

Plot_OSZICAR_MD_Demo

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1 Plot OSZICAR Script

Plot_OSZICAR_MD.py is a Python script which allows to read and plot all quantites of OSZICAR VASP file. Pylab package is needed for plotting. [Script source](#)

```
In [1]: %matplotlib inline
```

```
In [2]: %run Plot_OSZICAR_MD.py
```

```
OSZICAR File Name ? > OSZICAR_MD
```

```
T : is the current temperature.
```

```
E : is the total free energy (including the kinetic energy of the ions and the energy of the No
```

```
F : is the total free energy (at this point the energy of the reference atom has been subtract
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```
E0 : is the energy for sigma-> 0 .
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```
EK : is the kinetic energy.
```

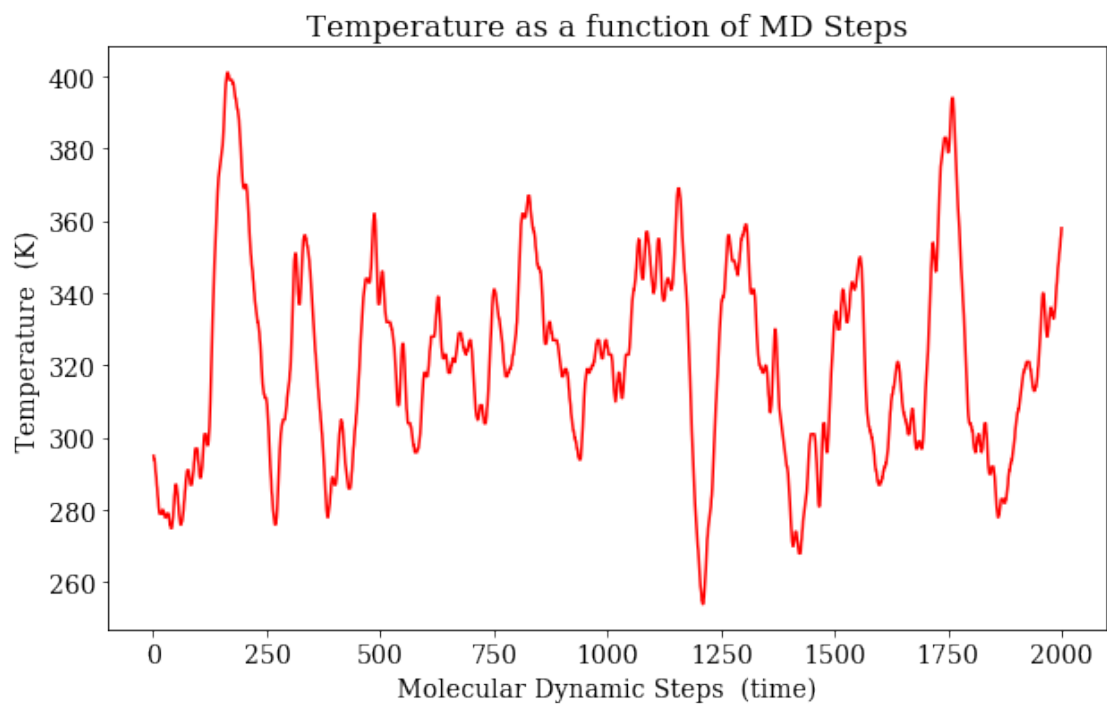
```
SP : is the potential energy of the Nosé thermostat.
```

```
SK : is the corresponding kinetic energy.
```

```
more infos : https://cms.mpi.univie.ac.at/vasp/vasp/stdout\_OSZICAR\_file.html
```

```
Yplot (T, E, F, E0, EK, SP or SK ) > T
```

