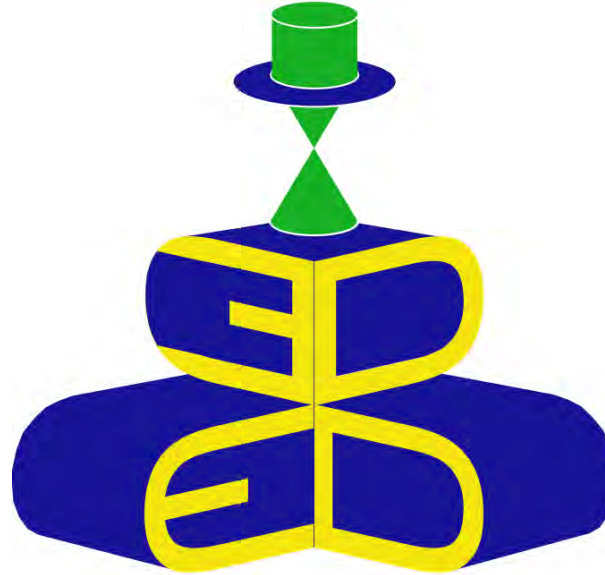




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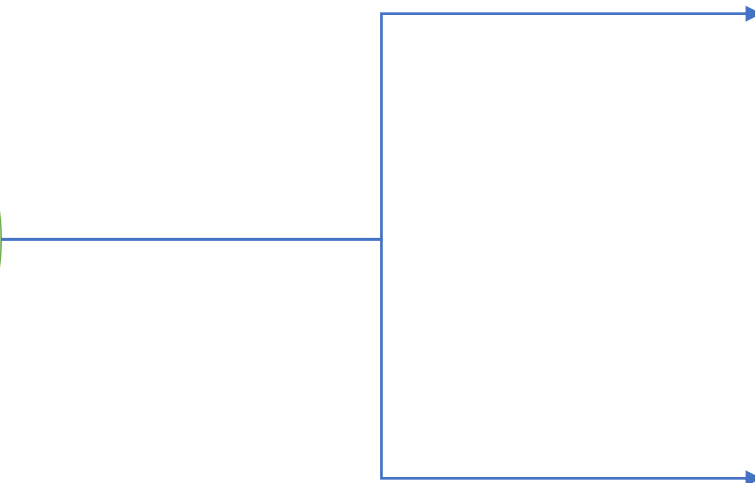
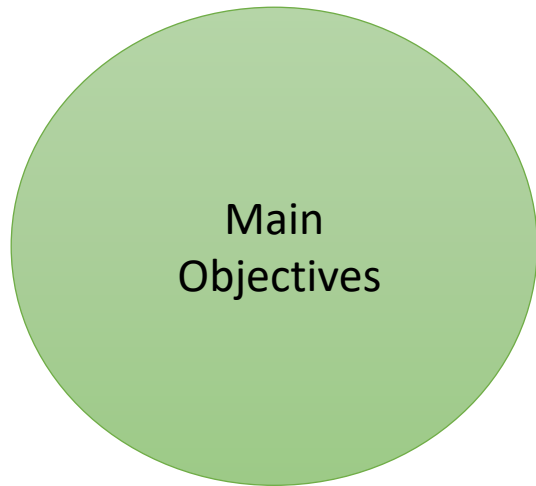


Nan ED

ESR 1:

