**Bash shell command practice/ data process (extraction of "energy without entropy = ")**

**Use of grep and awk command to extract the data of energy without entropy in the OUTCAR\_project file. While also making a new file with the extracted data .**[**¶**](http://localhost:8888/notebooks/OUTCAR_project_MorganRhinehart.ipynb#Use-of-grep-and-awk-command-to-extract-the-data-of-energy-without-entropy-in-the-OUTCAR_project-file.-While-also-making-a-new-file-with-the-extracted-data-.)

grep -i "energy without entropy=" OUTCAR\_project | awk '{printf "%s\n",$4}'>>Extract\_Energy.dat

### greps all iterations after the first 27 and for the Free energy of the ion-electron system (eV)

### >> Extract\_energy.dat command at the end of the above pipe command to create the .dat file

#### chmod the file to .sh with chmod +x filename.sh this will show the grep commands in the new executable file

touch Extract\_Energy.sh #### to make an empty file for the grep command

chmod u+x Extract\_Energy.sh

####This executable will hold my grep and awk commands and allow one to execute it on RCC

#### Copy and paste the grep and awk command into the newly made Extract\_Energy.sh file on Cygwin

### note to make the new .sh an active executable to run on Cygwin ou need to use RCC

### put commands below into an Energy\_Plot.py folder

import numpy as np

from matplotlib import pyplot as plt

values = np.loadtxt("Extract\_Energy.dat") ### load the text from the .dat file

plt.plot(values)

plt.savefig("EnergyPlot.png") ##### save the plot as the set name "EnergyPlot.png"

plt.show() ####Shows the plot of extracted energy without energy points

A picture containing text, antenna

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