How to calculate Fermi-Softness *via* VASP

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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)

3. You can install ASE from the website:
Installation — ASE documentation (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)

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

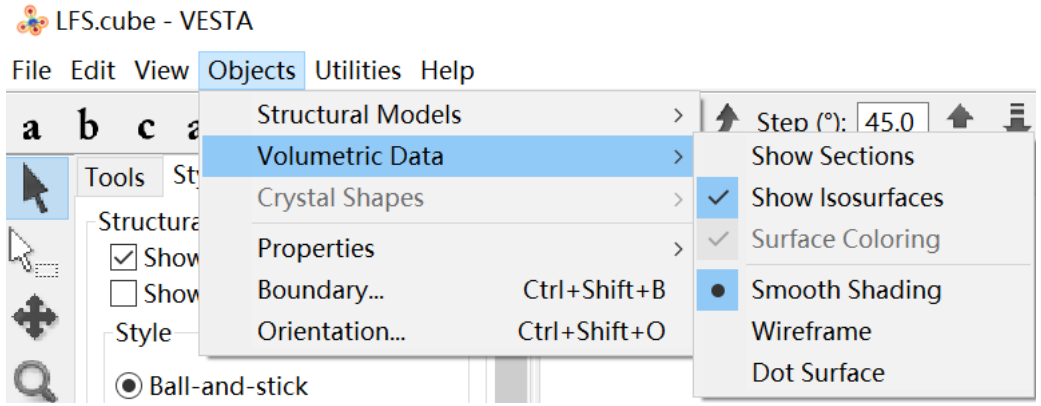
5. In *FSCAR*, you can find Total Fermi-Softness and Projected Fermi-Softness, the grid datas of Local Fermi-Softness were recorded in *LFS.cube*.