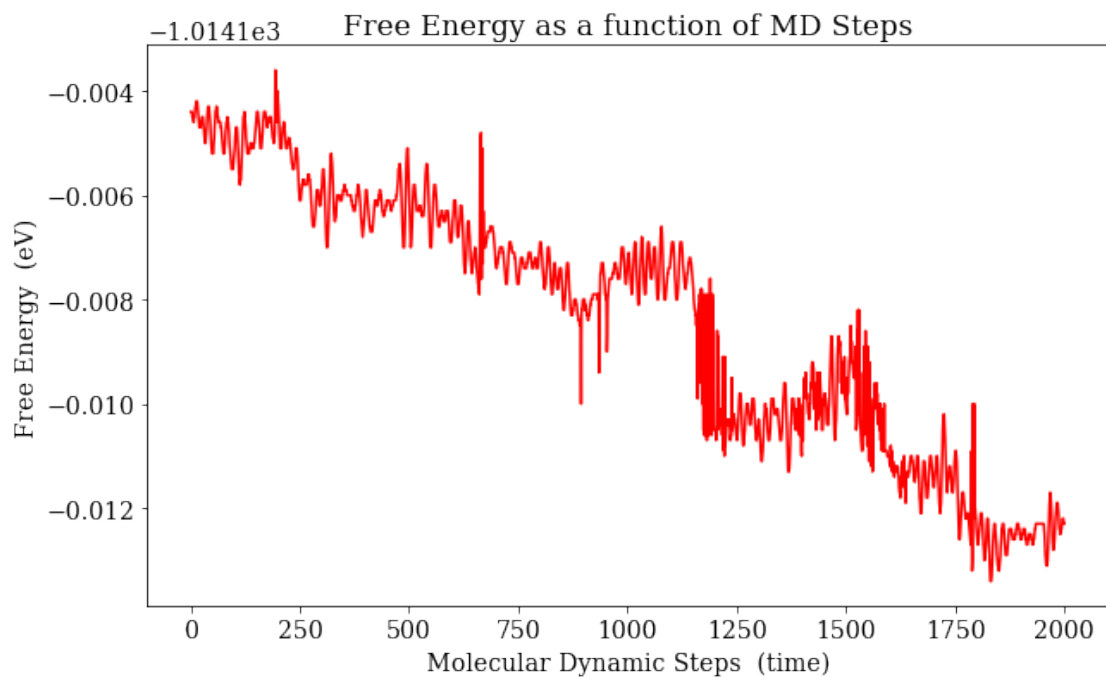
```
Mean Temperature = 321.018 (K)
```



Plot Other Quantities (yes/no)? > yes

Yplot (T, E, F, E0, EK, SP or SK) > E

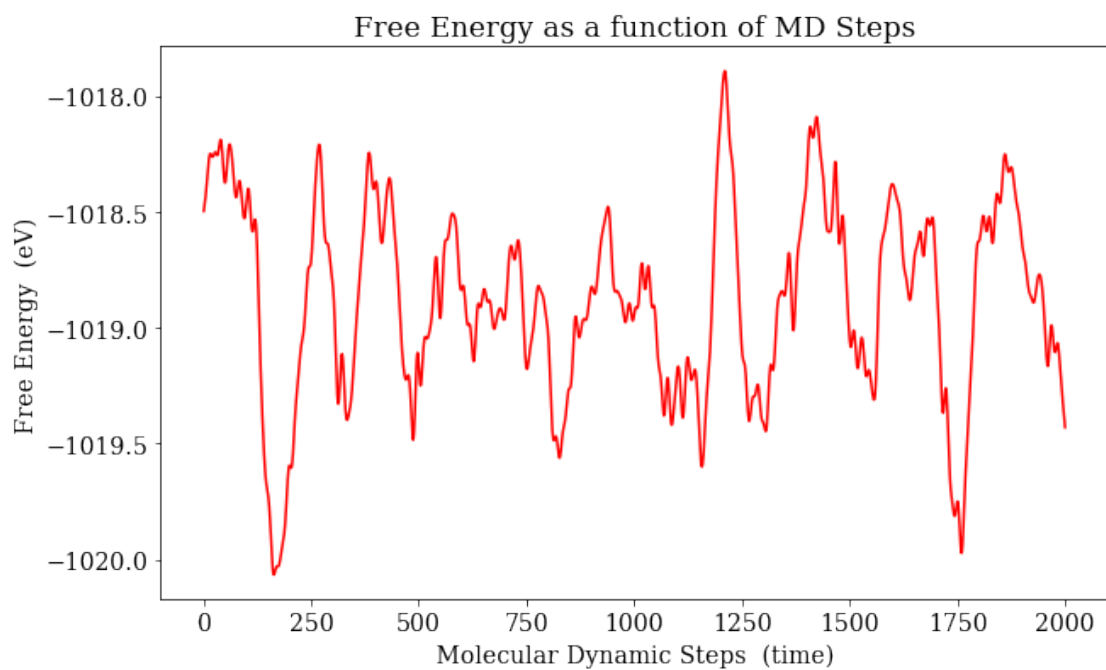
Mean Free Energy = -1014.1083702 (eV)



