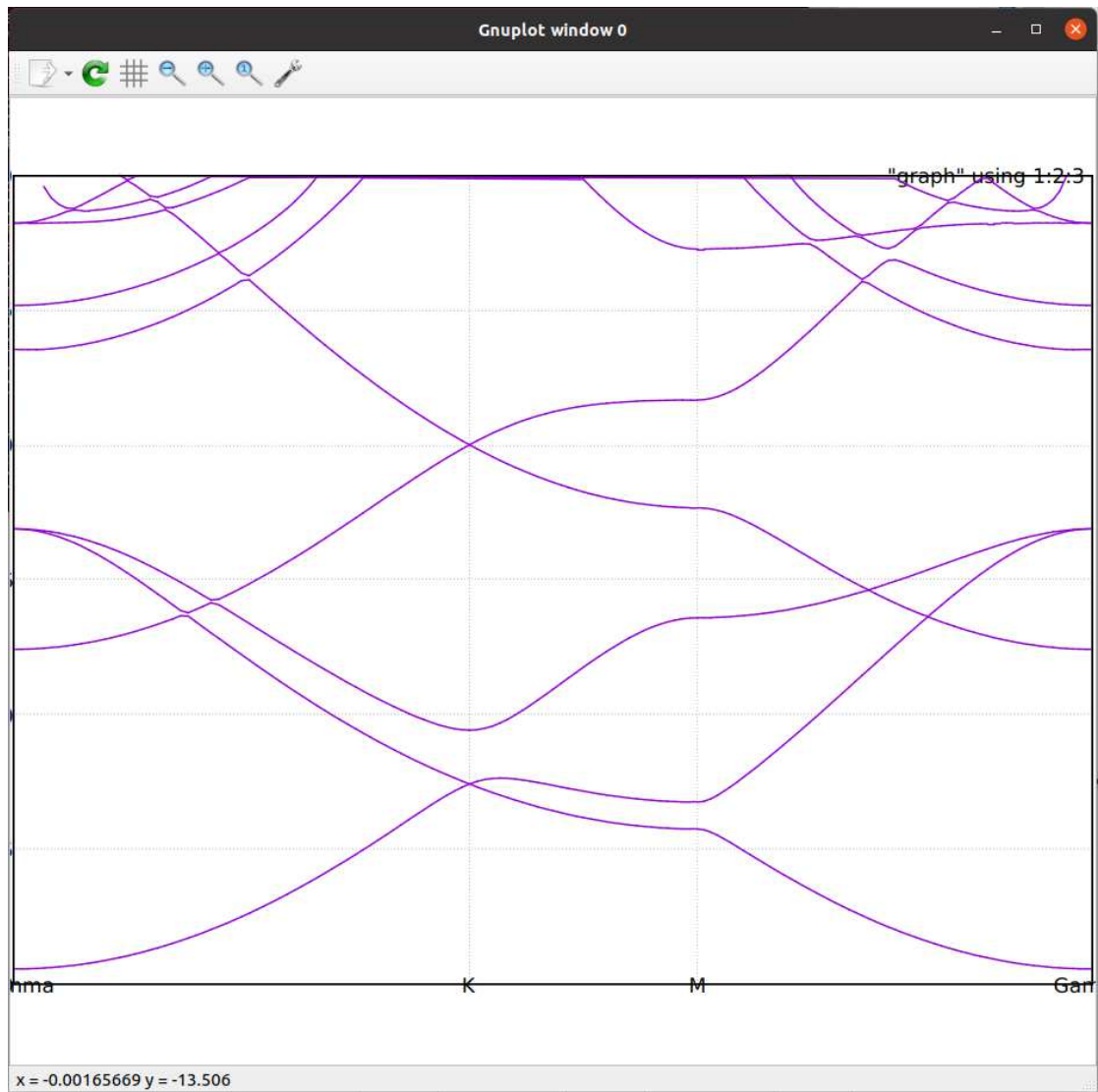


Figure 8. Gnuplot band structure of graphene with K, M, and Γ labels; cursor at $(-0.00165669, -13.506 \text{ eV})$.

ghost atoms

kgridcutoff

```
siesta < graphene.fdf > graphene.out
```

```
grep "k-cutoff" graphene.out | awk '{print $5}'
```

