ICSM

Institut de Chimie Separative de Marcoule

Marcoule Institute in Separation Chemistry

Ph.D. Thesis 2025

Last update: December 20, 2024

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Presentation of ICSM

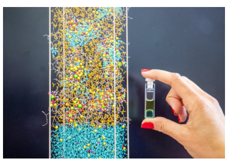
Created in January 2007, the Marcoule Institute in Separation Chemistry (ICSM) is a Joint Research Unit (UMR 5257) between the French Atomic Energy Commission (CEA), the French National Center for Scientific Research (CNRS), the University of Montpellier (UM) and the National Graduate School of Chemistry in Montpellier (ENSCM). ICSM is composed of 3 research axes gathering 8 research teams working in close collaboration:

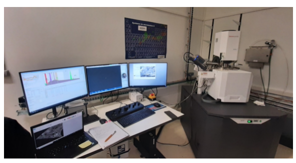
- Hybrid Systems for the Separation (LHYS)
- Ions at Active Interfaces (L2IA)
- Ion Separation using supra-Molecular self-assembled colloids (LTSM)
- Sonochemistry in Complex Fluids (LSFC)
- Adaptive Nanomaterials for eneRgy (LNAR)
- Interface of materials in Evolution (LIME)
- Study of Matter in Environmental Conditions (L2ME)
- Mesoscopic Modelling and Theoretical Chemistry (LMCT)

It is also attached to the Balard chemistry cluster, which brings together the four Montpellier chemistry institutes, including the Institut Européen des Membranes (IEM), the Institut Charles Gerhardt de Montpellier (ICGM) and the Institut des Biomolécules Max Mousseron (IBMM).

As part of the Pôle de Chimie from the University of Montpellier and the Institut des Sciences et Technologies pour une Economie circulaire des énergies bas Carbone (ISEC) within the CEA Energy Division (CEA/DES), the ICSM aims to develop fundamental research whose main objective is to "propose choices" for the development of separative chemistry processes applied to the field of decarbonized energies, by integrating the challenges of sustainable nuclear energy and the circular economy.

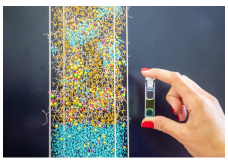


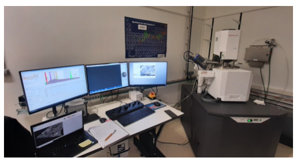




LIST OF PH.D. THESIS







AI BASED PREDICTION OF SOLUBILITIES FOR HYDROMETALLURGY APPLICATIONS

Starting date: 01/10/2025

HYbrid Systems for the Separation Laboratory (LHYS)

Contacts Marie SIMONNET – marie.simonnet@cea.fr
Christophe RAYNAUD – christophe.raynaud1@umontpellier.fr

Doctoral School Sciences Chimiques Balard (EDSCB), University of Montpellier

Funding CEA **Reference** SL-DES-25-0176

Abstract

Finding a **selective and efficient extractant** is one of the main challenges of **hydrometallurgy**. A comprehensive screening is impossible by the synthesis/test method due to the high number of possible molecules. Instead, more and more studies use quantum calculations to evaluate the complexes stabilities. Still, some important parameters such as solubility are lacking in this model.

This project thus aims to **develop an AI-based tool** that provides **solubility values from the molecular structure** of any ligand. The study will first focus on 3 solvents: water, used as a reference as AI tools already exist, 3 mol L^{-1} **nitric acid** to mimic nuclear industry applications and ***n*-octanol**, organic solvent used to measure the partition coefficient log(P). The methodology follows 4 steps:

1. Bibliography on existing AI tools for solubility prediction yielding the choice of the most promising method(s)
2. Bibliography on existing databases to be complemented by the student's in-lab solubility experiments
3. Code generation and training of the neural network on the step 2 databases
4. Checking the accuracy of the predictions on molecules not included in the databases by comparing the calculated results with in-lab experiments

Candidate profile

You should hold a master's degree in **theoretical chemistry, data sciences** or **informatics**.

