```
In [5]:   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://github.com/Hari31416/PYL800/blob/main/Codes/Assignment2/data.csv?raw=tru
```

Run this code in Google colab and continue with the next cells.

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

```
In [7]:   df = pd.read_csv("data.csv")
```

```
In [8]:   df
```

Out[8]:

|    | 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 [9]:   #Setting global figure size
          mpl.rcParams['figure.figsize'] = (8, 6)
```

Making a rough plot of the data

```
In [10]:  df.plot(x='Distance', y='Energy', kind='scatter', color='green', s = 45)
          plt.title('Energy vs Distance for H2 Atom');
```
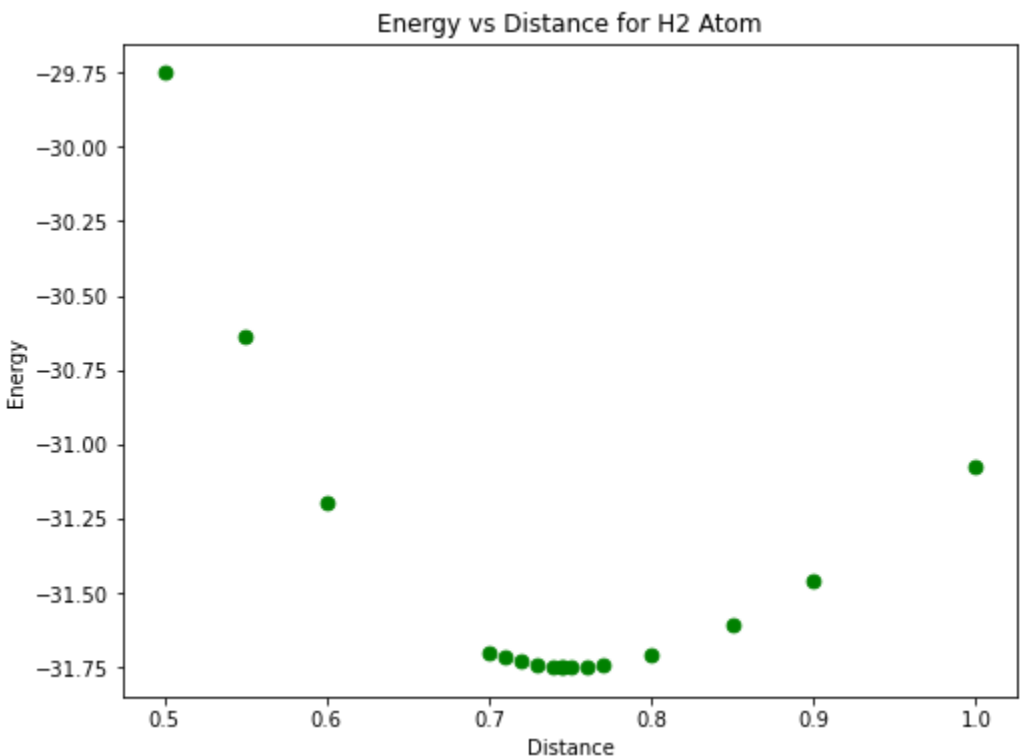

Getting the value of minimum energy and its corresponding distance

```
In [11]:  #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 [13]:  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} nm",
              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);
```