ICSM

INSTITUT DE CHIMIE SÉPARATIVE DE MARCOULE

MARCOULE INSTITUTE IN SEPARATION CHEMISTRY

PH.D. THESES 2026

Last update: February 23, 2026

Institut de Chimie Séparative de Marcoule
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https://www.icsm.fr

PRESENTATION OF ICSM

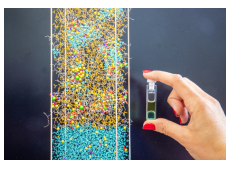
Created in January 2007, the Marcoule Institute in Separation Chemistry (ICSM) is a Joint Research Unit (UMR 5257) between the French Atomic Energy Commission (CEA), the French National Center for Scientific Research (CNRS), the University of Montpellier (UM) and the National Graduate School of Chemistry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

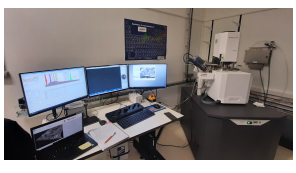
- Hybrid Systems for the Separation (LHYS)
- Ions at Active Interfaces (L2IA)
- Ion Separation using supra-Molecular self-assembled colloids (LTSM)
- Sonochemistry in Complex Fluids (LSFC)
- Adaptive Nanomaterials for eneRgy (LNAR)
- Interface of materials in Evolution (LIME)
- Study of Matter in Environmental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

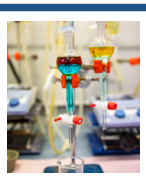
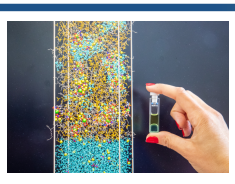
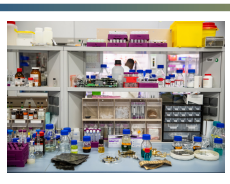
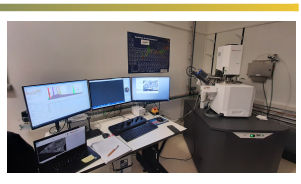
As part of the Pôle de Chimie from the University of Montpellier and the Institut des Sciences et Technologies pour une Economie circulaire des énergies bas Carbone (ISEC) within the CEA Energy Division (CEA/DES), the ICSM aims to develop fundamental research whose main objective is to "propose choices" 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.







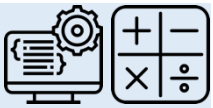
LIST OF PH.D. THESES

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

Starting date: 01/10/2026

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-26-0120

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

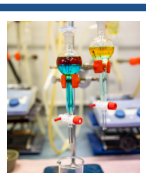
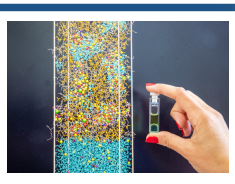
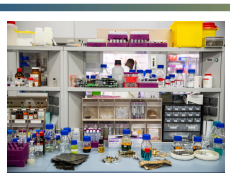
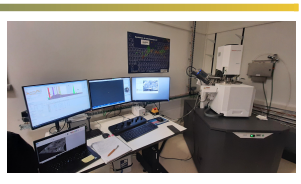
You are a highly motivated candidate holding a Master's degree in **physical chemistry, theoretical chemistry, physics**, or equivalent. You have a **strong interest in programming** (Python, Fortran) and possess good written and oral communication skills.

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).

MULTISCALE MODELLING OF UO_2 DISSOLUTION

Starting date: 01/10/2026

Mesoscopic Modelling and Theoretical Chemistry Laboratory (LMCT)

Contacts Katya GOLOVIZNINA – kateryna.goloviznina@cea.fr
Jean-François DUFRECHE – jean-francois.dufreche@icsm.fr

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

Funding University of Montpellier **Reference** -

Abstract

The **dissolution of UO_2 in nitric acid** has long been studied to optimize spent nuclear fuel recycling, yet the reaction mechanisms remain poorly understood. While atomistic simulations offer valuable insights, dissolution is a complex physico-chemical process that requires quantum-level modeling of surface chemical reactions. Recent advances in high-performance computing and the rapid evolution of artificial intelligence have transformed scientific discovery. ***Ab initio* molecular dynamics** (AIMD) is now capable of describing systems large enough to determine macroscopic thermodynamic data, while AI-driven techniques, such as machine learning force fields (MLFFs), enable larger timescales, higher resolutions, and more realistic conditions.