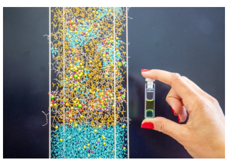
Benefit for the candidate

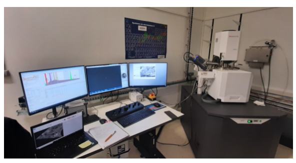
- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **technical skills in solution chemistry, data sciences, and computing chemistry**, in addition to **soft skills** such as **management through teamwork** and the **tutoring of intern students**, opening numerous **professional opportunities in both academic research and industrial R&D**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in a laboratory equipped with a rich array of advanced instruments, especially useful to characterize the solubility experiments.
- **High-Performance Computing**: You will gain experience working on high-performance computing centers, through access to the CEA Marcoule's cluster for the implementation of the AI code and the quantum calculations.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Marie Simonnet (marie.simonnet@cea.fr) and Dr. Christophe Raynaud (christophe.raynaud1@umontpellier.fr).







BIOSOURCED ALDITOL ANHYDRIDES, TUNABLE MOLECULAR ARCHITECTURES FOR A SUSTAINABLE APPROACH TO THE URANIUM EXTRACTION

Starting date: 01/10/2025

Ion Separation using self-assembled Molecular systems Laboratory (LTSM)

Contacts Fabrice GIUSTI – fabrice.giusti@cea.fr
Guilhem ARRACHART – guilhem.arrachart@cea.fr

Doctoral School Sciences Chimiques Balard (EDSCB), University of Montpellier

Funding CEA **Reference** SL-DES-25-0044

Abstract

Although current applied processes for extracting uranium in sulfuric, phosphoric and nitric media, are efficient enough to justify their large-scale application, they require improvements to increase their efficiency and reduce their environmental impact. This doctoral project aims to improve these performances by focusing **on the liquid-liquid extraction stage**. This consists of selectively transferring uranium, extracted after crushing, grinding and leaching rocks, to an oil phase containing a lipophilic ligand compatible with the leachate medium. The ambition here is to develop new extractants analogous to **trialkylamines** (AMEX process), **trialkylphosphines** and **phosphoric diesters** (URPHOS process), and **trialkylphosphates** (refining). The PhD student will synthesize **chiral amphiphilic extractants**, derived from bicyclic anhydrides of **biosourced alditols** (isosorbide, isomannide and isoidide). He will evaluate their affinity towards uranium and their selectivity in the presence of competing ions. He will then characterize the **molecular and supramolecular mechanisms** of these new extractants (coordination, aggregation) using state-of-the-art methods such as UV, IR, multinucleus NMR, X-ray scattering, and neutron scattering. The research will take place in the LTSM laboratory of the ICSM, renowned for its expertise in the chemistry and physical chemistry of extractants for hydrometallurgy.

Candidate profile

You should hold a Master's degree in **organic synthesis** and have **knowledge of characterization techniques**. Knowledge of the nuclear fuel cycle and small-angle x-ray/neutron scattering techniques would be an advantage.

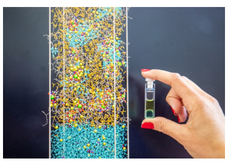
Benefit for the candidate

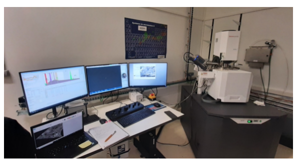
- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in hydrometallurgy, green chemistry, formulation, and nuclear research**, opening numerous **professional opportunities in both academic research and industrial R&D**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in a laboratory equipped with a rich array of advanced instruments.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Fabrice Giusti (fabrice.giusti@cea.fr) and Dr. Guilhem Arrachart (guilhem.arrachart@cea.fr).







IMPACT OF SOLVENT NANOSTRUCTURE ON URANIUM PRECIPITATION: A PHYSICOCHEMICAL APPROACH FOR NUCLEAR RECYCLING

Starting date: 01/10/2025

Ion Separation using self-assembled Molecular systems Laboratory (LTSM)

Contacts Sandrine DOURDAIN – sandrine.dourdain@cea.fr
Thomas DUMAS – thomas.dumas@cea.fr

Doctoral School Sciences Chimiques Balard (EDSCB), University of Montpellier

Funding CEA **Reference** SL-DES-25-0205

Abstract

Recycling nuclear fuel is a major challenge to ensure a sustainable energy future. The CEA, in partnership with Orano and EDF, has been developing a new process for separating plutonium-rich fuels for several years. The goal is to replace the current TBP/TPH system with a redox-free process, better suited for the reprocessing of MOX or fast neutron reactors (FNR).

