

How to calculate Fermi-Softness *via* VASP

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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-vasp.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

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.

3. Calculate Total, Condensed and Local Fermi-Softness

1. 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], # 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)
```

- 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

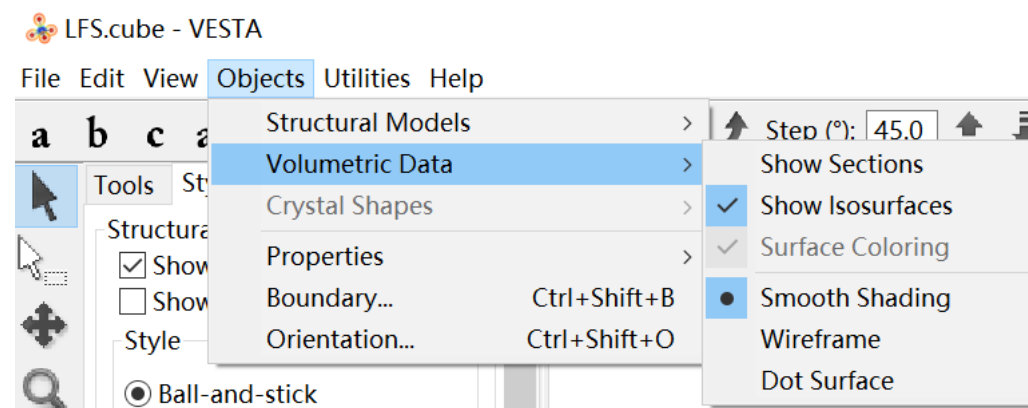
2. Copy *runfs-vasp.py* to the path where the non-SCF output of VASP is.
3. Run “*python runfs-vasp.py*” in terminal.
4. Wait ... it will take several minutes (depend on your k-point number).
5. Finished. You can find files *FSCAR* and *LFS.cube* in current path. (If the wavefunction is spin polarization, you can find *_UP*, *_DW* for different spin. If band gap exists, you can find *_CB*, *_VB* for holes and electrons.)
6. 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

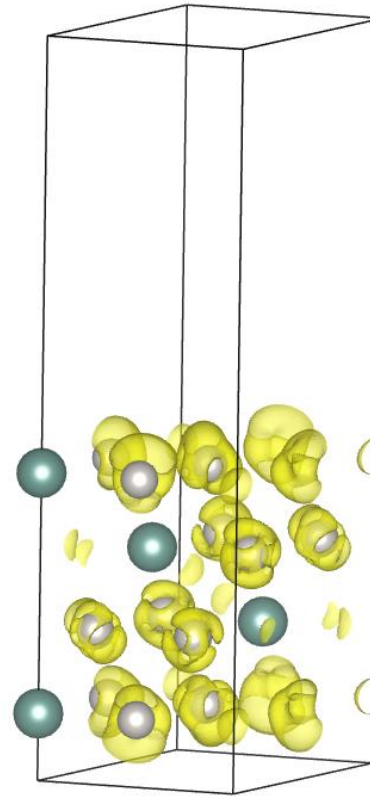
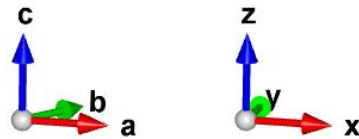
Delete

