Run on Google Colab View on Github

Assignment 2

Name: Harikesh Kushwaha

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Imports

In [1]:
```
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib as mpl
```

If you are running this file in Google colab, the associated csv file can be downloaded by using the command below:

In [ ]:
```
!wget https://raw.githubusercontent.com/Hari31416/Academic/main/Codes/Assignment2/data
```

Run the cell above in Google colab and continue with the next cells.

Also, the original excel file can be downloaded by clicking here.

In [2]:
```
df = pd.read_csv("data.csv")
```

In [3]:
```
df
```

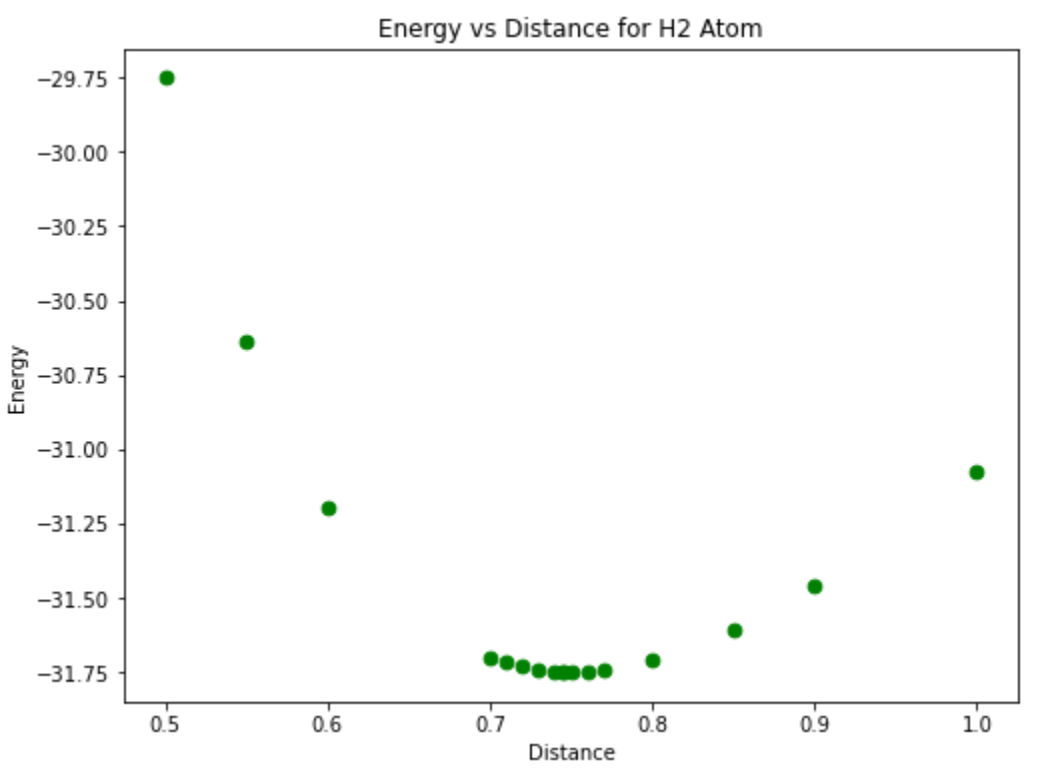
Out[3]:

	Distance	Energy
0	1.000	-31.078234
1	0.900	-31.460702
2	0.800	-31.710034
3	0.850	-31.608172
4	0.700	-31.700418
5	0.600	-31.199452
6	0.550	-30.636954
7	0.500	-29.751617
8	0.710	-31.718451
9	0.720	-31.732030
10	0.730	-31.741429
11	0.740	-31.746910
12	0.750	-31.748717
13	0.760	-31.747075
14	0.770	-31.742194
15	0.744	-31.748061
16	0.746	-31.748420

In [4]:
```
#Setting global figure size
mpl.rcParams['figure.figsize'] = (8, 6)
```

Making a rough plot of the data

In [5]:
```
df.plot(x='Distance', y='Energy', kind='scatter', color='green', s = 45)
plt.title('Energy vs Distance for H2 Atom');
```