In this context, this thesis proposes to **study the behavior of organic solvents** loaded with **uranium** to **understand and prevent the formation of precipitates**, a phenomenon that could i**mpact the performance of industrial processes.** The scientific approach will focus on the supramolecular scale and compare **different monoamides** to evaluate the **effect of alkyl chains** on the physicochemical properties and nanostructure of the solutions.

By joining this project, the candidate will become part of the CEA's cutting-edge laboratories (ICSM/LTSM and DMRC/SPTC/LILA), equipped with world-class facilities for studying radioactive samples. She/he will benefit from multidisciplinary supervision, including opportunities for international collaborations. This thesis represents a major scientific challenge with direct industrial applications, offering you valuable experience in the field of nuclear separation and processing technologies.

Candidate profile

You should hold a Master's degree (Master 2) in **chemistry, physical chemistry**, or **materials science**. **Skills in analytical chemistry, spectroscopy** (NMR, FTIR), and **scattering techniques** (SANS, SAXS) will be highly valued.

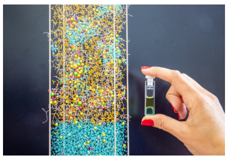
Benefit for the candidate

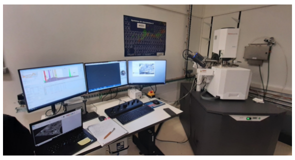
- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in the field of nuclear separation and processing technologies**, opening numerous **professional opportunities in both academic research and industrial R&D**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in laboratories equipped with a rich array of advanced instruments.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Sandrine Dourdain (sandrine.dourdain@cea.fr) and Dr. Thomas Dumas (thomas.dumas@cea.fr).







ULTRASOUND–ASSISTED DECONTAMINATION OF HG–BEARING SOLIDS

Starting date: 01/10/2025

Sonochemistry in Complex Fluids Laboratory (LSFC)

Contacts Rachel PFLIEGER – rachel.pflieger@cea.fr

Doctoral School Sciences Chimiques Balard (EDSCB), University of Montpellier

Funding CEA **Reference** SL-DES-25-0240

Abstract

Mercury is one of the most dangerous pollutants. Yet, it has been widely used in the industry, in particular in electrolyzers (chlor-alkali process), resulting in many contaminated facilities. Existing methods to stabilize or decontaminate are either energy-consuming or limited in terms of speciation. The aim here is to **develop a new method combining leaching and ultrasonic irradiation, to decontaminate porous solids** (e.g. mortar). The characterization of solids and liquids before/after decontamination will be performed using SEM-EDX, XRD, and XRF.

The PhD study will be performed in Marcoule Center, located 30 minutes from Avignon. The two host laboratories are the Laboratory of Supercritical Processes and Decontamination (DMRC/STDC/LPSD) and the Laboratory of Sonochemistry in Complex Fluids (ICSM/LSFC). Marcoule site is served by bus and hosts many PhDs and post-docs.

Candidate profile

You should hold a master's degree with a **chemical engineering background** and have desirable **skills in analytical chemistry and inorganic chemistry**.

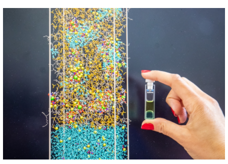
Benefit for the candidate

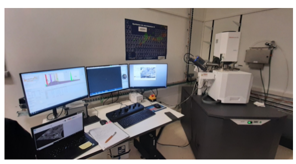
- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in materials science and physical chemistry**, opening numerous **professional opportunities in both academic research and industrial R&D, particularly in the field of environmental remediation**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in laboratories equipped with a rich array of advanced instruments.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Rachel Pflieger (rachel.pflieger@cea.fr).







NUCLEATION, GROWTH, AND MULTI-SCALE STRUCTURAL PROPERTIES OF COLLOIDAL NANOPARTICLES OF ACTINIDE OXIDES (PU, U, TH)

Starting date: 01/10/2025

Sonochemistry in Complex Fluids Laboratory (LSFC)

Contacts Matthieu VIROT – matthieu.virot@cea.fr

Doctoral School Sciences Chimiques Balard (EDSCB), University of Montpellier

Funding CEA **Reference** SL-DES-25-0201

Abstract

Nanocrystalline oxides possess unique physicochemical properties, modulated by their size and local structure, making them promising for various technological applications. However, **actinide oxide nanoparticles** remain underexplored due to their radioactivity and toxicity. Nonetheless, studies dedicated to these species are growing, driven by environmental and industrial considerations, particularly for their involvement in current and future nuclear fuel cycles. This thesis focuses on **plutonium**, a key element in nuclear reactors. Its behavior in solution is complex, particularly due to **hydrolysis reactions** that lead to the formation of highly stable **colloidal PuO_2 nanoparticles**. Although these species are now better described, the mechanisms leading to their formation remain largely unexplored.

