

How to calculate Fermi-Softness *via* CP2K

QIAOSONG LIN

FROM DALIAN INSTITUTE OF CHEMICAL PHYSICS, CAS

FEB 2022



Contents

1. How to **install program** ?
2. How to **run CP2K program** for calculating Fermi-Softness ?
3. How to **get Total, Condensed and Local Fermi-Softness** ?
4. How to **visualize Local Fermi-Softness** ?

1. Install program

Anaconda3, bader, and FermiSoftness is necessary.

1. You can install **Anaconda3** from the website:

[Anaconda | Individual Edition \(https://www.anaconda.com/products/individual#Downloads\)](https://www.anaconda.com/products/individual#Downloads)

2. You can download **bader** from the website:

[Bader Charge \(http://theory.cm.utexas.edu/henkelman/code/bader/\)](http://theory.cm.utexas.edu/henkelman/code/bader/)

3. You can install **FermiSoftness** by pip, ASE and Numpy will be installed automatically:

```
$ pip install FermiSoftness
```

2. Run CP2K program

1. Build a Slab model.
2. Relaxation calculation.
3. Do a single point energy calculation with **gamma only**, and following key words should be in your input:

&DFT

.....

```
&PRINT
  &MO_CUBES
    STRIDE 1
    NHOMO -1
    NLUMO -1
  &END MO_CUBES
&END PRINT
&END DFT
```

3. Calculate Total, Condensed and Local Fermi-Softness

1. Generate input file runfs.py :

```
$ python -c "from FermiSoftness import gen; gen(software='cp2k');"
```

2. Copy runfs.py to the path where the input of CP2K is.

3. Calculate Total, Condensed and Local Fermi-Softness

3. Modify the parameters in *runfs.py* :

```
filename='pt3y.out'  
project_name='pt3y'  
kbT=0.4                # Electron temperature (eV)  
dfdd_threshold=0.001  # Derivation of Fermi-Dirac distribution threshold  
bader_dir='bader'      # Path of bader  
band_gap={'VBM':[0.0], # If band gap exists, set as  $E_{\text{VBM}}, E_{\text{CBM}}$  (Do not minus  $E_{\text{Fermi}}$ );  
          'CBM':[0.0]} # Otherwise set as 0.0 0.0 (eV)
```

- filename is the single point energy output file, project_name should be the same as the value after the PROJECT keyword in the input file
- If *bader* is in your *\$PATH*, you don't need to change `bader_dir`

3. Calculate Total, Condensed and Local Fermi-Softness

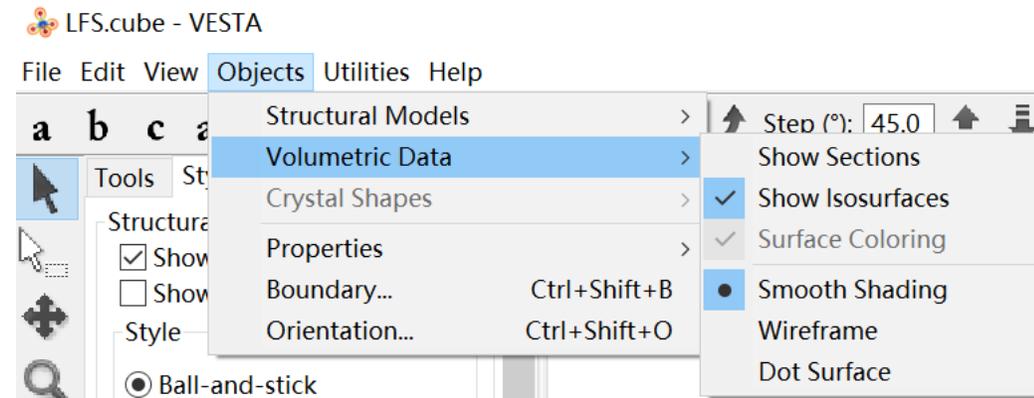
4. Run “*python runfs.py*” in terminal.
5. Wait ... it will take several minutes.
6. Finished. You can find files *FSCAR* and *LFS.cube* in current path. (If the wavefunction is spin polarization, you can find *_UP*, *_DW* for different spin. If band gap exists, you can find *_CB*, *_VB* for holes and electrons.)
7. In *FSCAR*, you can find Total Fermi-Softness (NUMBER OF ELECTRONS) and Condensed Fermi-Softness (CHARGE), the grid data of Local Fermi-Softness were recorded in *LFS.cube*.

