

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

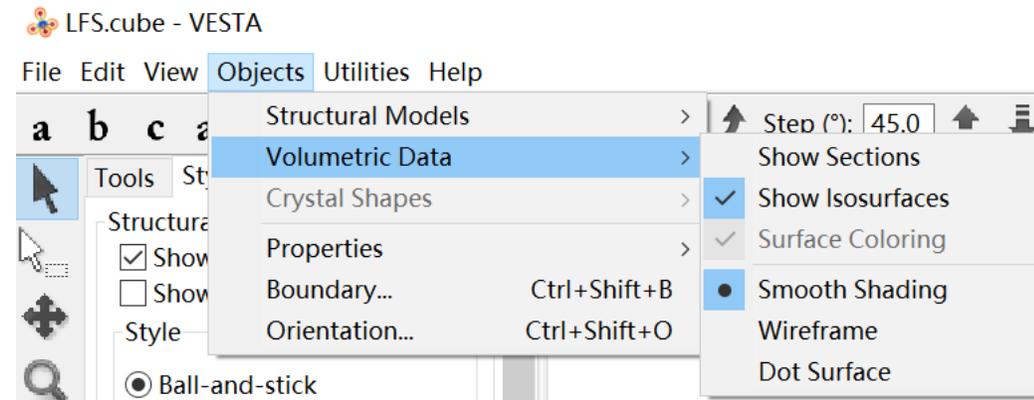
4. Run “*python runfs.py*” in terminal.
5. Wait ... it will take several minutes.
6. Finished. You can find files *FSCAR* and *LFS.cube* in current path. (If the wavefunction is spin polarization, you can find *_UP*, *_DW* for different spin. If band gap exists, you can find *_CB*, *_VB* for holes and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

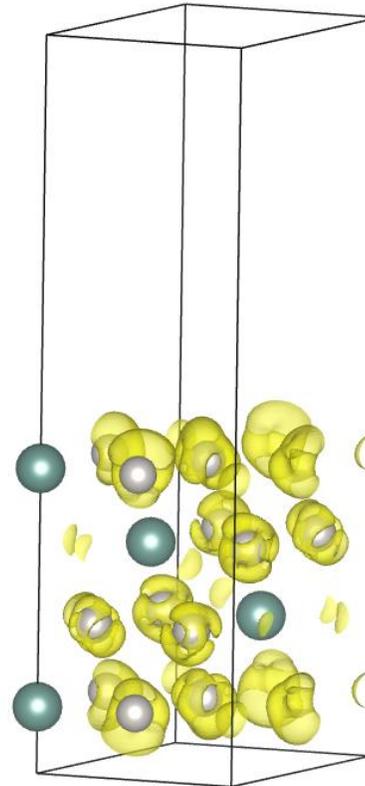
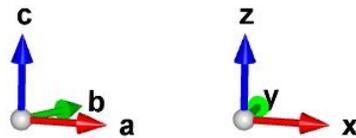
New Delete

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

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

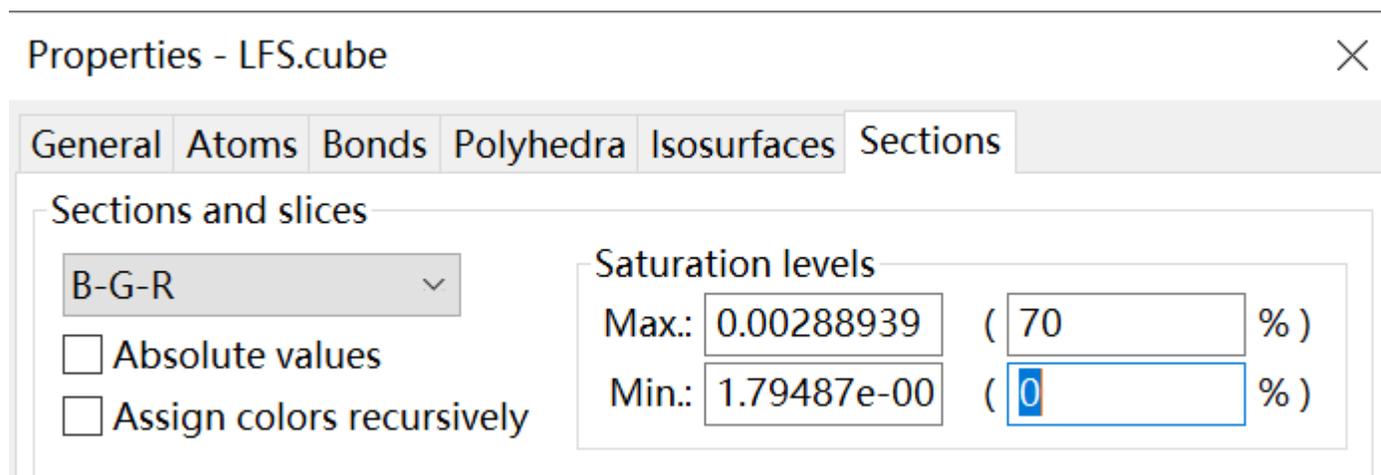
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4. Visualize Local Fermi-Softness