Electron nanocrystallography of heterometallic MOFs





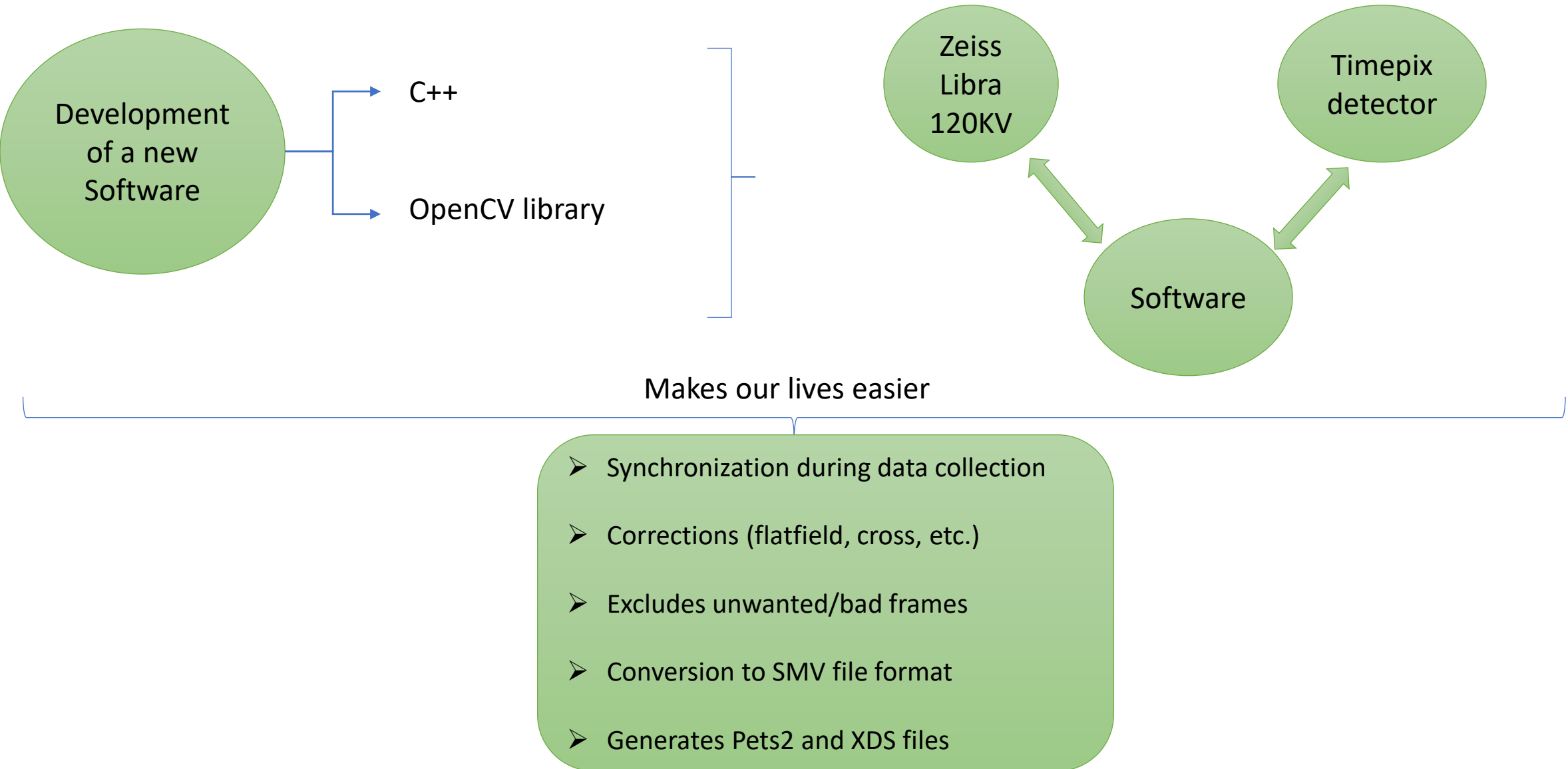
Design a protocol for characterization of beam sensitive porous materials

Structural characterization of new heterometallic MOFs



Design a protocol for characterization of beam sensitive porous materials

Making our lives easier



Design a protocol for characterization of beam sensitive porous materials

Crystal tracking

Pre-recording
crystal
movement

Take images every x degrees

Reproduce

Doesn't
always
work

- Movement is not always reproducible
- Tends to go to the center of the crystal (thick)



