



## 2020\_2021\_France\_Montpellier\_University of Montpellier\_Chemistry *Erasmus+ Internship Report*

My study program is MaMaSELF (Materials science using large scale facilities), a master program for students with backgrounds in chemistry, physics, or metallurgy who are interested in specializing in material sciences for energy applications. During my third exchange semester I took part in a research traineeship at the university of Montpellier in France. The traineeship was performed under the supervision of Prof. P. W and his team at the Charles Gerhart Institute (ICGM).

During this internship I worked on the project entitled : Structure and magnetism of transition metal oxides. The project focused on a specific structure type of perovskite oxide mineral called Brownmillerite. The perovskite class of compounds has a general formula of  $ABO_3$  (e.g.,  $CaTiO_3$ ) where the B cations are coordinated by six oxygens and are arranged with A cations in alternated layers .

The specificity of the Brownmillerite class is the deficiency in Oxygen atoms, the typical general formula is ABO<sub>2.5</sub>. These O-deficiencies induces changes in the B cation coordination, and we get two types : octahedra's and tetrahedron's and thus different valence states. This aspect is very interesting because it leads to a change of the structure's symmetry as a function of temperature. It also creates canals for oxygen to pass through which makes this class of materials of great interest for different kind of technological applications (e.g., oxygen superconducting effects, magnetism).

To study the ordering and disordering of the chains as a function of temperature, along with magnetic phase transitions in this non stochiometric oxides, I used different techniques: Powder X-ray diffraction technique PXRD for structure determination, Thermogravimetric Analysis TGA coupled with mass spectrometry to confirm the phase transition after 500°C. My main tasks were about structure analysis using the Rietveld refinement Process with Fullprof software. For X-ray refinements were the PXRD experiments data were used as for the Neutron Rietveld analysis I used data that was collected from D2B@ILL.



Fig. 1 Rietveld refinement performed on the neutron diffraction obtained from D2B@ILL for samples at room temperature a), and at 500°C c). the tetrahedral chains orientation when viewed along the b-axis in I2mb b), and in Imma d).

The hosting research group was very helpful and professional, regular discussions about phase transition problems and structure analysis were carried out. I recommend any future trainee to engage in discussions with mentors and post-doctoral who work in the same research group as they can provide helpful tips and information based on their experiences and previous works. My supervisor gave me many high-quality resources to learn about my research topic such as books, scientific articles that are related to this class of materials.

I learnt many things about oxide materials during this traineeship, but also how to investigate the phases problems and analyze compounds structures using sophisticated techniques like PXRD and Neutron diffraction and how to use software like Fullprof, Jana and vesta professionally to get the best results. I also improved my scientific language which I consider one the most assets I gained from this enriching experience.

This traineeship was organized while I was still in summer semester between my host institution represented by my supervisor Prof. P. W, the sending institution represented by Mrs. K. K coordinator of the MaMaSELF master at LMU university, and the Praktika services of LMU who were very fast and efficient during the process. This traineeship was financed by the Erasmus+ Traineeship grant.

I did not participate in the intercultural seminar nor a preparatory course of the French language since I already had an experience in France and that I also speak the French language perfectly. I highly recommend future students to take part in these kind of events as they prepare you to integrate the society smoothly and taking a language course since the French people speak no to less English in day-to-day life. Montpellier is seen as student's city in France so you will for sure find and should make friends who will most likely speak English and French.

The accommodation was arranged prior to my departure with CROUS hosing services of Montpellier University. It was easily done with the help of the supervisor who prepared everything with the CROUS. I was housed in a studio type room inside of the Triolet student residency located just In-front of the faculty of the sciences campus. Of course, other type of housing can be found, such as private housing but it is more expensive and takes more time to get the paperwork done. It can usually be found on websites like Leboncoin or even on dedicated Facebook pages but cautious is needed.

Transportation system in Montpellier is very good, I was using the tramway and the bus services, you can get the monthly TAM card for about 30 euro. This grants you the free usages of bus and all tram lines. To get to the city center the best way is via the tram line 1. You can also use the bike, either by buying it or loaning it from the TAM services. As for coming to Montpellier, the fastest way is by airplane, the best way is by train and the cheapest but longest trip is using the Bus like Flixbus.

One piece of advice since we do not live in a perfect world, be aware of pickpocket's thieves whenever you are in a crowed place or a tram station, especially in the city center stations (i.e., Gare saint-rock, comedy station, observatoire, and Occitanie).

I had a good experience in terms of social interactions whether it is inside of the hosting institution or outside. In Montpellier there are a lot of places to visit and many things to discovers, like museums beach, the historic city center, etc. During my spare time I was practicing sport (in my case judo). Practicing a sport activity is a very good way to interact with the natives and making friends easily. For this you can get a stamp from the university sport center called SUAPS. This allows to try and practice a wide range of sports and activities for free.



Fig. 2 City Center Comédie

I also was able to attend the 9<sup>th</sup> young researcher and chemists congress hosted in Montpellier from the 28<sup>th</sup> to 29<sup>th</sup> of October. This event was organized by the French Society of Chemistry and Doctoral School of Chemistry Sciences Ballard (ED SCB), during this event many PHD and post-doc students presented their work, and some of the famous chemists gave conferences about their hot topic research of the present.

This internship allowed me to use my knowledge in the fields of chemistry, physics, and materials sciences that I accumulated during my study cycles so far. It also allowed me to gain skills in X-ray and Neutron diffraction techniques along with the usage of refinements software's. I also developed many soft skills and critical thinking which will be of a great importance later in my scientific career. During this internship I found the area of research in which I intend to do a PHD studies. One of the biggest gains was the strong network that i formed with great scientists.

If I get the chance for another research mobility experience, I will certainly take it, and I highly recommend any student to do so. This experience was only possible because of the Erasmus + traineeship grant otherwise I would not have been able to enjoy my time during this internship and stay focused on my work and nothing else.

I would like to thank my supervisor Prof. P. W for organizing this project and for all his support and guidance the entire period and all his team of research from whom I learnt a lot of things. I also thank the coordinator Mrs. K.K in LMU and all the Praktika service who made this internship possible.