

# How to calculate Fermi-Softness *via* VASP

---

QIAOSONG LIN

FROM WUHAN UNIVERSITY

SEP 2021



# Contents

---

1. How to **install program** ?
2. How to **run VASP program** for calculating Fermi-Softness ?
3. How to **extract Total, Projected and Local Fermi-Softness** ?
4. How to **visualize Local Fermi-Softness** ?

# 1. Install program

---

**VASP, Anaconda3, vaspkit, ASE and *runfs.py* is necessary.**

1. VASP needs to be compiled in advance, VASP 5.4.4 is better.

2. You can install Anaconda3 from the website:

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

3. 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)

4. You can install vaspkit from the website, and make sure vaspkit is in your \$PATH, vaspkit 1.3 is better:

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

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.

### 3. Extract Total, Projected 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 *FSCAR\_UP*, *FSCAR\_DW*, *LFS\_UP.cube* and *LFS\_DW.cube* for different spin.)
5. In *FSCAR*, you can find Total Fermi-Softness and Projected Fermi-Softness, the grid datas of Local Fermi-Softness were recorded in *LFS.cube*.

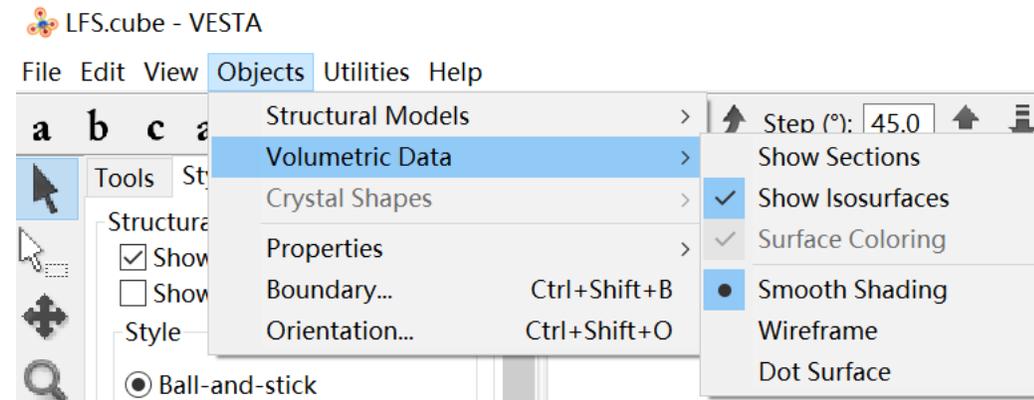
# 4. Visualize Local Fermi-Softness

---

## 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

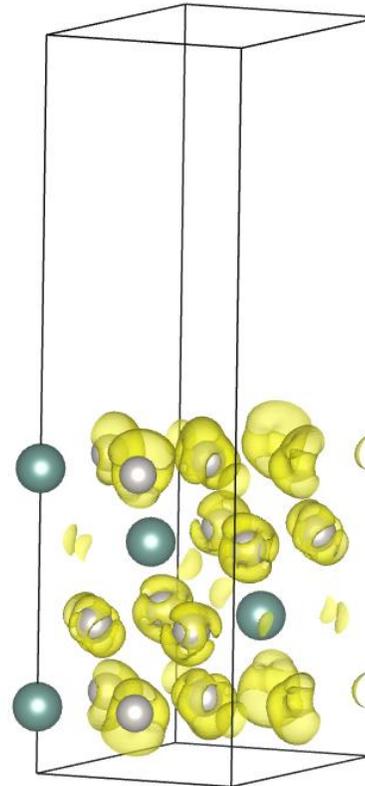
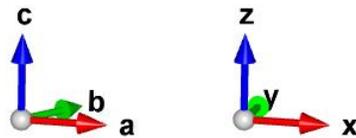
# 4. Visualize Local Fermi-Softness

