

PostDoctoral position at the CEA Saclay / LSDRM in Tritium Solid State NMR and DFT-Molecular Modeling

One postdoctoral position is available in the LSDRM group (<http://iramis.cea.fr/nimbe/lsdrm/>) at CEA Saclay (20 km south-west of Paris) on a project funded by a French national agency ANR (http://www.agence-nationale-recherche.fr/projet-anr/?tx_lwmsuivibilan_pi2%5BCODE%5D=ANR-15-CE32-0015)

We are currently seeking a motivated postdoctoral fellow to work on the methodology development based on Solid State NMR, Molecular Dynamics and DFT-computation of NMR shifts to investigate the structural conformation of small molecules in self-assembled nanotubes. The project focuses on diphenylalanine (PhePhe) and aims at first to validate new concepts based on long-range distance measurements using ^3H MAS NMR (see <https://pubs.acs.org/doi/abs/10.1021/ja908915v>). ^3H is a radioactive isotope of ^1H but possess the highest gyromagnetic ratio among the NMR-active nuclei (532 MHz at 11.75T); therefore, ^3H can be used in high dilution to form ideal spin pairs. The low radiation from ^3H permits 'safe' application in MAS NMR experiments by using the tightly sealed inserts in standard MAS NMR probe (sample are prepared in dedicated installations in CEA Saclay). A 500WB DOTY 3H/1H/X XC4 MAS NMR probe is available for these non-standard experiments which has been now routinely performed in our lab. For improving the NMR performance, we are currently acquiring a new probe 3H/1H with optimized 1H decoupling, the recruited postdoctoral fellow will develop and optimize NMR experiments for 3H-3H distance measurements. The 3H-results will be complemented by conventional ^{13}C and ^{15}N NMR experiments from the corresponding labelled samples. In addition to NMR experiments, MD simulations and computations of NMR shifts (DFT-GIPAW and Machine Learning methods) will be carried out to assist in the data interpretation, including the determination of the molecular conformation within the nanotubes.

Applicants are expected to have a PhD degree in Physical Chemistry or Physics, and a strong experience in solid-state NMR experiments. Knowledge in computational methods for NMR is a clear asset.

The postdoctoral fellow will mainly work with Thibault Charpentier (<http://www.researcherid.com/rid/A-3557-2010>) and Yves Boulard (<https://www.i2bc.paris-saclay.fr/spip.php?article180>). The successful candidate will be recruited for 12 months. The net monthly salary will be between 2000 and 2500 €, depending on experience.

Preferred starting date: March 2019 (3 months are required for an administrative clearance in CEA).

For queries about the position and/or the lab, please send an email to Thibault Charpentier (Thibault.charpentier@cea.fr)