**WEEK 3 – Geometric properties of pores**

After learning how to clean the structures, we will now learn how to perform a simple analysis of pore diameter in an organic framework.

**PART 1: Installing and compiling Zeo++**

1. Make sure you are in the environment you created for this project

conda activate myproject

2. Easy installation with conda

conda install -c conda-forge zeopp-lsmo

3. Compiling

Unzip the folder zeopp-lsmo and access it with

cd zeopp-lsmo

Now, since zeo++ is based on C++ language, we will need a library for algebra calculations called Eigen

wget https://gitlab.com/libeigen/eigen/-/archive/3.2.7/eigen-3.2.7.tar.bz2

tar xf eigen-3.2.7.tar.bz2 (you can also unzip using another software you have installed)

Check if you have a make compiler installed

make -h

If not, install it with

xcode-select --install (Mac)

For windows, if not available, check the file setup\_tutorial.pdf

Now, access the folder

cd voro++

And run

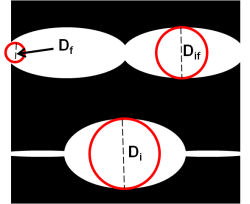
make

Do the same for the zeo++ folder

cd ../zeo++

make

**PART 2: Running zeo++ to get information about the pore diameter**



We can get information about pore diameter by running the following command on zeo++

./network -ha -res output\_file.res input\_structure.cif

To run this command, you need to be in the folder “zeo++” and have the input structure in this folder. Another way of doing this is just adding the path to your structure, for example:

./network -ha -res ../../structures/output\_file.res ../../structures/input\_structure.cif

In this example, I am in the “zeo++” folder and getting my structure from a “structures” folder that is in the same path as the “zeopp-lsmo” folder.

You should replace “input\_structure” with the name of your structure and the name you specify in “output\_file” will be the name of your out file.

Reading the out file, you can see that you have the name of your structure and three columns with values. They correspond to the largest included sphere (Di), the largest free sphere (Df) and the largest included sphere along free sphere path (Dif), respectively.

To get more information about what you can do with Zeo++, you can visit the page:

<http://zeoplusplus.org>

PART 3: Choosing our structures

Starting on week 5, we will run calculations on a selected structure. You can suggest MOFs and COFs you want to work with, they can be related to applications you are interested in. So for now you can think about structures that might interest you, keeping in mind that they should be:

* Relatively small regarding the total number of atoms we are working with (less than 200 atoms) – we will discuss this
* They shouldn’t have open shell metals (like Cu, Fe, Co) – we will discuss this