

# Energy\_CellParam\_Plot\_Demo

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## 1 Energy Vs Cell Parameters Plotting

Sort\_Energy\_CellPara.sh is a Shell and Python script. It allows to extract and plot cell parameters ( $a$ ,  $b$ ,  $c$  and  $volume$ ) as a function of energy from VASP OUTCAR File. python packages need: pylab & scipy

[Script source](#)

### 1.1 Usage

Sort\_Energy\_CellPara.sh takes a list of OUTCAR file name as input file. In each **Calc\_\*** directory a SCF calculation has been performed for a defined cell parameters values. To execute Sort\_Energy\_CellPara.sh, one must create a file.txt which lists all outcar name and their path. It can be done as below:

```
ls -C1 Calc_*/OUTCAR > list.txt
```

- Print to terminal :

```
In [1]: %%bash
```

```
ls -C1 Calc_*/OUTCAR
```

```
Calc_01/OUTCAR
Calc_02/OUTCAR
Calc_03/OUTCAR
Calc_04/OUTCAR
Calc_05/OUTCAR
Calc_06/OUTCAR
Calc_07/OUTCAR
Calc_08/OUTCAR
Calc_09/OUTCAR
Calc_10/OUTCAR
Calc_11/OUTCAR
Calc_12/OUTCAR
Calc_13/OUTCAR
Calc_14/OUTCAR
Calc_15/OUTCAR
Calc_16/OUTCAR
```

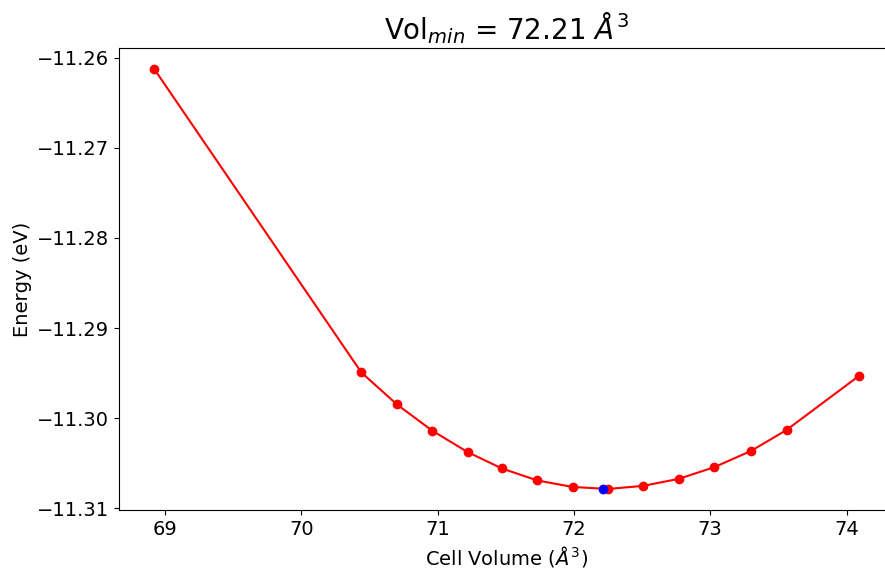
- Create the list.txt file:

```
In [2]: %%bash
ls -Cl Calc_*/OUTCAR > list.txt
```

## 1.2 Execution of Sort\_Energy\_CellPara.sh

```
./Sort_Energy_CellPara.sh
```

```
List name which contains all OUTCAR Files names ? > list.txt
OUTPUT file name to save data ? > data.out
X plot ( Energy, A, B, C or Vol ) ? > Vol
Y plot ( Energy, A, B, C or Vol ) ? > Energy
Calculate the Optimized Value (yes/no)? > yes
All Data are saved to file : data.out
```



E\_Vol.png