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 tackes a list of OUTCAR file name as input file. In each **Calc_**** directory a SCF calcultaion has been performed for a defined cell parameters values. To execute Sort_Energy_CellPara.sh, ones 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
```
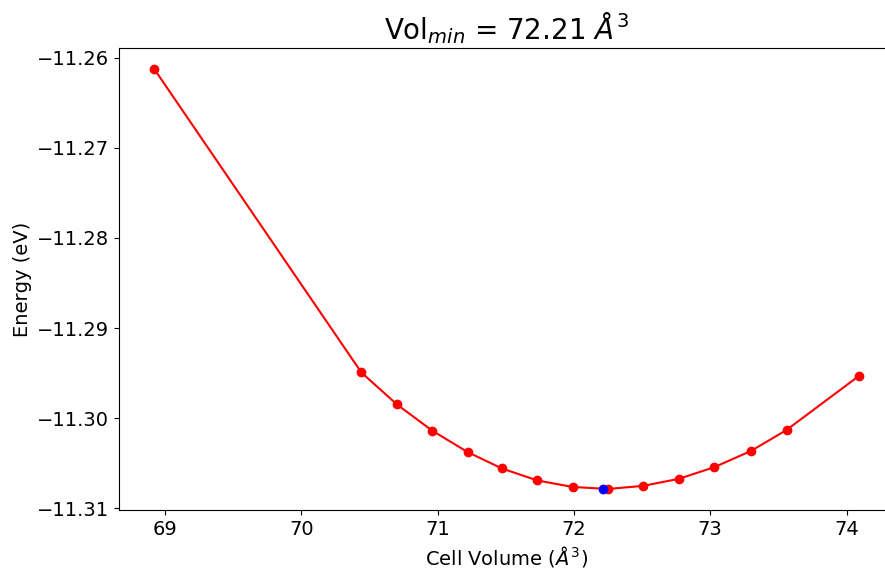
- Create the list.txt file:

```
In [59]: %%bash
         ls -C1 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