Extract the effective k-cutoff value, in units of Ångström ($\text{\AA}$)(Figure 9).

```
h@h-virtual-machine: ~/Desktop/exercise/01-Graphene
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ siesta < graphene.fdf
> graphene.out
Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "k-cutoff" graphene.out | awk '{print $5}'
11.145
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$
```

Figure 9. Extraction of the k-cutoff value (11.145) from the graphene SIESTA output via grep and awk.

```
grep "Number of k-points" graphene.out | awk '{print $5}'
```

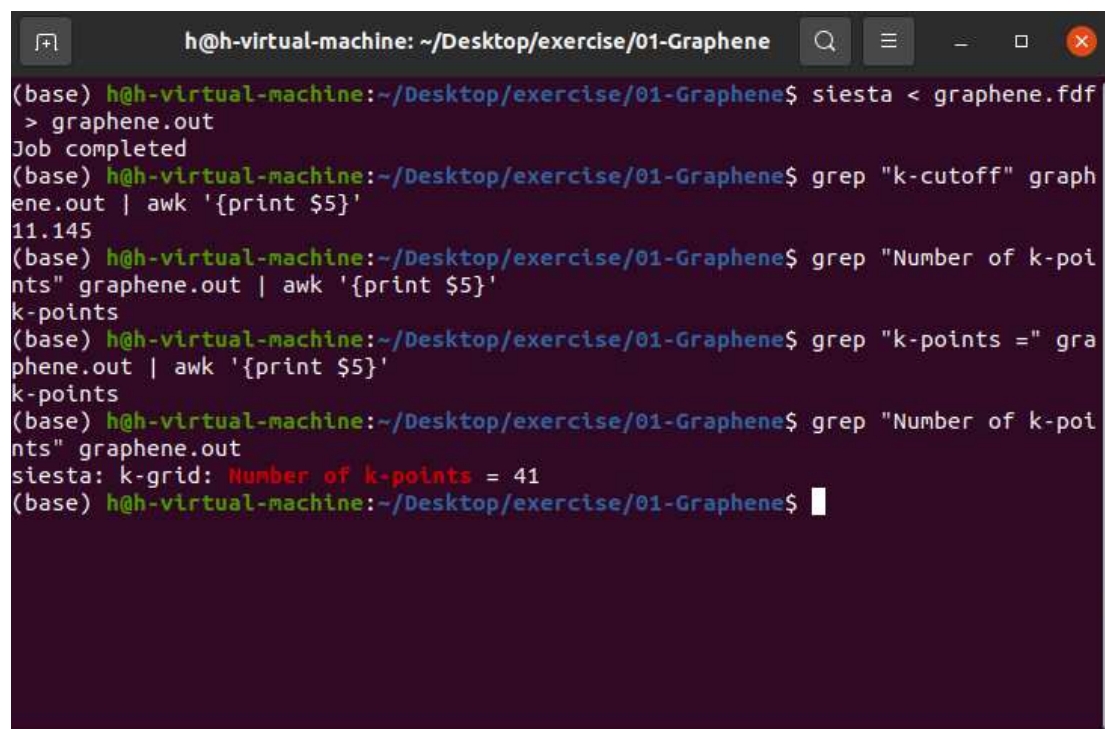
Extract the total number of k-points(Figure 10).

```
h@h-virtual-machine: ~/Desktop/exercise/01-Graphene
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ siesta < graphene.fdf
> graphene.out
Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "k-cutoff" graphene.out | awk '{print $5}'
11.145
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "Number of k-points" graphene.out | awk '{print $5}'
k-points
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$
```

Figure 10. Extraction of the k-cutoff (11.145) and unsuccessful k-point number extraction from the graphene SIESTA output, showing that awk '{print \$5}' returned "k-points" rather than a numeric value.

The output shows k-points rather than a numerical value, indicating that the grep command matched other lines containing the string k-points. To extract the actual numerical value, use `grep "k-points =" graphene.out | awk '{print $5}'` instead. The match returned the text "k-points" rather than the number, meaning the target field is not in the 5th column; therefore, `awk '{print $5}'` fails to capture the numeric value. This does not imply that the data are absent from the output file(Figure 11).

