Introduction to Modeling and Simulation
Part II : Quantum Modeling

Problem Set #5

The following problem set is to be solved as a group. Each group should hand in only one set of solutions containing the names of all group members.

1. Simulation of Crystalline Silicon using Density Functional Theory

For this problem, perform the required simulations using "MIT Atomic Scale Modeling Toolkit" on the nanoHUB. Select the "SIESTA" tool from the menu. In all simulations, use `GGA/PBE` for "XC functional" and `DZP` for "Basis". Also, take `100` for "Mesh cutoff".

(a) Using the `Si diamond structure`, find the equilibrium lattice constant and verify that your value is converged with respect to k-point density.

(b) Using the equilibrium lattice constant found in (a), plot the band structure.

(c) Perform the same calculations as in (a) and (b) for `Zincblende(GaAs)`. Discuss how GaAs is different than Silicon. In particular what are the differences between the two band structures? How might these differences be relevant to solar cells?

(d) Use the same tool to compute the binding energies of each material. Compare your values with experiments. You'll need to have "spin polarized" selected for calculating the energies of the atoms. Be sure to specify what your convergence settings were – namely your k-point mesh and basis set.

(e) Calculate the bulk modulus (in GPa) for both Si and GaAs and verify which of these two materials is harder. Be sure your computed values are converged with respect to k-points. Compare your results with the experimental data. Note that the bulk modulus (B) is defined as: $B = V\frac{d^2E}{da^2}\left(\frac{da}{dV}\right)^2 = \frac{4}{9a}\frac{d^2E}{da^2} = \frac{8k}{9a}$ where k is the quadratic coefficient and a is the lattice constant.

2. Simulation of Aluminum and Metalization of Silicon by Aluminum

Unlike the materials in problem 1, here we will consider a metal system.

(a) Calculate the equilibrium lattice constant and the bulk modulus of aluminum. Compare your results with the experimental data. Keep I mind that the k-point convergence may be different than for Si and GaAs.

(b) At the equilibrium lattice constant, calculate the density of states (DOS) of aluminum – show how the DOS converges with k-points. Comment on the difference in the DOS between a metal such as Al and the semiconductors you simulated in problem 1 above.

(c) Metalization of a semiconductor like silicon can happen near the metal contacts in a device such as a solar cell. This means that the metal atoms have diffused into the semiconductor, which can cause undesirable effects. Compute the effects of substituting one silicon atom with an aluminum atom, starting from the original bulk silicon calculation. You will need to re-optimize the lattice and also be sure to converge the k-points. What happens to the DOS for such a material? Is it still a good semiconductor?

(d) Now use a larger unit cell, with a larger lattice constant and more basis atoms in the unit cell, to simulate crystalline silicon. Using this larger cell, you can make substitutions of Al for Si atoms at lower concentrations than the 50% in part (c). Show your predicted dependence of the DOS on percent Al substitution. Discuss the significance of your results.

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