598SCM Fall 2004 Homework 3 - PART I

Handed out Tuesday, September 28, 2004
Due Tuesday, October 12, 2004
    There will be an "Office hour" session before the due date. Anyone is welcome to come to discuss the solutions to the problems. Time to be announced.

1. Download the ABINIT code

2. Work the Tutorial, parts 1 - 4

   Additional calculations:

3. For Si, calculate the change with pressure of the fundamental gap (the lowest energy gap between filled and empty states). Do this by finding the gap at the lattice constant used in tutorial, and also the gap with a slightly compressed lattice constant.

   To complete the homework, turn in your results for the fundamental gap and the lattice constant for the two cases.

4. Now distort the lattice by reducing the lattice constant in the x direction, and expanding in the y and z directions to keep the volume constant. What happens to the top of the valence bands at the Γ point? Do the three band split so that they are not degenerate?

   To complete the homework, turn in your results for the splitting of the top of the valence bands at the Γ point and the values of the lattice constants that you chose. Describe why you expect the bands to split in this case.

5. Carry out a calculation for Si in the fcc structure (the close-packed structure with one atom per cell, the same structure as many elemental metals). Do the calculation using the LDA and at a volume similar to that for the minimum energy of Si in the fcc structure given in Figure 2.4. Calculate the difference in the energy per atom in the fcc structure compared to that for Si in the diamond structure at its equilibrium volume. Is the energy difference similar to that shown in Figure 2.4?

   To complete this homework, email to Prof. Martin the two output files for Si in the diamond structure at its equilibrium volume and for Si in the close-packed fcc structure near its equilibrium volume (The volume does not have to be the exact equilibrium volume).

Optional Problems
Good for understanding - Prof. Martin will be happy to discuss the solution of these problems

6. Any other example you choose using ABINIT.