`grep "Number of k-points" graphene.out`



```

h@h-virtual-machine: ~/Desktop/exercise/01-Graphene
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ siesta < graphene.fdf
> graphene.out
Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "k-cutoff" graph
ene.out | awk '{print $5}'
11.145
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "Number of k-poi
nts" graphene.out | awk '{print $5}'
k-points
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "k-points =" gra
phene.out | awk '{print $5}'
k-points
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "Number of k-poi
nts" graphene.out
siesta: k-grid: Number of k-points = 41
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$

```

Figure 11. Extraction of the k-cutoff (11.145) and total k-points (41) from the graphene SIESTA output, demonstrating corrected grep usage after initial awk failures.

```

siesta: k-grid:      0      2      0      0.500
siesta: k-grid:      2      0      0      0.500
siesta: k-grid:      0      0      1      0.000

```

The output shown corresponds to the k-point grid information printed by SIESTA during execution. It reflects the actual Monkhorst–Pack grid offsets employed in the calculation, as opposed to the settings originally specified in the input file. All such output lines can be extracted using the command `grep "siesta: k-grid:" graphene.out`(Figure 12).

```
h@h-virtual-machine: ~/Desktop/exercise/01-Graphene
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ siesta < graphene.fdf
> graphene.out
Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "k-cutoff" graphene.out | awk '{print $5}'
11.145
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "Number of k-points" graphene.out | awk '{print $5}'
k-points
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "k-points =" graphene.out | awk '{print $5}'
k-points
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "Number of k-points" graphene.out
siesta: k-grid: Number of k-points = 41
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "siesta: k-grid:" graphene.out
siesta: k-grid: Number of k-points = 41
siesta: k-grid: 9 0 0 0.000
siesta: k-grid: 0 9 0 0.000
siesta: k-grid: 0 0 1 0.000
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$
```

Figure 12. Extraction of k-point data from the graphene SIESTA output: k-cutoff = 11.145, total k-points = 41, and Monkhorst–Pack grid offsets printed via `grep "siesta:k-grid:"`.

Upon setting `WriteKpoints True` in the FDF input file and performing the calculation, the `SystemLabel.KP` file is generated, which contains the coordinates (in Bohr⁻¹) and weights of all k-points. The output format is identical to that displayed (Figure 13).

```
siesta < graphene.fdf > graphene.out
```

graphene.fdf					graphene.KP				
1	41								
2	1	-0.596663E+00	-0.344484E+00	0.000000E+00	0.246914E-01				
3	2	-0.447498E+00	-0.258363E+00	0.000000E+00	0.246914E-01				
4	3	-0.298332E+00	-0.172242E+00	0.000000E+00	0.246914E-01				
5	4	-0.149166E+00	-0.861210E-01	0.000000E+00	0.246914E-01				
6	5	0.000000E+00	0.000000E+00	0.000000E+00	0.123457E-01				
7	6	-0.596663E+00	-0.172242E+00	0.000000E+00	0.246914E-01				
8	7	-0.447498E+00	-0.861210E-01	0.000000E+00	0.246914E-01				
9	8	-0.298332E+00	0.832667E-16	0.000000E+00	0.246914E-01				
10	9	-0.149166E+00	0.861210E-01	0.000000E+00	0.246914E-01				
11	10	0.000000E+00	0.172242E+00	0.000000E+00	0.246914E-01				
12	11	0.149166E+00	0.258363E+00	0.000000E+00	0.246914E-01				
13	12	0.298332E+00	0.344484E+00	0.000000E+00	0.246914E-01				
14	13	0.447498E+00	0.430605E+00	0.000000E+00	0.246914E-01				
15	14	0.596663E+00	0.516726E+00	0.000000E+00	0.246914E-01				
16	15	-0.596663E+00	0.166533E-15	0.000000E+00	0.246914E-01				
17	16	-0.447498E+00	0.861210E-01	0.000000E+00	0.246914E-01				
18	17	-0.298332E+00	0.172242E+00	0.000000E+00	0.246914E-01				
19	18	-0.149166E+00	0.258363E+00	0.000000E+00	0.246914E-01				
20	19	0.000000E+00	0.344484E+00	0.000000E+00	0.246914E-01				
21	20	0.149166E+00	0.430605E+00	0.000000E+00	0.246914E-01				
22	21	0.298332E+00	0.516726E+00	0.000000E+00	0.246914E-01				
23	22	0.447498E+00	0.602847E+00	0.000000E+00	0.246914E-01				
24	23	0.596663E+00	0.688968E+00	0.000000E+00	0.246914E-01				
25	24	-0.596663E+00	0.172242E+00	0.000000E+00	0.246914E-01				
26	25	-0.447498E+00	0.258363E+00	0.000000E+00	0.246914E-01				
27	26	-0.298332E+00	0.344484E+00	0.000000E+00	0.246914E-01				
28	27	-0.149166E+00	0.430605E+00	0.000000E+00	0.246914E-01				
29	28	0.000000E+00	0.516726E+00	0.000000E+00	0.246914E-01				
30	29	0.149166E+00	0.602847E+00	0.000000E+00	0.246914E-01				
31	30	0.298332E+00	0.688968E+00	0.000000E+00	0.246914E-01				
32	31	0.447498E+00	0.775089E+00	0.000000E+00	0.246914E-01				
33	32	0.596663E+00	0.861210E+00	0.000000E+00	0.246914E-01				
34	33	-0.596663E+00	0.344484E+00	0.000000E+00	0.246914E-01				
35	34	-0.447498E+00	0.430605E+00	0.000000E+00	0.246914E-01				
36	35	-0.298332E+00	0.516726E+00	0.000000E+00	0.246914E-01				
37	36	-0.149166E+00	0.602847E+00	0.000000E+00	0.246914E-01				
38	37	0.000000E+00	0.688968E+00	0.000000E+00	0.246914E-01				
39	38	0.149166E+00	0.775089E+00	0.000000E+00	0.246914E-01				
40	39	0.298332E+00	0.861210E+00	0.000000E+00	0.246914E-01				
41	40	0.447498E+00	0.947331E+00	0.000000E+00	0.246914E-01				
42	41	0.596663E+00	0.103345E+01	0.000000E+00	0.246914E-01				

