How to calculate Fermi-Softness *via* VASP

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1. Install program

Anaconda3, vaspkit, 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 install vaspkit from the website:

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

3. 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/)

4. You can install FermiSoftness by pip, ASE and Numpy will be installed automatically:

   $ *pip install FermiSoftness*

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. Generate input file runfs.py :

$ *python –c “from FermiSoftness import gen; gen(software=‘vasp’);”*

2. Copy runfs.py to the path where the non-SCF output of VASP is.

3. Calculate Total, Condensed and Local Fermi-Softness

3. 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_VBM,E_CBM (Do not minus E_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

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.)

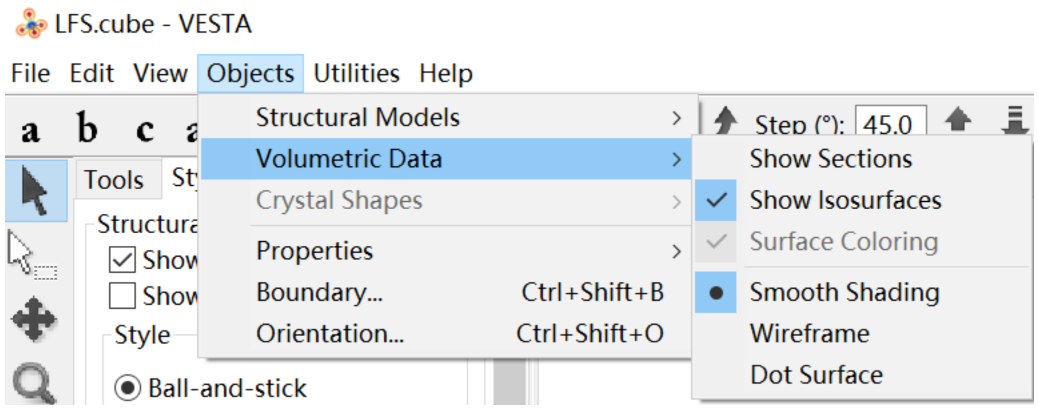
7. In FSCAR, you can find Total Fermi-Softness (NUMBER OF ELECTRONS) and Condensed Fermi-Softness (CHARGE), the grid data of Local Fermi-Softness were recorded in LFS.cube.

