This code performs data processing and analysis of chemical reactions related to a CVD (Chemical Vapor Deposition) process obtained from DFT calculations by invoking different libraries, specifically, ‘cclib’ and ‘ASE’.

The main loop iterates through different temperatures (T\_CVD) and different input files within the specified range (start\_range to end\_range). It reads data from these files, processes the data, and calculates various parameters related to the reactions.

Some of the key tasks performed in this loop include:

Reading atom data from log files using ‘cclib’.

Calculating Gibbs free energy using ASE (Atomic Simulation Environment).

Calculating differences in Gibbs free energy for different reaction steps.

Determining reaction types based on changes in atom counts.

After processing the data, the code prints out various arrays and lists that store the results of the analysis. Finally, the code also generates potential energy surface by taking results from these arrays.

**Execution of the code (Mo1-Mo22\_Nuc-Phase-Growth.ipynb):**

**Step 1**. Execute the section “Thermodynamics of main gaseous species”. Main gaseous species are: MoCO3, CO, H2S and H2.

Change “init = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/gaseous-species/"” path with the appropriate one

**Step 2**. Execute the “Main Code”

For example, the mechanistic pathway for the formation of Mo(SH)4, MoS4H2 and Mo3S8H4 (T3) cluster formation related data are kept inside “Mo1-Mo3” directory. The Gaussian output files are arranged with numerical values such as 5.log, 6.log, and so on. Invoke the main code by using the following command (for Figure 3 in the manuscript):

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo1-Mo3/" # change the path as per need**

**CVD\_process(initial,5,52,' Mo1-Mo3\_N')**

Similarly, execute the following command to extract data related to the cluster expansion process from Mo3S8H4 (T3) to Mo10S22 (T10) (for Figure 4 in the manuscript)

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo3-Mo10/" # change the path as per need**

**CVD\_process(initial,52,130,'N2')**

Execute the following command to extract data related to the cluster expansion process from Mo10S22 (T10) to Mo19S42 (T19) (for Figure 6c in the manuscript)

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo10-Mo19/" # change the path as per need**

**CVD\_process(initial,130,237,'N3')**

Execute the following command to extract data related to the T to H phase transition at Mo19S42 (for Figure 8 in the manuscript)

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo19\_T-H/" # change the path as per need**

**CVD\_process(initial,237,271,'TH')**

Execute the following command to extract data related to the population of the Szz edge vacancies by S atoms at the H phase of Mo19S42 (for Figure S7 in the supporting information)

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo19S42-Mo19S45/" # change the path as per need**

**CVD\_process(initial,271,300,'Mo19S42-45')**

Execute the following command to extract data related to the growth of Szz edge from Mo19S45 to Mo22S51 (for Figure 10 in the manuscript)

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo19-Mo22\_Szz/" # change the path as per need**

**CVD\_process(initial,300,334,'Szz')**

Execute the following command to extract data related to the growth of Mozz edge from Mo19S45 to Mo22S51 (for Figure 10 in the manuscript)

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo19-Mo22\_Mozz/" # change the path as per need**

**CVD\_process(initial,300,336,'Mozz')**

Execute the following command to extract data related to the cluster expansion process from Mo13S28 (T10) to Mo15S32 (T15) to compare triangular and hexagonal shaped clusters.

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo10-Mo19/" # change the path as per need**

**CVD\_process(initial,160,180,'Mo13-15')**

**initial = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Mo13-15\_tri/" # change the path as per need**

**CVD\_process(initial,160,185,'Mo13-15-t')**

**Step 3:** Execute the plotting function. For generation of plots provided in the manuscript, consider “Plotting PES from the genrated dataset at 1023.15 K” section.

Execute the following command to generate the plot of the mechanistic pathway for the formation of Mo(SH)4, MoS4H2 and Mo3S8H4 (T3) cluster formation (Figure 3 in the manuscript). Before that, please also execute “To add direct H2 removal path separately in the plot” section. Change “initial\_ts = "/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/direct\_H2-removal/"” path with the real one.

**import matplotlib.pyplot as plt**

**plotting(5, 52, ' Mo1-Mo3\_N ', -650, -100) #please consider line 110 to 142 from "Plotting PES from the genrated dataset at 1023.15" section K**

**plt.savefig('/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Fig/ Mo1-Mo3\_N.png', dpi=500) # change the path as per need**

Similarly, execute the following command to generate the plot for the cluster expansion process from Mo3S8H4 (T3) to Mo10S22 (T10) (Figure 4 in the manuscript)

**import matplotlib.pyplot as plt**

**plotting(52, 130, 'N2', -650, -100)**

**plt.savefig('/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Fig/N2.png', dpi=500) # change the path as per need**

Execute the following command to generate the plot for the cluster expansion from Mo10S22 (T10) to Mo19S42 (T19) (Figure 6c in the manuscript)

**import matplotlib.pyplot as plt**

**plotting(130, 237, 'N3', -1200, -500)**

**plt.savefig('/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/N3.png', dpi=500) # change the path as per need**

Execute the following command to generate the plot for T to H phase transition at Mo19S42 (Figure 8 in the manuscript)

**import matplotlib.pyplot as plt**

**plotting(237, 271, 'TH', -1200, -900)**

**plt.savefig('/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Fig/TH.png', dpi=500) # change the path as per need**

**Step 4**. Consider “Comparing Mozz and Szz edge growth” section to compare Szz and Mozz edge growth on the same plot by executing the following command (Figure 10 in the manuscript):

**plot\_reactions(300, 336, 300, 334, -1200, -900)**

**plt.savefig("/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Fig/Mozz-Szz\_edge-growth.jpg", dpi=500) # change the path as per need**

**Step 5**. Consider “Mo13-Mo15 hexagonal shape vs triangular shape” section to compare hexagonal vs triangular shape on the same plot by executing the following command (Figure S4 in the supporting information):

**plot\_reactions(160, 180, 160, 185, -900, -600)**

**plt.savefig("/home/chesagar/CVD\_sagar/reacion\_plotting/CVD-manuscript\_data/Fig/Mo13-15\_hex-tri.jpg", dpi=500) # change the path as per need**

**Execution of the code (Nucleation.ipynb): Execute all cells and change the directories as per need.**