How to calculate Fermi-Softness *via* Quantum-Espresso

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1. Install program

Anaconda3, bader, and FermiSoftness is necessary.

1. You can install Anaconda3 from the website:

Anaconda | Individual Edition (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/)

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

$ *pip install FermiSoftness*

2. Run QE 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**.

3. Calculate Total, Condensed and Local Fermi-Softness

1. Generate input file runfs.py :

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

2. Copy runfs.py to the path where the non-SCF input of QE is.

3. Calculate Total, Condensed and Local Fermi-Softness

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

```
prefix='pwscf'
outdir='./tmp'
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
pp_laucher='pp.x'                    # Laucher of pp.x, e.g.: 'pp.x' or 'mpirun -np 4 pp.x'
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)
```

- The prefix and outdir need to be set the same as those in the nscf input file. If these keywords are defaulted in nscf, the default values should also be filled in. If outdir is the current directory, you should enter './', which cannot be abbreviated as ' '.
- If *bader* is in your *$PATH*, you don't need to change bader_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.)

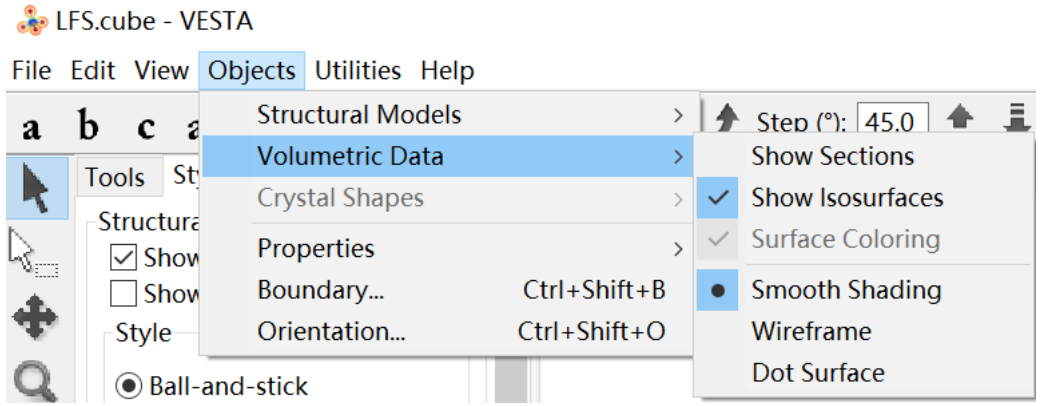
7. In *FSCAR*, you can find Total Fermi-Softness (NUMBER OF ELECTRONS) and Condensed Fermi-Softness (CHARGE), the grid data of Local Fermi-Softness were recorded in *LFS.cube*.

