CVL867: Atomistic and multiscale modelling

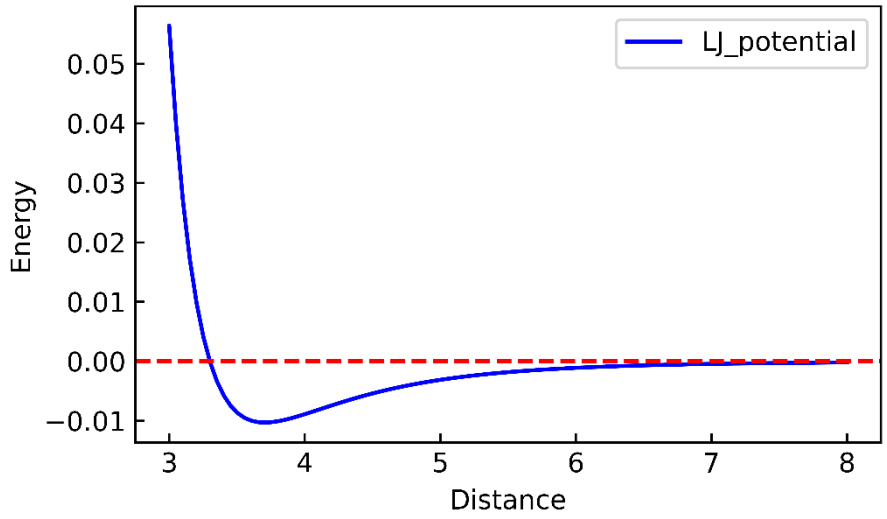
Assignment – 03

Submitted by: Aman Pawar

[Note: All the code is available in CVL867_Assignment_03_AmanPawar.ipynb]

Answer 01)

LJ Potential computation:



Answer 02)

Potential energy of the cluster is -795.21

Answer 03)

Potential energy of the cluster is -795.21
Potential energy of the cluster after energy minimization is -807.31

Picture to show the last few epochs of energy minimization.

```
Step: 85, New Potential: -807.1552400212980
Step: 86, New Potential: -807.1659141076868
Step: 87, New Potential: -807.1781092107356
Step: 88, New Potential: -807.2061834215338
Step: 89, New Potential: -807.2420403898442
Step: 90, New Potential: -807.253119079725
Step: 91, New Potential: -807.2637838165309
Step: 92, New Potential: -807.274063005796
Step: 93, New Potential: -807.2676669562857
Step: 94, New Potential: -807.277255478643
Step: 95, New Potential: -807.286507689351
Step: 96, New Potential: -807.2954404237282
Step: 97, New Potential: -807.2714446688112
Step: 98, New Potential: -807.2798153704106
Step: 99, New Potential: -807.3123933351335
```

Answer 04)

As the output is too large the results are shown in the code.

Answer 05)

As the output is too large the results are shown in the code.

Answer 06)