

Assignment 4

Name: Harikesh Kushwaha

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Imports

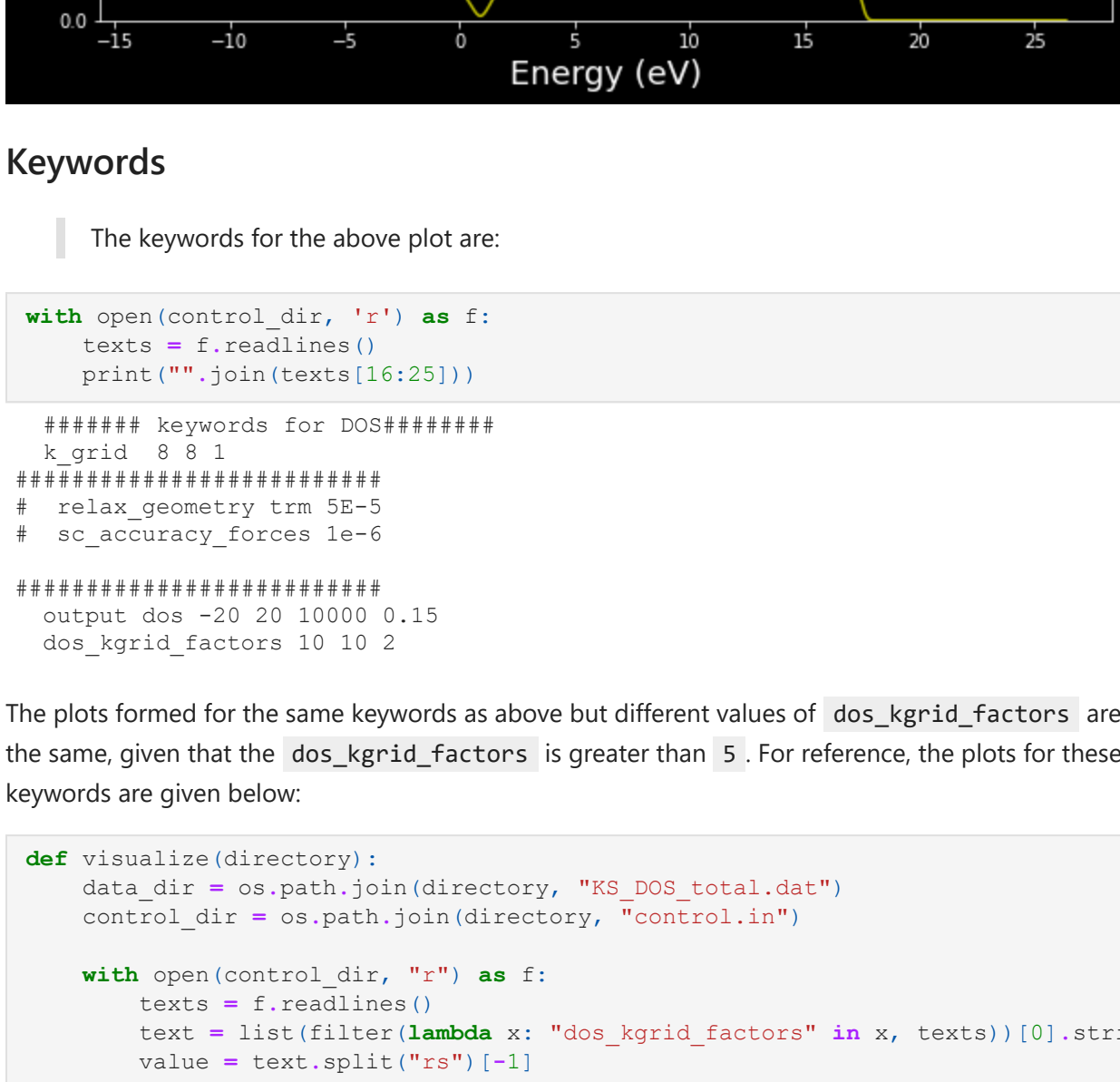
```
In [1]: import numpy as np
import matplotlib.pyplot as plt
import os
import pandas as pd
import seaborn as sns
```

Plot

```
In [4]: #directory for the dat file
data_dir = os.path.join('kgrid5', 'run4', 'KS_DOS_total.dat')
#directory for the control file
control_dir = os.path.join('kgrid5', 'run4', 'control.in')

#Extracting the data from the dat file
data = np.loadtxt(data_dir)
#Ignoring the last column which gives DOS for spin down and is exactly the same as spin up