4. Visualize Local Fermi-Softness

1. Isosurfaces

Load LFS.cube by VESTA

- Objects->Volumetric Data-> Show Isosurfaces

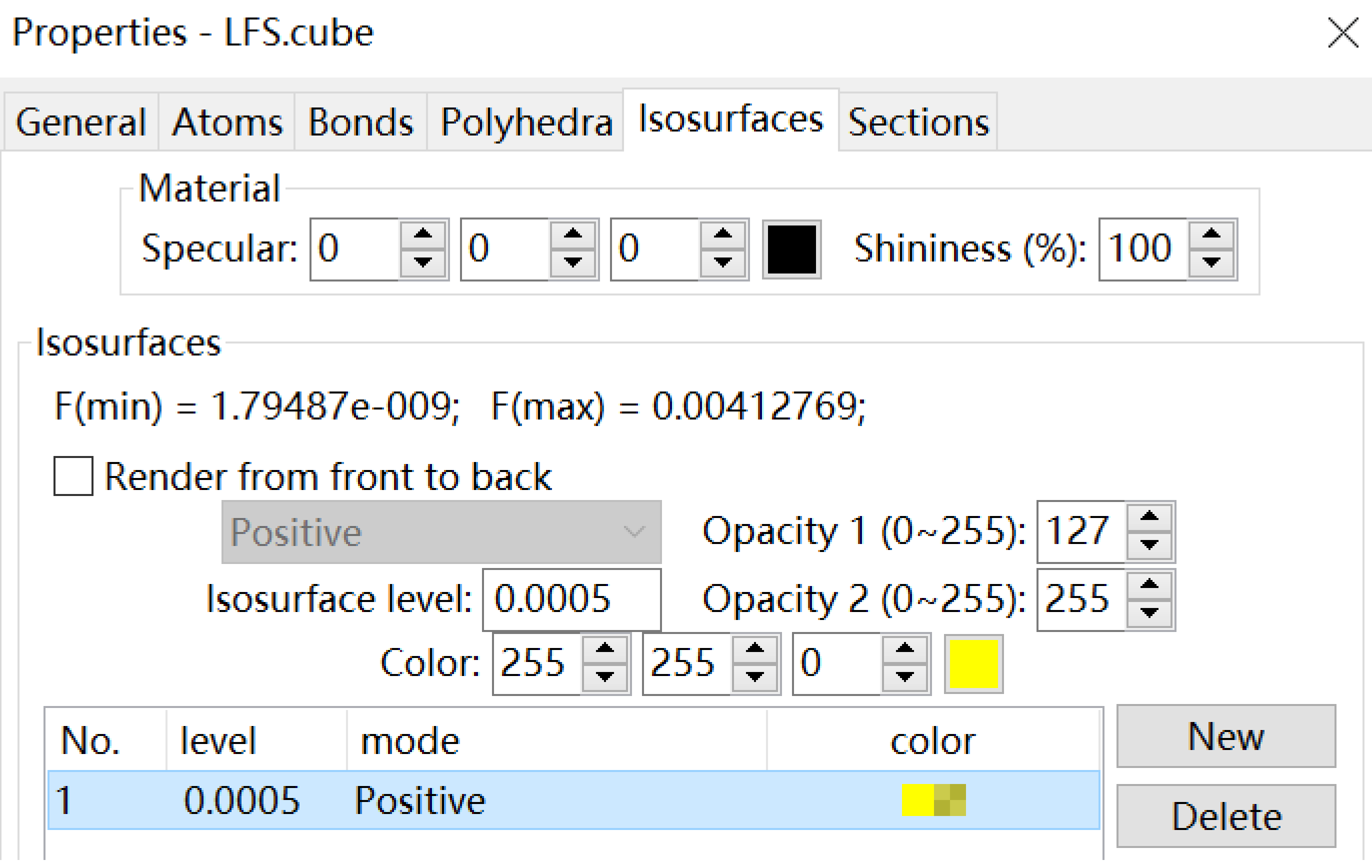


4. Visualize Local Fermi-Softness

1. Isosurfaces

Objects->Properties-> Isosurfaces

- Set appropriate isosurface level

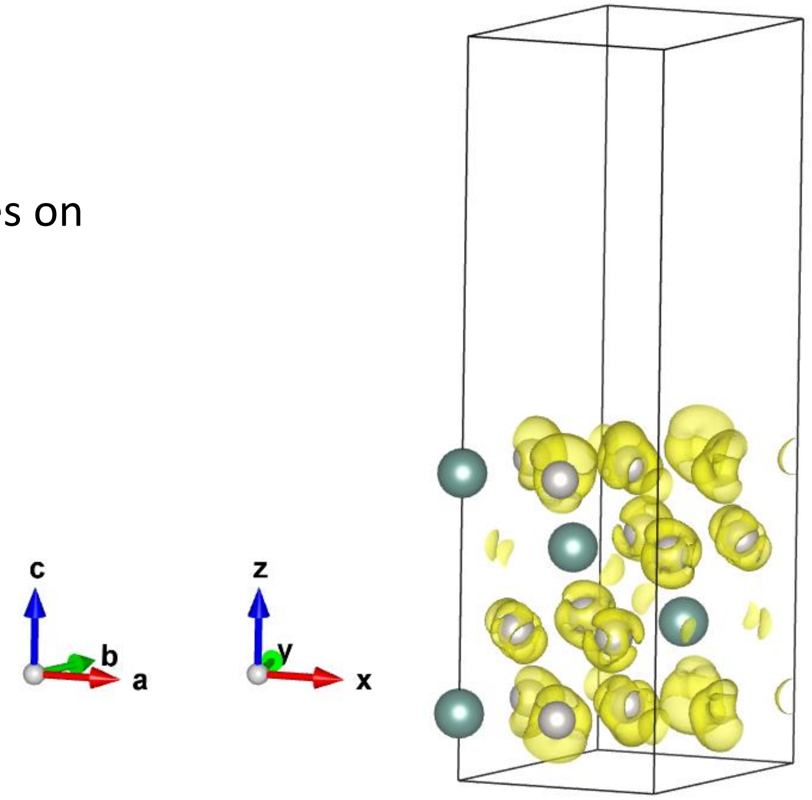


4. Visualize Local Fermi-Softness

1. Isosurfaces

Local Fermi-Softness mainly distributes on

Pt atoms in $Pt_3Y(111)$ surface.



