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3.021J / 1.021J / 10.333J / 18.361J / 22.00J Introduction to Modeling and Simulation  
Spring 2008

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# Introduction to Modeling and Simulation

## Thonhauser, Spring 2008

### Part III, Quantum Modeling

#### Problem Set 2

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**Post date: 05/05/08**

**Due date: 05/09/08**

The following problem set is to be solved in groups of 2–3 students. Each group should hand in only one set of solutions containing the names of all group members.

- 1. Diamond:** Using PWscf and the input files `diamond.*` perform calculations on diamond, which is the hardest material that exists. Determine the equilibrium lattice constant  $a_{\text{lat}}$  and from that find the density of a diamond in  $\text{kg}/\text{m}^3$ . Further, calculate the bulk modulus of diamond and verify that it is harder than silicon and iron. Confirm that diamond is an insulator by calculating the density of states (DOS). Explain in a simple picture why diamond is transparent in the visible range of light.
- 2. Silicon:** Using PWscf and the input files `silicon.*` perform calculations on silicon—one of the most important materials of the last century. Calculate the equilibrium lattice constant  $a_{\text{lat}}$ , the density, and the bulk modulus of silicon. For  $a_{\text{lat}}$  calculate the band structure along the lines in the appropriate input files. Determine the gap by calculating the DOS and explain why silicon is considered a semiconductor.
- 3. Iron:** Using PWscf and the input file `iron.input` perform a spin-polarized calculation and find the equilibrium lattice constant  $a_{\text{lat}}$  and the bulk modulus of iron. Determine the ground state magnetization and show that iron is a ferromagnetic metal.

Show that all results from above are converged with respect to all applicable simulation parameters.