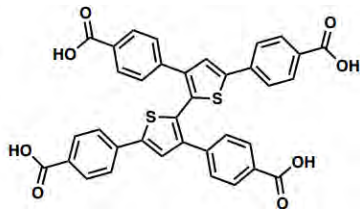
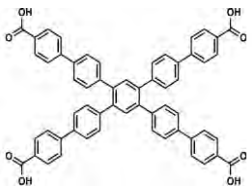
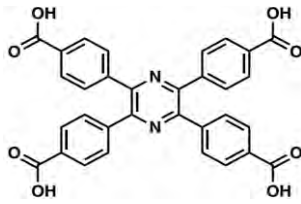
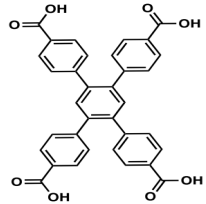
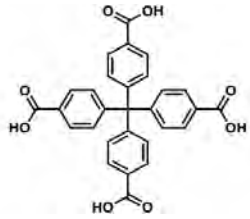
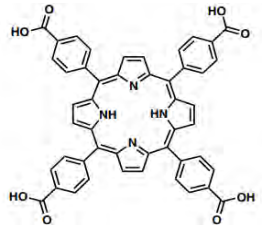
Structural
characterization of new
heterometallic MOFs



Structural characterization of new heterometallic MOFs



Dr. Carlos Martí-Gastaldo



Tetracarboxylated ligands

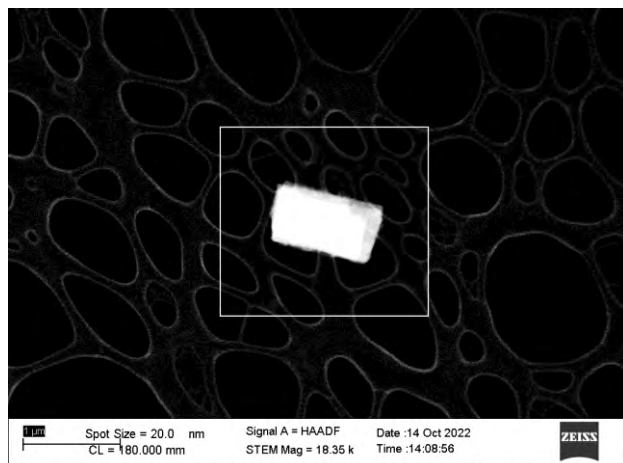
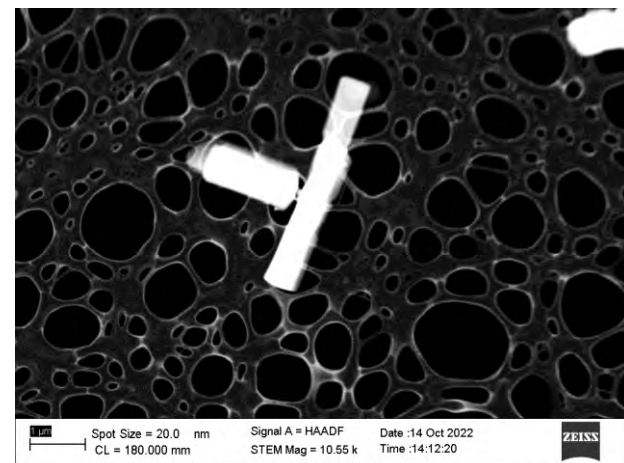
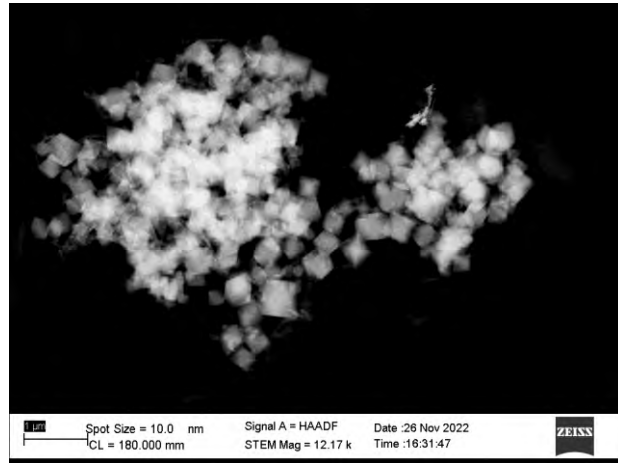
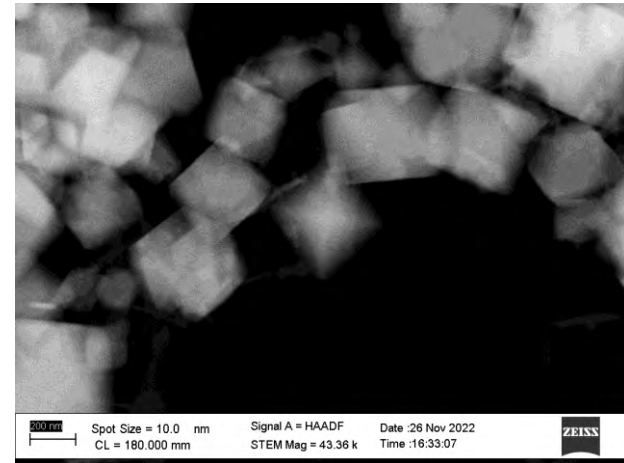
Form different networks with different topologies, using the same metallic cluster (Ca:Ti)



