EXERCISE 7

MOLECULAR DYNAMICS

In this exercise you will play with different MD options. The system under study is a cubic supercell of 8 atoms of Si in the diamond structure. In order to make the runs fast, we use a single-Z basis set with short orbitals (energy shift 300 meV).

Verlet dynamics

Go to the directory *verlet*. Edit the *si8.fdf* file and study it. It is an input file for a simple (microcanonical) MD simulation with the Verlet algorithm. The initial positions correpond to the ideal crystal structure. The inicial velocity is 300 K. The time step is 3 fs, and the simulation is run for 200 steps.

Run the simulation and analyze the result. Look at the *si8.MDE* file, and plot:

- total energy and KS energy versus time. Check the energy conservation
- temperature versus time.

Why is the average temperature smaller than the initial one?

Nose dynamics

In directories *nose-X-Y* you have input files for different Nose runs, for the same si8 system. *X* indicates the target temperature, and *Y* the mass of the Nose thermostat.

Run each of the simulations, and analyze the results, again plotting the different physical quantities versus time. Look at how the results change with different target temperatures and Nose masses

Cell vectors relaxation

In directories *Relax-CG* and *Relax-PR*, you have input files to relax the lattice vectors of the same Si8 system. In this case, the initial configuration is such that the lattice vectors are distorted with respect to those of the diamond structure. *Relax-CG* does the simulation using conjugate gradients minimizations, whereas *Relax-PR* uses Parrinello-Rahman dynamics, with the *MD.Quench* option.

Run both cases. Plot the evolution of the lattice constant and angles versus time. Which method is more efficient?

Parrinello-Rahman dynamics.

In directory PR you have an input file for a Parrinello-Rahman run. The system starts from a distorted geometry. The target pressure is cero. Run the simulation and analyze the results. In particular, look at the evolution of the lattice constants and angles versus simulation time. If you have time, you can run another simulation with a target pressure of 10 GPa, and see the differences.