

EXERCISE 4

CONVERGENCE WITH RESPECT TO THE GRID: THE MESH-CUTOFF

The purpose of this exercise is to see the importance of the *MeshCutoff* parameter, which determines the fineness of the real space grid on which some of the integrals are computed. In particular, we will see:

- how the properties of your system are affected by the *MeshCutoff* value, and
- how to get a good *MeshCutoff* value.

We will use the Methane (CH₄) molecule.

1) Signs of an insufficient *MeshCutoff*

Check the input file named *ch4-0.fdf* in directory *mesh-30ry*

The system is a methane molecule, inside a cubic cell of 10 Ang side. The carbon atom is localized at the origin.

Now, look for the mesh cutoff chosen in the input file. Run SIESTA with this input file, using the pseudopotential file *C.ps* located in the directory Pseudos

Read the output, paying special attention to:

- The mesh used in the calculation (look for the line starting with: *InitMesh: MESH =*)
- Total energy
- Max atomic force
- Total CPU execution time

Can you calculate what is the distance between mesh points?

Now, we do a small displacement in the position of the molecule inside our "box". With SIESTA, you can do a rigid translation of the system, by using the input block:

```
%block AtomicCoordinatesOrigin  
x y z  
%endblock AtomicCoordinatesOrigin
```

This is done in the input file *ch4-d.fdf*, which is exactly the same as the former one (*ch4-0.fdf*) but with a rigid translation of (0.127,0.745,-0.33) Ang.

Run again SIESTA using this new input file. Analyze your output file and compare with the former. Do you see anything strange? You should notice some signs that tell you that the *MeshCutoff* that has been used is too small for this system.

2) The “eggbox effect”

We will now do a series of calculations to see the so-called 'eggbox' effect. Go to directory *egg* and use the input file *ch4.fdf*. We will plot a profile of the total energy as a function of the displacement of the molecule with respect to the mesh, by displacing it in small steps in the x direction. The eggbox (as a function of the displacement of the molecule) will be periodic, with a period that correspond to the distance between meshpoints (why?).

Do a few (say, about ten) calculations to see one of these periods. How much do you need to displace the molecule? Of course, this depends on the spacing between mesh points, which you should have calculated before.

Plot the total energy and the total force versus the displacement of the molecule. You should be able to reproduce the results shown in *egg/Out/e.ps*.

Why are the properties of the molecule changing so much with this translation? Of course, the answer is that the meshcutoff is not sufficiently large for this system, and therefore the integrals are not converged, producing a variation of the results when the position of the grid changes with respect to the atomic positions.

3) Finding the right *MeshCutoff*.

Go to the directory *mesh-cutoff*. Use the *ch4.fdf* input file, and the same pseudopotential file as before.

Do a series of calculations increasing the value of the *MeshCutoff* parameter, by steps of 10 Ry. From the output files, extract:

- The actual *MeshCutoff* used (which is usually different from the one required in the input file!)
- The total energy
- The total force
- The CPU time

Plot the total energy and total force versus the requested meshcutoff and the used meshcutoff. Try to decide what would be a reasonable value for a real calculation in this system.

An important issue: realize how the total time of your calculation has grown with the increment of *MeshCutoff* value. Always take this into account, in trying to reach a compromise between accuracy and computational time.

You have plots with the results that you should obtain in *mesh-cutoff/Out*

Once that you have chosen a meshcutoff which you consider as converged, you can again plot the eggbox effect. (Notice that the mesh spacing has now changed!).

4) Effect of the inclusion of Core Corrections in the Pseudopotential.

Core corrections often make convergence with the *MeshCutoff* slower. As a matter of example, we will do the same calculation as before, but using a C pseudopotential that has a large core correction term (note that this is not necessary for C, but we do it as a matter of example).

Go to directory *core*. In file *core.ps* you can see the valence charge and the core correction included in the pseudopotential. You have the pseudopotential file in *C.pe.psf*. Note that we have included a very hard core correction, just as a matter of illustration.

Do similar tests as you did in Section 3. See how the convergence of the total energies and forces change with the inclusion of this large core correction.

You have plots with the results that you should obtain in *core/Out*.