Structural characterization of new heterometallic MOFs



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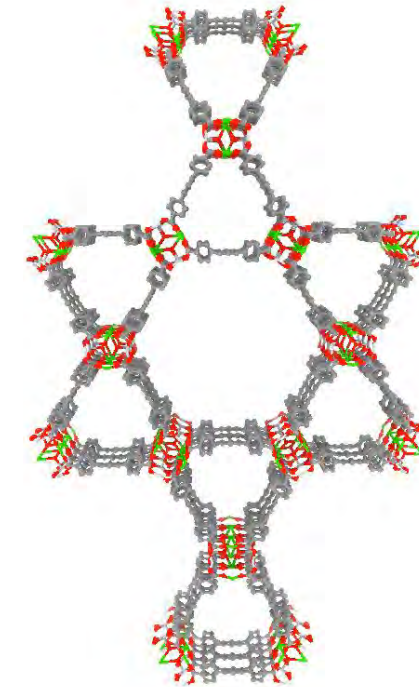
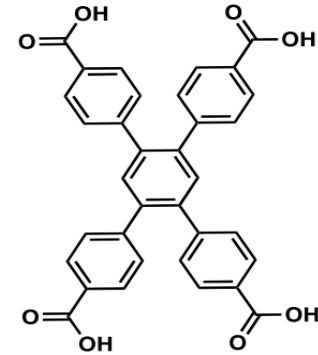
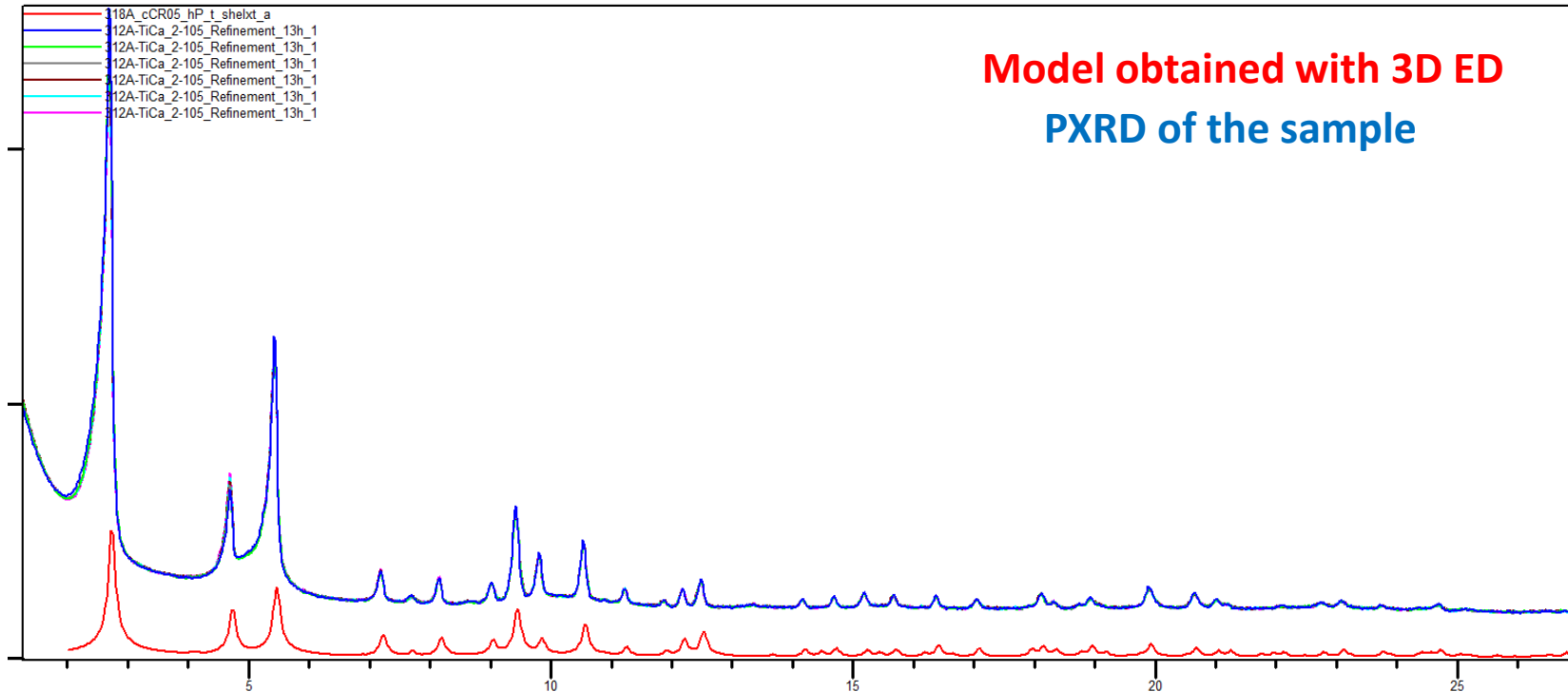
- Small crystals ~200nm – 300nm
- Continuous Rotation Electron Diffraction
- Data processed with XDS
- Data refined with ShelXL



