

How to calculate Fermi-Softness *via* VASP

QIAOSONG LIN

FROM WUHAN UNIVERSITY

SEP 2021



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1. Install program

Anaconda3, vaspkit, bader, ASE and *runfs.py* 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 install ASE from the website:

[Installation — ASE documentation \(https://wiki.fysik.dtu.dk/ase/install.html\)](https://wiki.fysik.dtu.dk/ase/install.html)

3. You can install vaspkit from the website:

[Installation — vaspkit documentation \(https://vaspkit.com/installation.html\)](https://vaspkit.com/installation.html)

4. 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/)

5. You can download *runfs.py* from the website:

[runfs.py \(https://github.com/Linqiaosong/Fermi-Softness-for-VASP\)](https://github.com/Linqiaosong/Fermi-Softness-for-VASP)

2. Run VASP program for calculating Fermi-Softness

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**, reading CHGCAR generated by SCF.

2. Run VASP program

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

```
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
vaspkit_dir='vaspkit' # Path of vaspkit
band_gap={'VBM':0.0, 'CBM':0.0} # If band gap exists, set as  $E_{\text{VBM}}, E_{\text{CBM}}$  (Do not subtract  $E_{\text{Fermi}}$ );
# Otherwise set as 0.0 0.0 (eV)
```

- Save intermediate files can make calculation become faster sometime, but need more disk space
- If *bader* and *vaspkit* are in your *\$PATH*, you don't need to change `bader_dir` and `vaspkit_dir`

3. Calculate Total, Condensed and Local Fermi-Softness

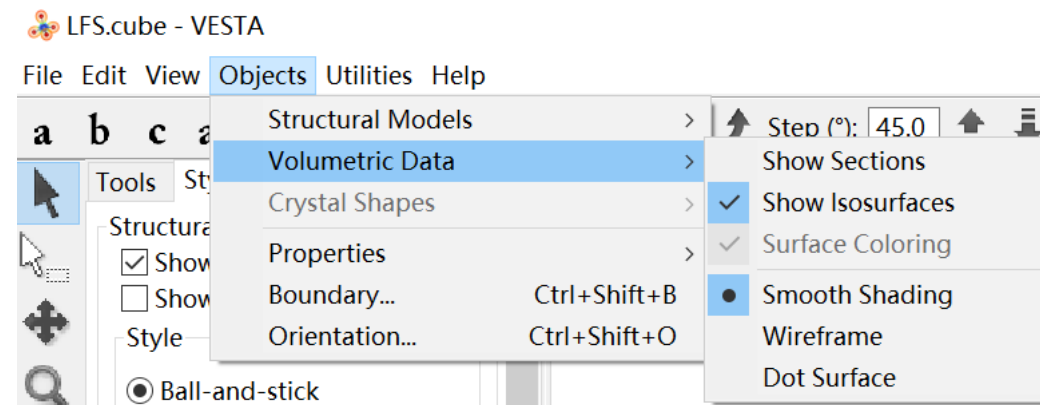
1. Copy *runfs.py* to the path where the non-SCF output of VASP is.
2. Run “*python runfs.py*” in terminal.
3. Wait ... it will take several minutes (depend on your k-point number).
4. Finished. You can find files *FSCAR* and *LFS.cube* in current path. (If the wavefunction is spin polarization, you can find *_UP*, *_DW* for different spin. If band gap exists, you can find *_CB*, *_VB* for holes and electrons.)
5. In *FSCAR*, you can find Total Fermi-Softness (NUMBER OF ELECTRONS) and Condensed Fermi-Softness (CHARGE), the grid datas 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	

