DRF: Thesis SL-DRF-17-0314

RESEARCH FIELD

Ultra-divided matter, Physical sciences for materials / Physique de l'état condensé, chimie et nanosciences

TITLE

Advanced atomic-scale structural characterization of functional materials

ABSTRACT

INAC (Institute for Nanoscience and Cryogenics, CEA Grenoble) has a PhD opening for a physicist/chemist. This position will deal with the development and implementation of an emerging and powerful atomic-level characterization technique, namely high magnetic field Dynamic Nuclear Polarization (DNP), thus bridging fundamental and application-driven research. DNP is used to hyperpolarize nuclei such that high sensitivity can be attained for solid-state NMR (Nuclear Magnetic Resonance) experiments, allowing the extraction of important structural information, such as surface functionalization and internuclear distances, as well as crystallographic data.

Since the potential of this technique is only just beginning to be realized, and mainly for organic-based systems, the aim of this PhD will be to further develop the methodology and apply it to characterize functional (nano)materials of significant importance for both CEA as well as external collaborators/industry, which could not have been otherwise investigated in such a manner. The studied materials will arise from diverse but related fields including fuel cells (CEA/INAC), photovoltaics (CEA/INAC + external), hybrid organic/inorganic polymers (CEA/LETI + industry), and functionalized nanoparticles (CEA/LITEN).

This PhD will take place in the highly dynamical environment of the MINATEC campus (CEA Grenoble) and more specifically in the nanocharacterization platform (PFNC) where the DNP group, in collaboration with Bruker Biospin (world leader in DNP and NMR instrumentation), is currently pushing the development and use of DNP far beyond its current state-of-the-art. The group is working with the first high-field DNP system installed in France (since September 2011) and has successfully conducted theoretical, methodological, and instrumental developments over the last 5 years.

The work of the PhD candidate represents an interdisciplinary project that will involve:

- mastering sample preparation for DNP of the various systems under investigation (30 %)

- performing spin-dynamics simulations to improve NMR methodology (20 %)

- conducting advanced solid-state MAS-DNP experiments (50 %)

The PhD candidate will thus attain an understanding of quantum mechanics for the spin dynamics at stake in MAS-DNP experiments and for the development and implementation of innovative pulse sequences. A sound knowledge of chemistry and materials science will also be acquired as commanding DNP sample preparation and data interpretation will be paramount to the success of the project.

LOCATION

Institut nanosciences et cryogénie
Modélisation et Exploration des Matériaux

Laboratoire de Résonance Magnétique
Place: Grenoble
Start date of the thesis: 01/09/2017

CONTACT PERSON

Daniel LEE
CEA
DRF/INAC/MEM/RM
INAC/MEM/RM
CEA Grenoble
17 rue des Martyrs
38054 Grenoble cedex 9
Phone number: +33 4 38 78 65 84
Email: daniel.lee@cea.fr

UNIVERSITY / GRADUATE SCHOOL

Université Grenoble Alpes
Chimie et Sciences du Vivant (EDCSV)

FIND OUT MORE

http://inac.cea.fr/Pisp/daniel.lee/
http://inac.cea.fr/en/Phocea/Vie_des_labos/Ast/ast_visu.php?id_ast=1111

THESIS SUPERVISOR

Gaël DE PAEPE
CEA
DRF/INAC/MEM/RM
INAC/MEM/RM
CEA Grenoble
17 rue des Martyrs
38054 Grenoble cedex 9