**WEEK 4 – Building hypothetical MOFs**

**Part 1. Installing ToBaCCo**

The Topologically Based Crystal Constructor (ToBaCCo), developed by Colón *et. al.*, [1] is a computational algorithm that generates MOFs taking into consideration edge-transitive topological nets for subsequent evaluation via molecular simulation.

[1] Cryst. Growth Des. 2017, 17, 5801-5810, DOI: 10.1021/acs.cgd.7b00848

1. Create a new conda environment just for ToBaCCo, with python 3.7

conda create --name my\_tobacco python=3.7

conda activate my\_tobacco

2. Install the dependencies we will need

conda install numpy

conda install networkx

conda install scipy

3. Uncompress the folder tobacco\_3.0-master.zip if not already uncompressed

**Part 2. Designing hypothetical MOFs**

1. On the folders “edges”, “nodes” and “templates”, keep the ones you want to use to construct your MOFs. Don’t keep a lot of files there, otherwise the script on step 2 will take forever to run. You can delete files in this folder, as it’s all in the folders “edges\_database”, “nodes\_database”, “templates\_database”. You can also copy specific files you want to use from the respective \*\_database folders into the “edges”, “nodes” and “templates”.

Questions:

1. What is it that’s referred to as “edges”, “nodes” and “templates”? You can visualize the .cif files with Avogadro to have a better understanding.
2. Can you tell in advance which templates are more common for MOFs? You can have a look at this paper: [**https://doi.org/10.1039/C4QI00236A**](https://doi.org/10.1039/C4QI00236A)

2. Now, on your terminal, make sure you are in the folder “tobacco\_3.0-master”

python tobacco.py

Note: if it’s taking too long, you can cancel it with ctrl+c after some MOFs have been constructed.

Questions:

1. Do you understand what the code is doing?
2. Take a look at what is being printed in the terminal: what kind of information can you get?

You can use several strategies to explore the building of MOFs: keep one template and one edge and many nodes; one node and one edge and many templates; and so on.

3. On the “output\_cifs” you will find the .cifs for the MOFs you constructed.

Questions:

1. How are they named?
2. Open some with Avogadro: do they look clean? You can check with mofchecker (just remember to activate the other environment: myproject).

**Part 3. Next steps…**

Now that you’ve built hypothetical MOFs, the next step is to perform an optimization of the structure, since the code (tobacco.py) itself cannot tell the configuration which minimizes the energy.

Optimizations can be done in different ways, and we will explore the ones that use force fields and DFT.

Before we do that, I would suggest you have a look on the following:

Density functional theory – a practical introduction (pdf in this week’s folder) – starting on page 73 (or 88 in the pdf)

<https://www.cp2k.org/howto:geometry_optimisation>

<https://docs.lammps.org/minimize.html>

You don’t need to do anything yet – just read a bit to get acquainted and ask questions if you have them.