The Institut de Chimie Radicalaire of Aix-Marseille University a PostDoc opening for physical chemists.

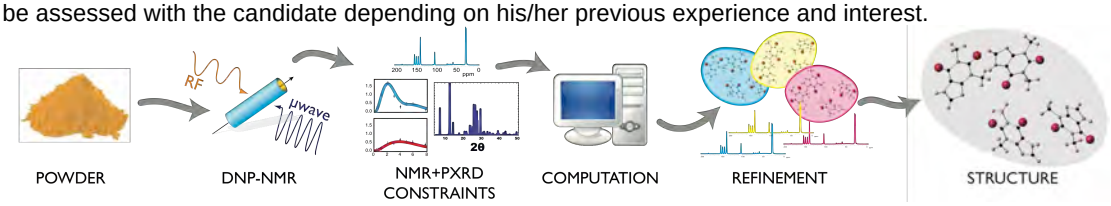
We are seeking motivated candidates to work on an exciting project for excellent research funded by the European Research Council (ERC). The project is aimed at the development and application of an emerging hyperpolarization technique, *high field MAS-DNP* (Magic Angle Spinning Dynamic Nuclear Polarization). This approach is used to increase the sensitivity of solid-state Nuclear Magnetic Resonance (SSNMR), enabling the extraction of unique structural information on solid materials at atomic length scale without the need for isotopic enrichment.

- Project description

The aim of the project is the development of a new experimental and computational approach to achieve *de novo* structural determination of organic molecular crystals used as functional materials in fields ranging from pharmaceutical science, to electronics and energy. These materials, essentially composed of small organic molecules, can assume different crystalline arrangements, a phenomenon known as polymorphism, whose physical origins are still not fully understood. Because different polymorphs of the same chemical compound can display radically different physico-chemical properties, polymorphism could constitute a precious opportunity to tailor the properties of the material for specific applications. The main limitation towards a complete understanding of structure-properties relationships comes from the experimental difficulty in accessing the structure of such materials with atomic-scale accuracy. In fact, because of the harsh manufacturing conditions typically employed for their preparation, in their end-use form these materials exist as powders, for which diffraction techniques are far from being the optimal choice, but remain the most popular option. The use of MAS-DNP is expected to have a significant impact in this field because it offers the advantages of SSNMR (atomic-scale resolution, no need for long-range structural order, noninvasiveness) without the usual sensitivity limitations.

In recent years very powerful computational approaches have been proposed that allow prediction of the structure of a material and, from this, its properties. Typically, when prediction methods are used for the generation of structural models, the candidate structures are ranked and then selected uniquely on the basis of their global lattice energy. However, energy accuracies can be insufficient to resolve polymorphs whose global lattice energies only differ by a few kJ/mol. For this reason, the quality of predicted crystal models is often assessed with the help of experimental - including NMR - data providing complementary structural information. However, until present, experimental data are only used to validate or reject structural model proposed by computational methods.

The postdoctoral researcher recruited on this project will work at combining the structural data obtained through MAS-DNP experiments with computational tools for crystal structure search with the aim of developing a new approach to crystal structure determination of organic powders. The level of his/her implication in the experimental acquisition of MAS-DNP data will be assessed with the candidate depending on his/her previous experience and interest.



- Host institution

Research in the framework of this project will be carried out at the *Institut de Chimie Radicalaire* (ICR UMR7273). Located in the south of France in Marseille, ICR is internationally recognized for its double expertise in i) the development of new DNP approaches for the characterization of organic solids and ii) the synthesis of radical species currently used as the most effective polarizing agents for solid DNP. Through the analytical facility Spectropole, ICR has access to a vast range of instrumentation for X-ray diffraction, mass spectrometry, IR, elemental analysis, as well as several NMR spectrometers for liquids and solids with fields ranging from 300 to 600 MHz. Notably, the candidate will access two 400 MHz wide-bore NMR spectrometers equipped with the latest hardware and numerous solid-state probes for spinning speeds up to 60 kHz. A MAS-DNP spectrometer is on its way and will be installed in Marseille in 2019.

The postdoctoral position will be funded for **1 year**, renewable depending on results.

- Candidate profiles

Candidates should have strong skills in mathematics/physics or computational chemistry. Previous experience with the use of software for DFT calculations and crystal structure prediction will be a plus. This work will be supported by collaboration with theoretical chemists at the University of Oxford.

- Application procedure

CNRS has the label HR Excellence for research (HRS4R) and promotes transparency of the recruitment process and equal opportunities.

The candidate should send a motivation letter, at least two names for recommendation, CV (with list of publications and communications) to:

Dr. Giulia Mollica,
CNRS researcher

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