

## Fundamentals of Energy Materials

### HW#3 Quantum Espresso practice.

Total: 100점, 4 problems

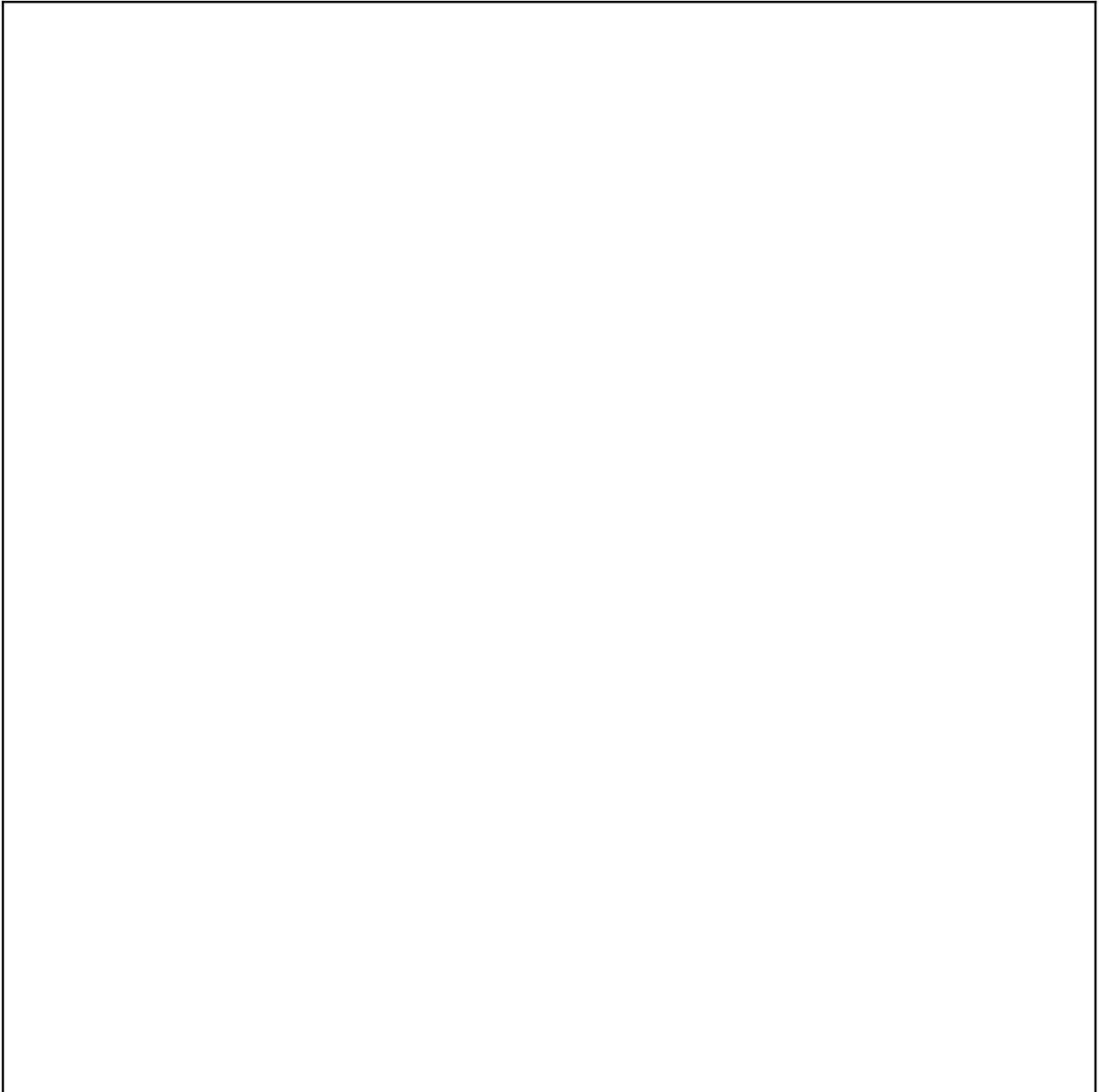
1. (25 points) Please answer the following questions.
  - (a) Briefly describe SCF calculation and geometry optimization.
  - (b) Explain the difference between SCF and geometry optimization.

2. (25 points) Describe the difference between the structures of C-graphite and C-diamond.

3. (25 points) Determination of C-graphite and C-diamond after geometric optimization
  - (a) Lattice constants
  - (b) Volume of structures,
  - (c) Comparison of theoretical and calculated densities,  $\rho$ .



(25 points) Determine Optimization curve of structure (Each student should set different intervals for the lattice constant) (changing x-axis only for C-graphite)



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