4. Visualize Local Fermi-Softness

1. Isosurfaces

Load *LFS.cube* by VESTA

- Objects->Volumetric Data-> Show Isosurfaces

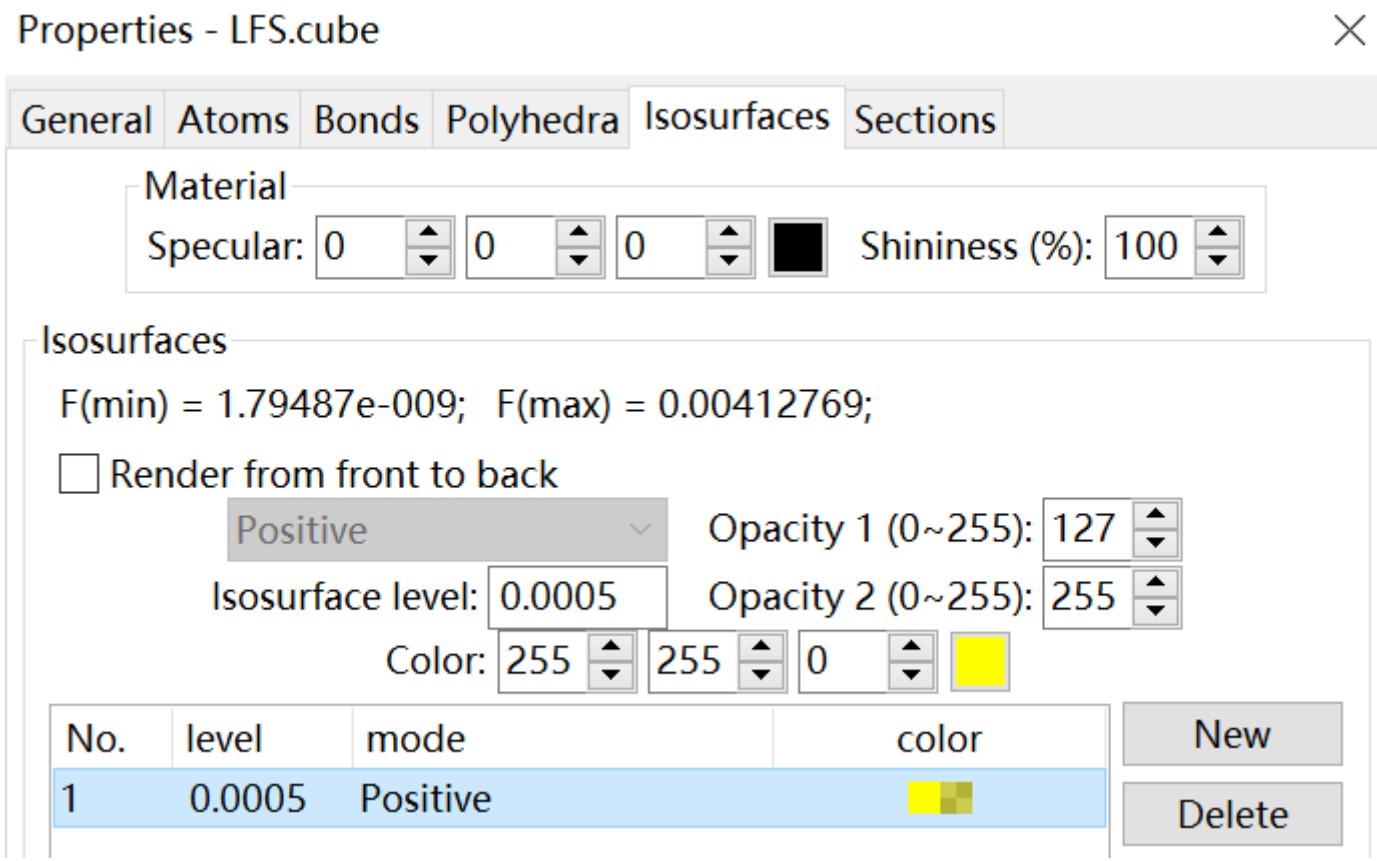


4. Visualize Local Fermi-Softness

1. Isosurfaces