data = data[:, :2]

#Plotting the figure
plt.figure(figsize=(10,6))
plt.plot(data[:, 0], data[:, 1], "y")
plt.xlabel("Energy (eV)", fontdict={"size": 18})
plt.ylabel("Density of States", fontdict={"size": 18})
plt.title("Density of States for Graphene",
          fontdict={"size": 18, "weight": "bold"})
plt.ylim(0, 0.9)
```



Keywords

The keywords for the above plot are:

```
In [5]: with open(control_dir, 'r') as f:
        texts = f.readlines()
        print("".join(texts[16:25]))

##### keywords for DOS#####
k_grid 8 8 1
#####
# relax_geometry trm 5E-5
# sc_accuracy_forces 1e-6

#####
output dos -20 20 10000 0.15
dos_kgrid_factors 10 10 2
```

The plots formed for the same keywords as above but different values of `dos_kgrid_factors` are almost the same, given that the `dos_kgrid_factors` is greater than 5. For reference, the plots for these keywords are given below:

```
In [8]: def visualize(directory):
        data_dir = os.path.join(directory, "KS_DOS_total.dat")
        control_dir = os.path.join(directory, "control.in")

        with open(control_dir, "r") as f:
            texts = f.readlines()
            text = list(filter(lambda x: "dos_kgrid_factors" in x, texts))[0].strip()