---

## 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 plane

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

↑ ↓

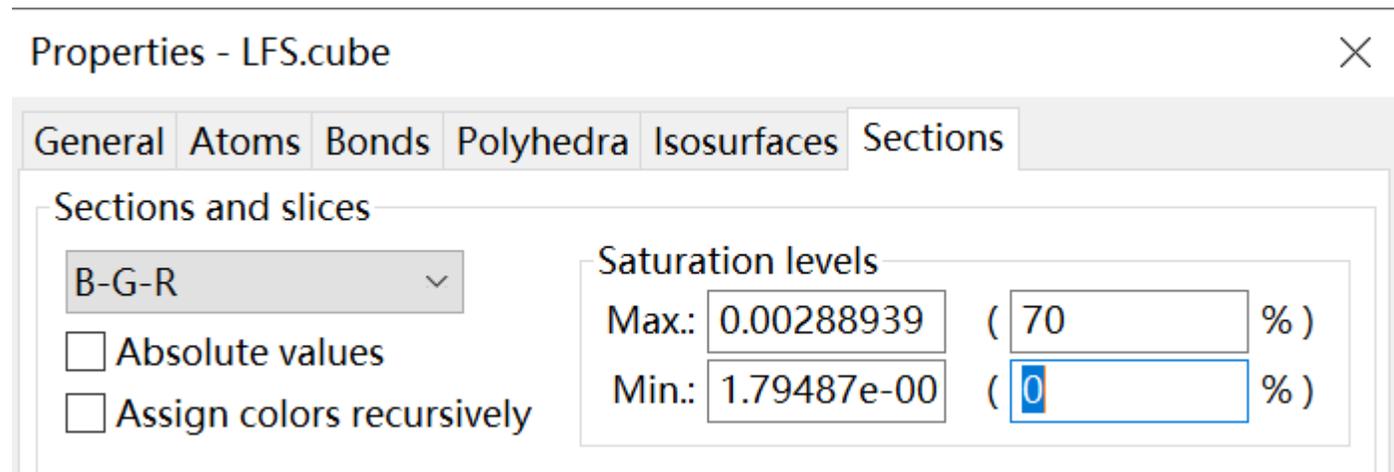
## 4. Visualize Local Fermi-Softness

---

### 2. Contour plane

Objects->Properties-> Sections

- Set appropriate Saturation level



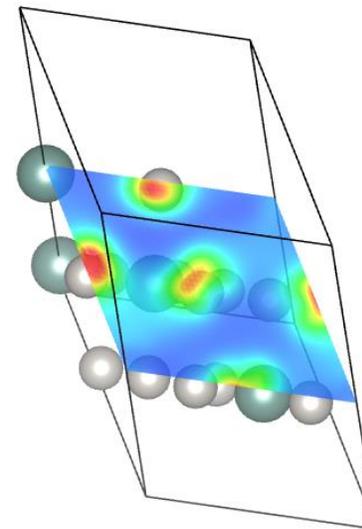
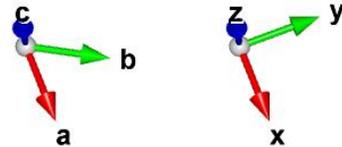
# 4. Visualize Local Fermi-Softness

---

## 2. Contour plane

Local Fermi-Softness mainly distributes on

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



## 4. Visualize Local Fermi-Softness

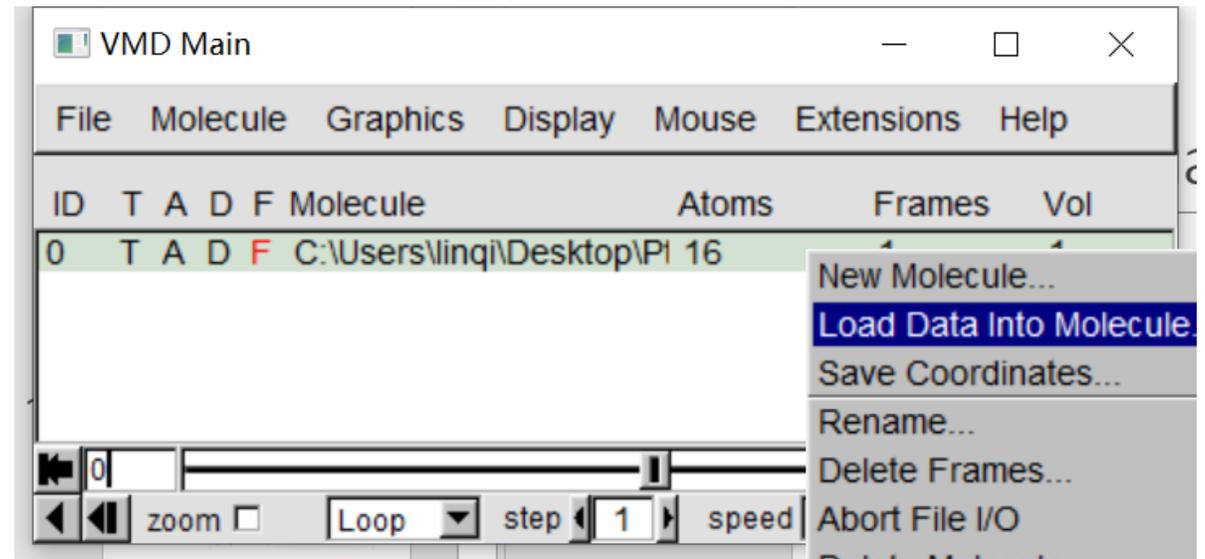
---

### 3. Projected isosurface

Load *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

Create Rep Delete Rep

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

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Volume 1: C Material: Opaque

Drawing Method: Isosurface Default

Range:  $1e-007$  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.