4. Visualize Local Fermi-Softness

1. Isosurfaces

Load *LFS.cube* by VESTA

- Objects->Volumetric Data-> Show Isosurfaces



4. Visualize Local Fermi-Softness

1. Isosurfaces

Objects->Properties-> Isosurfaces

- Set appropriate isosurface level

Properties - LFS.cube ✕

General Atoms Bonds Polyhedra **Isosurfaces** Sections

Material

Specular: 0 0 0  Shininess (%): 100

Isosurfaces

F(min) = 1.79487e-009; F(max) = 0.00412769;

Render from front to back

Positive Opacity 1 (0~255): 127

Isosurface level: 0.0005 Opacity 2 (0~255): 255

Color: 255 255 0 

No.	level	mode	color
1	0.0005	Positive	

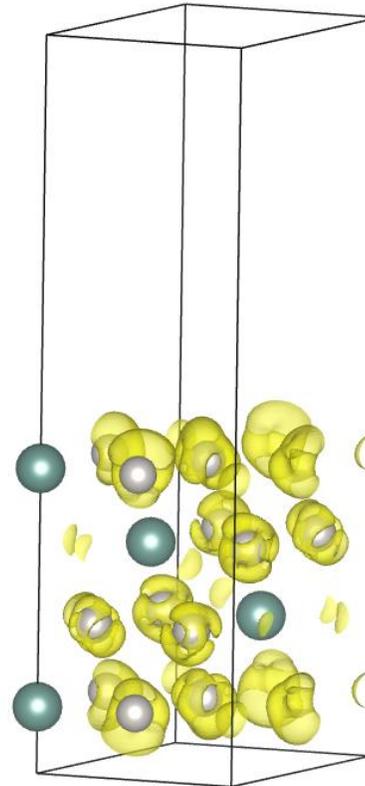
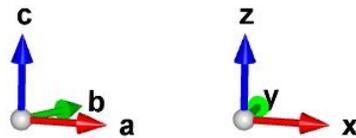
New
Delete

4. Visualize Local Fermi-Softness

1. Isosurfaces

Local Fermi-Softness mainly distributes on

Pt atoms in $\text{Pt}_3\text{Y}(111)$ surface.



4. Visualize Local Fermi-Softness

2. Contour plante

Load *LFS.cube* by VESTA

Edit->Lattice Planes

- Set Miller indices (001)
- Set appropriate Distance from origin

Lattice Planes - LFS.cube

Phase: 1 Fermi_Softness

Material

Specular: 255 255 255 Shininess (%): 100

Edges

Show edges Line width: 1.0

Add lattice planes

Miller indices (hkl): 0 0 1

Distance from origin: 9.85863 Å (0.445004 x d)