4. Visualize Local Fermi-Softness

1. Isosurfaces

Load *LFS.cube* by VESTA

- Objects->Volumetric Data-> Show Isosurfaces

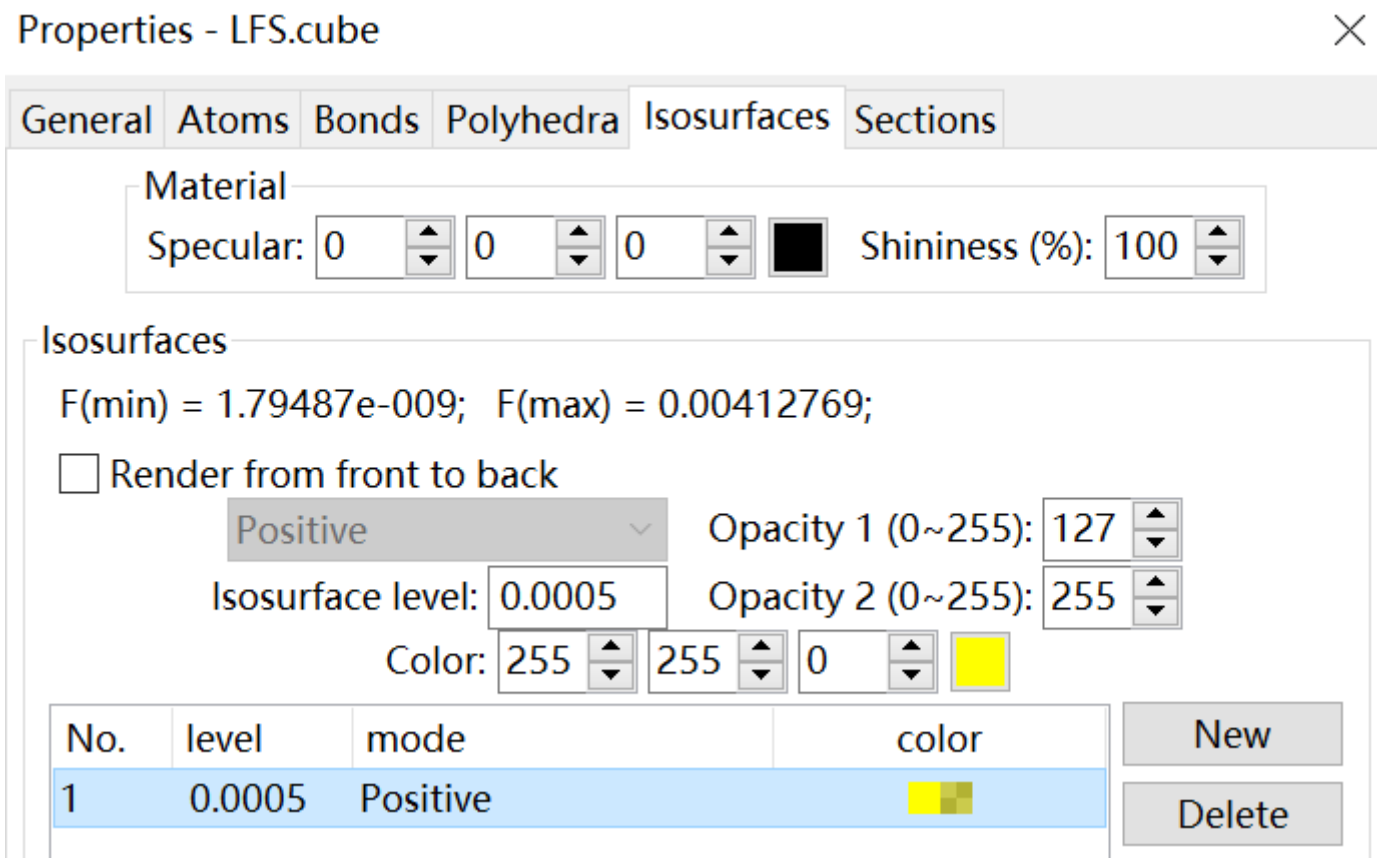


4. Visualize Local Fermi-Softness

1. Isosurfaces

Objects->Properties-> Isosurfaces

- Set appropriate isosurface level

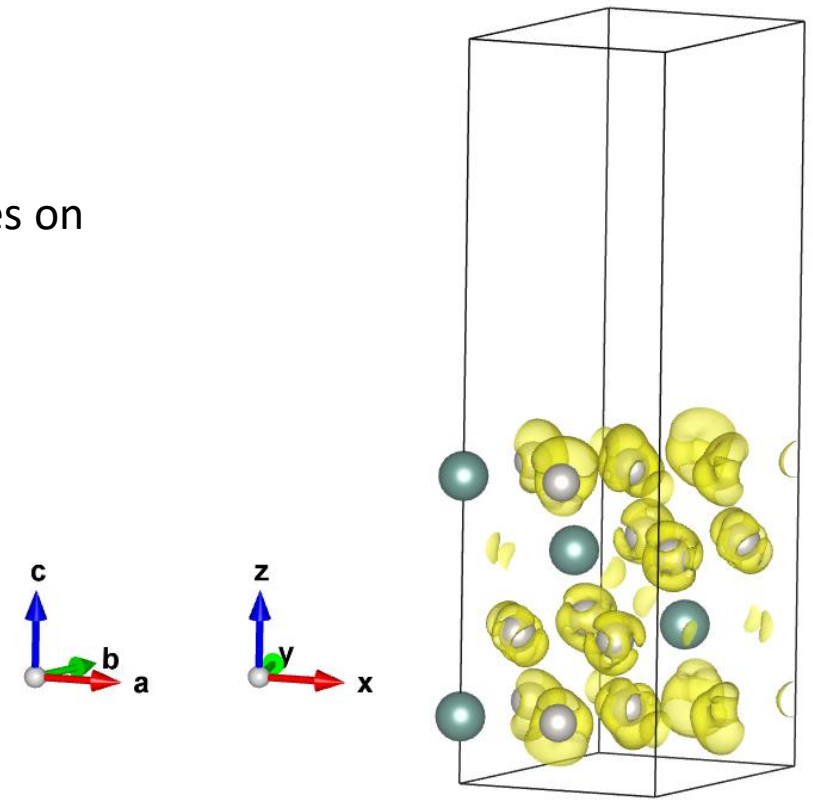


4. Visualize Local Fermi-Softness

1. Isosurfaces

Local Fermi-Softness mainly distributes on

Pt atoms in $Pt_3Y(111)$ surface.



