Week 1 – Introduction

Good morning, everyone. I’m Beatriz, nice to meet you all. I’m a 1st year PhD student in the group of prof. Berend Smit – Laboratory of Molecular Simulations (LSMO). I am one of the TAs of this course and I’ll be supervising one of the 4 projects, which I will present soon. Here is my email address where you can contact me if needed.

Just for a bit of background, I will tell you about LSMO. We are based in Sion. The ongoing research in the group is interdisciplinary, so it’s hard to define, but we can say that the common topic is Molecular Simulations. The group is mainly computational, which allows us to explore different topics since we don’t even need to change the computer for that. Such topics revolve around different applications of metal organic frameworks (MOFs) and covalent organic frameworks (COFs). For example, with different approaches such as molecular dynamics, density functional theory and machine learning, the group has been exploring the areas of carbon capture, photocatalytic hydrogen generation and materials design and discovery.

It is within this context that in this course we propose the following project: exploring the properties of MOFs and COFs. I know the name sounds broad, but hopefully in the end you’ll come to realize that so are the application possibilities of those materials. That being said, the main motivation for this project is to think over the following questions: why are those materials interesting?; and how can we use computers to assess their properties and retrieve chemical information?

In the end of the project the goal is to be able to analyze some of the electronic properties of the material and the geometric properties of its pores, in such a way that you can think about how MOFs and COFs can be explored from an application point of view.

The way to get there is getting familiarized with computational tools and programs to visualize and handle the materials structure, for example seeing the difference between experimental structure and a structure we can do computations with; and learning how to evaluate electronic properties using open-source software for quantum calculations.