



Postdoctoral position available in solid state NMR spectroscopy and DFT modeling

The joint CEMHTI (CNRS, Orléans) - IMPMC (Sorbonne Université, Paris) team is recruiting a full-time Post-Doctoral research associate in the context of the MeLiCa ANR project. The contract is managed by Sorbonne Université and runs for 24 months with remuneration depending on the experience.

The project has been designed to explore the mechanisms controlling the incorporation and isotope fractionation of Li in calcite and aragonite. It is centered on the comprehension of the Li chemical and isotopic effects associated with the coprecipitation of Li in carbonates in the cases of Li sorption and Li inorganic precipitation with the most common CaCO_3 minerals calcite and aragonite by coupling the state-of-the-art concepts and tools in experimental and computational chemistry, Li isotope measurements and NMR spectroscopy.

The Post-Doctoral research associate will be in charge of the high-resolution solid-state ^7Li MAS NMR measurements of synthetic and natural Li-bearing calcium carbonate samples prepared by the project partners. The experiments will be conducted on a Bruker AVANCE III 850 MHz-20T (one of the highest magnetic fields in France) spectrometer in Orléans. Different acquisition conditions will be tested to discriminate the various Li local environments. In parallel, the Post-Doctoral research associate will investigate theoretical models of Li-bearing CaCO_3 accounting for different local environments of Li at the atomic scale. The structure and NMR spectroscopic properties of these different models will be determined within the density functional theory framework and compared with the new experimental data. Dissemination of the findings through publications in leading international journals and presentations at international scientific conferences is anticipated.

The successful candidate should hold a PhD in Chemistry, Physics or Material Sciences or closely related fields and should have experience in solid-state NMR spectroscopy. Experience with the use of plane-wave/pseudopotential DFT codes is a plus. Writing skills in English are important.

The experimental NMR part of the work will be performed at the high temperature site of CEMHTI in the MatRMag team of CEMHTI in Orléans (<https://www.cemhti.cnrs-orleans.fr>) under V. Montouillout direction. The CEMHTI is a CNRS research unit located on two nearby sites (High Temperature and Cyclotron) in Orléans, with about 110 people. The laboratory develops expertise and original tools on the national and international level to study in situ the physicochemical properties of materials under extreme conditions.

The modeling part will be conducted in the Environmental Mineralogy team of IMPMC (Sorbonne Université - CNRS - MNHN) (<http://impmc.sorbonne-universite.fr/fr/index.html>) in Paris under the direction of E. Balan in collaboration with J. Aupart. The IMPMC (Institut de Minéralogie, Physique des Matériaux et Cosmochimie) is a joint Sorbonne Université - CNRS - MNHN unit in Paris which develops inter-disciplinary experimental and theoretical approaches in condensed matter physics, Earth and environmental sciences and biology.

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To submit applications, the candidate should send a CV, a list of publications, and the names and e-mail addresses of potential referees to Etienne.Balan@sorbonne-universite.fr and valerie.montouillout@cnrs-orleans.fr.

The closing date for the receipt of applications is 02/04/2023, but delayed submissions may be considered until the position is filled. The intended start is in June 2023.