The ambitious goal of this thesis is to uncover the **fundamental mechanisms** involved in the formation of these nanoparticles by adopting a systematic approach that combines a wide range of experimental parameters. These include the synthesis medium, temperature, reactant concentration, reaction time, and the contribution of sonochemistry. The focus will be on studying the **nucleation and growth stages of these nanoparticles**, as well as their **structural properties** in relation to the **physico-chemical conditions that influence their formation**. Studies will be conducted at ICSM with Th, U, and Zr as analogs, and at the **Atalante** facility for Pu. In addition to standard laboratory techniques necessary for characterizing these systems, complementary experiments will be carried out on synchrotron lines (SOLEIL and ESRF) to thoroughly investigate the structural and reactive properties of these species and their precursors.

Candidate profile

You should hold a master's or degree or engineer in **chemistry** with knowledge of **radiochemistry**.

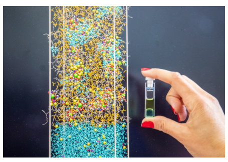
Benefit for the candidate

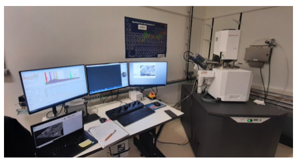
- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in materials chemistry, actinide chemistry and handling, and related characterization techniques**, including synchrotron radiations, opening **numerous professional opportunities in both academic research and industrial R&D**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in a laboratory equipped with a rich array of advanced instruments.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Matthieu Virot (matthieu.virot@cea.fr).







DEVELOPMENT OF SOLID POROUS SILICEOUS SUPPORTS FOR ACTINIDE SORPTION – BEHAVIOUR UNDER IRRADIATION

Starting date: 01/10/2025

Adaptive Nanomaterials for eneRgy Laboratory (LNAR)

Contacts Xavier DESCHANELS – xavier.deschanels@cea.fr
Cyrielle REY – cyrielle.rey@cea.fr

Doctoral School Sciences Chimiques Balard (EDSCB), University of Montpellier

Funding CEA **Reference** SL-DES-25-0302

Abstract

The aim of this research project is to study **the densification of a mesoporous structure under radiation damage produced by the presence of an actinide (^{238}Pu)** in the porous structure. To achieve this, siliceous materials based on mesoporous silicas modified by the addition of additive elements (B, Al, etc.) will be used. The purpose of adding these elements is to weaken the mesoporous structure in order to promote densification. The characteristics of the mesoporous structure (pore diameter, wall size, symmetry of the pore network) will be other parameters of the study. These materials will be functionalized with phosphonate ligands for actinide adsorption: thorium as a simulant in a preliminary stage, followed by plutonium. The final part of this work, which will continue beyond the thesis, will involve using various techniques (SAXS, BET, microscopy, etc.) to study the evolution of the mesoporous structure under the effect of irradiation damage as the material ages. This fundamental research work could have spin-offs in the field of nuclear waste conditioning materials: ageing of gels on the surface of nuclear glass, support material for decontaminating radioactive effluents. Part of the work will be carried out at CEA Marcoule's Atalante facility.

Candidate profile

Master CSMP, ENSCM other engineering schools, Master Nuclear Energy (Paris-Saclay)

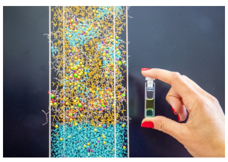
Benefit for the candidate

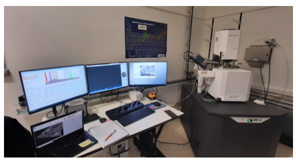
- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in materials synthesis, mesoporous materials, and radiation damage in material**, opening numerous **professional opportunities in both academic research and industrial R&D**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in laboratories equipped with a rich array of advanced instruments.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Xavier Deschanels (xavier.deschanels@cea.fr) and Dr. Cyrielle Rey (cyrielle.rey@cea.fr).