Structural characterization of new heterometallic MOFs



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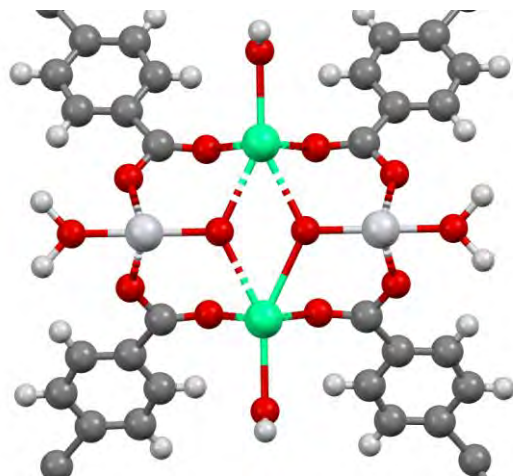
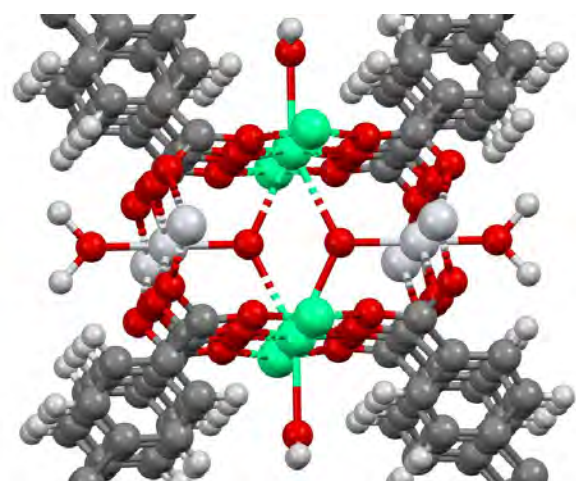
Bravais Class: **hP**