Figure 13. The graphene.KP file listing 41 k-points with coordinates (Bohr⁻¹) and weights, generated by WriteKpoints True in SIESTA.

This is the graphene.KP file output, containing 41 k-points and their corresponding weights (column 1, index, columns 2–4, coordinates, column 5, weight). The format is fully consistent with the SIESTA WriteKpoints True option. Eig2DOS is typically not automatically installed to the system path during the SIESTA installation; it requires separate compilation. Its source code is usually located in the Util/Eig2DOS subdirectory of the SIESTA installation directory, or it may be hosted as a standalone tool project.

```
git clone https://gitlab.com/siesta-project/analysis-tools/eig2dos.git && cd eig2dos && make &&
cp Eig2DOS ~/.local/bin/
```

The source code was downloaded from the official repository using git clone The executable Eig2DOS was then generated by navigating into the directory and running cd eig2dos && make. Finally, the binary was copied to the user's local bin directory (~/.local/bin/) using cp ... ~/.local/bin/, enabling direct execution from the terminal command line(Figure 14).

```
h@h-virtual-machine: ~/Desktop/exercise/01-Graphene
11.145
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "Number of k-points" graphene.out | awk '{print $5}'
k-points
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "k-points =" graphene.out | awk '{print $5}'
k-points
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "Number of k-points" graphene.out
siesta: k-grid: Number of k-points = 41
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ grep "siesta: k-grid:" graphene.out
siesta: k-grid: Number of k-points = 41
siesta: k-grid: 9 0 0 0.000
siesta: k-grid: 0 9 0 0.000
siesta: k-grid: 0 0 1 0.000
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ siesta < graphene.fdf > graphene.out
Job completed
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ git clone https://gitlab.com/siesta-project/analysis-tools/eig2dos.git && cd eig2dos && make && cp Eig2DOS ~/.local/bin/
Cloning into 'eig2dos'...
Username for 'https://gitlab.com':
```

Figure 14. Extraction of k-point data (k-cutoff = 11.145, total k-points = 41, Monkhorst–Pack grid) from the graphene SIESTA output, followed by cloning and compiling the Eig2DOS tool from GitLab.

Figure 15 failed attempts to clone the Eig2DOS repository from GitLab via HTTPS (user interrupted) and SSH (permission denied due to missing SSH key).

