Partial Charge density

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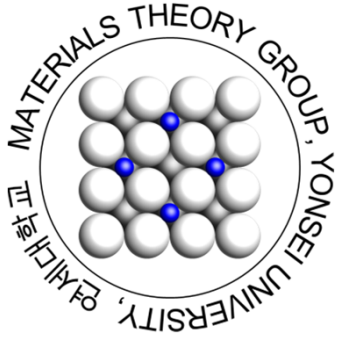


Partial density of state (PDOS)

Firstly, in order to find the energy range that you want to plot the partial charge density, PDOS should be calculated.

The geometry optimization is supposed to have been done.

Files for PDOS calculation

mv CONTCAR POSCAR

KPOINTS could be are twice with that in geometry optimization.

POTCAR file is same with that in geometry optimization.

❖INCAR file

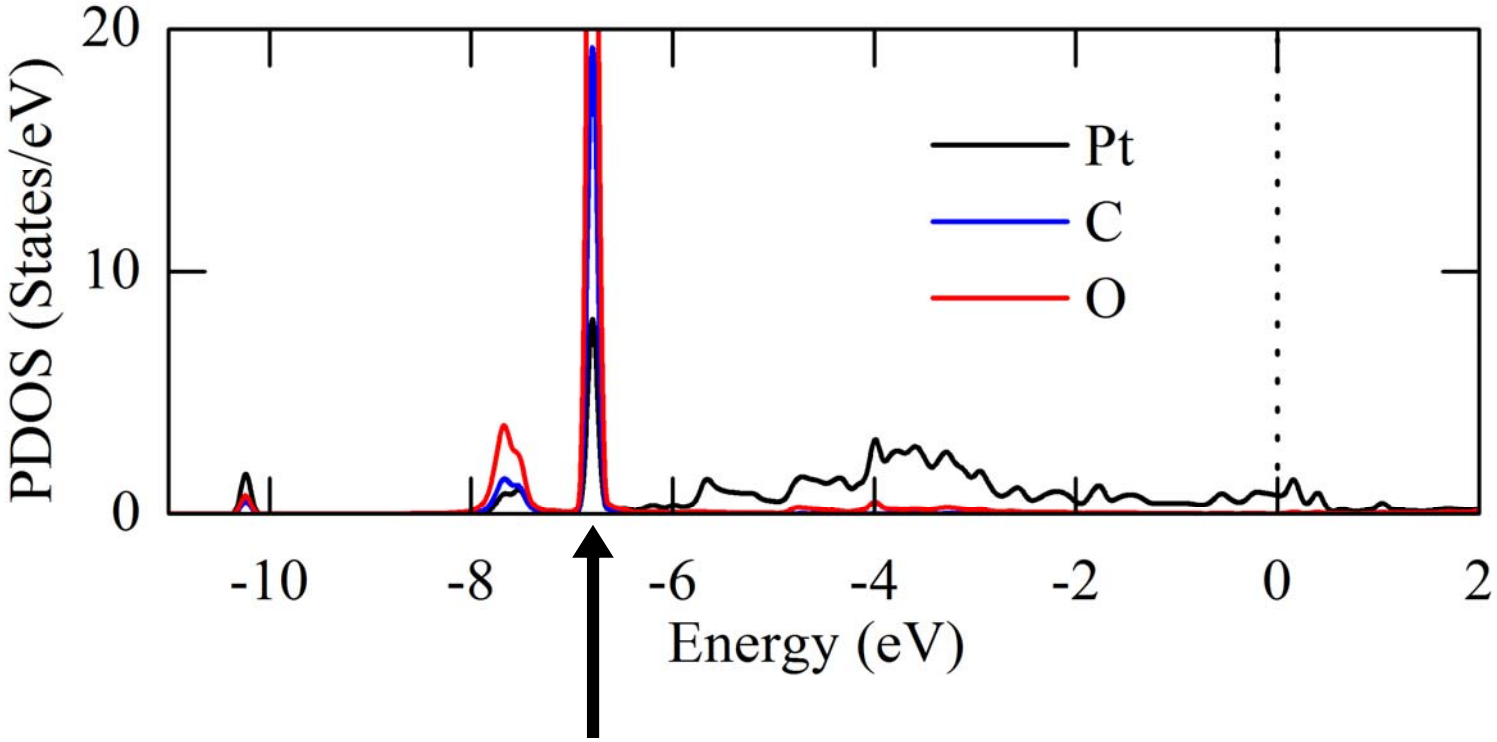
```
PREC=accurate
ENCUT=500
NELMIN=4
EDIFF=1E-5
NSW=0
IBRION=-1
ALGO=Fast
ISMEAR=-5
SIGMA=0.01
ADDGRID=T
LWAVE=T
LCHARG=F
LREAL=F
LASPH=T
LORBIT=10
EMIN=-20.00
EMAX=20.00
NEDOS=501
```

Only electronic-SC loops are performed

WAVECAR is written for the next run

DOSCAR is written

When the calculation is finished, DOSCAR file is obtained. Take CO adsorbed Pt (111) surface for example.



