JOB DESCRIPTION

Functions: **PhD position in material chemistry (W/M) – Exploring new inorganic Mg^{2+} solid electrolytes with high room-temperature conductivity for post-Li batteries applications**

Activities in the job description may evolve with knowledge of the position and the service requirements.

Presentation of Sorbonne University

Sorbonne University is a multidisciplinary, research-intensive, world-class university. Located in the heart of Paris, with a regional presence, it is committed to the success of its students and to meeting the scientific challenges of the 21st century. Thanks to its 54 000 students, 6 300 academic researchers and partner researchers, and 3,600 administrative and technical staff who make it a daily reality, Sorbonne University promotes diversity, creativity, innovation and openness to the world.

The university is structured in three faculties: « **Art and Humanities** », « **Medicine** » et « **Science and Engineering** » each disposing of an important autonomy in the application of the university's strategy.

To learn more about Sorbonne University: https://www.sorbonne-universite.fr/en

This position is available within the Faculty of Science and Engineering: http://sciences.sorbonne-universite.fr

Within Sorbonne University, **the Faculty of Science and Engineering** covers a large spectrum of scientific disciplines.

It is composed of **79 research laboratories**, 22 teaching departments and 6 UFR (Formation and Research Units) in chemistry, engineering, mathematics, physics, life sciences as well as Earth, Environment and Biodiversity. It also comprises the university's engineering school - Polytech Sorbonne -, the Paris Astrophysic Institute, the Henri Poincaré Institute, three marine stations located in Banyuls-sur-Mer, Roscoff and Villefranche-sur-Mer.

It is hosting 20 800 students among which 2 700 doctoral researchers and accounts for 4 800 academic and research staff and 3 252 administrative and technical staff.

Laboratoire de Chimie de la Matière Condensée de Paris (UMR 7574)

Laboratoire de Chimie de la Matière Condensée de Paris (UMR 7574) : https://lcmcp.upmc.fr/

within the **Reactive Materials for Energy deviceS (RMES) team:** https://lcmcp.upmc.fr/site/rmes

The PhD researcher will integrate the LCMCP, laboratory internationally recognized in the field of Material Sciences for the elaboration of **functional inorganic and hybrid materials**, and the evaluation of their physico-chemical properties at multiple scales. The lab brings together all facets of chemistry of materials with a strong coupling between synthesis methods and processing of materials. These materials target applications with a strong societal impact in the fields of **energy**, **health,** and **environment**.

The **RMES team's** expertise covers organic/inorganic/hybrid materials, processing and sintering of ceramics and electrochemical characterization methods that place it in an ideal position to develop innovative ideas at the crossroads of material science disciplines, a scientific culture largely developed at the LCMCP. The RMES team is part of the French Network on Energy Storage (https://www.energie-rs2e.com/en) which nurtures strong scientific connections between research labs to accelerate the development of energy storage through dynamic collaborations and the development and mutualization of advanced in situ/operando characterization techniques, including at synchrotron facilities.

Project and main Activities

This project deals with the **development of new crystalline inorganic solids with high Mg^{2+} mobility** at room temperature (> 10^{-4} $S.cm^{-1}$) for the **development of next generation (post lithium) all-solid-state batteries**. Our goal is to develop a new generation of multivalent cation electrolytes based on safe, inexpensive and earth-abundant elements which would have the potential to alleviate resource issues with Li-ion systems. The success of this project would be a significant milestone for the development of an all-solid-state magnesium battery.