STUDY OF MOX AND MODEL COMPOUNDS LEACHING IN UNDERWATER STORAGE CONDITIONS

Starting date: 01/10/2025

Interfaces of Material in Evolution Laboratory (LIME)

Contacts Nicolas DACHEUX – nicolas.dacheux@cea.fr
Laurent CLAPAREDE – laurent.claparede@cea.fr

Doctoral School Sciences Chimiques Balard (EDSCB), University of Montpellier

Funding CEA **Reference** SL-DES-25-0216

Abstract

This thesis deals with **nuclear fuel recycling** in France, with a focus on the **multi-recycling of uranium and plutonium** from **MOX fuels**, planned for 2040. Spent fuel is **stored underwater in pools**, where a cladding defect could lead to water contamination and complicate reprocessing. This thesis proposes to study the **leaching** of these fuels and the appearance of **secondary phases** under conditions simulating storage. The work is divided into three parts: the **preparation of model compounds**, the study of the **chemical durability** of model and industrial materials, and the **analysis of secondary phases** forming on the surface of irradiated fuels. The aim is to gain a better understanding of the stability of these phases as a function of chemical and **irradiation conditions**, as well as their **transformation mechanisms**. The results will enable us to develop models for the behavior of defective rods over several decades, contributing to the safer and more efficient management of irradiated fuels.

Candidate profile

You should hold a Research Master's degree or an Engineering School degree in **Radiochemistry** and/or **Materials Chemistry**.

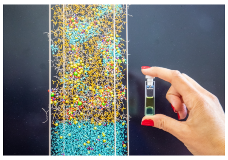
Benefit for the candidate

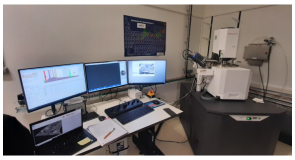
- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in physical chemistry in relation to ceramic materials, their characterization and aging**, opening numerous **professional opportunities in both academic research and industrial R&D (EDF)**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in a laboratory equipped with a rich array of advanced instruments.

How to apply

Please send a cover letter, a detailed CV, and references to Pr. Nicolas Dacheux (nicolas.dacheux@cea.fr) and Dr. Laurent Claparède (laurent.claparede@cea.fr).







MICROEMULSION MODEL: TOWARDS THE PREDICTION OF LIQUID-LIQUID EXTRACTION PROCESSES

Starting date: 01/10/2025

Mesoscopic Modelling and Theoretical Chemistry Laboratory (LMCT)

Contacts	Magali DUVAIL – magali.duvail@cea.fr Jean-François DUFRECHE – jean-francois.dufreche@icsm.fr		
Doctoral School	Sciences Chimiques Balard (EDSCB), University of Montpellier		
Funding	CEA	**Reference**	SL-DES-25-0263

Abstract

This **multi-scale modeling** thesis aims to **develop innovative theoretical approaches and numerical tools** to revolutionize **strategic metal extraction processes**, such as **liquid-liquid extraction**, whose underlying mechanisms remain poorly understood. To address these challenges, solvent phases will be represented as microemulsions through a **synergy of mesoscopic and molecular modeling approaches**.

The **mesoscopic approach** will involve the **development of a code** based on microemulsion theory using a **random wavelet basis**. This code will enable the characterization of the **structural and thermodynamic properties** of the solutions. The **molecular approach** will rely on **classical molecular dynamics simulations** to evaluate the **extractants' curvature properties**, which are essential for bridging the two scales. The **new high-performance computational code** may integrate **artificial intelligence techniques** to accelerate the minimization of the system's free energy while accounting for all chemical species present with a minimal number of parameters. This will pave the way for **new research directions**, such as predicting speciation and calculating thermodynamic instabilities in ternary phase diagrams, thereby identifying unexplored experimental conditions.

This PhD thesis will have applications in the **recycling domain** and extend to the broader field of **nanoscience**, thereby expanding the impact of this work. The PhD candidate will be encouraged to disseminate his/her scientific results through publications and presentations at national and international conferences.

Candidate profile

You are a highly motivated candidate holding a Master's degree in **physical chemistry, theoretical chemistry, physics**, or equivalent. You have a **strong interest in programming** (Python, Fortran) and possess good written and oral communication skills.

Benefit for the candidate

- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in modeling and physical chemistry**, opening numerous **professional opportunities in both academic research and industrial R&D**.
- **International Environment**: You will work in an international environment, fostering cross-cultural collaboration and communication.
- **High-Performance Computing**: You will gain experience working on high-performance computing centers, enhancing computational and data analysis skills.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Magali Duvail (magali.duvail@cea.fr) and Pr. Jean-François Dufrêche (jean-francois.dufreche@icsm.fr).