WEEK 2: Visualizing experimental structures

1. (Check if they have conda installed) Download software (Avogadro and maybe VESTA and managecrystal?)

2. Talk – what is their background and what do they want to learn apart from what was proposed

3. Explain a bit about MOFs and COFs

4. Show them a paper and teach them how to get the cif file from the paper (or maybe just give them cif files)

5. Do one myself first (6-…)

6. Open cif file, get properties like cell parameters, volume… check what else we can get

7. Build a supercell

8. Maybe teach them to impose stackings for COFs?

9. Ask them if they can identify something that is wrong with the structure

10. Point it out myself – maybe a missing hydrogen

\*show them simple use of jupyter notebook

\*show them …

For the exercises:

1. structure1 - 1246903\_missing\_H
2. structure2 – missing\_h\_on\_c

3. structure3 – MOF-74-Zn

4. structure4 – ABAVIJ\_clean

5. structure5 – HKUST\_floating

6. structure6 – floating\_check