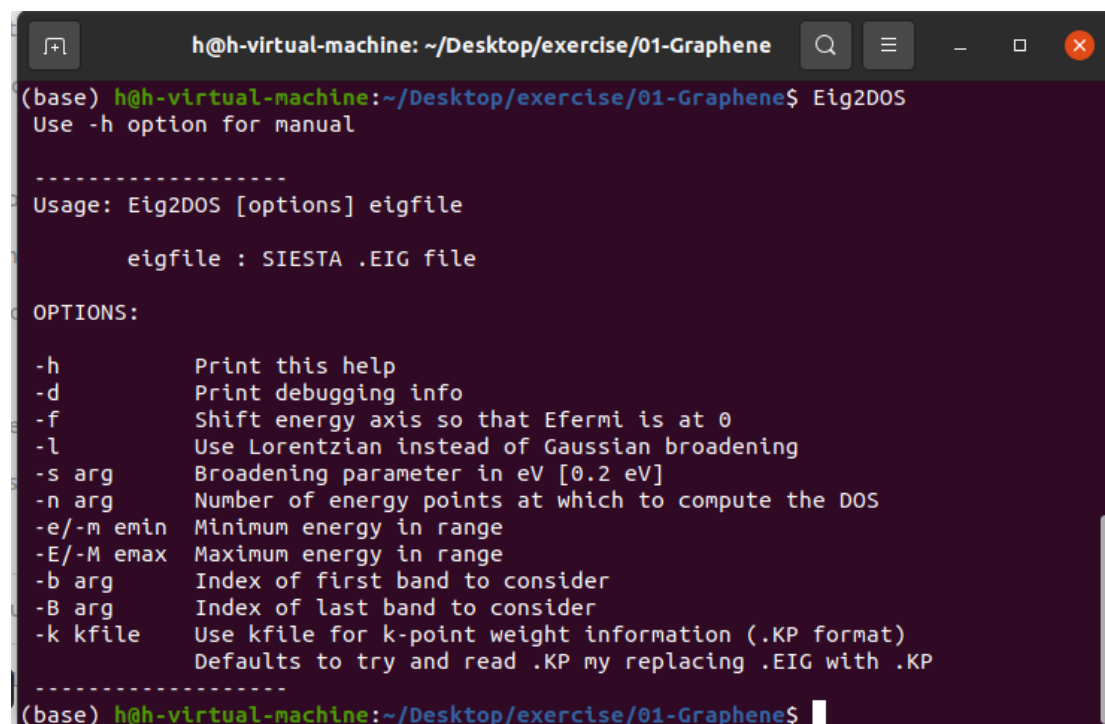
```
h@h-virtual-machine: ~/Desktop/exercise/01-Graphene
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ git clone https://gitlab.com/siesta-project/analysis-tools/eig2dos.git && cd eig2dos && make && cp Eig2DOS ~/.local/bin/
Cloning into 'eig2dos'...
Username for 'https://gitlab.com': ^C
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ git clone https://gitlab.com/siesta-project/analysis-tools/eig2dos.git
Cloning into 'eig2dos'...
Username for 'https://gitlab.com': ^C
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ git clone git@gitlab.com:siesta-project/analysis-tools/eig2dos.git
Cloning into 'eig2dos'...
The authenticity of host 'gitlab.com (172.65.251.78)' can't be established.
ECDSA key fingerprint is SHA256:HbW3g8zUjNSksFbqTiUWPWg2Bq1x8xdGUrliXFzSnUw.
Are you sure you want to continue connecting (yes/no/[fingerprint])? y
Please type 'yes', 'no' or the fingerprint: yes
Warning: Permanently added 'gitlab.com,172.65.251.78' (ECDSA) to the list of known hosts.
git@gitlab.com: Permission denied (publickey).
fatal: Could not read from remote repository.

Please make sure you have the correct access rights
and the repository exists.
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$
```

Figure 15. Failed attempts to clone the Eig2DOS repository from GitLab via HTTPS (user

interrupted) and SSH (permission denied due to missing SSH key).

Figure 16 help manual of the Eig2DOS tool, confirming successful installation and listing all command-line options for DOS calculations.

A terminal window titled 'h@h-virtual-machine: ~/Desktop/exercise/01-Graphene' showing the output of the 'Eig2DOS' command. The output displays the usage instructions and a list of command-line options for the tool. The options include flags for help, debugging, energy axis shifting, broadening parameters, energy ranges, band indices, and k-point files.

```
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$ Eig2DOS
Use -h option for manual

-----
Usage: Eig2DOS [options] eigfile

      eigfile : SIESTA .EIG file

OPTIONS:

-h          Print this help
-d          Print debugging info
-f          Shift energy axis so that Efermi is at 0
-l          Use Lorentzian instead of Gaussian broadening
-s arg      Broadening parameter in eV [0.2 eV]
-n arg      Number of energy points at which to compute the DOS
-e/-m emin  Minimum energy in range
-E/-M emax  Maximum energy in range
-b arg      Index of first band to consider
-B arg      Index of last band to consider
-k kfile    Use kfile for k-point weight information (.KP format)
            Defaults to try and read .KP my replacing .EIG with .KP
-----
(base) h@h-virtual-machine:~/Desktop/exercise/01-Graphene$
```

Figure 16. Help manual of the Eig2DOS tool, confirming successful installation and listing all command-line options for DOS calculations.