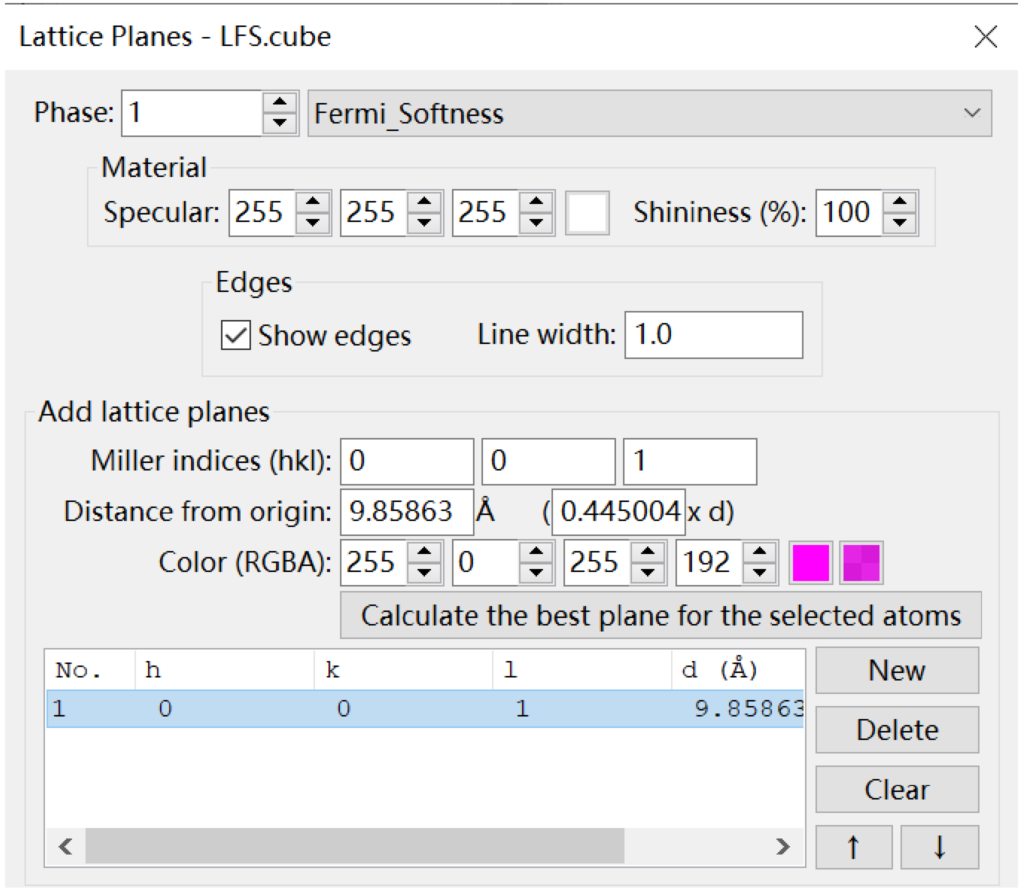
4. Visualize Local Fermi-Softness

2. Contour plante

Load LFS.cube by VESTA

Edit->Lattice Planes

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

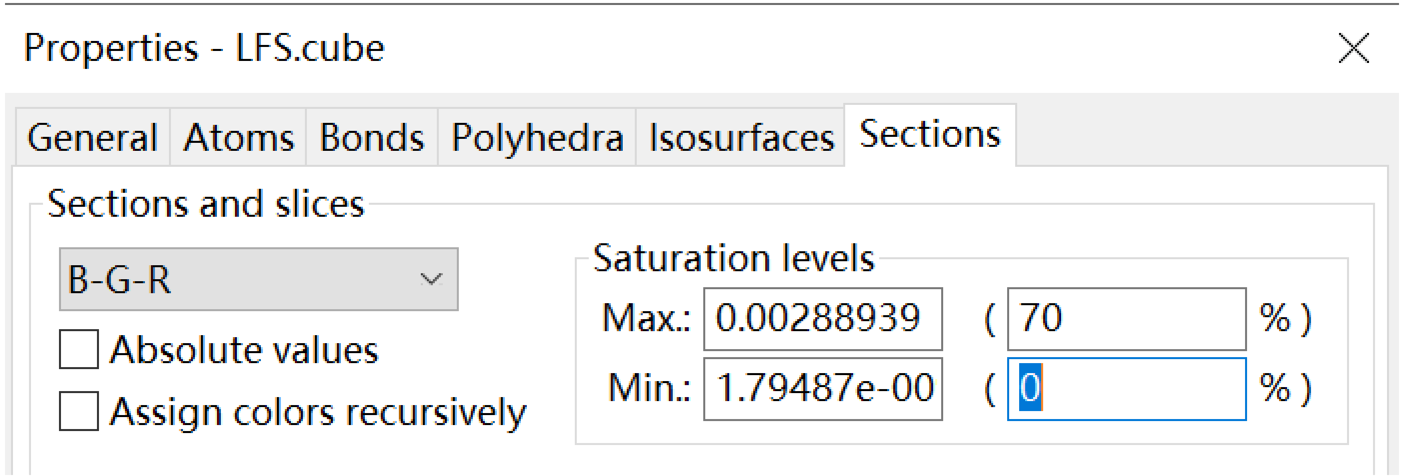


4. Visualize Local Fermi-Softness

2. Contour plante