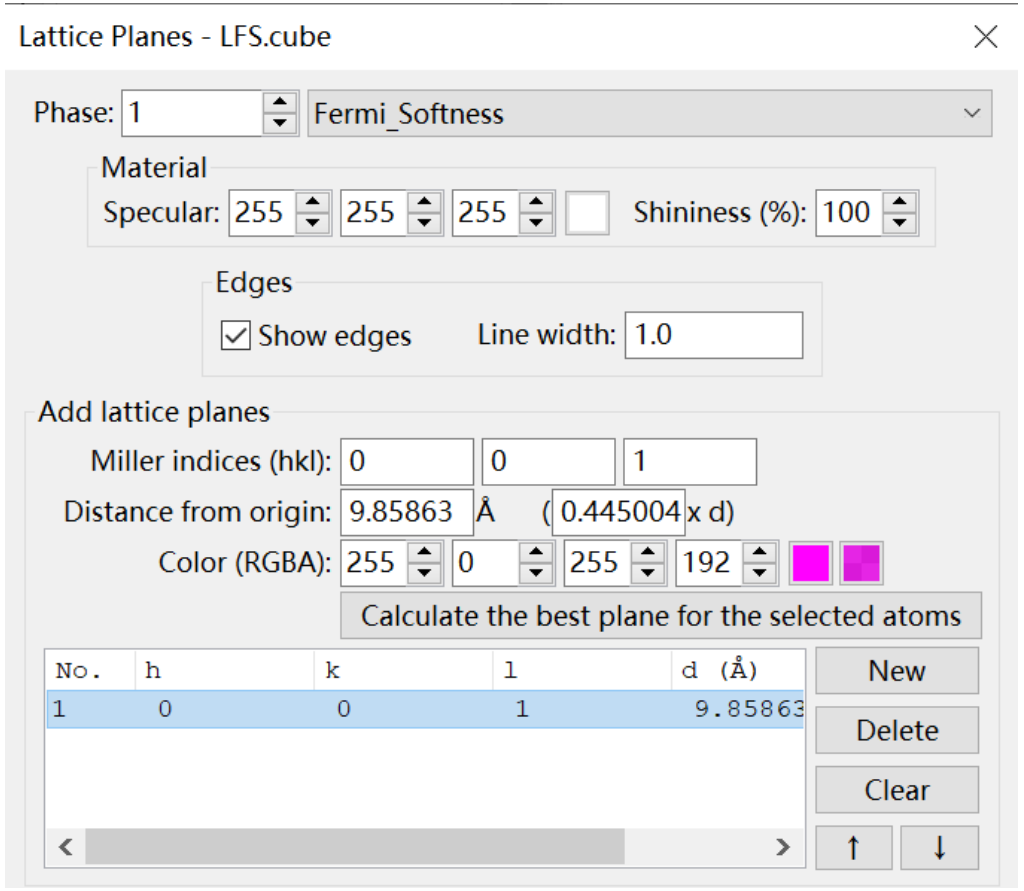
4. Visualize Local Fermi-Softness

2. Contour plante

Load *LFS.cube* by VESTA

Edit->Lattice Planes

- Set Miller indices (001)
- Set appropriate Distance from origin

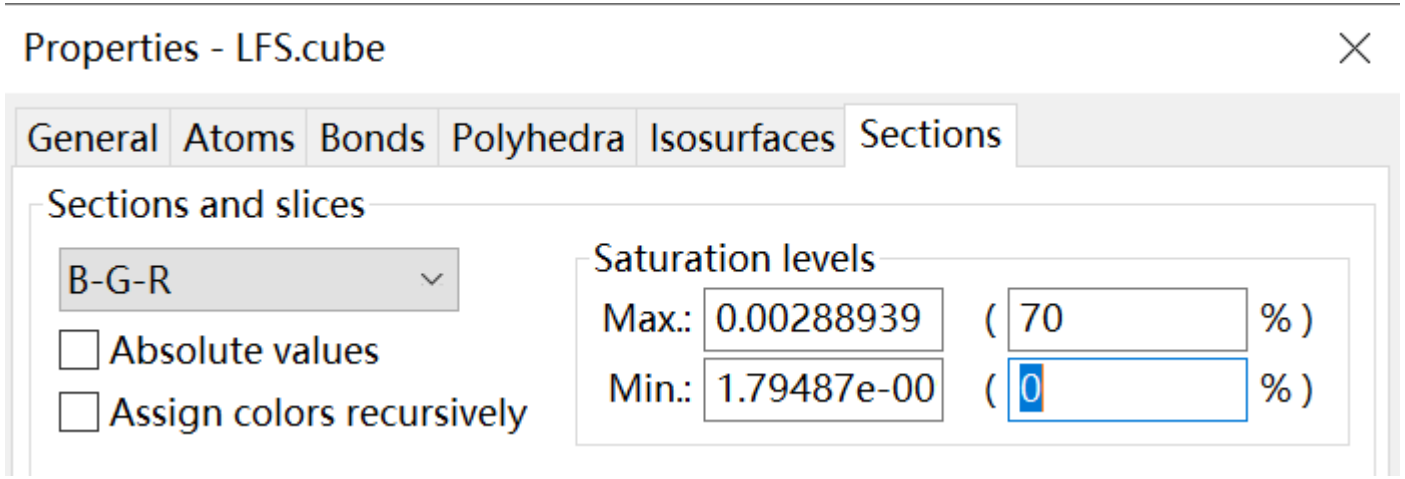


