

How to calculate Fermi-Softness *via* Quantum-Espresso

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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 QE program

Usually, the process of calculating Fermi-Softness is the same as calculating density-of-state (DOS):

1. Build a Slab model.
2. Relaxation calculation.
3. Static calculation (SCF) with small k-points.
4. Static calculation (non-SCF) with **large k-points**.

3. Calculate Total, Condensed and Local Fermi-Softness

1. Generate input file runfs.py :

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

2. Copy runfs.py to the path where the non-SCF input of QE is.

3. Calculate Total, Condensed and Local Fermi-Softness

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

```
prefix='pwscf'
outdir='./tmp'
kbT=0.4                                     # Electron temperature (eV)
dfdd_threshold=0.001                       # Derivation of Fermi-Dirac distribution threshold
intermediate_file_options=False            # Save intermediate files?
bader_dir='bader'                          # Path of bader
pp_launcher='pp.x'                         # Launcher of pp.x, e.g.: 'pp.x' or 'mpirun -np 4 pp.x'
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)
```

- The prefix and outdir need to be set the same as those in the nscf input file. If these keywords are defaulted in nscf, the default values should also be filled in. If outdir is the current directory, you should enter './', which cannot be abbreviated as '.'.
- If *bader* is in your *\$PATH*, you don't need to change `bader_dir`

3. Calculate Total, Condensed and Local Fermi-Softness

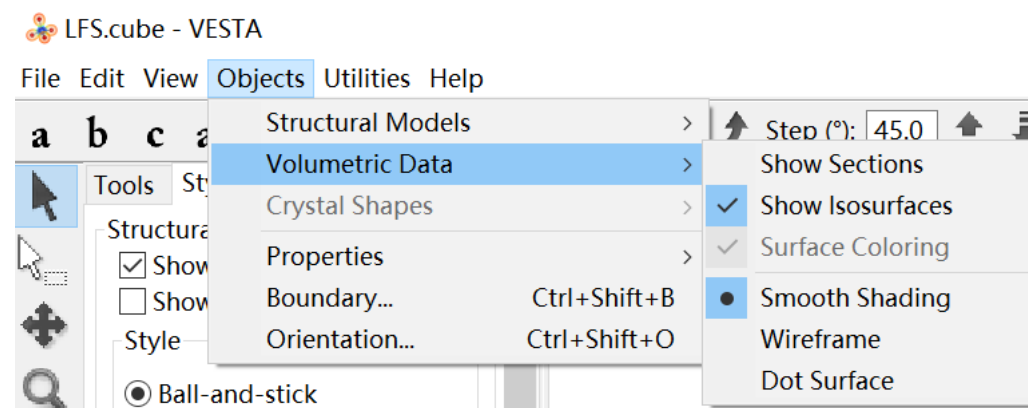
4. Run “*python runfs.py*” in terminal.
5. Wait ... it will take several minutes.
6. Finished. You can find files *FSCAR* and *LFS.cube* in current path. (If the wavefunction is spin polarization, you can find *_UP*, *_DW* for different spin. If band gap exists, you can find *_CB*, *_VB* for holes and 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