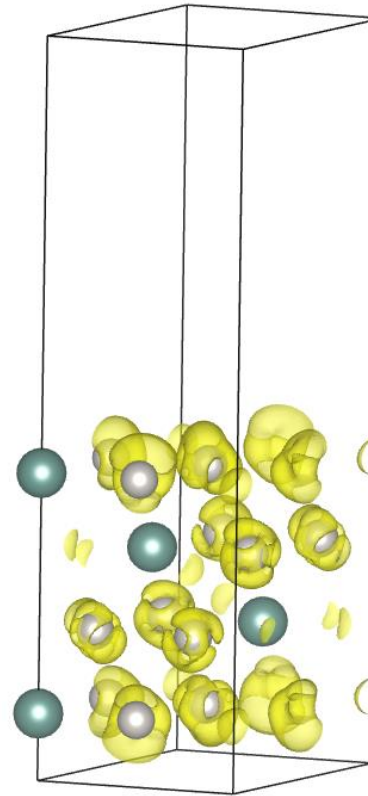
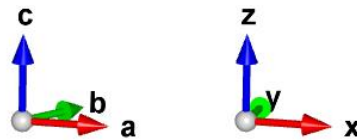
New

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

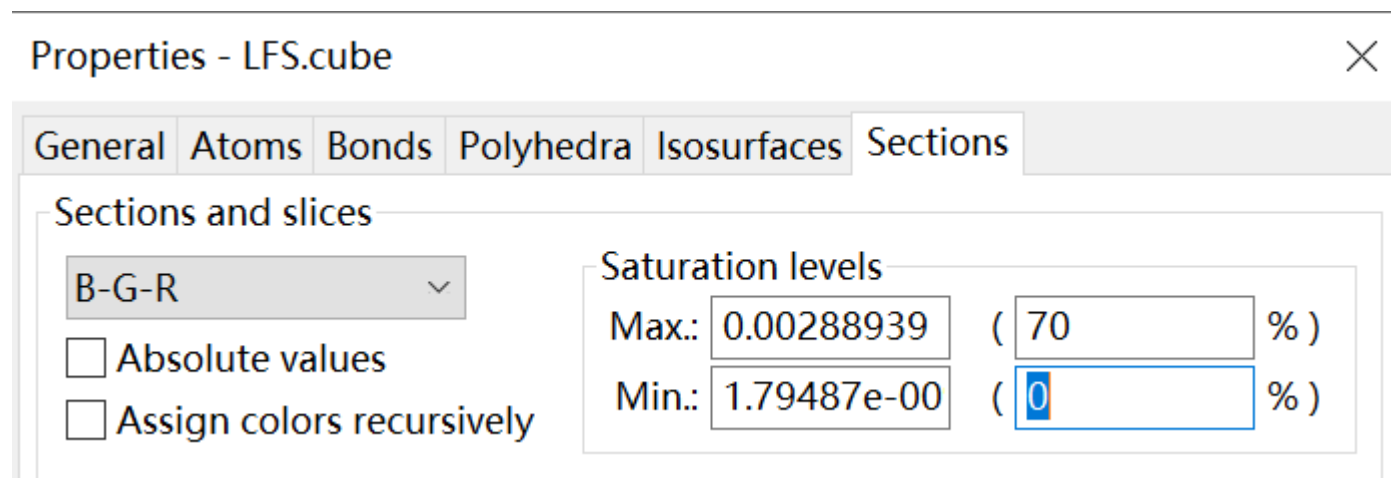
< > ↑ ↓

4. Visualize Local Fermi-Softness

2. Contour plante

Objects->Properties-> Sections

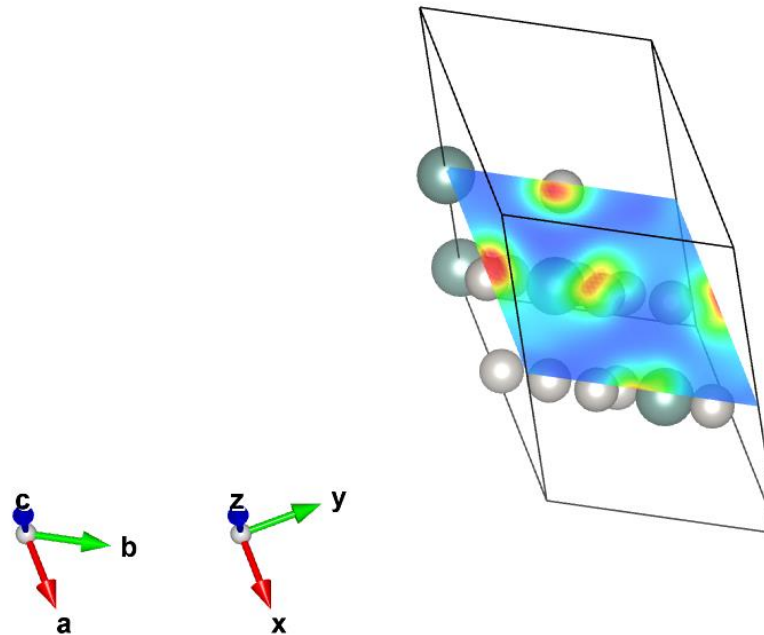
- Set appropriate Saturation level



4. Visualize Local Fermi-Softness

2. Contour plane

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



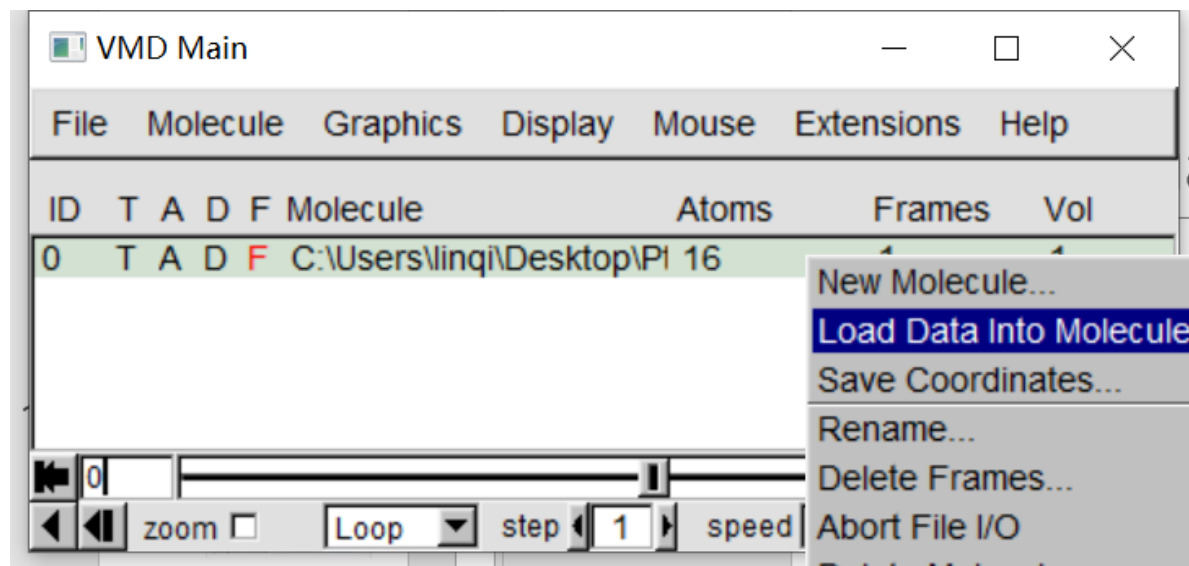
4. Visualize Local Fermi-Softness

3. Projected isosurface

Load *CHGCAR* by VESTA and save as *CHGCAR.cube*

Load *CHGCAR.cube* 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 projected isosurfaces. It features a table with columns for Style, Color, and Selection. The first row is 'CPK' with 'Name' and 'all'. The second row is 'Isosurface' with 'Volume 1' and '<volume>'. 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 dropdowns for 'Coloring Method' (set to 'Volume'), 'Material' (set to '1: C'), and 'Drawing Method' (set to 'Isosurface'). There are also buttons for 'Default' and 'Wireframe'. At the bottom, there are input fields for 'Range' (set to 'e-007' and '72804'), 'Isovalue' (set to '0.0276'), 'Step' (set to '1'), and 'Size' (set to '1'). There are also dropdowns for 'Vol' (set to 'vol0: CHGCAR') and 'Show' (set to '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 | 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.