1. *Description of the project*

Since their inception onto the market in 1991, Lithium-ion Batteries (LiBs) have been a key-enabling electrochemical energy solution for a hand full of applications. Nevertheless, LiBs are relatively expensive, usually involve the use of rare and toxic transition metals (Co, Ni, *etc.*) and suffer from safety limitations, both due to the flammable nature of liquid electrolytes and the tendency of the lithium anode to form dendrites in the lithium-metal batteries. As asserted by a recent report of the World Economic Forum, searching for alternatives to lithium batteries is both a societal and scientific challenge [1]. Batteries based on other monovalent or multivalent cations (*e.g.* Na^{+}, K^{+}, Ca^{2+}, Mg^{2+}, Zn^{2+}, Al^{3+}) appear to be promising alternative technologies to consider if scientific and technological roadblocks can be lifted to reach the required performance targets for authorizing their commercialization. Among alternatives to Li^{0} for alkali metal-based batteries, Mg^{0} is considered as an interesting metal anode due to **i)** its high abundance and higher accessibility in the terrestrial crust, **ii)** its theoretical volumetric capacity of 3833 $mAh{\cdot}cm^{-3}$, and **iii)** its relatively low reduction potential (− 2.37 V *vs.* SHE) [2]. Despite these obvious advantages, development of rechargeable Magnesium batteries is lagged because of low Room Temperature ionic conductivity of stable (*vs.* both electrodes), non-toxic, sustainable and cost-effective Mg^{2+} electrolytes. Developing a suitable electrolyte remains thus a big challenge.

Recently, the discovery of the first generation of crystalline solids, *i.e.*, **spinel MgX_2Z_4**, with *X* = (In, Y, Sc) and *Z* = (S, Se), which possess **high Mg^{2+} cation mobility at room temperature** (*ca.* 0.1 mS cm^{-1} for $MgSc_2Se_4$) opens exciting perspectives for the development of Li-free all-solid-state batteries [3]. The high Mg^{2+} mobility in this compound is explained by the unfavorable anion coordination environment, *i.e.* ≠ 6. Although very interesting, **$MgSc_2Se_4$ has small interest for a large-scale implementation** because of price and toxicity of Sc and Se, respectively. Based on preliminary analysis, we expect that **the spinel structure can be stabilized by substituting some Sc and Se by suitable non-toxic and abundant trivalent ions.** If their Mg^{2+} transport properties are good enough, these new compounds will be an excellent alternative to $MgSc_2Se_4$ for large-scale applications in Mg all-solid-state batteries, opening a new era in the search for high performance multivalent-ion solid conductors.

2. *Specific techniques or methods*

We propose, within the framework of this PhD, to investigate the **relationship between crystal structure, composition and Mg^{2+} ion transport in the MgX_2Z_4 solid solution**, in the range of room temperature to *ca.* 150 °C. Compounds will be synthesized at LCMCP by solid state reaction at high temperature of elemental elements. Phase purity of the synthesized powders will be checked by **X-ray diffraction** (iMat platform). **Advanced structural characterization** will be performed on the best samples at the CRISTAL beamline of **Soleil Synchrotron**; complementary **neutron powder diffraction** will be also performed at the Institut Laue Langevin (ILL, Grenoble) to accurately determine cation atomic positions and Mg diffusion paths. The crystallographic structure and microstructure insights (crystallite size and microstrain) will be obtained from **Rietveld refinements** of these powder patterns. Potential nanoscale (inter)metallic phases (responsible of electronic conductivity) will be searched by **TEM** (iMat platform). Ionic and electronic conductivity will be measured at room temperature and *vs.* temperature (for activation energy calculation) by **impedance spectroscopy** at LCMCP.

3. *References*

[1] A. Ponrouch *et al.*, Phil. Trans. R. Soc. A 377 (2019) 20180297. DOI: 10.1098/rsta.2018.0297 [Open access]
[2] R. Dominko et al., J. Power Sources 478 (2020) 229027. DOI: 10.1016/j.jpowsour.2020.229027
[3] P. Canepa et al., Nature Com. 8 (2017) 1759. DOI: 10.1038/s41467-017-01772-1

Knowledge and Skills*

Education, Qualifications and Training :

- Master in Chemistry or Materials Science (or very close to completion)

General and interpersonal skills :

- Ability to work as a team member and foster positive relationships.
- Demonstrate proactivity, availability, and reactivity in leading research projects.
- Excellent communication skills.

- Clear reporting and scientific writing.

Specific dispositions related to the position and exposure to occupational hazards

Contract: *36 months CDD contract*

Salary: *28 k€/year*

Expected starting date: *October 2023*

Application deadline: 10th April 2023

Interested candidate should send a CV, cover letter and contact information for two references (PhD advisor, supervisor) to Dr. Arnaud Perez (damien.bregiroux@sorbonne-universite.fr).

**Conformément à l'annexe de l'arrêté du 18 mars 2013 (NOR : MENH1305559A)*