

Fundamentals of Energy Materials

HW#2 Quantum Espresso practice.

Total: 100 points, 4 problems

General computational instructions

- Use BURAI as the GUI for Quantum ESPRESSO.
- Use the same pseudopotential, energy cutoff, and k-point mesh for comparable calculations unless otherwise instructed.
- Use the same computational settings as the in-class example; a separate convergence study is not required for this assignment.
- For Problem 4, use consistent DOS calculation settings for C-diamond and C-graphite and set the Fermi level as the common energy reference ($E_f = 0$ eV).
- Submit screenshots/plots that clearly show the model, main input settings, and final results.

1. (20 points) Basic concepts

- Briefly describe the purpose of an SCF (self-consistent field) calculation.
- Briefly describe geometry optimization.
- Explain the difference between an SCF calculation and geometry optimization.

2. (20 points) Crystal structures of carbon

Compare C-graphite and C-diamond in terms of crystal structure, atomic arrangement, coordination number, and bonding characteristics. Include one structure image from BURAI for each material.

3. (25 points) Geometry optimization of C-graphite and C-diamond

Perform geometry optimization for both C-graphite and C-diamond using BURAI/Quantum ESPRESSO. Summarize the following results in a table:

- Optimized lattice constant(s)
- Unit-cell volume
- Calculated density
- Comparison with a reference/experimental value and the percent error

Note: For graphite, the interlayer spacing is strongly affected by van der Waals interactions. In this assignment, do not use the c-axis agreement as the main criterion for grading unless specifically instructed.

4. (35 points) Electronic structure of carbon allotropes

Using BURAI/Quantum ESPRESSO, compare the electronic structures of C-diamond and C-graphite using Density of States (DOS) calculations.

- Calculate and plot the DOS of C-diamond and C-graphite. Indicate the Fermi level ($E_f = 0$ eV) in each plot. (15 points)
- Compare the DOS near the Fermi level and explain the difference in their electronic behavior. (10 points)
- Based on literature or reliable databases, explain how sp^2 and sp^3 bonding lead to the different electronic structures of graphite and diamond. Cite at least one reference. (10 points)

Recommended report contents

For each problem, include the necessary BURAI/QE screenshots, numerical results, plots, and a short interpretation. For Problem 4(c), include at least one properly cited reference. The objective is not only to obtain a result, but also to explain what the calculated quantity physically means.