Solid-State NMR, Paramagnetic NMR and First-Principles Calculations on Rare Earth Element Complexes

The NMR Research Unit of the University of Oulu, Finland, in collaboration with Chemistry of Interfaces research group at Luleå University of Technology (LTU), Sweden, are looking for a PhD student within the research subjects Molecular and Materials Physics (UO) and Chemistry of Interfaces (LTU).

Project description

In 2010, European Raw Material Initiative placed Rare Earth Elements (REE) on the list of leading strategic metals, since they have a wide range of important high-technology applications in materials engineering and the demand for REE is increasing globally with the development of green technologies. Currently, it is a challenging task to extract, concentrate and separate REE, because they are usually spread at low quantities in different minerals and have very similar physico-chemical properties. Present processing methods involve many extraction and separation steps, which use toxic solvents and reagents having a large negative impact on human health and the environment. Another challenge is that most of REE are paramagnetic, which makes calculations and experimental studies of REE -complexes challenging.

The proposed project will combine solid-state Nuclear Magnetic Resonance (ssNMR) and paramagnetic NMR (pNMR) spectroscopies and first-principles quantum-mechanical calculations to obtain detailed information on REE complexes with commonly used flotation collectors, as well as with anionic ligands from novel ionic liquids, recently developed at LTU. The NMR Research Unit at UO has recently developed novel methodology for calculating pNMR parameters. Validation of the new methods is currently in progress with success at both UO and LTU. Using the chemical shift predictions facilitated by theory, we will further study how different ligands interact with mineral surfaces and leach REE. Hyperpolarization NMR techniques will be used to enhance NMR signals from surface-adsorbed species. The outcome will be useful for development of novel greener technologies for the extraction, concentration and separation of REE.

The project has importance for mining industries (in Finland and Sweden) and is adjoined to another project on REE co-funded by the Centre of Advanced Mining and Metallurgy (CAMM) at LTU.

The theoretical calculations will mainly take place in Oulu, while the experimental (synthesis, liquid and ssNMR and hyperpolarisation NMR) work will be performed both in Oulu and in Luleå and the student is expected to spend approximately half the time (two + two years, *i.e.*, four years in total) at each university.

The student is expected to take part in teaching activities at the two institutions. The student will be awarded with both a Swedish and a Finnish doctoral degree.

Qualifications

The PhD student positions belong to I4Future doctoral programme, funded by the European Commission Marie Skłodowska-Curie COFUND action. Applicants must fulfil the eligibility criteria described in the programme call text (see http://www.oulu.fi/i4future/node/34377).

The candidate should have a MSc degree in (Organic or Inorganic) Chemistry, Physics or Materials Science. Previous experience with NMR spectroscopy or first-principles electronic structure calculations is an advantage. The candidate should be able to productively communicate in English (both written and spoken).

Information

Academy Researcher Ville-Veikko Telkki (Ville-Veikko.Telkki@oulu.fi) and Professor Juha Vaara (juha.vaara@iki.fi), NMR Research Unit, University of Oulu, Finland
Professor Oleg N. Antzutkin (olan@ltu.se) and Assoc. Prof. Anna-Carin Larsson (acla@ltu.se), Chemistry of Interfaces, Luleå University of Technology, Sweden

Application

Expressions of interest should be directed (in English) to: Academy Researcher Ville-Veikko Telkki (Ville-Veikko.Telkki@oulu.fi) and Professor Juha Vaara (juha.vaara@iki.fi), NMR Research Unit, University of Oulu, Finland, as soon as possible

Deadline

Due date for the final application is July 31, 2016, interviewing process will be carried out during August 2016, and the project is planned to start in September 2016.