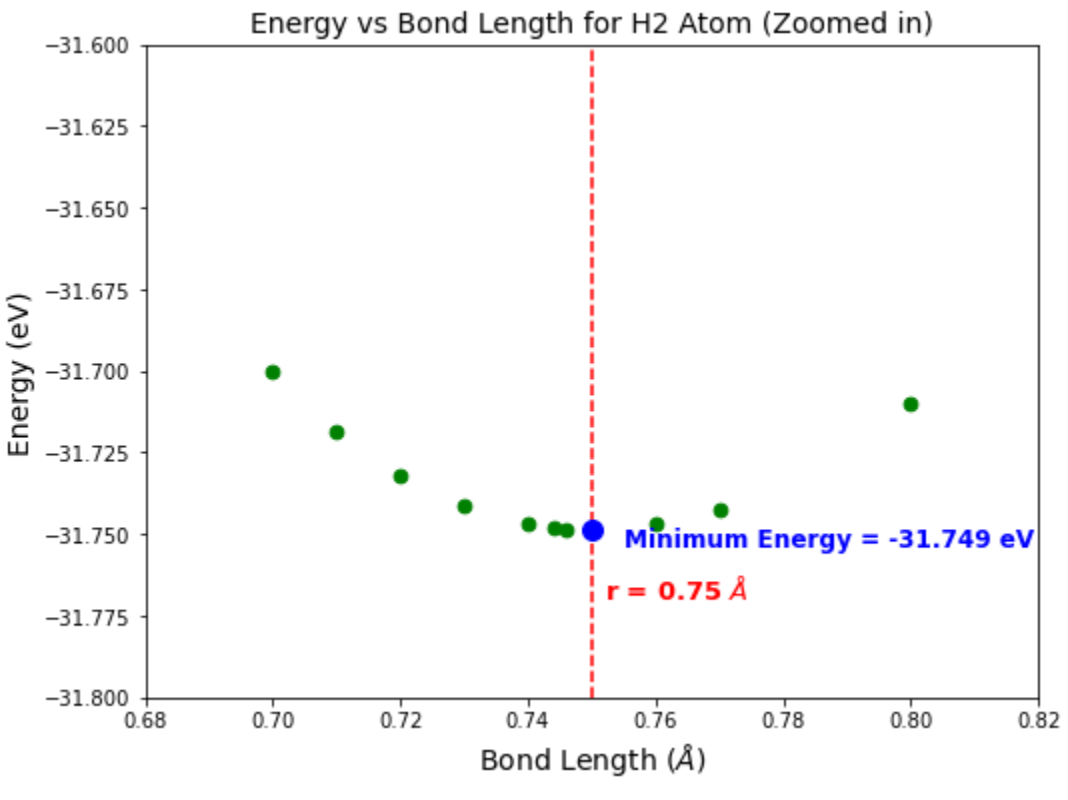


Getting the value of minimum energy and its corresponding distance

In [6]:
```
#Getting the value of minimum energy and its corresponding distance
min_position = df[df['Energy'] == df['Energy'].min()].values
min_energy = float(min_position[:,1])
min_energy_position = float(min_position[:,0])
```

The Final Plot

In [15]:
```
df.plot(x='Distance', y='Energy', kind='scatter', color='green', s = 45)
#The point corresponding to minimum energy
plt.plot(min_energy_position, min_energy, 'bo', markersize=10)
#Text describing the minimum energy
plt.text(min_energy_position+0.005, min_energy-0.005,
    f'Minimum Energy = {round(min_energy,3)} eV',
    fontdict={'size': 12, 'color': 'blue', 'weight': 'bold'})
#Vertical line at the distance corresponding to minimum energy
plt.vlines(min_energy_position, -32, -29, linestyles='dashed', colors='red')
#Text describing the minimum distance
plt.text(min_energy_position+0.002, -31.77,f"r = {min_energy_position} $\AA$",
    fontdict={'size': 13, 'color': 'red', 'weight': 'bold'})
#Modifying the lables
plt.xlabel('Bond Length $(\AA)$', fontsize=14)
plt.ylabel('Energy (eV)', fontsize=14)
#Zooming in on the minimum energy
plt.ylim([-31.8, -31.6])
plt.xlim([0.68,0.82])
#Adding a title
plt.title('Energy vs Bond Length for H2 Atom (Zoomed in)', fontsize=14);
```



In [ ]:
```
```