This thesis proposes a **multiscale modelling approach,** combining AIMD to understand dissolution mechanisms with classical molecular dynamics (CMD) using state-of-the-art MLFFs to explore larger systems and longer timescales. AIMD will help to identify the most probable reaction path for interactions with nitric acid and the radiolysis-generated metastable agents. Enhanced sampling methods will be used to accelerate the exploration and to establish reliable MLFF training. Then, CMD with MLFF will be used to investigate **solid-liquid equilibrium**, system dynamics, ion transport in solution, and oxidation kinetics. Larger simulation boxes will also make achievable the modelling of imperfect systems due to the presence of surface defects.

This PhD thesis should have a dramatic **impact on the recycling domain** because dissolution is a crucial stage to perform sustainable separation processes of strategic materials. In addition, this work at the nanoscale will also be important for 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

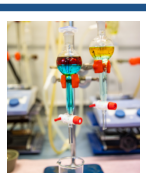
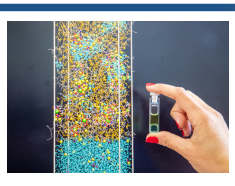
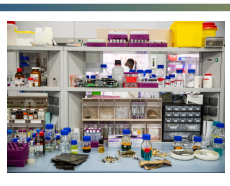
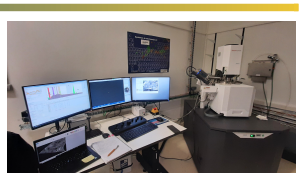
You are a highly motivated candidate holding a Master's degree in **theoretical chemistry**, **physical chemistry**, **physics**, or equivalent. You have a **strong interest in programming** (e.g. Python, Fortran, C++) and possess good written and oral communication skills.

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 Pr. Jean-François Dufrêche (jean-francois.dufreche@icsm.fr) and Dr. Katya Goloviznina (kateryna.goloviznina@cea.fr). Please submit your application via the Sciences Chimiques Balard doctoral school website at https://adum.fr/as/ed/voirproposition.pl?langue=&site=edscb&matricule_prop=68590, and click the button "Candidater" (bottom of page).

EXTRACTION OF URANIUM FROM REFRACTORY ORES BY SONOCHEMICAL ACTIVATION: APPLICATION TO BRANNERITE AND U–TI ASSOCIATIONS

Starting date: 01/10/2026

Interfaces of Material in Evolution (LIME) & Sonochemistry in Complex Fluids (LSFC)

Contacts Stéphanie SZENKNECT – stephanie.szenknect@cea.fr
Matthieu VIROT – matthieu.virot@cea.fr

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

Funding University of Montpellier **Reference** -

Abstract

Faced with growing global energy needs, the nuclear power industry must develop **innovative methods to exploit unconventional uranium sources**, particularly brannerite (UTi_2O_6). Although this ore has a high uranium content, its dissolution is limited by the formation of a passivating layer of TiO_2, making conventional processes (high-temperature acid leaching) less effective and more costly. An alternative approach, based on **sonolysis of the leaching solution**, could improve extraction yields by combining the mechanical and chemical effects of ultrasound in a heterogeneous system.

This thesis aims to **evaluate the potential of sonochemistry to optimize the extraction of uranium** from brannerite and other minerals containing uranium and titanium. The main objectives are:

- To characterize the sonolysis reactions in leaching media (production of oxidizing species, influence of ultrasonic parameters).
- To study the dissolution kinetics of synthetic and natural brannerite under ultrasound, comparing the effects with conventional methods.
- To determine the optimal conditions (frequency, power, temperature, acidity) for maximizing extraction yields.
- To evaluate the environmental impact of this method compared to conventional processes.

This thesis will contribute to the **development of a more efficient and sustainable extraction method**, thereby reducing the energy and environmental constraints associated with current processes. The results could pave the way for the application of sonochemistry to the treatment of refractory ores.

Candidate profile

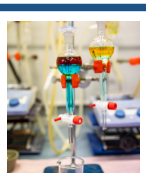
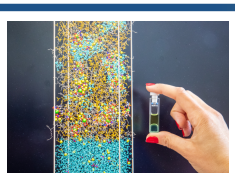
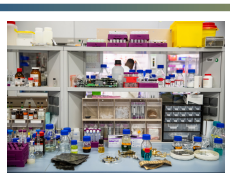
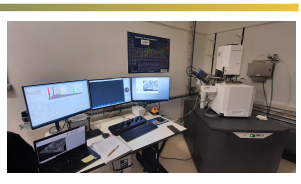
This PhD subject is intended for candidates with a Master's degree in **materials chemistry**, **geochemistry**, or **process engineering**, who have a strong interest in experimental research with practical applications in an academic context.