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

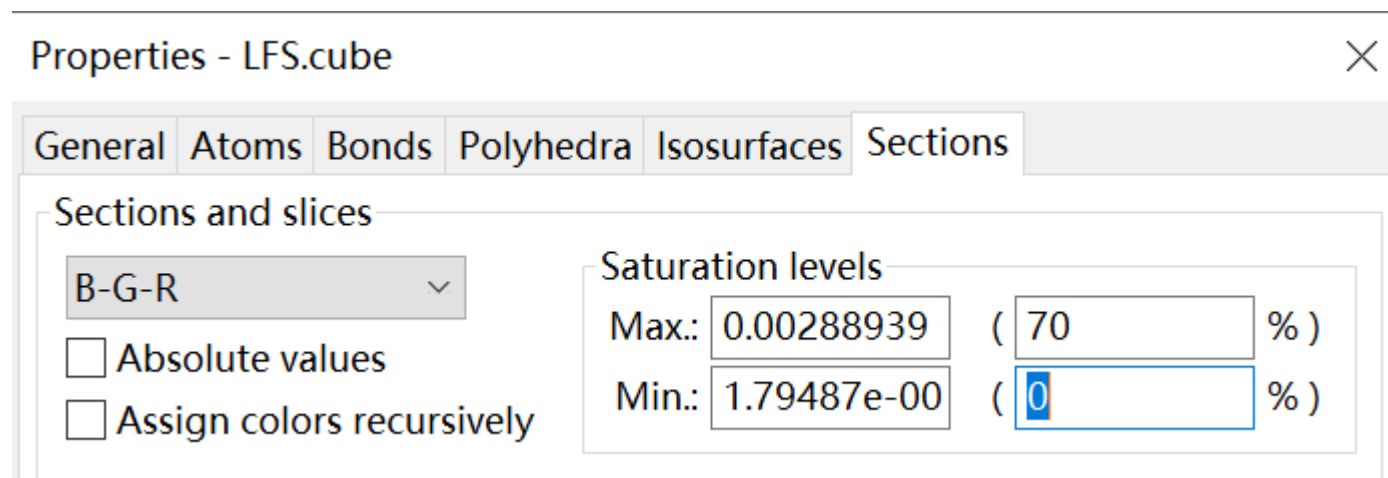
< > ↑ ↓

4. Visualize Local Fermi-Softness

2. Contour plante

Objects->Properties-> Sections

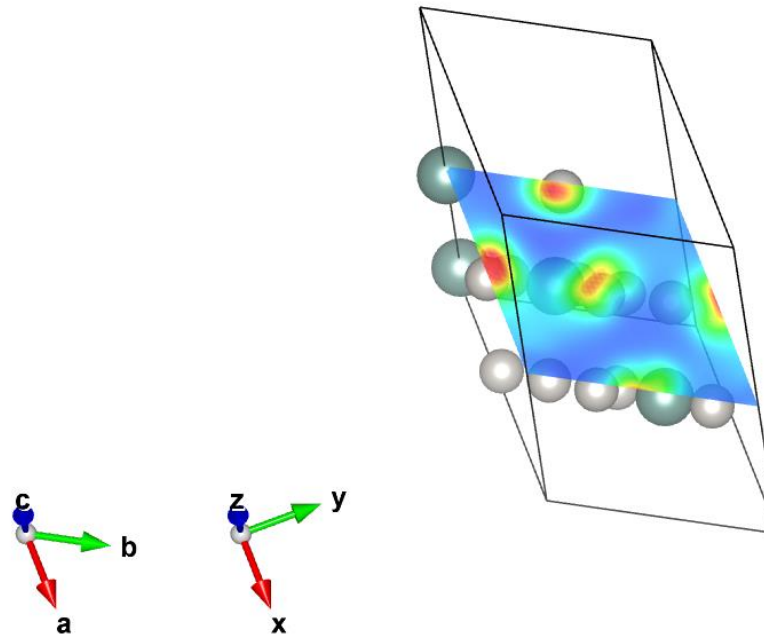
- Set appropriate Saturation level



4. Visualize Local Fermi-Softness

2. Contour plane

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



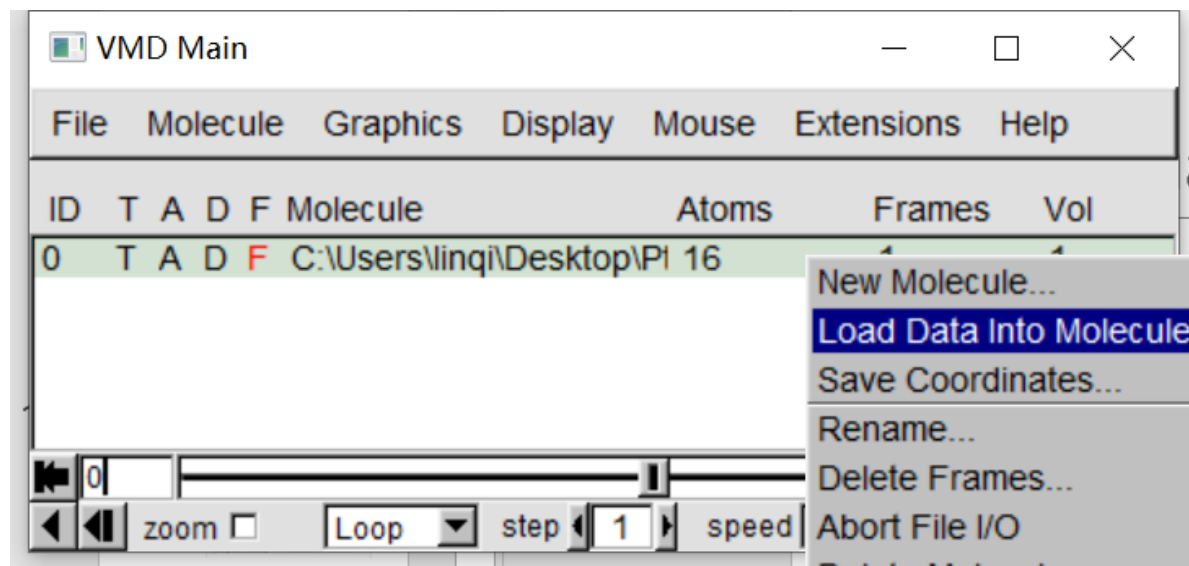
4. Visualize Local Fermi-Softness

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 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' in the 'Selection' column, and 'Isosurface' with 'Volume 1' and '<volume>' in the 'Selection' column. 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) and 'Material' (1: C, Opaque). Below these is a 'Drawing Method' (Isosurface) and a 'Default' button. There is a 'Range' field (e-007, 72804) and a 'Vol' field (vol0: CHGCAR). Below these is an 'Isovalue' field (0.0276) and a 'Step' field (1). At the bottom, there is a 'Size' field (1) and a 'Show' field (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 | 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.