2. Contour plane

Objects->Properties-> Sections

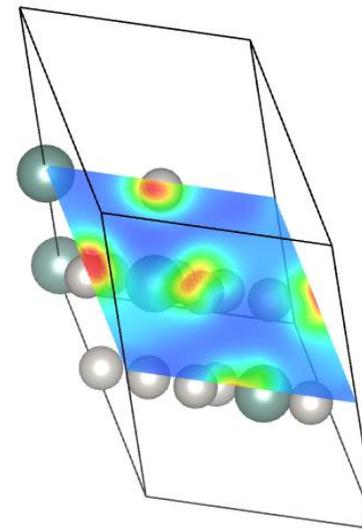
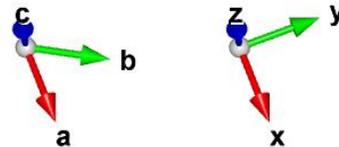
- Set appropriate Saturation level



4. Visualize Local Fermi-Softness

2. Contour plane

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

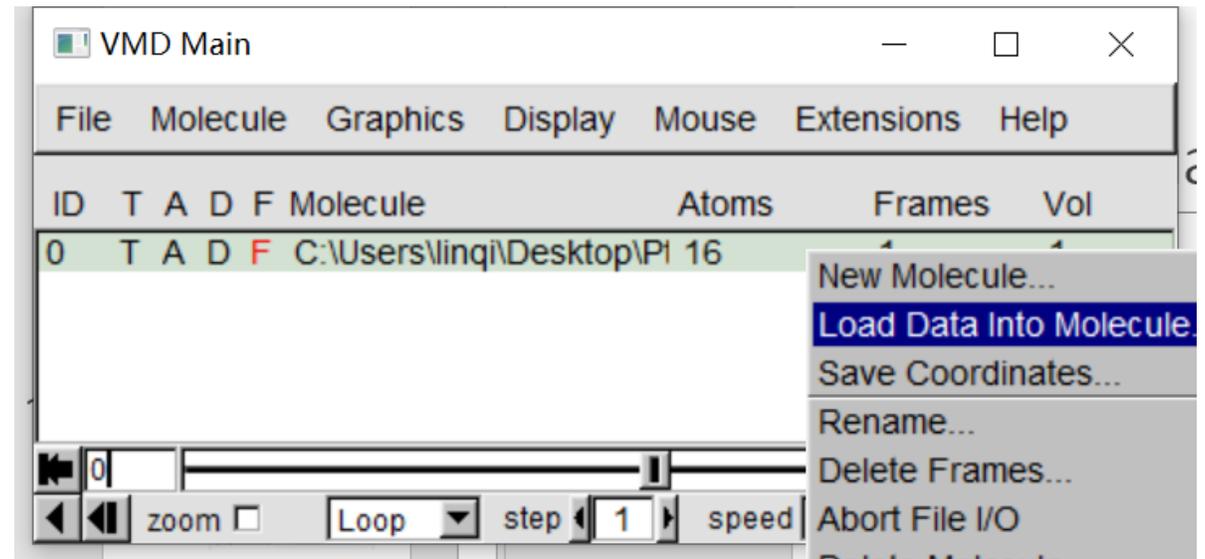


4. Visualize Local Fermi-Softness

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

The screenshot shows a software interface for visualizing local Fermi-softness. It features a table with columns for Style, Color, and Selection. Below the table is a 'Selected Atoms' field containing 'all'. The interface also includes tabs for 'Draw style', 'Selections', 'Trajectory', and 'Periodic'. Under 'Draw style', there are dropdowns for 'Coloring Method' (set to 'Volume'), 'Material' (set to '1: C'), and 'Drawing Method' (set to 'Isosurface'). A 'Range' field is set to 'e-007 72804', and a 'Vol' dropdown is set to 'vol0: CHGCAR'. An 'Isovalue' field is set to '0.0276'. There are also 'Step' and 'Size' fields, both set to '1', and 'Draw' and 'Show' dropdowns set to 'Wireframe' and 'Box+Isosurface' respectively.

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: 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.