Benefit for the candidate

- **Skill Development:** Upon completion of the thesis, you will have acquired a **recognized expertise** in the field of **uranium sonochemistry**, **chemistry**, and **geochemistry**, opening numerous **professional opportunities in both academic research and industrial R&D**.
- **Working Environment:** The **LIME-LSFC shared supervision** of the thesis will ensure scientific monitoring of all aspects of the subject. Both teams welcome several doctoral students in a dynamic working environment conducive to the production of original results.
- **Equipment:** You will have the opportunity to work in a laboratory equipped with a rich array of advanced instruments. All of these devices are available at the ICSM and enable the analysis of radioactive samples.

How to apply

Please send a cover letter, a detailed CV, and references to Dr. Stéphanie Szenknect (stephanie.szenknect@cea.fr) and Dr. Matthieu Virot (matthieu.virot@cea.fr). Please submit your application via the Sciences Chimiques Balard doctoral school website at https://adum.fr/as/ed/voirproposition.pl?langue=&site=edscb&matricule_prop=68510, and click the button "Candidater" (bottom of page).

STEREOSELECTIVE SYNTHESIS OF CHIRAL ORGANOPHOSPHORUS COMPOUNDS FOR THE STRUCTURE–ACTIVITY RELATIONSHIP INVESTIGATION AT THE FRONT-END OF THE FUEL CYCLE

Starting date: 01/10/2026

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

Contacts Fabrice GIUSTI – fabrice.giusti@cea.fr
Stéphane PELLET-ROSTAING – stephane.pellet-rostaing@cea.fr

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

Funding CEA **Reference** SL-DES-26-0397

Abstract

This PhD project, part of the CEA's accelerated research program on nuclear energy front-end technologies, focuses on optimizing **uranium recovery** through **liquid-liquid extraction (LLE)**. The process involves selectively transferring uranium—extracted from crushed, ground, and leached ore—into an immiscible oil phase using lipophilic ligands.

Building on prior laboratory research, the project explores the relationship between **the stereochemistry of organophosphorus ligands** (phosphoric diesters, amido-, and aminophosphonates) and their uranium extraction efficiency. Previously, these ligands were only available in stereo-enriched forms. The PhD candidate will **synthesize diastereopure versions**, evaluate their uranium affinity and selectivity against competing ions, and investigate their molecular and supramolecular mechanisms (coordination, aggregation) using advanced techniques: **UV**, **IR**, **multinuclear NMR**, **DFT**, **EXAFS**, **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

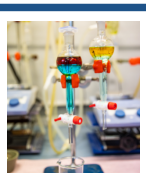
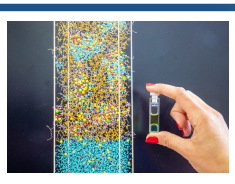
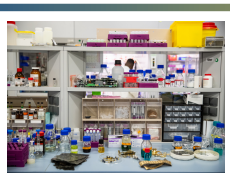
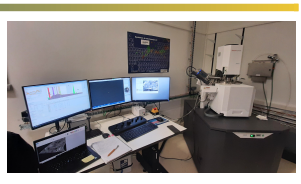
We are looking for a **highly motivated organic chemist** with **a strong foundation** in organic synthesis—both theoretical and practical. Experience in **asymmetric induction** and **DFT calculations** is highly desirable. The successful candidate will be **eager to work in an interdisciplinary environment** and will have the opportunity to expand their skill set by learning **small-angle scattering analysis** (X-ray/neutron scattering). This project offers a unique chance to contribute to cutting-edge research in nuclear chemistry within a dynamic and collaborative team.

Benefit for the candidate

- **Skill Development**: Upon completion of the thesis, you will have acquired a wide range of **skills in the fields of nuclear fuel cycle and separation 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 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. Stéphane Pellet-Rostaing (stephane.pellet-rostaing@cea.fr).

IONIC COACERVATION FOR NANO-ION ASSISTED SEPARATION

Starting date: 01/10/2026

Ions at Active Interfaces Laboratory (L2IA)

Contacts Pierre BAUDUIN – pierre.bauduin@cea.fr
Maria BOLTOEVA – maria.boltoeva@cea.fr

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

Funding CEA **Reference** SL-DRF-26-0440

Abstract

In the context of increasing demands for efficient and sustainable metal recovery, there is a strong need for **new separation systems** capable of selectively extracting metal ions from complex aqueous media, beyond the limits of conventional solvent-based approaches. This PhD focuses on developing innovative, organic solvent-free methods for the **selective separation of metal ions** using nanometric sized ions (nano-ions). **Nano-ions**, such as the superchaotropic anion cobalta-bis-dicarbollide (COSAN) a well-known ionic extractant of Cs^+ and Sr^{2+}, exhibit exceptionally low solvation while retaining high water solubility. Superchaotropic nano-ions display unusually strong interactions with **hydrated polymers** (e.g., polyethylene glycol) and **non-ionic surfactants**. These interactions induce a liquid-liquid phase separation between a dilute and a surfactant rich phase (referred to as a **coacervate**), which we propose to exploit to selectively concentrate and separate metal ions from complex aqueous solutions.

