Entry Number: 2021PHS7181 **Imports** import numpy as np In [1]: import matplotlib.pyplot as plt import os import pandas as pd import seaborn as sns Note: All the combinations I have done and output files related to them can be found on github: Assignment4. **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 whch gives DOS for spin down and is exactly the same as spin 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); **Density of States for Graphene** 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0.0 -5 -io 20 25 -i5 Energy (eV) 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 This completes the assignment. Some more details are provided below but you might ignore them. **Extras** 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) data = data[:, :2] 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); for dir in os.listdir("kgrid4"): In [9]: if "." not in dir: try: directory = os.path.join("kgrid4", dir) visualize(directory) except BaseException as 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 DOS = 1120.9 0.8 0.7 Density of States 0.2 0.1 10 15 20 25 Energy (eV) DOS = 2 2 2 0.9 0.8 0.7 Density of States 0.6 0.5 0.4 0.3 0.2 0.1 0.0 -5 Energy (eV) -15 -10 10 15 20 25 DOS = 332 0.9 0.8 0.7 Density of States 0.6 0.5 0.4 0.3 0.2 0.1 -5 Energy (eV) -15 15 -10 ò 10 20 25 442 DOS = 0.9 0.8 0.7 Density of States 0.6 0.5 0.2 0.1 -5 15 -15 -10 ò 10 20 25 Energy (eV) DOS = 5520.9 0.8 0.7 Density of States 0.6 0.5 0.4 0.3 0.2 0.1 5 10 Energy (eV) -5 -15 -10 ò 10 15 20 25 DOS = 6620.9 0.8 0.7 Density of States 0.2 0.1 0.0 -5 Energy (eV) -15 ò 15 -10 10 20 25 DOS = 7720.9 0.8 0.7 Density of States 0.6 0.5 0.4 0.2 0.1 0.0 -i5 -io <u>-</u>5 ò 10 15 20 25 Energy (eV) for dir in os.listdir("kgrid5"): In [11]: if "." not in dir: try: directory = os.path.join("kgrid5", dir) visualize(directory) except BaseException as 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 DOS = 7720.9 0.8 0.5 0.3 0.2 0.1 0.0 --15 -10 -5 ò 10 15 20 Energy (eV) DOS = 16 16 2 0.9 0.8 Density of States 0.6 0.5 0.4 0.3 0.2 0.1 0.0 -15 -5 -io 15 Energy (eV) 0.9 0.8 0.7 Density of States 0.6 0.5 0.4 0.3 0.2 0.1 0.0 --10 -5 -15 10 15 20 25 Energy (eV) DOS = 9920.9 0.8 0.7 Density of States 0.5 0.3 0.2 0.1 0.0 Energy (eV) -5 -10 ò 10 15 20 25 DOS = 10 10 2 0.9 0.8 Density of States 0.5 0.3 0.2 0.1 0.0 Energy (eV) -5 -10 10 15 20 25 11 11 2 0.9 0.8 0.7 Density of States 0.5 0.3 0.2 0.1 0.0 --10 -5 -15 10 15 20 25 Energy (eV) DOS = 12 12 2 0.9 0.8 0.7 Density of States 0.5 0.3 0.2 0.1 0.0 Energy (eV) -5 -10 ò 10 15 20 25 DOS = 13 13 2 0.9 0.8 Density of States 0.5 0.3 0.2 0.1 0.0 Energy (eV) -5 -10 10 15 20 25 0.9 0.8 0.7 Density of States 0.6 0.5 0.4 0.3 0.2 0.1 0.0 -15 -10 -5 20 25 10 15 Energy (eV) DOS = 15 15 2 0.9 0.8 0.7 Density of States 0.6 0.5 0.4 0.3 0.2 0.1

0.0 -15

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Energy (eV)

As you can see the plot starts to smoothen after dos\_kgrid\_factors attains the value of 5 5 2 and

becomes very smooth at 10 10 2. This is why I chose this value of dos\_kgrid\_factors.

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**Assignment 4** 

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