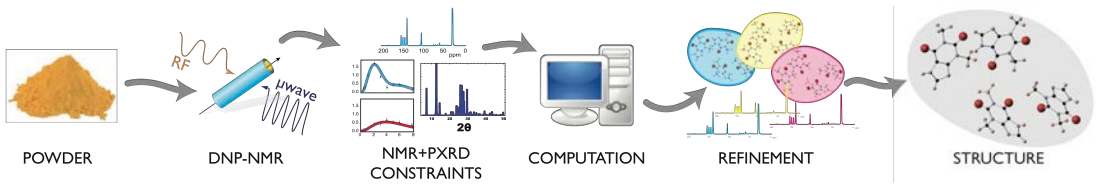
ERC-funded PhD position on the structural investigation of functional organic materials by DNP and NMR

Project title: "Structural investigation of polymorphic organic powders at natural isotopic abundance"

A 3-year PhD position is available at the CNRS/University of Aix-Marseille on the development of new experimental and theoretical approaches in dynamic nuclear polarization (DNP) NMR for the structural investigation of functional organic powders at natural isotopic abundance.

Context: Functional organic materials have been successfully used as active components in many applications, going from light emitters to optical devices, flexible photovoltaic devices, printed electronic inks, molecular machines, pigments, pharmaceuticals, etc. Such compounds can be used to produce low-cost, easily manufacturable, and lightweight materials that can replace traditional inorganic functional materials in energy-related applications (*e.g.* as semiconductors in solar cells or light emitter diodes), bringing significant economic and practical benefits. Moreover, they can be easily chemically modified to respond to specific application requirements (*e.g.* as active principle ingredients in pharmacy). In view of obtaining new functional materials with tailored properties, the true challenge in this field is the ability to establish a clear two-way relationship between the structure and the properties of the functional material in its end-use solid form. Because, in their end-use form, materials for the mentioned applications generally form particles with nanometer to micrometer-size dimensions, the main actual limitation to the rational development of new functional materials is the lack of a widely applicable methodology able to characterize fully and unambiguously the structure of functional organic powders lacking long-range order.

Aim and job description: The aim of the thesis is to devise new analytical routes for accessing "*ab initio*" the structure of polymorphic organic microcrystalline powders at natural isotopic abundance through a combination of DNP NMR experiments and computational methods. The selected candidate will actively develop and optimize new NMR experiments for accessing dipolar and scalar couplings on functional materials for energy or pharmaceutical applications at natural isotopic abundance. The candidate will also use first principle calculations of NMR observables (in collaboration with the University of Oxford), as well as analytical (Mathematica, MatLab) or numerical (SIMPSON) simulations to help interpretation of experimental data.



Details: The PhD project will be performed 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.

The PhD studentship will be funded by a European contract (ERC Starting grant, STRUCTURE project, G. Mollica) for a duration of **3 years**, starting **October 1st 2018**. In the framework of ongoing collaborations, the candidate will be in contact with researchers from other European groups. He/she is expected to communicate the results of his/her work at international conferences.

Candidate profile: The candidate should have a Master degree in Chemistry or Physics. Previous experience in NMR spectroscopy and/or computational methods is an advantage. Skills in organic chemistry are not required, but experience with crystallization procedures will be a plus. He/she is expected to be a motivated, imaginative, independent hard worker, with an interest in understanding fundamental aspects of NMR and polymorphism. He/she should have no issues with mobility and demonstrate excellent communication skills in English (knowledge of French is not required).

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

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