Objects->Properties-> Sections

- Set appropriate Saturation level



4. Visualize Local Fermi-Softness

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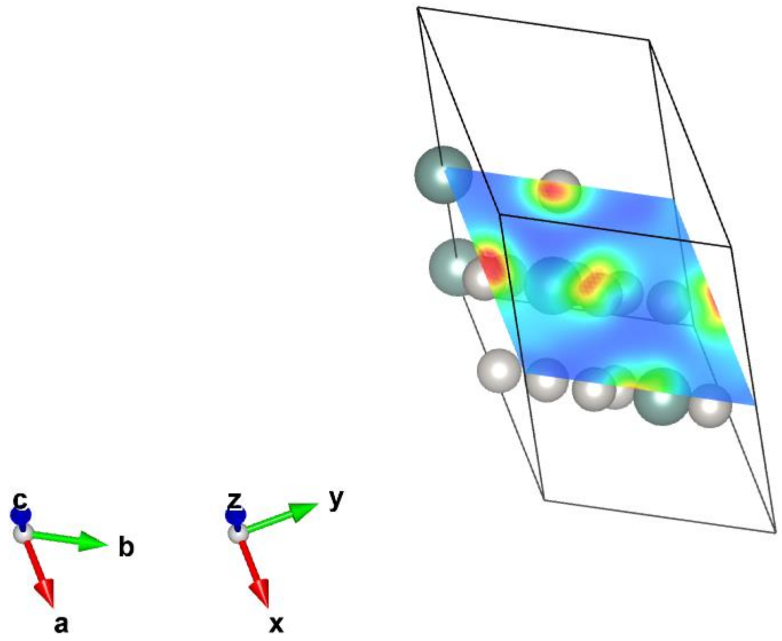
Local Fermi-Softness mainly distributes on

Pt atoms in $Pt_3Y(111)$ surface.

