# Postdoctoral fellowship in parahydrogen NMR for the study of hydrogen storage

Laboratoire de Chimie de Coordination - CNRS UPR 8241
205 route de Narbonne, 31077 TOULOUSE Cedex 4 – France

Type of offer: Post-doctoral fellow 12 months
Financing: "Green Hydrogen Key Challenge", RHYO research cluster
Salary: determined upon experience (roughly between 2800 and 4000 € per month)
Position immediately available, to be filled before end 2023
Deadline for application is 1st May 2023

## Missions

A postdoctoral position is available in the field of nuclear magnetic resonance spectroscopy (NMR), in the following specific topic: Development of parahydrogen-NMR hyperpolarization techniques for studying storage of H2 in liquid or solid-state.

The storage of hydrogen ($H_2$) in organic liquids or solids is an alternative to compressed $H_2$ storage at high pressure. The need to know the mechanisms that allow storage within these materials is important in order to create new materials with the necessary properties to store and release $H_2$ efficiently. The objective of the project is to explore use of parahydrogen induced polarisation (PHIP) NMR based protocols as potential characterization technique of chemical reactions associated with hydrogen storage. The PHIP effect that significantly increase NMR sensitivity can allow the detection of very low concentration or short-lived products, including reaction intermediates, and therefore has many applications in monitoring hydrogenation reactions and elucidating reaction mechanisms.

## Activities

The research associate will have particular responsibility for the development of parahydrogen hyperpolarisation experiments for high-field NMR, focusing on the design and implementation of novel NMR methods and data analysis strategies as well as instrumentation development. This position would suit a candidate with experience in magnetic resonance research, particularly in the development of NMR instrumentation and methods. Experience in parahydrogen hyperpolarisation methods is highly desirable. We believe that, NMR spectroscopy can provide an in-depth physico-chemical characterisation of hydrogene storage mechanism and will become a valuable technique in this research field.

Your tasks are:

- Installation and optimization of an in-house system for the production of 50% enriched para-H2 under pressure (50 bar).
- The development of systems for transferring para-H2 under pressure to the samples to be studied in situ inside the NMR spectrometers.
- The development of specific NMR experiments for the study of hyperpolarised molecules.

- The application of this technology to the study of chemical reactions involved in hydrogen storage in the liquid and solid state.

## Expected skills

The successful applicant must have a completed PhD in physics, chemistry, materials science, or a related field. Significant experience in experimental NMR spectroscopy are to be documented for this position. Strong skills in parahydrogen hyperpolarisation methods are valuable to the project. The postdoc will be part of a NMR facility implying that in addition to proven individual scientific excellence a collaborative mindset and good skills in English is required. The candidate should be independent, creative, and dependable.

## Context of the work

You will be appointed as a postdoctoral researcher at the Laboratory of Coordination Chemistry (LCC, UPR8241) in Toulouse. LCC is a CNRS research center whose research areas are: Chemistry and catalysis, Chemistry and materials and Chemistry and health. The project will be carried out under the supervision of Dr Yannick Coppel, manager of the NMR facility within the context of a broader project involving researchers at the University of Toulouse and external partners.

The facility covers complementary research activities in the area of liquid-state NMR and solid-state NMR. It is equipped with 6 NMR spectrometers operating from 600 MHz to 300 MHz suited for an unusually broad variety of studies (wide range of nuclei, gas/liquid/solid…). In addition, the facility is part of the "RMN midi-pyrénées" network allowing access to complementary NMR spectrometers ranging from 300 to 800 MHz. We develop experimental, methods based on NMR spectroscopy and apply those methods to topical problems in molecular and materials sciences. Our particular strength is in the tight connection between state-of-the-art measurements and applications.

For information about our laboratory, activities is available here: https://www.lcc-toulouse.fr/

## Formalities and salary range

Salary depends on seniority as agreed by CNRS. The salary is thus in practice roughly between 2800 and 4000 € per month, depending on the appointee's qualifications, experience and the progress in the research. The length of the position is one year.

## Application Procedure

The candidate must apply via the site https://emploi.cnrs.fr (https://emploi.cnrs.fr/Offres/CDD/UPR8241-YANCOP-001/Default.aspx).

At the same time, he/she should contact Yannick Coppel (yannick.coppel@lcc-toulouse.fr) and send a CV including publications, cover letter with statement of future research plans

Applicants seeking further information are invited to contact Yannick Coppel