

# How to calculate Fermi-Softness *via* CP2K

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1. How to **install program** ?
2. How to **run CP2K program** for calculating Fermi-Softness ?
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4. How to **visualize Local Fermi-Softness** ?

# 1. Install program

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**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 CP2K program

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1. Build a Slab model.
2. Relaxation calculation.
3. Do a single point energy calculation with **gamma only**, and following key words should be in your input:

&DFT

.....

```
&PRINT
&MO_CUBES
  STRIDE 1
  NHOMO -1
  NLUMO -1
&END MO_CUBES
&END PRINT
&END DFT
```

### 3. Calculate Total, Condensed and Local Fermi-Softness

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1. Generate input file runfs.py :

```
$ python -c "from FermiSoftness import gen; gen(software='cp2k');"
```

2. Copy runfs.py to the path where the input of CP2K is.

### 3. Calculate Total, Condensed and Local Fermi-Softness

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

```
filename='pt3y.out'
project_name='pt3y'
kbT=0.4                                # Electron temperature (eV)
dfdd_threshold=0.001                  # Derivation of Fermi-Dirac distribution threshold
bader_dir='bader'                     # Path of bader
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)
```

- filename is the single point energy output file, project\_name should be the same as the value after the PROJECT keyword in the input file
- If *bader* is in your *\$PATH*, you don't need to change `bader_dir`

### 3. Calculate Total, Condensed and Local Fermi-Softness

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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*.

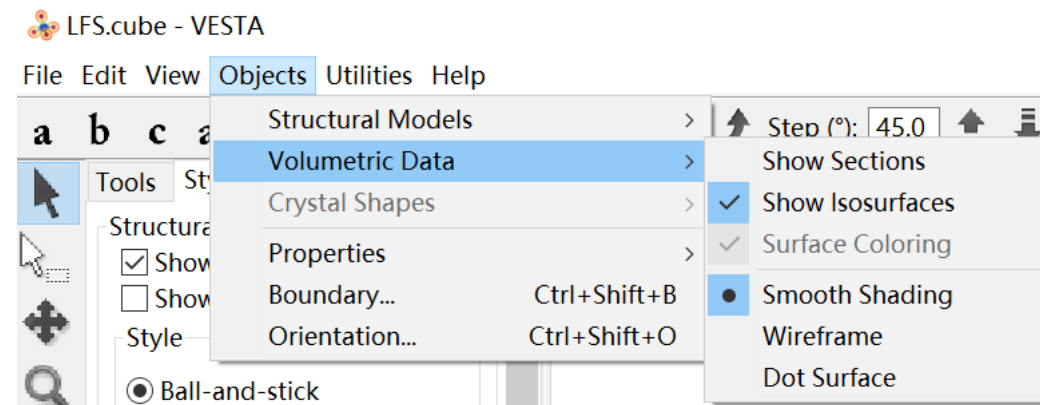
# 4. Visualize Local Fermi-Softness

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## 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

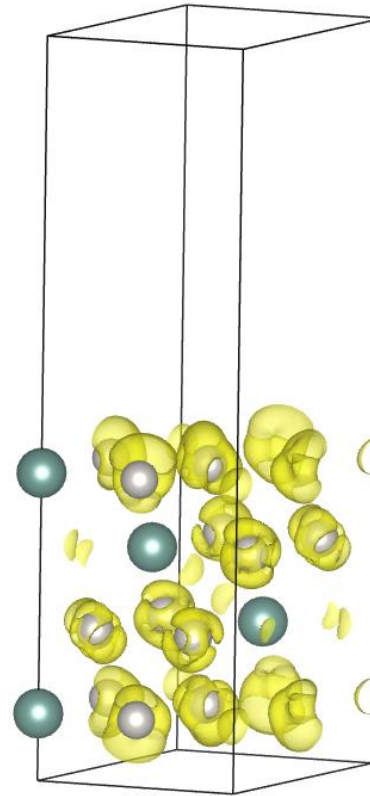
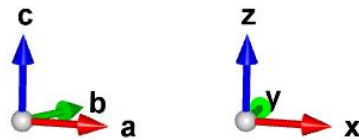
Delete

## 4. Visualize Local Fermi-Softness

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### 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

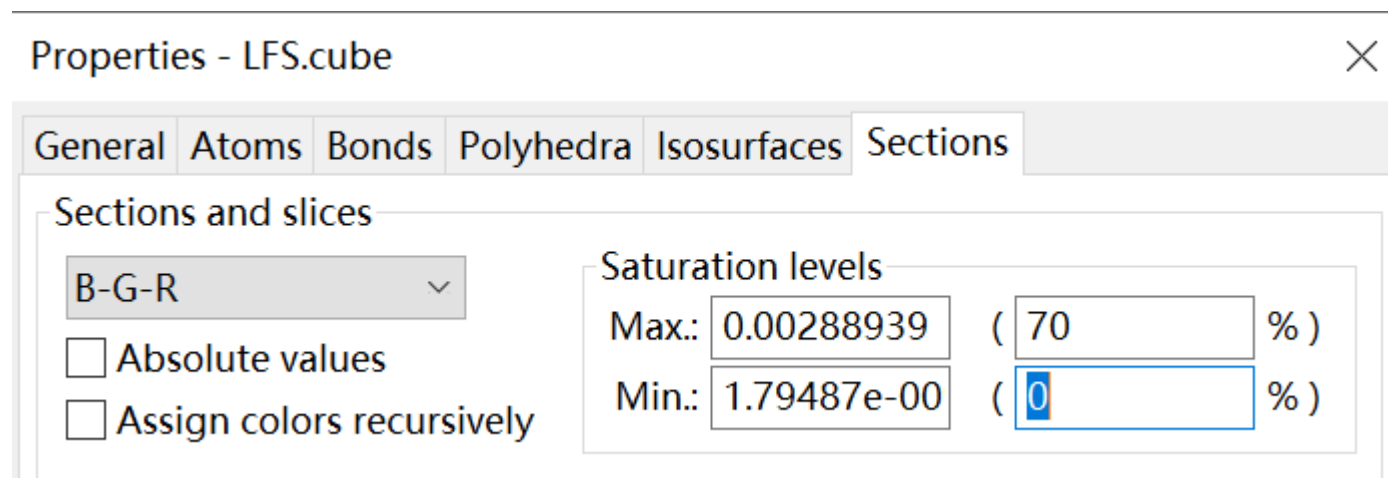
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## 4. Visualize Local Fermi-Softness

