Introduction to Modeling and Simulation: Part II : Quantum Modeling

Problem Set #6

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. Increasing the mobility in crystalline silicon

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) For many applications, such as next-generation computer chips, solar cells or thermoelectrics, we would like to be able to control the mobility of a material – that is, the drift velocity of electrons and holes in response to an applied electric field. Startomg from your converged calculations in the last homework of crystalline silicon, compress and stretch the Si unit cell. You can do so by changing the lattice constant. How does this pressure (or negative pressure in the case of stretching) affect the mobility of charge carriers in Si? Discuss your findings for both positive and negative carriers.
(b) Can you think of other ways to change the mobility in silicon? Try at least one such "materials design" idea out (apart from applying pressure) using the simulation tool and show and discuss your findings.

2. Simulation of the electronic structure of graphene

For this problem use the same tool as for problem #1, and the same basis and XC functional.

(a) Design the graphene honeycomb structure for your input, and optimize its lattice parameters. Keep in mind you will need to test k-point convergence. Report your lattice constant and converged k-point values.
(b) Calculate the cohesive (formation, or binding) energy of graphene. Compare with experimental data.
(c) From your computed band structure of grapheme, state whether this material is a metal, semiconductor, or ...?
(d) Compare the obtained properties (lattice structure, cohesive energy and band structure) with the diamond form of carbon and comment on the differences.
(e) Using your insights and previous experience, see if you can come up with a way to "open" (that is, increase) the gap of graphene. Explain your motivation and show your results.

3.021J / 1.021J / 10.333J / 18.361J / 22.00J Introduction to Modeling and Simulation
Spring 2011