Objects->Properties-> Isosurfaces

- Set appropriate isosurface level

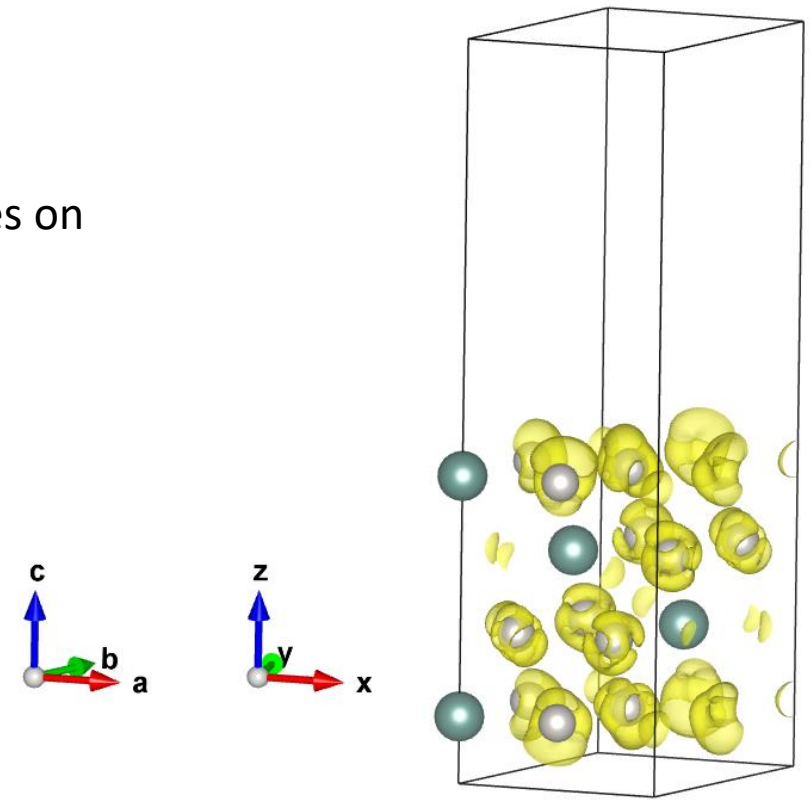


4. Visualize Local Fermi-Softness

1. Isosurfaces

Local Fermi-Softness mainly distributes on

Pt atoms in $Pt_3Y(111)$ surface.