Plot Other Quantities (yes/no)? > yes

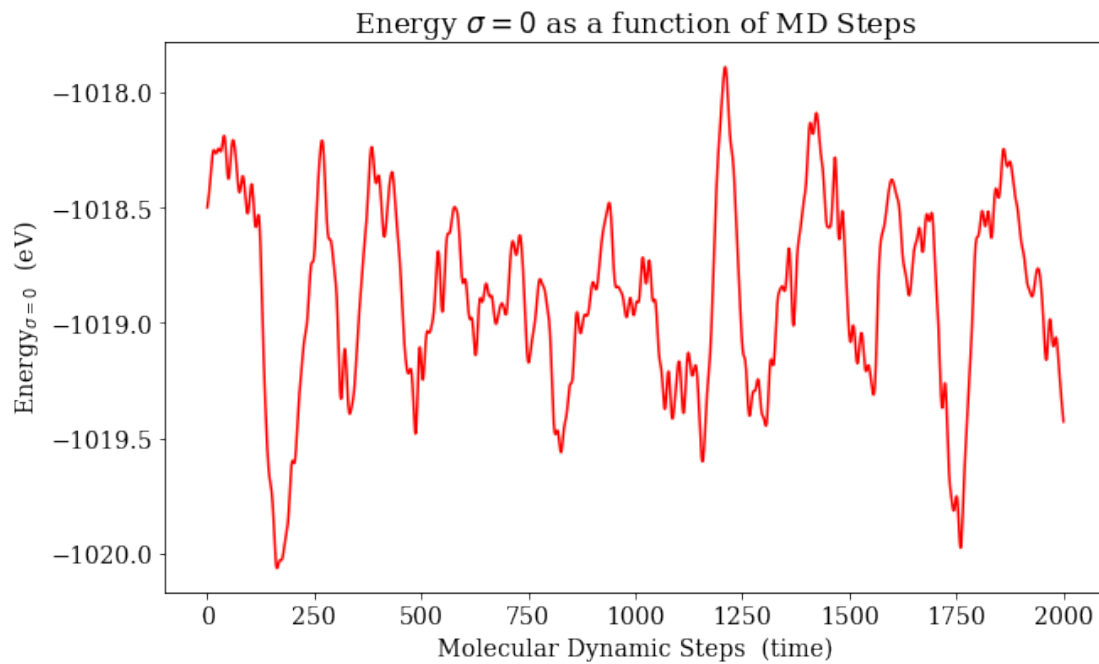
Yplot (T, E, F, E0, EK, SP or SK) > F

Mean Free Energy = -1018.8802606 (eV)



```
Plot Other Quantities (yes/no)? > yes
Yplot (T, E, F, E0, EK, SP or SK ) > E0
```

Mean Energy $_{\sigma=0}$ = -1018.88000705 (eV)



```
Plot Other Quantities (yes/no)? > no
```

Exit!..