Space group: **P6/mmm**





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- Green = Calcium, coordinated to 7 Oxygens
- White, Titanium coordinated to 6 Oxygens
- Other MOFs with similar cluster geometry (Mn:Ti)



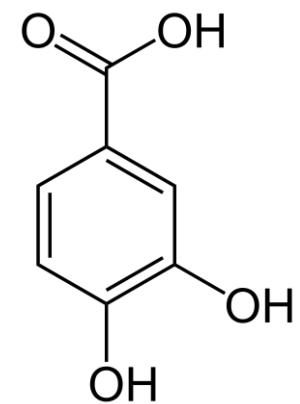
Structural characterization of new heterometallic MOFs



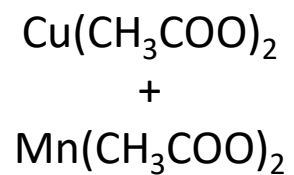
Dr. Andrea Sala



Danilo Marchetti



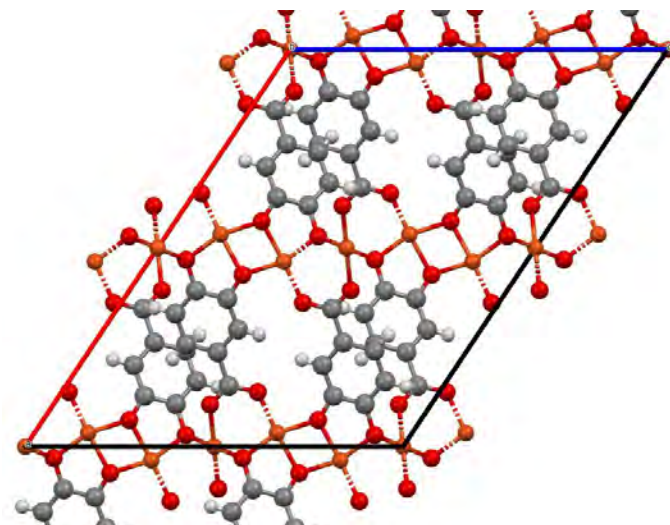
Protocatechuic acid



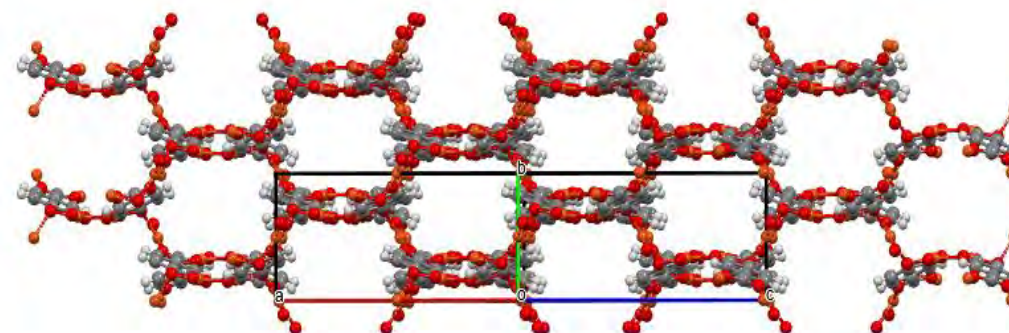
Mechanosynthesis



LAG (H₂O)



Only one metal site, monometallic



Bravais Class: **mC**

Space group: **c2/c**



Main difficulties
&
Future work



- Low resolution (1.3Å – 1.6Å) → Unmodelled molecules/solvents in the pores → High Rvalues
- Try refinement vs PXRD (Rietveld)
- Correct for elliptical distortions
- Different approaches for crystal tracking





Electron Crystallography Group



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Grant n. 956099





Thank you for your attention!