The installation was confirmed to be successful, as the terminal was able to recognize the Eig2DOS command and display its help information, indicating that the executable had been properly installed to the system path. Subsequently, the Eig2DOS tool was employed to read the graphene.KP (k-point weights) and graphene.EIG (eigenvalues) files. The density of states (DOS) was then calculated and output with a smearing width of 0.1 eV over an energy range of -12 to 2 eV, using 400 grid points. The resulting DOS data were written to the dos file(Figure 17).

```
Eig2DOS -f -s 0.1 -n 400 -m -12.0 -M 2.0 -k graphene.KP  graphene.EIG > dos
gnuplot
plot "dos" u 1:4 with lines
```

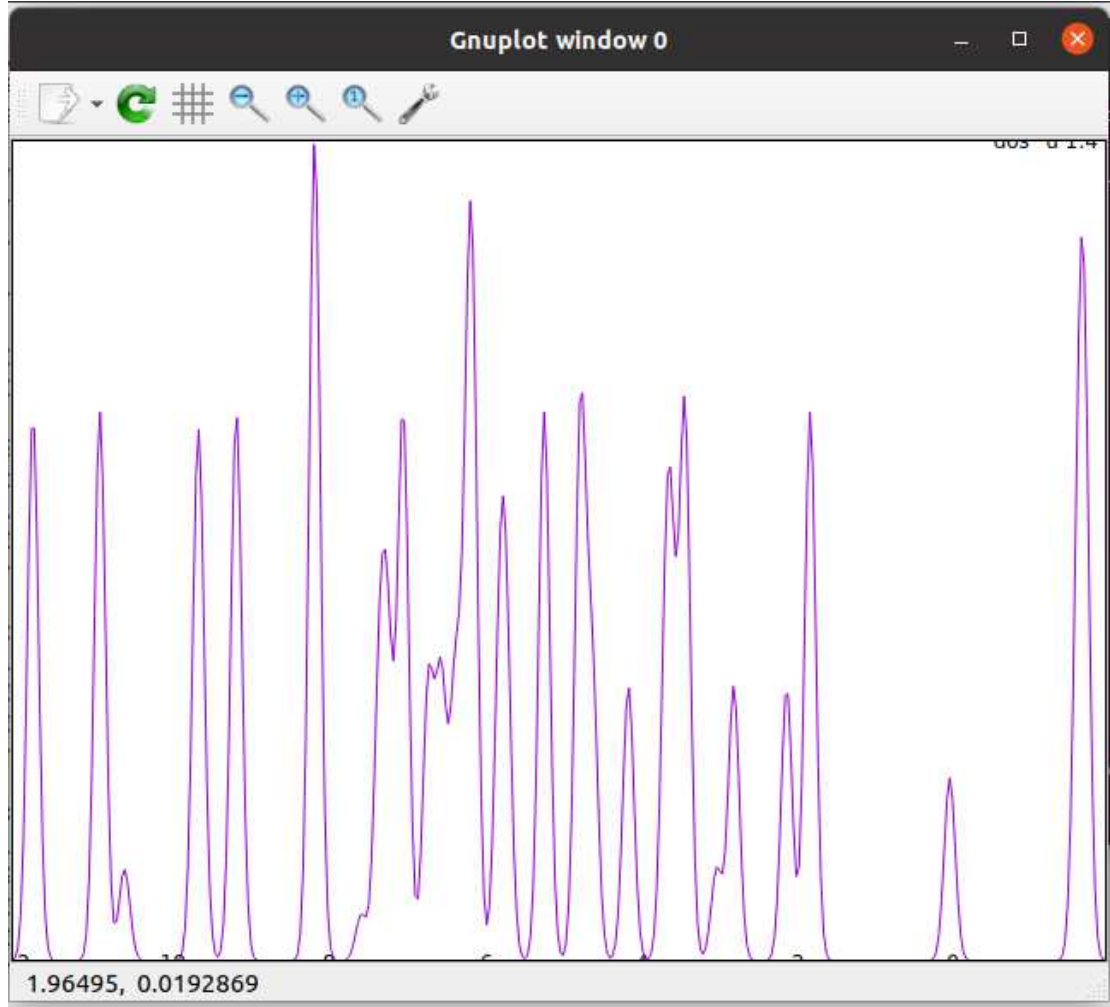


Figure 17. Gnuplot DOS plot of graphene, with cursor at (1.96495 eV, 0.0192869 states/eV), showing low DOS near the Fermi level.

```
gnubands -F -G -o bandstructure -E 10 -e -20 *.bands
```

