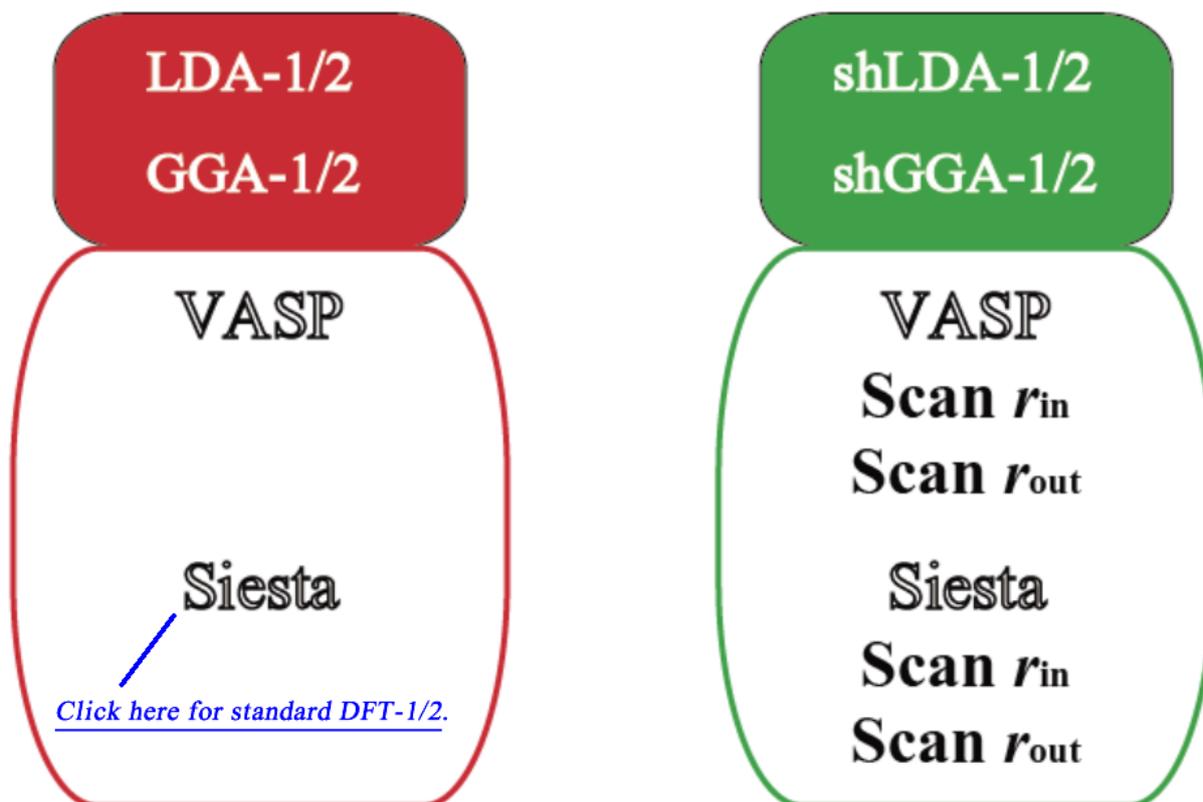


User Manual for online DFT-1/2 or shDFT-1/2 corrections

---- For SIESTA

1. Visit <http://www.eedevic.com/dft-half/>



2. Select DFT-1/2 input settings as shown below. We use LDA-1/2 calculation for cubic Li_2S as an example. Select the local “S.ion” file, and click the “Upload” button in order to trigger the online calculation. Our initial guess for the cutoff radius is in the range of 2.5 bohr to 4.0 bohr.

The “*.ion” file should be taken from the output of a previous LDA/GGA run for the same system. **If you have used the old 2.0.2 version of Siesta, the “S.ion” file shows a normal charge-neutral nature**, see figure below.

The head part of “S.ion”:

```
<basis_specs>
=====
S                               Z= 16   Mass= 32.070   Charge= 0.0000
```

with “Charge = 0.0000”. On the other hand, **the newer versions of Siesta yield divergent charge value** here, thus the “*.ion” file taking from Siesta 3.* or 4.* runs cannot be used for DFT-1/2 calculation.

