**Running RMG Job Exercise –**

**CO2 hydrogenation on Ni(111)**

**Step 1: Open the input file**

1. The input species are CO2, H2
2. We want to investigate Ni(111) as the active site, which is defined by the following binding energies for the descriptor species:
   1. 'H':(-2.76, 'eV/molecule')
   2. 'C':(-6.45, 'eV/molecule')
   3. 'O':(-4.70, 'eV/molecule')
   4. Surface site density 3.16e-9 mol/cm2
3. The reaction library ‘Surface/Methane/Deutschmann\_Ni’ is loaded
4. Conditions for the mechanism generation
   1. T=673 K, p=1 bar
   2. Initial composition H2= 4 mol, CO2=1 mol
   3. Termination criterion: 90% CO2 conversion

**Step 1: Run the input file**

1. Open the terminal in the folder that contains the ‘input.py’ file.
2. Activate rmg\_env by typing the below line on your terminal

conda activate rmg\_env

1. Since you are already in the folder containing the input file, you can simply type the line below to run the RMG input file.

rmg.py input.py

The minimal example should take 2 minutes to finish. If it ran successfully, you should be able to see the following messages at the end (termination time will be different):

MODEL GENERATION COMPLETED

The final model core has 35 species and 255 reactions

The final model edge has 254 species and 865 reactions

RMG execution terminated at Mon Aug 8 18:27:42 2022

If the RMG simulation is taking too long, you can stop it by pressing ctrl + z.

**Step 2: Explore the output files**

If your RMG job ran successfully, you will see various output files in your folder like this. Let’s look at some of the results.

1. Open the folder “Solver” and look at the last produced image. What are the main products?
2. Open the output.html and output\_edge.html file. Explore the discovered species and reactions.

**Step 3: Modify the input file**

Now it’s your time to play around with the input file to see how the mechanism and the generation procedure changes.

1. Change the temperature by +100 or -100 K. How does this affect the speed of the generation? (Easy)
2. Move to a different metal by using the linear scaling relations. Ru is also a catalyst that is often used for hydrogenation reactions. Let’s build a mechanism for the Ru0001 surface (Ru is an hcp crystal). You can do this by uncommenting the block “catalystProperties” (add # in front of each line) or deleting the block. Add the following command instead:

catalystProperties(

metal = ‘Ru0001’

)