



PhD fellowship funded by the European Research Council

Project title: "New methods in nuclear magnetic resonance for the structural analysis of functional materials at natural isotopic abundance" (M/W)

A 3-year PhD contract funded by the European Research Council ([ERC](#)) is available at the CNRS / Aix-Marseille University for the development of a new method for the characterization of functional materials. This PhD thesis will be carried out in an international environment and will benefit from privileged access to advanced equipment for hyperpolarized nuclear magnetic resonance.

Background: Functional organic materials have been successfully used as active components in many applications ranging from light emitters to optical devices, flexible photovoltaic devices, printed electronic inks, molecular machines, pigments, pharmaceuticals, and so on. These are lightweight, easy-to-manufacture materials that can replace traditional inorganic functional materials in energy-related applications (for example, as semiconductors in solar cells or light-emitting diodes), with significant economic and practical benefits. In order to obtain new functional materials for targeted applications, the real challenge is the ability to establish a clear relationship between the structure and properties of the material. At present, the main limitation to the rational development of new functional materials is the absence of a method capable of fully and unambiguously characterizing their structure at an atomic level.

Aim and description: Research carried out in the framework of this PhD contract focuses on the design of new analytical approaches based on nuclear magnetic resonance (NMR) coupled with nuclear dynamic polarization (DNP) to access the structure of functional materials with applications in energy or in pharmacy. In-between chemistry and physics, the work will combine the design of new NMR experiments with the use of computational methods (e.g. based on density functional theory). To realize this challenging project, the candidate will benefit from a stimulating scientific framework, as well as from the access to state-of-the-art MAS DNP equipment that will be fully operational in our laboratory by September 2019. More specifically, the selected candidate will:

- develop new approaches for studying functional materials via hyperpolarized NMR (DNP NMR)
- use *ab-initio* methods for calculating NMR properties (e.g. CASTEP)
- perform analytical simulations (Mathematica, MatLab) or numerical simulations (SIMPSON) to assist the interpretation of experimental data.

The computational work will be supported by collaborations with theoretical chemists in France and abroad (Oxford University).

Location: The thesis project will be carried out within the Institute of Radical Chemistry ([ICR UMR7273](#)), a joint research unit between Aix-Marseille University and the CNRS¹. 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 efficient polarizing agents for the analysis of solid materials by DNP. Our laboratory also has access to a wide range of supercomputers and instruments for materials analysis, e.g. X-ray diffraction, mass spectrometry, IR, elemental analysis, as well as several NMR spectrometers for liquid and solid analysis with magnetic fields ranging from 300 to 600 MHz. In particular, the candidate will have access to a new 400 MHz Bruker solid state DNP NMR spectrometer, which will be installed in the laboratory in September 2019, as well as to a second solid-state NMR spectrometer equipped with a state-of-the-art console and many probes for sample spinning speeds up to 60 kHz.

The thesis will be funded by the European Research Council (ERC) for a period of 3 years, starting in September / October 2019 and will be supervised by Dr. G. Mollica. In the framework of ongoing collaborations, the candidate will be in contact with researchers from other European groups. He / she will be part of the ED 250 doctoral school of Aix-Marseille University. **Net salary:** ~1700 €/month.

Candidate profile: Candidates must have a background in chemistry or physics. Previous experience with NMR spectroscopy and / or computational methods is an advantage. Knowledge of crystallization procedures will also be an asset. Candidates will have to prove motivation, imagination and independence, with an interest in understanding the fundamental aspects of NMR and polymorphism. He / she will have excellent communication skills in English to disseminate the results of his / her work in international journals and conferences.

Application procedure: Applicants must send:

- cover letter
- CV (with names of one or two references)
- Master's grades (with ranking)

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

¹ The Centre National de la Recherche Scientifique ([CNRS](#)) is among the world's leading research institutions.