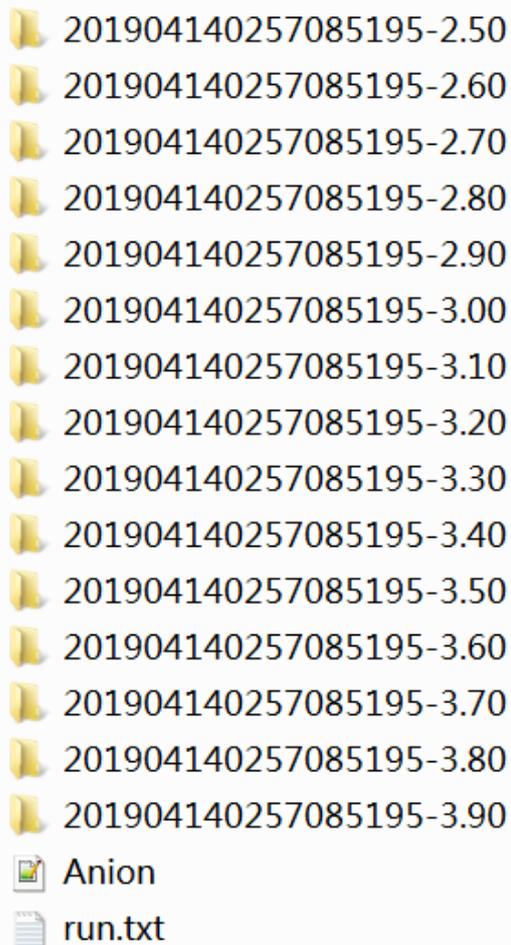
A suggested solution is to do self-energy correction using the “*.ion” file generated by Siesta 2.0.2, but use the self-energy corrected “*.ion” new files for Siesta 3.* / 4.* calculations.

LDA(GGA)-1/2 program for Siesta		
*Please use Siesta 2.0.2 to generate *.ion file, in order to avoid charge divergence. Yet, the new *.ion files with self-energy correction can be used for Siesta 3.* and 4.* calculations.		
Element: <input type="text" value="S"/>	Strip - <input type="text" value="0.50"/> e	Power index <input type="text" value="8"/>
Scan cutoff radii from <input type="text" value="2.5"/> bohr to <input type="text" value="4.0"/> bohr		
XC <input type="text" value="LDA (Ceperley-Alder)"/>		
Upload *.ion file and start the run:		
<input type="button" value="选择文件"/> S.ion	<input type="button" value="Upload"/>	
Click here to download the user manual ...		

3. After a short while, the webpage will refresh and afford you a zip-format output file. Download it to local computer.

Upload *.ion file and start the run:		
<input type="button" value="选择文件"/> 没有选择文件	<input type="button" value="Upload"/>	
Processed with self-energy potential: S-050p.		
Download zipped file at: http://www.eedevic.com/pub-ion/201904140257085195.zip		
Click here to download the user manual ...		

4. Unzip this file and you will obtain the following files:



Here the “Anion” file contains the pseudopotential of the anion element before self-energy correction. The “run.txt” file includes some parameters regarding this DFT-1/2 run. All these files are just for your information. **The remaining folders ending up with the cutoff radius (unit: bohr, or a. u.) are the key outputs.** Each folder contains a self-energy corrected *.ion file, which should replace the old “*.ion” file in DFT-1/2 runs.

5. For each cutoff radius, run Siesta in the “User Basis mode”. This means that you have to specify explicitly:

UserBasis yes

in your input *.fdf file. Otherwise, Siesta will neglect your renewed “S.ion” input, and the calculation remains to be conventional LDA.

6. Compare the band gap values obtained using various anion self-energy potential cutoff radii. Choose the “*.ion” file that renders the maximum band gap, whose corresponding cutoff radius is thus the optimal anion self-energy potential cutoff radius.
7. The “S.ion” file with the optimal cutoff radius can be used in the following large supercell calculations involving Li₂S.
8. In shDFT-1/2 calculations, you may scan either the inner cutoff radius, or the outer cutoff radius. In each case, you need to fix the other cutoff radius. Hence, it may take two or three rounds before you confirm the final optimal set of cutoff radii.