Let’s plot the charge density distribution of these peaks. The rang is from -6.88 to -6.56 eV.

Files for Partial charge density

KPOINTS, POSCAR and POTCAR files could be same with that in previous calculation.

After running the job, you will find the PRACAR file, the structure of which is the same as that of CHGCAR.

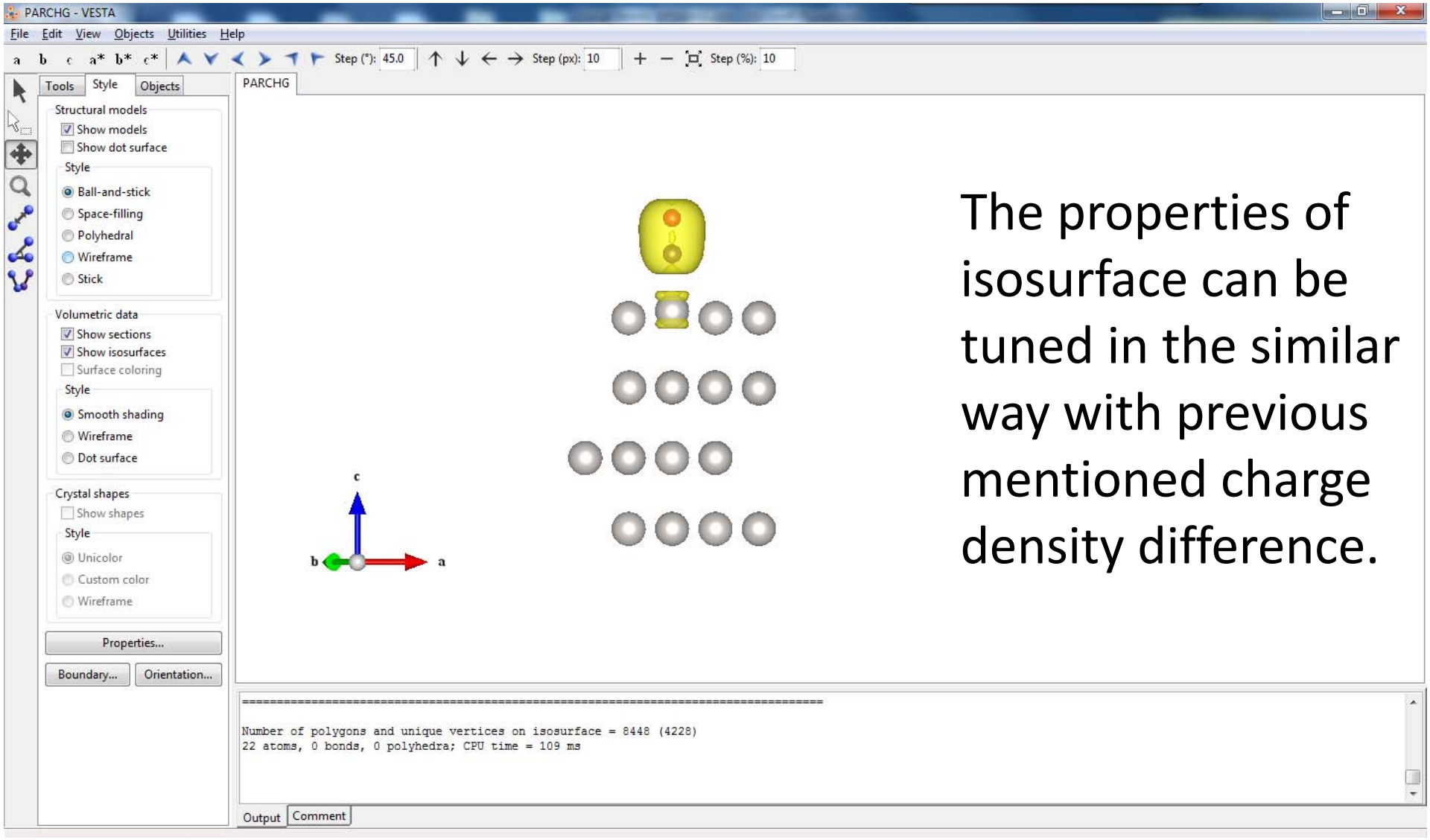
❖INCAR file

```
PREC=accurate
ISTART=1
ICHARG=1
LPARD=T
NBMOD=-2
EINT=-6.88 -6.56
ENCUT=500
NELMIN=4
EDIFF=1E-5
NSW=0
IBRION=-1
ALGO=Fast
ISMEAR=-5
SIGMA=0.01
ADDGRID=T
LCHARG=F
LREAL=F
LASPH=T
LORBIT=10
```

Read the calculated WAVECAR

PARCAR is written

Open PARCAR by VESTA



The properties of isosurface can be tuned in the similar way with previous mentioned charge density difference.

Final figure