Color (RGBA): 255 0 255 192

Calculate the best plane for the selected atoms

No.	h	k	l	d (Å)
1	0	0	1	9.85863

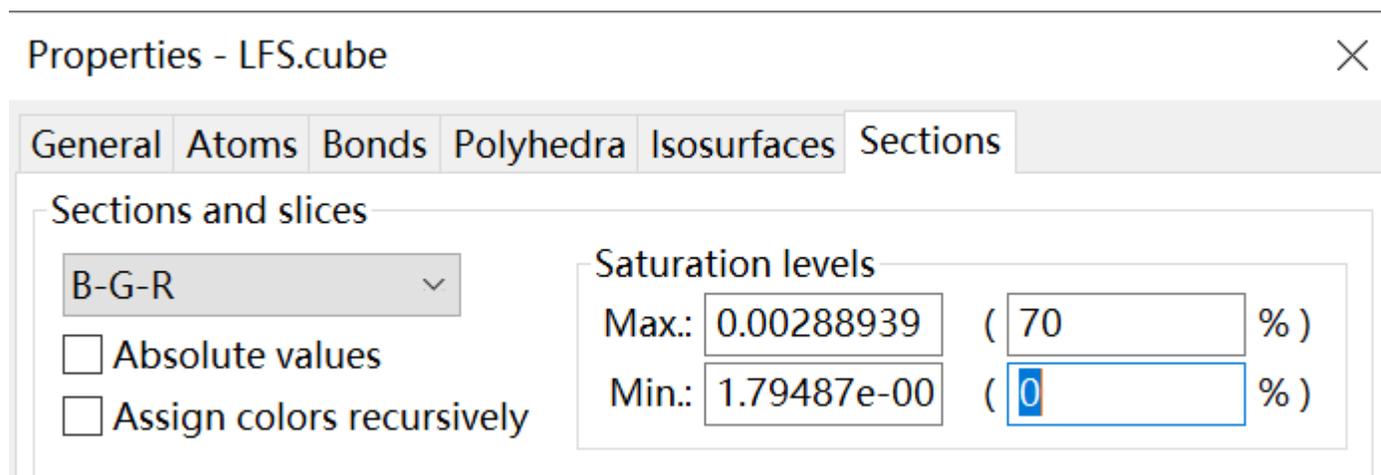
New Delete Clear ↑ ↓

4. Visualize Local Fermi-Softness

2. Contour plane

Objects->Properties-> Sections

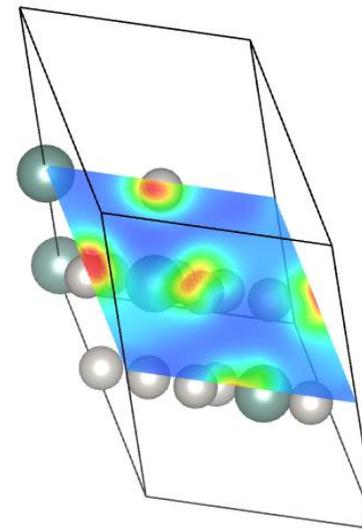
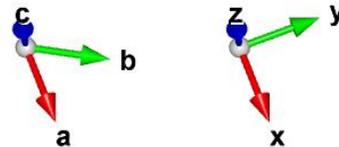
- Set appropriate Saturation level



4. Visualize Local Fermi-Softness

2. Contour plane

Local Fermi-Softness mainly distributes on
Pt atoms in $\text{Pt}_3\text{Y}(111)$ surface.

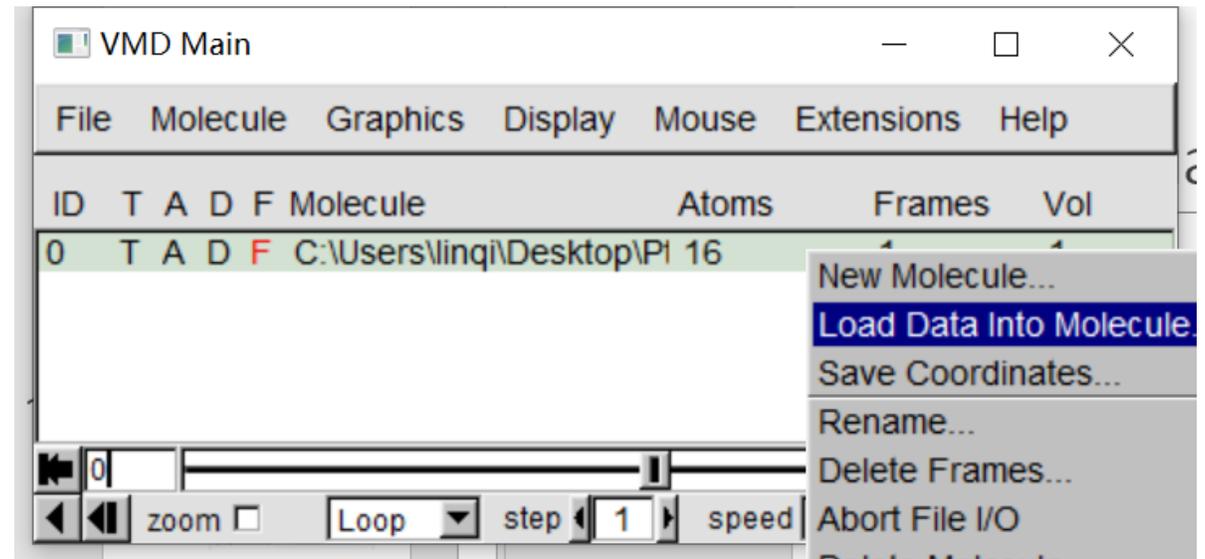


4. Visualize Local Fermi-Softness

3. Projected isosurface

Load *charge density files* by VMD

Load Data Into Molecule: *LFS.cube*



4. Visualize Local Fermi-Softness

3. Projected isosurface

Graphics->Colors->Color Scale->Method: BWR

Graphics->Representation

- Make first Rep: CPK Name all
- Make second Rep: Isosurface Volume 1

Graphics->Representation->Trajectory

- Set appropriate Color Scale Data Range

Style	Color	Selection
CPK	Name	all
Isosurface	Volume 1	<volume>

Selected Atoms: all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Volume | Material: 1: C | Opaque

Drawing Method: Isosurface | Default

Range: Vol:

Isovalue:

Step: Draw:

Size: Show:

4. Visualize Local Fermi-Softness

3. Projected isosurface

Local Fermi-Softness mainly distributes on Pt atoms in Pt₃Y(111) surface.

