SORBONNE UNIVERSITÉ

MASTER DE CHIMIE DE SORBONNE UNIVERSITE
Proposition de stage 2025-26
Internship Proposal 2025-26

Parcours type(s) / *Specialty(ies) :*

☐ Chimie Analytique, Théorique, Spectroscopies et Electrochimie/ *Analytical, Theoretical Chemistry, Spectroscopies, Electrochemistry*
☐ Chimie Moléculaire / *Molecular Chemistry*
☒ Chimie des Matériaux / *Materials Chemistry*
☐ Ingénierie Chimique / *Chemical Engineering*

Laboratoire d'accueil / *Host Institution*
Intitulés / *Name* : Laboratoire de chimie de la matière condensée de Paris (LCMCP)
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Directeur / *Director (legal representative) :* Corinne Chaneac
Tél / *Tel* :
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Equipe d'accueil / *Hosting Team :* RMES
Adresse / *Address :* Sorbonne Université - Tour 44-43 / Et.4, 4, Place Jussieu 75005 PARIS
Responsable équipe / *Team leader* : Christel Laberty-Robert
Site Web / *Web site :* https://lcmcp.science/rmes/
Responsable du stage (encadrant) / *Direct Supervisor :* Elyes Labidi
Fonction / *Position :* PhD Candidate
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Période de stage / *Internship period* * : February - July

***Title :* Synthesis and characterization of chalcogenide materials as electrolytes for rechargeable magnesium batteries**

Projet scientifique du stage / *Internship scientific Project :*

Multivalent-based batteries, such as magnesium ion batteries could prove to be a promising complementary solution to current lithium and sodium ion technology. This relies on the ability to develop room-temperature ionic conductors for Mg^{2+}. As discussed in a theoretical study by Canepa *et al.* using DFT[1], high Mg^{2+} mobility could be reached if Mg^{2+} is located in an unfavorable coordination environment, i.e. different than 6. With Mg^{2+} occupying tetrahedral sites, cubic direct spinel structure MgB_2X_4 perfectly meets this requirement (figure a). Indeed, $MgSc_2Se_4$ experimentally shows good RT-ionic conductivity ($\sigma_i = 10^{-4}$ S.cm^{-1}). Unfortunately, selenium and scandium are, respectively, toxic and an expensive rare earth. Therefore, MgB_2S_4 (*B* = Al, Y, In) are proposed as an interesting alternative.

* **min. 5 mois, maximum 6 mois à partir du 26 janv 2026 / *min. 5 months and max. 6 months not earlier than January, 26th 2026.***
Fin des conventions de stage au plus tard le 15/07/2026 ou le 15/09/2026 et le 15 novembre 2026.
End of internship at the latest July 15th, 2026 or September. 15th, 2026 and November 15th, 2026.

In this internship, the aim is to try to stabilize the spinel phase in aforementioned compositions (MgB_2S_4, *B* = Al, Y, In) through different synthesis routes, such as sealed quartz ampule solid-state reactions, spark plasma sintering and, if possible, high temperature high pressure synthesis[2]. Potential solid solutions, where a fraction of B atoms are replaced with other available elements could also be explored. Stabilized structure is highly dependant on trivalent (*B*) ionic radii (figure b). Materials will then be structurally characterized using X-Ray diffraction and subsequent refinement to obtain cell parameters, atomic positions and site occupation. Spinel inversion coefficient is either obtainable with XRD or with complimentary ^{27}Al / ^{89}Y solid state NMR. XRF and SEM-EDS measurements will confirm composition. If beamtime is available, high resolution angle dispersive X-Ray synchrotron measurements will be acquired. Finally, materials' ionic conductivities will be measured using variable temperature Electrochemical Impedance Spectroscopy.

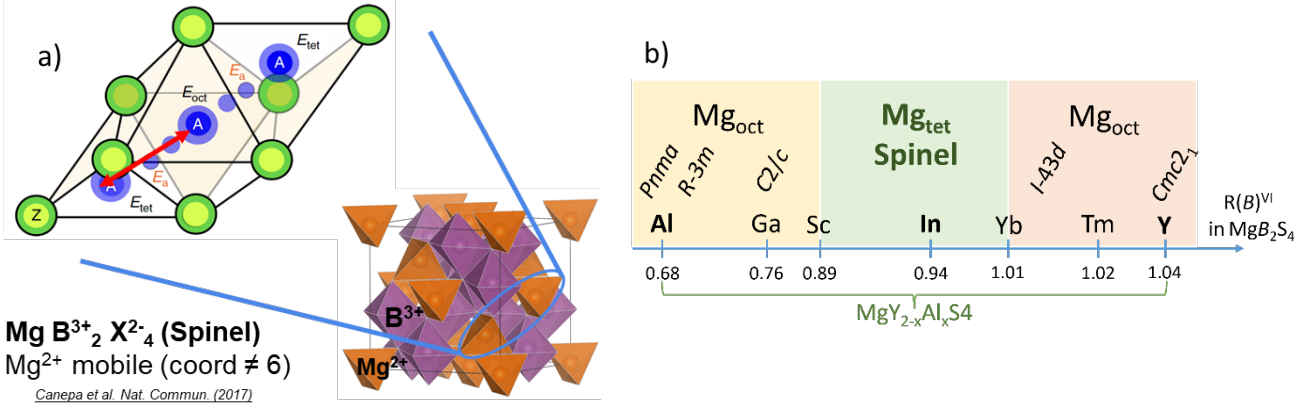

Figure: a) Mg^{2+} migration path in spinel type structure [1] b) Structure dependance on trivalent octahedral ionic radii

Specific techniques and methods:
- Synthesis via solid-state reaction and spark plasma sintering techniques.
- Powder X-Ray diffraction and subsequent profile matching and Rietveld refinement.
- Solid state NMR for ^{27}Al and ^{89}Y isotopes.
- X-Ray Fluorescence / Scanning electron microscopy - Energy dispersive spectroscopy elemental composition determination.
- Electrochemical impedance spectroscopy measurements with temperature variation

References:

[1]. Canepa, P.; Bo, S.-H.; Sai Gautam, G.; Key, B.; Richards, W. D.; Shi, T.; Tian, Y.; Wang, Y.; Li, J.; Ceder, G. High Magnesium Mobility in Ternary Spinel Chalcogenides. Nat Commun 2017, 8 (1), 1759. https://doi.org/10.1038/s41467-017-01772-1.

[2]. Duan, L.; Wang, X.; Zhao, J.; Zhang, J.; Du, S.; Feng, Y.; Zhao, Z.; Wang, S.; Jin, C. High-Pressure Synthesis and Physical Properties of a Spinel Compound FeAl2S4. Inorg. Chem. 2022, 61 (33), 13184–13190. https://doi.org/10.1021/acs.inorgchem.2c02034.