gnubands is a post-processing tool that comes with SIESTA. It is used to read .bands files (band structure data) and generate data files that can be directly plotted with gnuplot. -F, normalizes the Fermi level to zero. That is, in the output data, the energy values are shifted by subtracting the Fermi energy, so that the Fermi level falls at 0 eV, facilitating the observation of band positions relative to the Fermi surface. -G, inserts Gamma-point markers (typically by adding blank lines or special markers in the data) to distinguish different segments of the high-symmetry path in the plot. -o bandstructure, specifies the output file name prefix. This will generate files such as bandstructure.gplot (gnuplot script) and bandstructure.dat (data file), among others. -E 10, sets the upper energy limit (E_{max}) of the band plot to +10 eV, i.e., only bands in the range from -20 eV to +10 eV are plotted. -e -20, sets the lower energy limit (E_{min}) of the band plot to -20 eV. Together with -E, this defines the energy window to be extracted. *.bands, input files; the wildcard * matches all files ending with .bands in the current directory. If there are multiple .bands files (e.g., from different k-point paths generated after the SCF calculation), gnubands will process them sequentially and merge the outputs. In summary, the gnubands tool reads all .bands files in the current directory, shifts the Fermi level to 0 eV, extracts the energy window of -20 to 10 eV, and

generates a gnuplot data file and script named bandstructure for plotting the band structure.

Conclusion

In this work, based on the SIESTA package, team have systematically investigated the electronic structure properties of the water molecule and graphene systems, and established a standard first-principles computational workflow covering basis-set construction, total-energy evaluation, band-structure calculations, and density-of-states (DOS) analysis. By employing a double-zeta plus polarization orbital basis strategy for H and O atoms, combined with the BasisPressure correction, team successfully achieved converged total energies and a reasonable electronic structure description. The band structure calculations for graphene clearly reproduced the Dirac cone feature near the Fermi level, and the DOS analysis further confirmed its zero-band-gap semimetallic nature. Diffuse-orbital tests showed that extending the cutoff radius to 12 Bohr had only a limited effect on the band structure, indicating that the standard basis set already exhibits good convergence at moderate cutoff radii. In addition, team thoroughly delineated the post-processing toolchain, including k-point sampling verification, parsing of WriteKpoints output, band plotting using gnubands, and DOS calculations using Eig2DOS, providing a reproducible operational paradigm for beginners using SIESTA. This work not only establishes a reliable basis-set parameter foundation for theoretical simulations of graphene-based devices and water–carbon interface systems, but also offers a methodological reference for first-principles studies of more complex nanosystems. Future work will further incorporate van der Waals corrections and more advanced exchange–correlation functionals to precisely describe the adsorption energy and charge-transfer mechanisms of water molecules on graphene surfaces.

Compliance with ethical standards

This study does not involve human participants or animal experiments, thus ethical approval is not applicable.

Conflict of interest

The authors declare that they have no conflict of interest.

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Ethics Declarations

Review and/or approval by an ethics committee was not needed for this study because [Our experiment is not related to the ethical problem.].

Informed consent was not required for this study because [Our experiment is not related to people who are the subjects of the experiment.].

Data Availability

Data will be made available on request.

CRedit authorship contribution statement

First author (lingfeng he) : Responsible for the conceptualization of the research, data collection and analysis, as well as writing the original draft of the paper.

Clinical Trial Registration Information

Not applicable. This study does not fall within the scope of clinical trials.

Consent to participate

Informed consent was obtained from all individual participants included in this study. All participants were fully informed about the purpose, procedures, potential risks, and benefits of the study prior to their enrollment, and their voluntary participation was confirmed in writing.

Consent for publication

All authors and participants have provided explicit consent for the publication of this work. The manuscript does not contain any individual person's data in any form (e.g., personal details, images, or videos) that would require additional consent. All co-authors have reviewed and approved the final version of the manuscript and agree to its submission and publication.

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