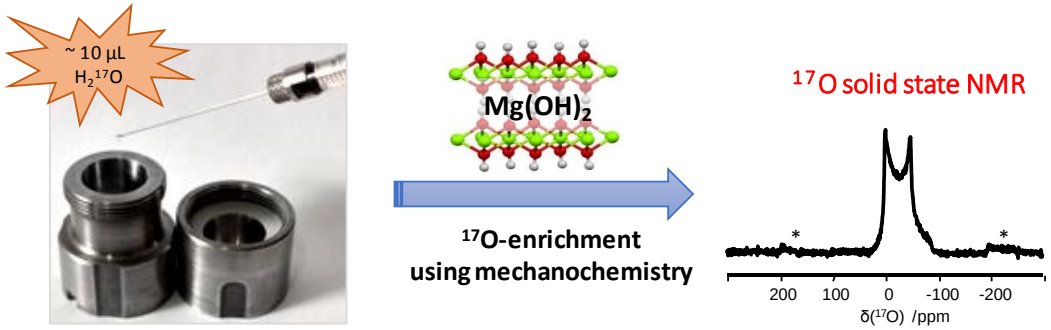
- Post-doctoral position -

"New approaches for ^{17}O solid state NMR spectroscopy"

Project :

Oxygen is everywhere: it is found in the vast majority of molecules and materials around us, whether they are natural or synthetic. Developing tools capable of analyzing precisely the local environment of this nucleus is thus essential to be able to understand the structure and reactivity of a large number of systems. In this context, Nuclear Magnetic Resonance (NMR) is a particularly powerful technique, which can provide detailed information about the local structure around oxygen. However, it is poorly sensitive and only occasionally used, mainly because the isotope which can be studied by NMR, oxygen-17, has a very poor natural abundance (0.04 %).

To counter the very poor sensitivity of oxygen-17 NMR spectroscopy, a CNRS research group in Montpellier (France), recently looked into new techniques for ^{17}O-isotopic labeling using mechanochemistry (https://doi.org/10.1002/anie.201702251). The advantage of this innovative approach is that it gives access to a much broader range of molecules and materials enriched in ^{17}O, thereby opening the way to structural investigations on a larger diversity of compounds, and to new developments in NMR spectroscopy.



In this context, a post-doctoral research position is currently available at the Institut Charles Gerhardt in Montpellier, on a 12 month contract (renewable) funded by a European ERC-CoG grant. The objective of the project is to implement analytical tools for the detailed study of a variety of materials enriched in ^{17}O using mechanochemistry, thanks to the development of novel solid state NMR experiments, and the use of combined experimental-computational approaches.

The work will consist in:

- NMR analyses of quadrupolar nuclei (mainly ^{17}O)
- Implementation of new ^{17}O…X heteronuclear correlation experiments
- *Ab initio* calculations of NMR parameters (GIPAW approach)
- Numerical simulations of NMR sequences (e.g. SIMPSON)
- Computational modeling of materials (molecular dynamics, DFT)
- Isotopic enrichment of inorganic and hybrid materials using mechanochemistry.

Requirements:

The candidate is expected to have a training in physical-chemistry or materials chemistry, and a PhD in solid state NMR. The knowledge of computational methods for solid state NMR and for the modeling of materials will be a definite asset.

More generally, the candidate needs to be highly motivated and capable of performing research in an autonomous and rigorous way. Given the multidisciplinarity and international-context of the project, the candidate is expected to have excellent team working skills and a very good level in English. He (she) will also be involved in the dissemination of the research, through publications and presentations at national and international conferences. Moreover, the selected candidate will participate to the supervision and NMR training of the undergraduate and graduate students involved in the project.

Host Ins titution / group:

The research will be performed at the Institut Charles Gerhardt (ICGM, UMR 5253) of the University of Montpellier (https://www.icgm.fr/). The ICGM is internationally recognised for its research in materials science, with an excellent environment for the synthesis and characterization of materials, notably by solid state NMR. The laboratory is equipped with 3 solid state NMR spectrometers (300, 400 and 600 MHz, all « wide bore »), and a very large range of MAS NMR probes (with rotor diameters between 1.2 and 9.5 mm), including one probe specifically for the development of high resolution ^{17}O NMR experiments.

The selected candidate will not only interact on a day-to-day basis with the team of researchers and students involved in the project (and more specifically with Drs Danielle Laurencin and Bruno Alonso), but also with scientists with whom the team has established collaborations, both nationally and internationally. Moreover, to gain in sensitivity and resolution, measurements at higher fields will be programmed, notably on the instruments of the French high-field NMR network.(IR-RMN - http://www.ir-rmn.fr/).

Application procedure:

The project is supported by the European Research Council (ERC consolidator program; MISOTOP project; PI: Danielle Laurencin). Funding for this post-doc position is available for 3 years, but the initial contract will be of 1 year (potentially renewable). The net monthly salary is between 2000 and 2900 euros, depending on experience.

For informal queries about the position and/or the project, please send an email to Danielle Laurencin (danielle.laurencin@umontpellier.fr) and Bruno Alonso (bruno.alonso@enscm.fr).

To formally apply for the position, please use the CNRS portal (http://bit.ly/2CxowBX); a CV, motivation letter, and the names of 2 references are requested.

Preferred starting date: April 15th, 2019