4. Visualize Local Fermi-Softness

2. Contour plante

Objects->Properties-> Sections

- Set appropriate Saturation level



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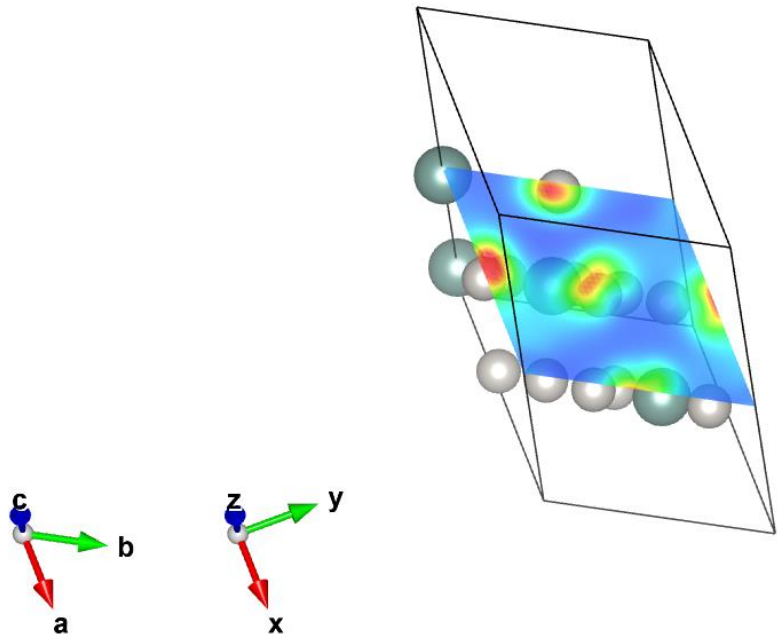