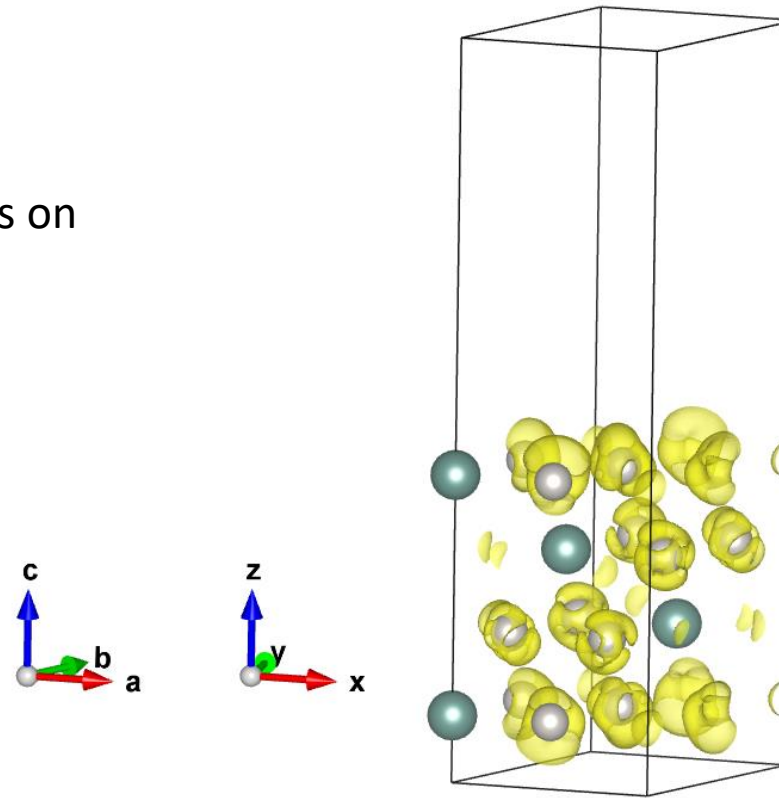
Delete

4. Visualize Local Fermi-Softness

1. Isosurfaces

Local Fermi-Softness mainly distributes on

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



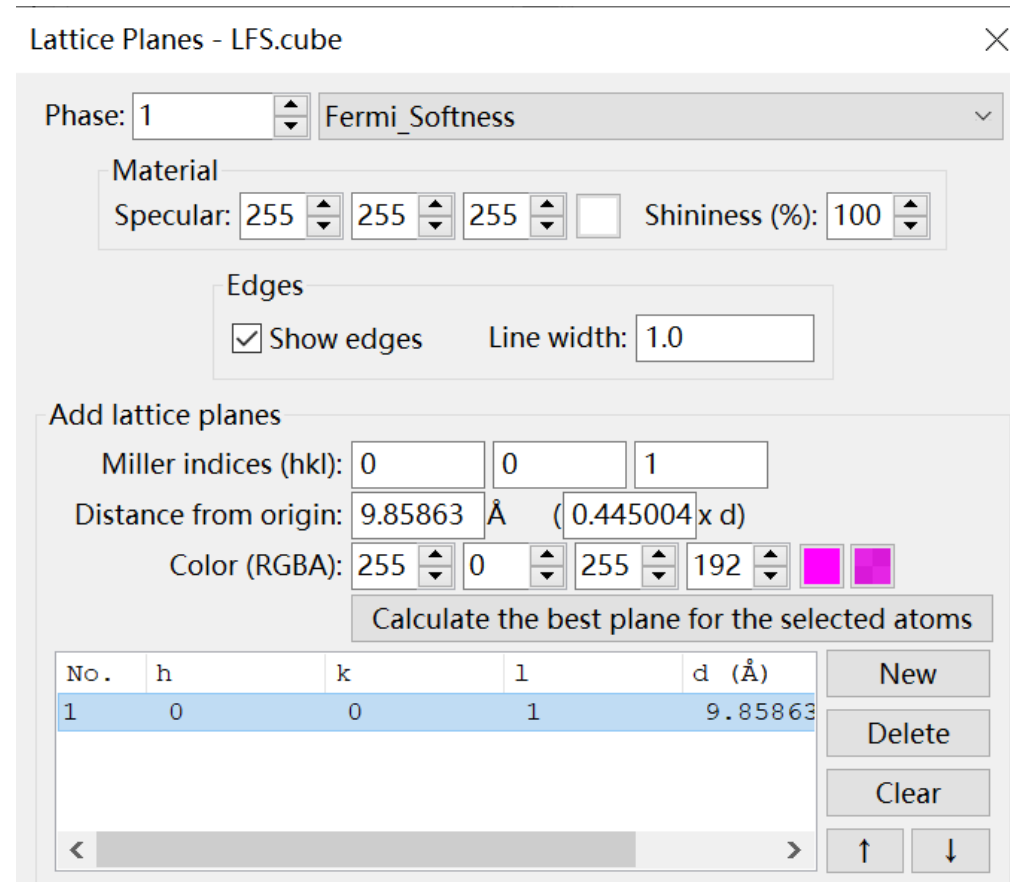
4. Visualize Local Fermi-Softness

2. Contour plante

Load *LFS.cube* by VESTA

Edit->Lattice Planes

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

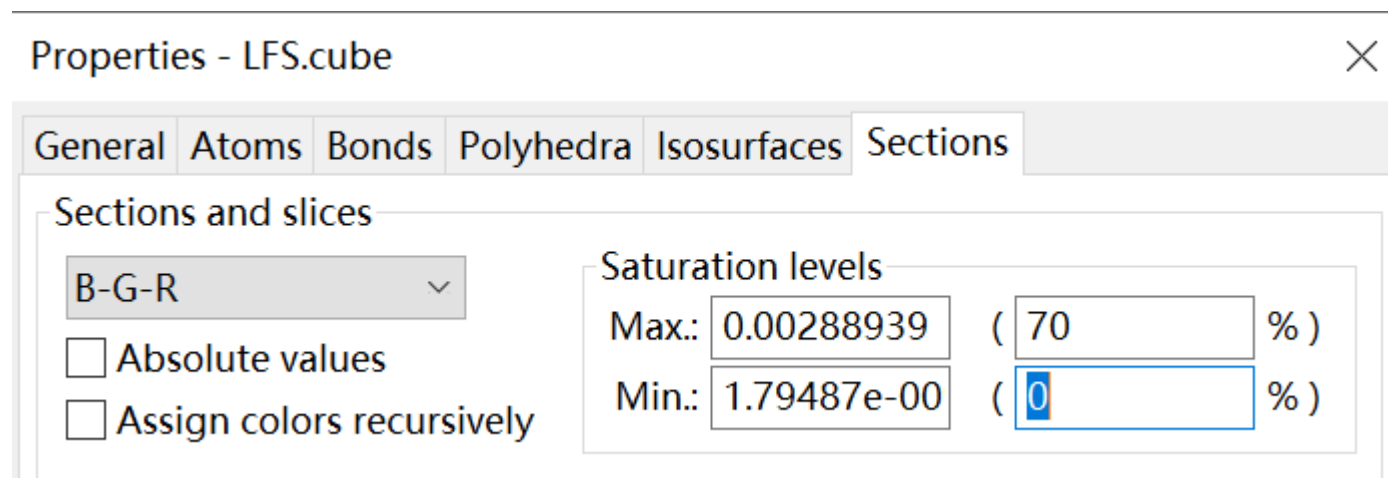


4. Visualize Local Fermi-Softness

2. Contour plante

Objects->Properties-> Sections

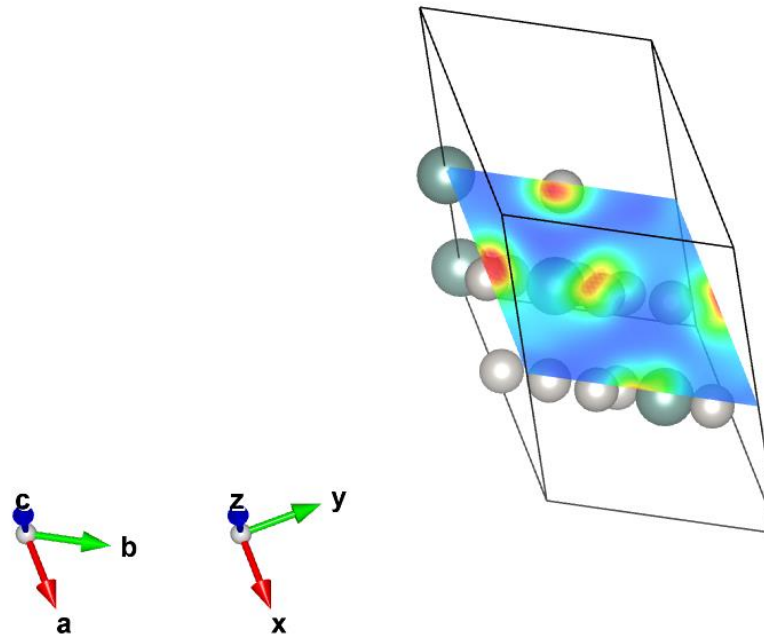
- Set appropriate Saturation level



4. Visualize Local Fermi-Softness

2. Contour plane

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

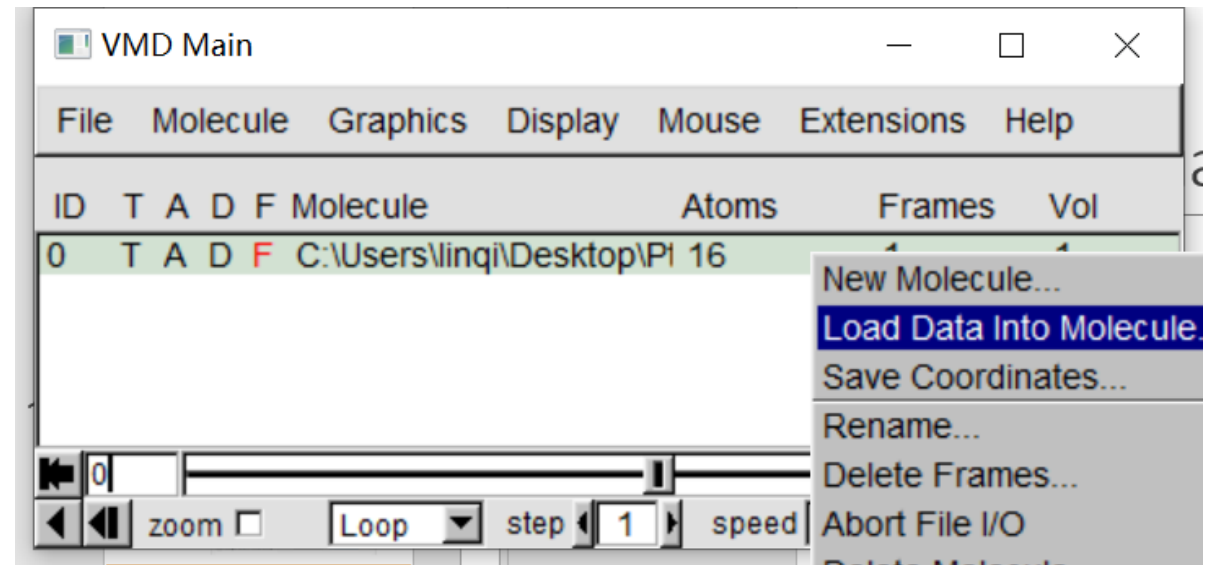