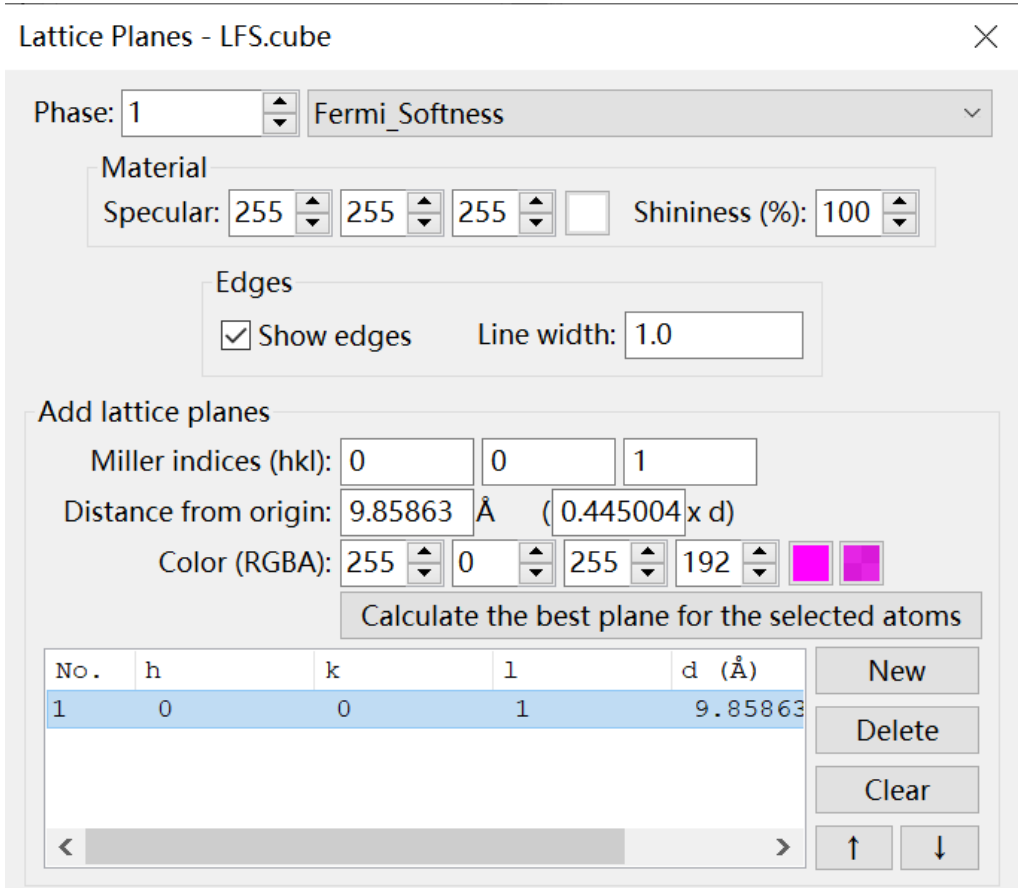
4. Visualize Local Fermi-Softness

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

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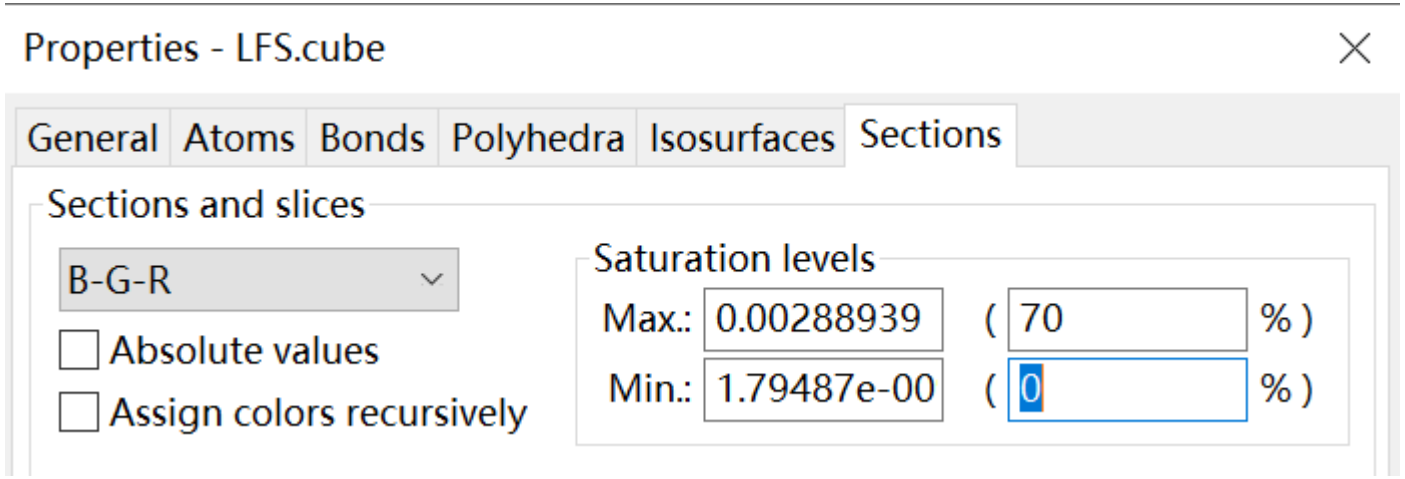
Objects->Properties-> Sections