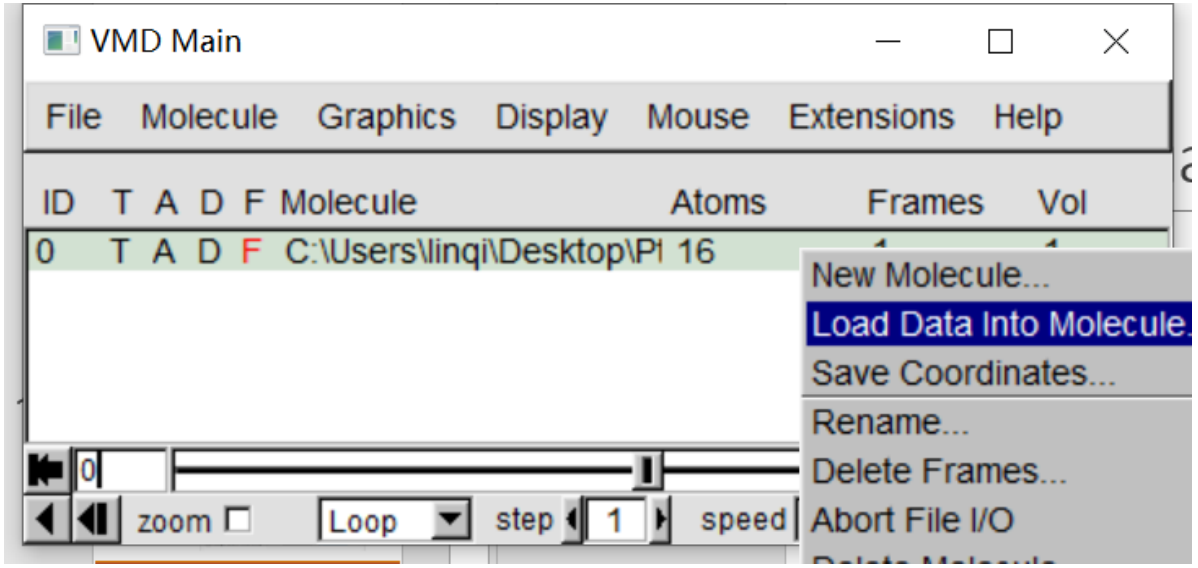
4. Visualize Local Fermi-Softness

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

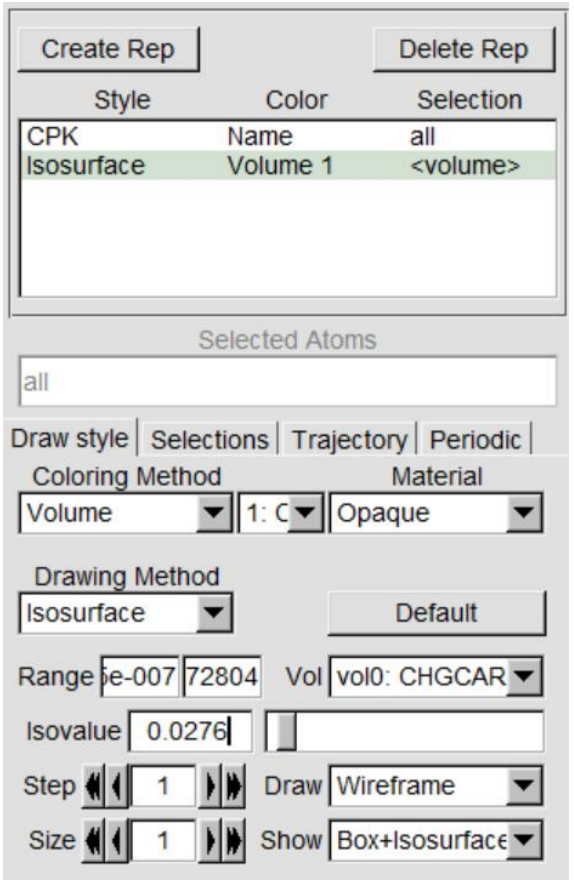
Graphics->Colors->Color Scale->Method: BWR

Graphics->Representation

- Make first Rep: CPK Name all
- Make second Rep: Isosurface Volume 1

Graphics->Representation->Trajectory

- Set appropriate Color Scale Data Range



4. Visualize Local Fermi-Softness

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