How to optimize a system using siesta

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Before the study of different properties of material/nanomaterial all system needs to be optimized. (Step-by-step optimization of Mesh-cutoff, kpoint, lattice constant and complete) . By using siesta this can be done using following 4 steps with the given scripts. Here I am using a single molecule of AgI as an example.

In the system directory (e.g. AgI-LDA here) make directories for mesh-cutoff, kpoint, latt_opt and tot_opt separately.

1. Step-1 : Mesh-cutoff optimization

In cutoff dir there are two scripts (*script_cutoff*.sh & *get_EvsC_script.sh*) and *.psf file for related elements. Now run first script i.e. script_cutoff.sh in cammand window using

```
$ sh script_cutoff.sh
```

This will create 10 folders after complete siesta rn u and then run second script using

```
$ sh get_EvsC_script.sh
```

(before running verify the data range and siesta output file name correctly)

This will generate a EvsC.dat file and show a plot for the same. You can find best mesh-cutoff value (lowest energy value).

2. Step-2 : kpoint optimization

In order to optimize kpointgo to kpoint directory where apart from *.psf file there are again two scripts *kpoint_script.sh* and *get_EvsK_script.sh*. Before running the scripts make a change in the the Cutoff value in the kpoint_script.sh as :

replace

MeshCutoff XXXXXXXXXXXXXX Ry by

MeshCutoff optimized value Ry (obtained from 1st step)

and run the scripts in following order :

```
$ sh kpoint_script.sh
```

(which gives you complete siesta run in different folders for respective K-values)

and then run second script using

$ sh get_EvsK_script.sh

(before running verify the data range and siesta output file name correctly)

This will create t a EvsK.dat file and show a plot for the same. You can find best K-point (lowest energy value).

3. Step-3: lattice constant optimization

In the 3rd dir lat_opt (containing *.psf for related species and two scripts : lat_opt_script.sh and get_Evsa_script.sh) for lattice constant optimization and make substitution for optimized mesh-cutoff and k-point in required place represented as XXX and XX in lat_opt_script.sh script and run

$ sh lat_opt_script.sh

This will give complete siesta run in different consecutive folders. And then run second script using

$ sh get_Evsa_script.sh

(before running verify the data range and siesta output file name correctly)

This will give a Evsa.dat file and show a plot for the same. You can find best lattice constant (lowest energy value).

4. Step-4 : total optimization

For complete optimization run go to dir optim substitute best mesh-cutoff, kpoint and lattice constant obtained from previous run and finally run the script using

$ sh script-run.x

Try this and give me feedback/suggestions in the forum. we can also discuss some problem regarding to this and related other.

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