4. Visualize Local Fermi-Softness

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

The screenshot shows a software interface for visualizing local Fermi-softness. It features a 'Create Rep' button and a 'Delete Rep' button. Below these is a table with columns 'Style', 'Color', and 'Selection'. The table contains two rows: 'CPK' with 'Name' and 'all', and 'Isosurface' with 'Volume 1' and '<volume>'. The 'Isosurface' row is highlighted. Below the table is a 'Selected Atoms' field containing 'all'. There are tabs for 'Draw style', 'Selections', 'Trajectory', and 'Periodic'. Under 'Draw style', there are 'Coloring Method' (Volume), 'Material' (1: C), and 'Material' (Opaque). Under 'Drawing Method', there is 'Isosurface' and 'Default'. There is a 'Range' field with 'e-007' and '72804', and a 'Vol' field with 'vol0: CHGCAR'. There is an 'Isovalue' field with '0.0276'. There is a 'Step' field with '1' and a 'Draw' field with 'Wireframe'. There is a 'Size' field with '1' and a 'Show' field with 'Box+Isosurface'.

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

Selected Atoms: all

Draw style | Selections | Trajectory | Periodic

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

Drawing Method: Isosurface | Default

Range: e-007 | 72804 | Vol: vol0: CHGCAR

Isovalue: 0.0276

Step: 1 | Draw: Wireframe

Size: 1 | Show: Box+Isosurface

4. Visualize Local Fermi-Softness

3. Projected isosurface

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