            value = text.split("rs")[-1]

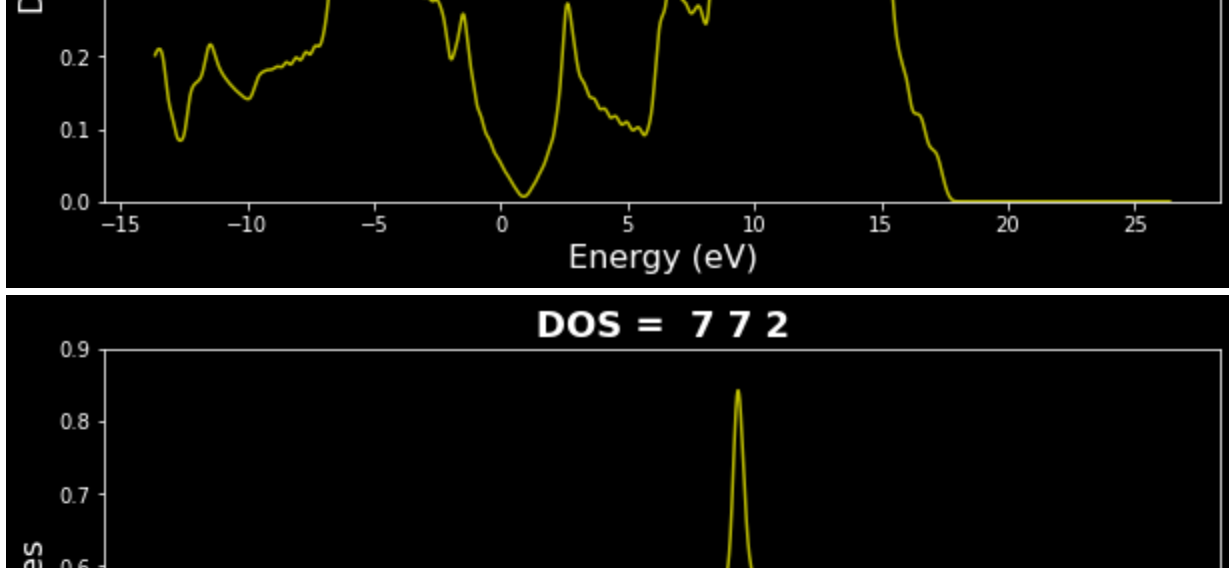
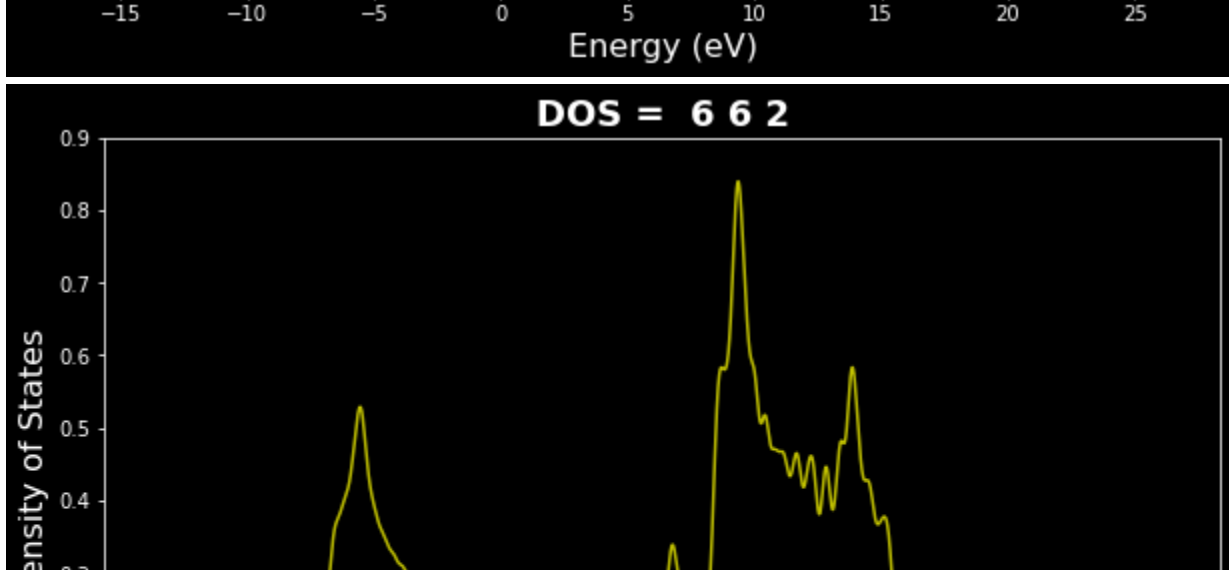
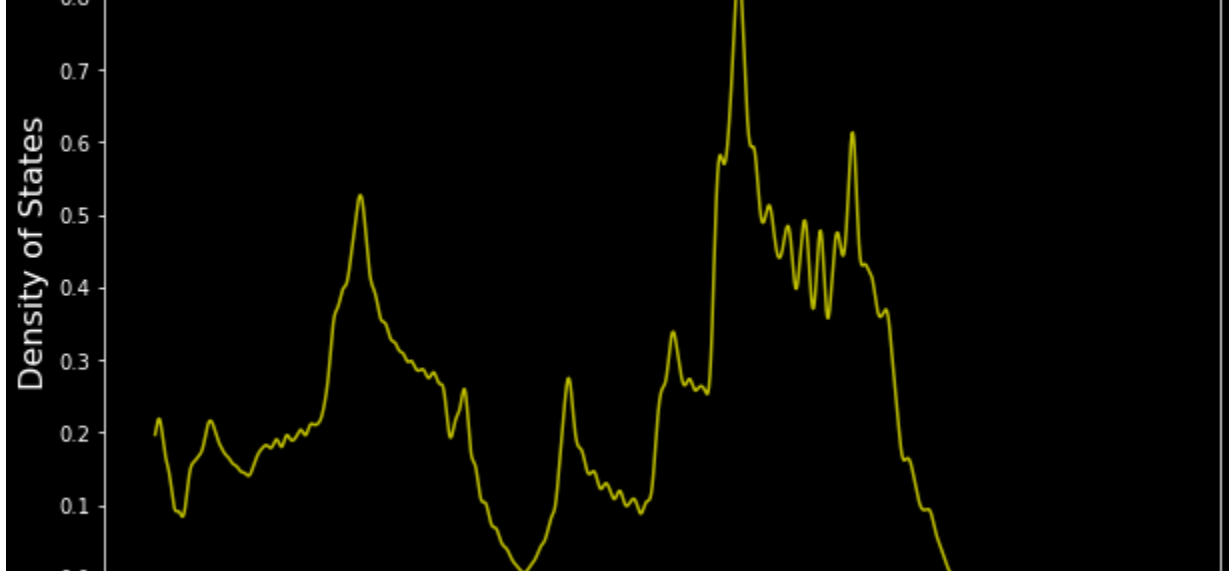
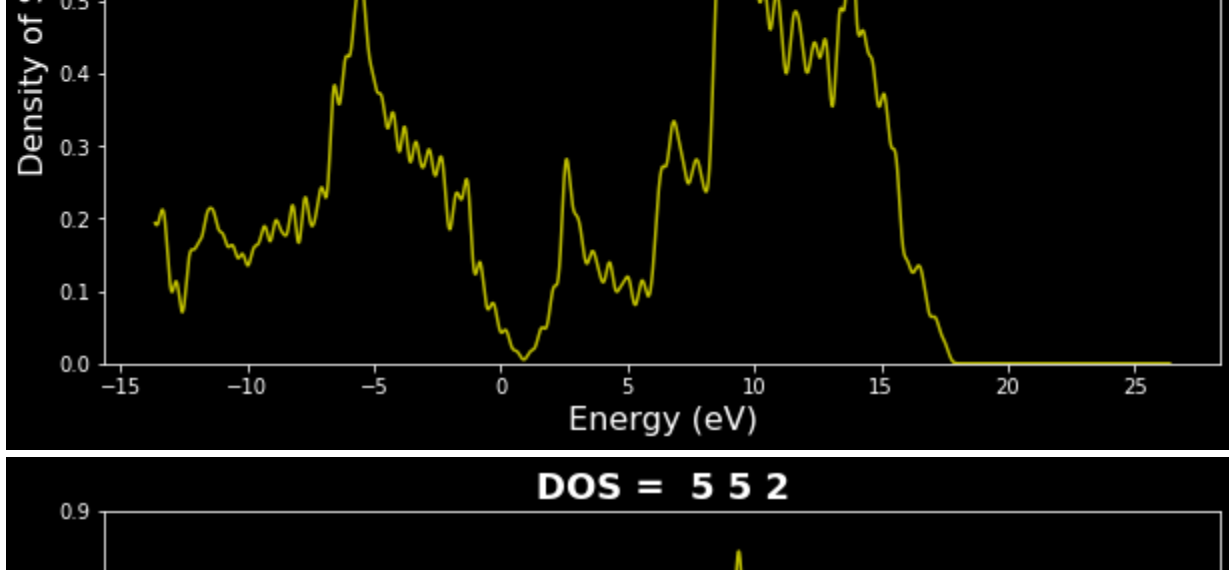
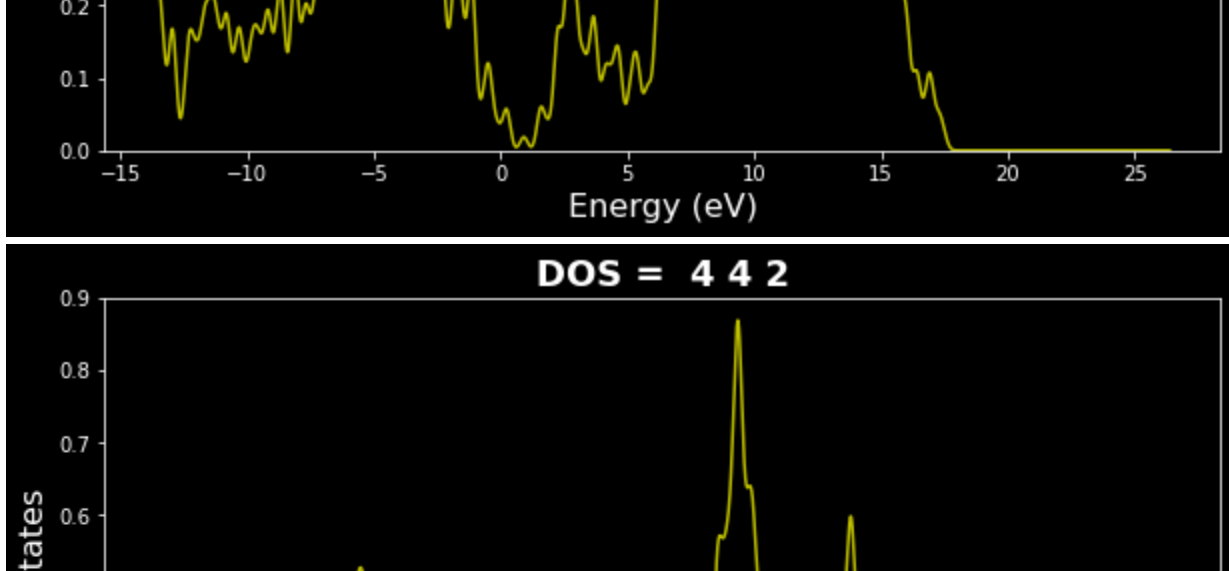
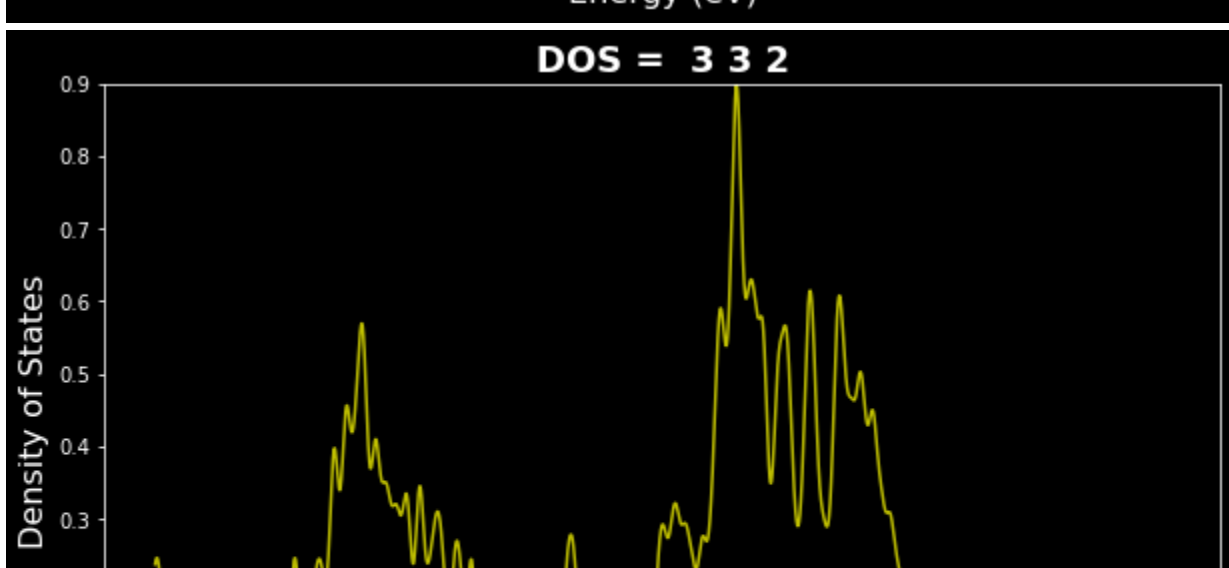
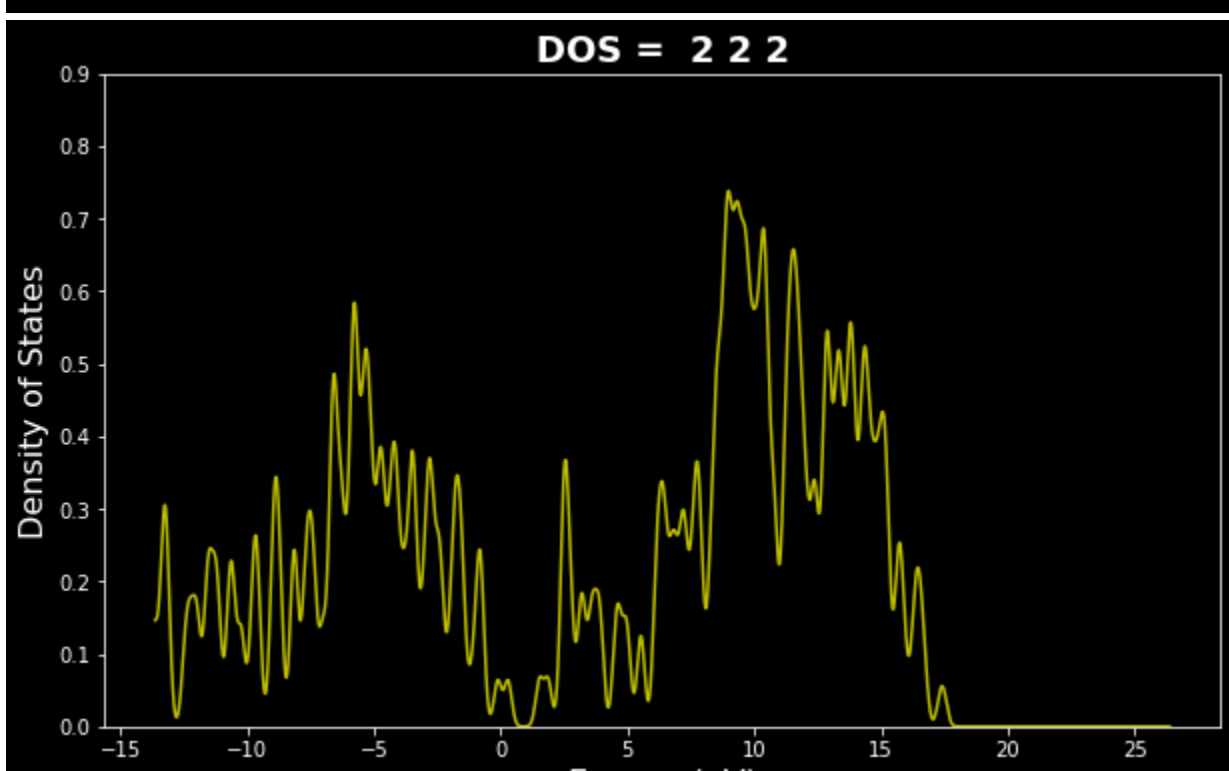
        data = np.loadtxt(data_dir)
        #Ignoring the last column which gives DOS for spin down and is exactly the same as spin up
        data = data[:, :2]

        #Plotting the figure
        plt.figure(figsize=(10,6))
        plt.plot(data[:, 0], data[:, 1], "y")
        plt.xlabel("Energy (eV)", fontdict={"size": 16})
        plt.ylabel("Density of States", fontdict={"size": 16})
        plt.title(f"DOS = {value}",
                  fontdict={"size": 18, "weight": "bold"})
        plt.ylim(0, 0.9)
```

```
In [9]: for dir in os.listdir("kgrid4"):
        if "." not in dir:
            try:
                directory = os.path.join("kgrid4", dir)
                visualize(directory)

            except BaseException as e:
                print(e)
                print("No Data File Found.")
            else:
                print(f"{dir} is Not a directory")
```

aims_sub.sh is Not a directory
control.in is Not a directory
geometry.in is Not a directory
tool.ipynb is Not a directory
visualize.ipynb is Not a directory



```
In [11]: for dir in os.listdir("kgrid5"):
        if "." not in dir:
            try:
                directory = os.path.join("kgrid5", dir)
                visualize(directory)

            except BaseException as e:
                print(e)
                print("No Data File Found.")
            else:
                print(f"{dir} is Not a directory")
```

aims_sub.sh is Not a directory
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visualize.ipynb is Not a directory