- Set appropriate Saturation level



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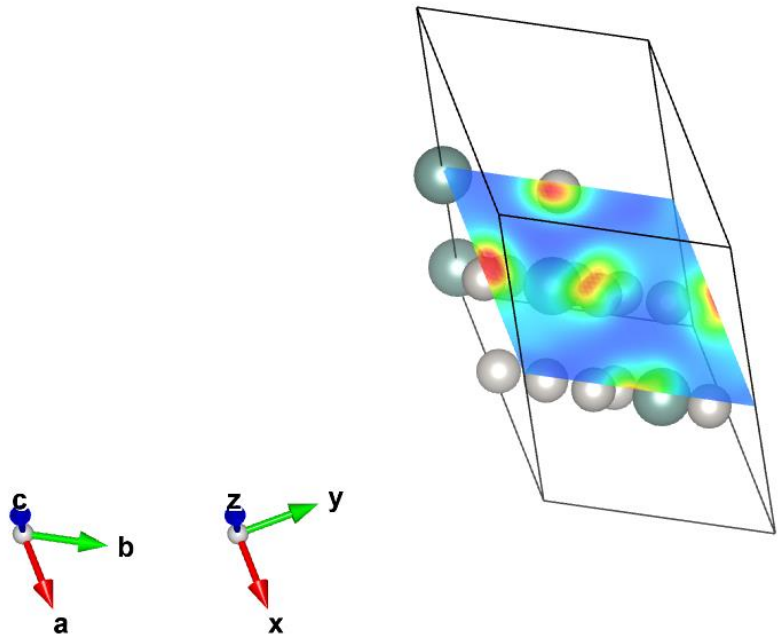
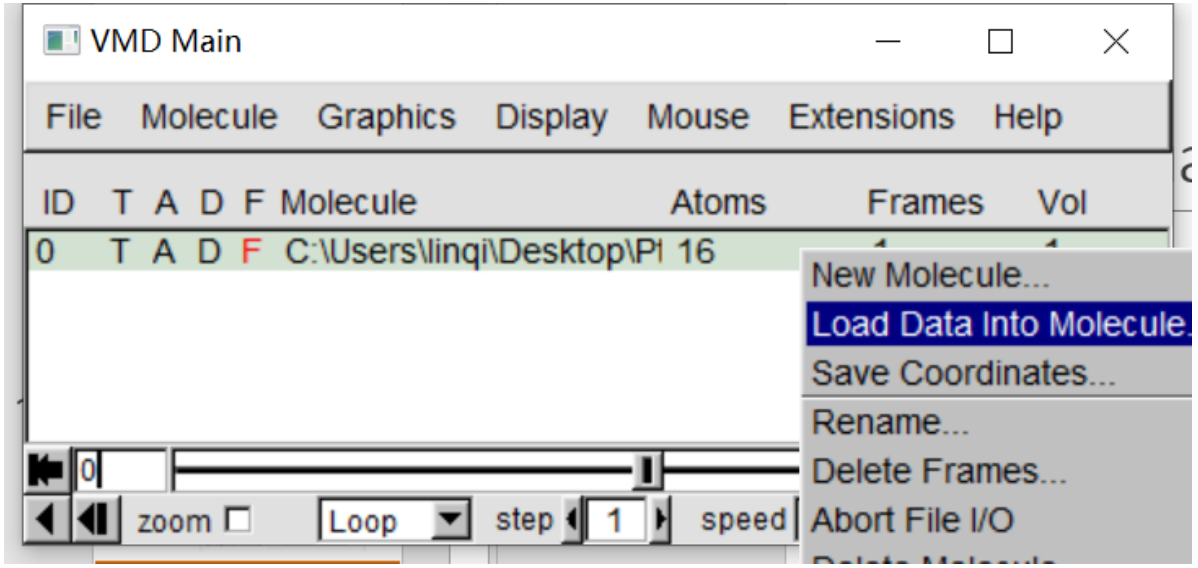


4. Visualize Local Fermi-Softness

3. Projected isosurface

Load *charge density files* by VMD

Load Data Into Molecule: *LFS.cube*



4. Visualize Local Fermi-Softness

3. Projected isosurface

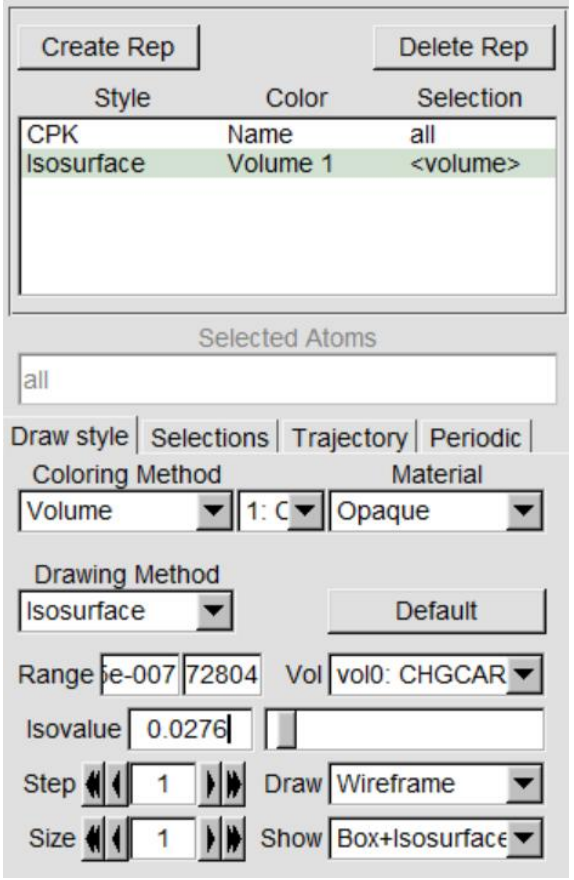
Graphics->Colors->Color Scale->Method: BWR

Graphics->Representation

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

Graphics->Representation->Trajectory

- Set appropriate Color Scale Data Range



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