ÉCOLE Normale Supérieure De Lyon

18 months Post-Doc position

Postdoctoral Research Assistant in DFT-based Geochemical Modeling

Context

As part of the European Research Council (ERC) Advanced Grant project DEEP-SEE, the Theoretical Chemistry and Molecular Thermodynamics axis of the "Laboratoire de Chimie" at the Ecole Normale Supérieure in Lyon (ENSL) seeks to appoint a full-time Postdoctoral Research Assistant (PDRA) to model the enrichment processes of rare earth elements (REE) in bioapatites (nominally Ca₅(PO₄)₃(OH,F,CI)) from marine deposits.

Background

REE are essential to modern life, yet we know little about how they concentrate at the Earth's surface, especially on the seafloor, which holds vast reserves. For example, Japanese researchers discovered recently a REE deposit that can supply the world for centuries. REE are concentrated in fossilized fish bones by post-mortem uptake from pore-waters all over the pelagic sediments of the global ocean. The DEEP-SEE project aims to elucidate geochemical processes that lead to the economic enrichments of REE through the characterization of their crystal chemistry using X-ray emission spectroscopy and the modeling of their incorporation mechanisms using computational chemistry.

Project

The PDRA will be office-based at the ENSL under the supervision of Dr. Stephan Steinmann, and will report to Dr. Alain Manceau, Principal Investigator of DEEP-SEE. Spectroscopic measurements will be performed at the European Synchrotron Radiation Facility (ESRF) in Grenoble by Alain Manceau and his colleagues, including an ERC-funded PDRA specializing in spectroscopy. While this position focuses on the modeling aspect of the DEEP-SEE project, close collaboration with the ESRF-based team and some travelling to Grenoble to attend meetings is anticipated. It is also anticipated that the PDRA will disseminate findings through publications in leading international journals and present the work at international scientific conferences and stakeholder events.

Applicant

The successful candidate should hold a PhD in Chemistry, Geosciences or closely related fields and should have knowledge of the fundamental processes that govern chemical reactions at the solid-water interface. Experience in combining process-based understanding with numerical/computational skills is essential. Experience with VASP, CP2K and/or Orca is a plus. Writing skills and proficiency in English are important.

The contract runs for 18 months, renewable for a further 6 or 18-months period, pending satisfactory progress. The salary depends on the experience of the PDRA, starting at a net salary of 2000 €/month for young graduates.

Workplace

The Theoretical Chemistry and Molecular Thermodynamics group benefits from the international recognition in the field of theoretical modeling of heterogeneous catalysis as well as processes at the





solid/liquid interface in general. Students from all-over the world have been or are part of the team, where English is the main language of scientific discussions. In addition, the team benefits from the international context of ENS Lyon, which welcomes hundreds of students each year. Lyon's listing by UNESCO as a World Heritage Site gives recognition to the long history heritage of the city. It is also recognized for its gastronomy and, last but not least, Lyon is a vivid city with thousands of students.

How to apply

Informal enquiries can be made to Dr. Stephan Steinmann.

To submit applications, please send your CV, list of publications, and names of potential referees to <u>stephan.steinmann@ens-lyon.fr</u> and <u>alain.manceau@ens-lyon.fr</u>

The closing date for the receipt of applications is 13/01/2023, but delayed submissions may be considered until the position is filled. The intended start-date is 1st April 2023.