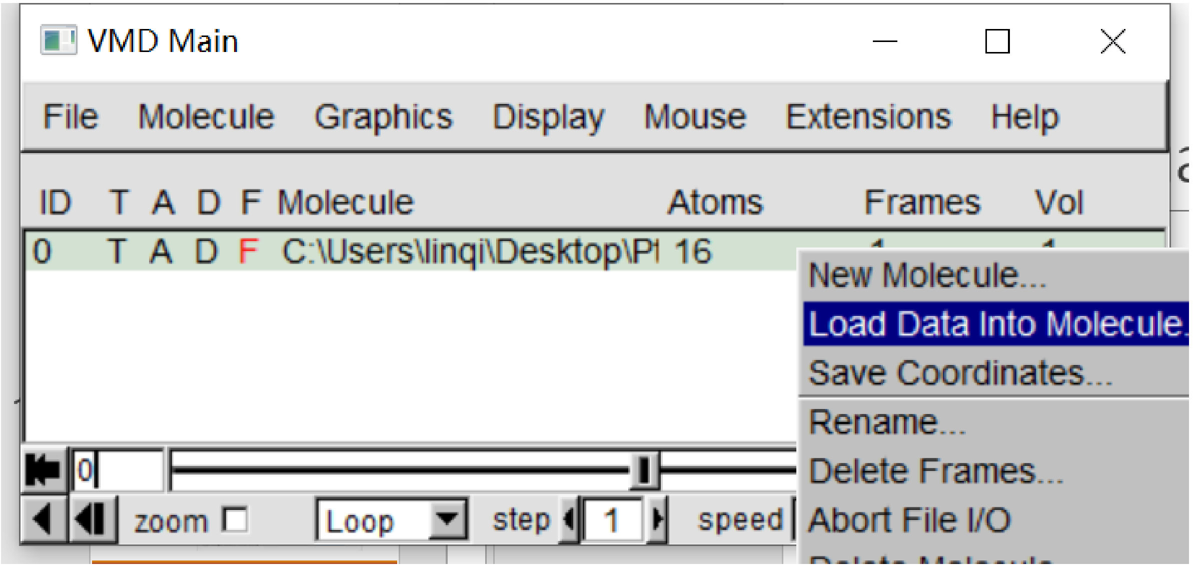


4. Visualize Local Fermi-Softness

3. Projected isosurface

Load CHGCAR by VMD

Load Data Into Molecule: LFS.cube



4. Visualize Local Fermi-Softness

3. Projected isosurface

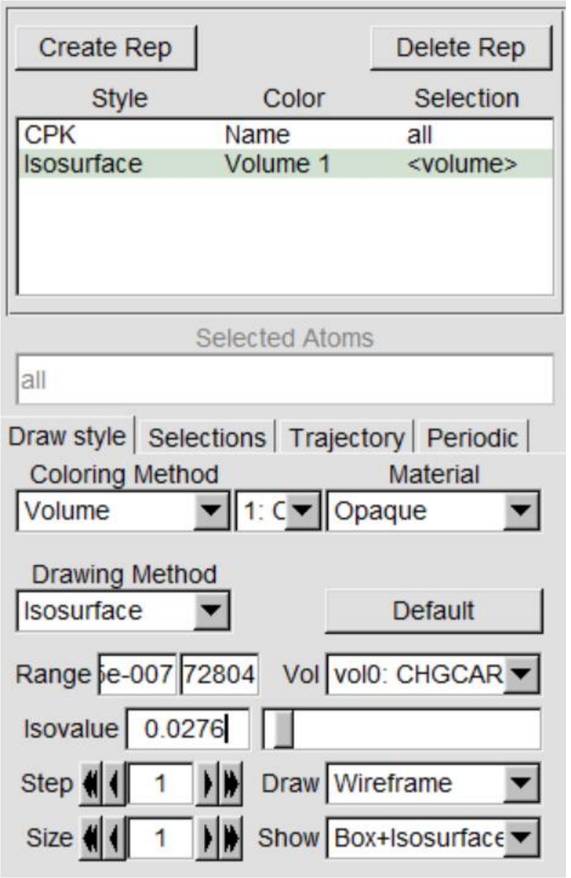
Graphics->Colors->Color Scale->Method: BWR

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

3. Projected isosurface

Local Fermi-Softness mainly distributes on

Pt atoms in $Pt_3Y(111)$ surface.