Running RMG Job Exercise – CO_2 hydrogenation on Ni(111)

Download the input.py file from GitHub
https://github.com/yunsiechung/RMG_workshop/tree/main/RMG_exercises

Step 1: Open the input file

1. The input species are CO_2, H_2
2. We want to investigate Ni(111) as the active site, which is defined by the following binding energies for the descriptor species:
    a. 'H':(-2.76, 'eV/molecule')
    b. 'C':(-6.45, 'eV/molecule')
    c. 'O':(-4.70, 'eV/molecule')
    d. Surface site density 3.16e-9 mol/cm^2
3. The reaction library 'Surface/Deutschmann_Ni' is loaded
4. Conditions for the mechanism generation
    a. T=673 K, p=1 bar
    b. Initial composition H_2= 4 mol, CO_2=1 mol
    c. Termination criterion: 90% CO_2 conversion

Step 1: Run the input file

5. Open the terminal in the folder that contains the '`input.py`' file.
6. Activate rmg_env by typing the below line on your terminal

```
conda activate rmg_env
```

7. 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 22 species and 39 reactions
The final model edge has 66 species and 162 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'
)
```