### 2. Contour plante

Objects->Properties-> Sections

- Set appropriate Saturation level

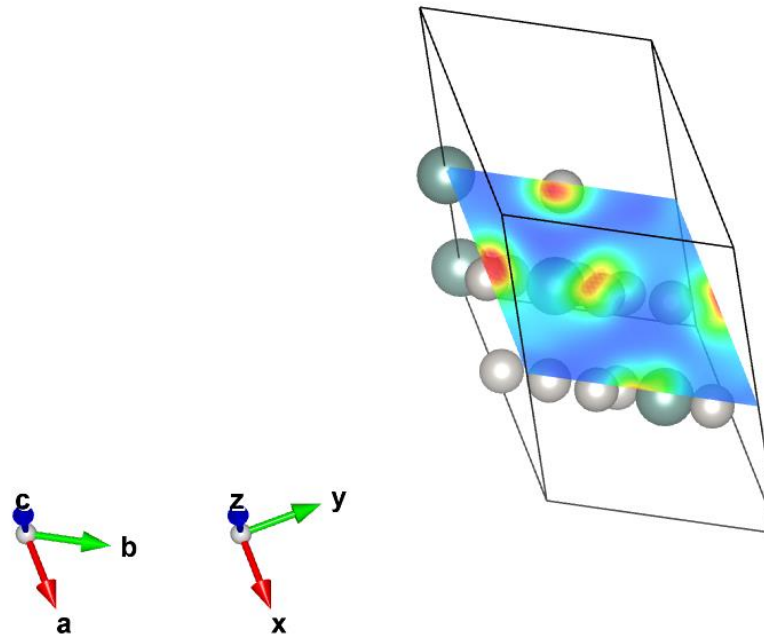


## 4. Visualize Local Fermi-Softness

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### 2. Contour plane

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



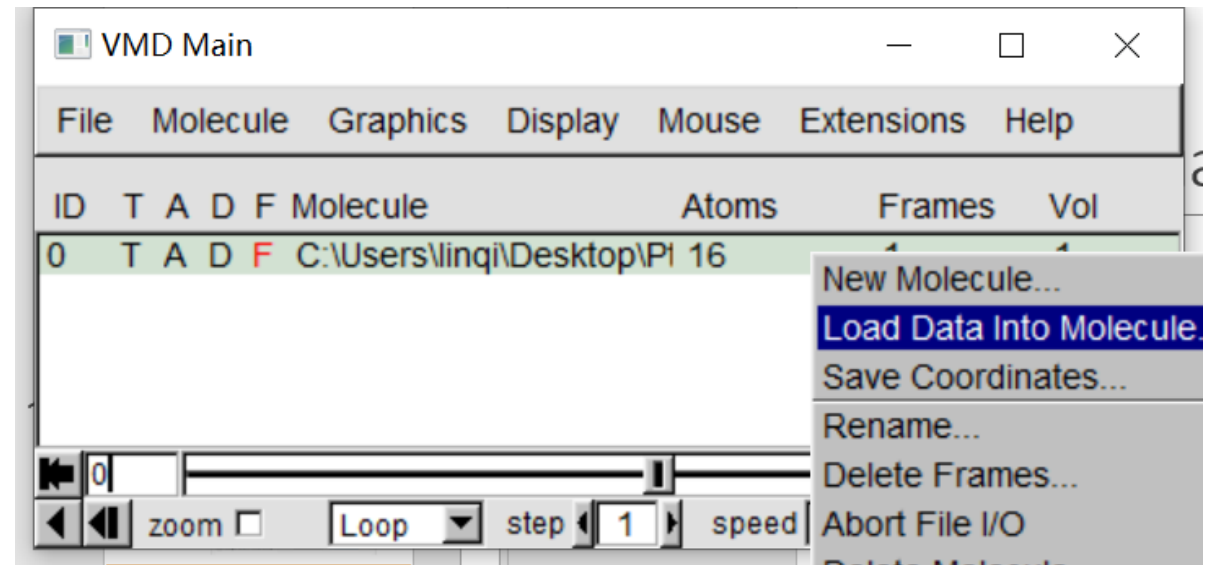
## 4. Visualize Local Fermi-Softness

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### 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 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

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### 3. Projected isosurface

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