Key objectives include:

- Investigating the formation and properties of coacervate phases in nano-ion/surfactant systems;
- Developing a high-throughput screening method to evaluate the selectivity of nano-ions toward various metal ions, including radionuclides (e.g., Cs^+, Sr^{2+}, UO_2^{2+}), transition and rare earth elements.
- Implementing an automated microfluidic screening platform with multi-element X-ray fluorescence detection.

This project addresses **critical challenges in nuclear waste treatment and strategic metal recovery**, offering a sustainable, solvent-free separation technology with broad industrial and environmental applications.

Candidate profile

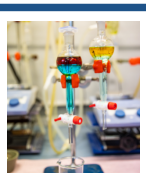
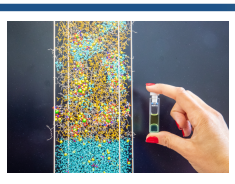
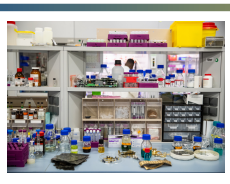
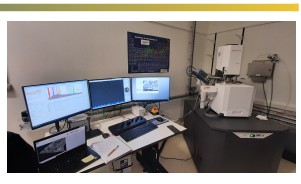
You should hold a **Master's degree** in **chemistry,** or **physical chemistry**, with **strong experimental skills** in colloid and interface science, soft matter, or separation processes. **Experience with scattering techniques** (X-ray, neutron), microfluidics, or spectroscopy is a plus. **Fluency in English** (written and spoken) and the ability to work in an international, interdisciplinary team.

Benefit for the candidate

- **Skill Development**: Upon completion of the thesis, you will have acquired **expertise in advanced separation techniques**, 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. Pierre BAUDUIN (pierre.bauduin@cea.fr) and Dr. Maria BOLTOEVA (maria.boltoeva@cea.fr).

DISSOLUTION OF MODEL MOX FUELS IN HYDROTHERMAL CONDITIONS

Starting date: 01/10/2026

Interfaces of Material in Evolution Laboratory (LIME)

Contacts Nicolas CLAVIER – nicolas.clavier@icsm.fr
Nicolas DACHEUX – nicolas.dacheux@umontpellier.fr

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

Funding CEA **Reference** SL-DES-26-0090

Abstract

The **dissolution of irradiated spent fuels** is a prerequisite step for their reprocessing and for closing the nuclear fuel cycle through the valorization of plutonium produced in reactors. However, irradiated fuels, particularly MOx, contain refractory phases that are difficult to dissolve, and which may include high plutonium concentrations, strategic elements (Ru, Pd, Rh), and/or complex phases that are challenging to manage.

This PhD project offers to **explore the use of mild hydrothermal conditions** (100–200 °C, under autogenous pressure) to i**mprove the dissolution of irradiated MOx fuels**, using model materials representative of the different phases: uranium matrix, plutonium-enriched zones, metallic precipitates (PGM), and perovskite-type oxides. The use of thorium as a surrogate for plutonium, along with stable isotopes of fission products, will enable the study of dissolution kinetics and mechanisms under unprecedented conditions, particularly the coupled influence of temperature and pressure.

The work will be structured in several stages, from the **dissolution of simple $(U,Th)O_2$ solid solutions** lightly doped with fission product simulants, to the **study of refractory phases** highly enriched in thorium or PGM, and finally to t**esting on a global fuel simulant**. The approach will combine **solution chemistry analyses with operando observations** of solid/liquid interfaces, in order to identify preferential attack zones, formed residues, and the role of microstructure. In addition, collaboration with CEA/ISEC/DMRC/SPTC/LSEM will ultimately allow the extension of the study to plutonium-bearing compounds at the ATALANTE facility of CEA Marcoule.

Candidate profile

This PhD subject is intended for candidates with a Master's or Engineering degree in **radiochemistry**, **separation chemistry**, or **materials chemistry**, with a **strong interest in experimental research** with practical applications in an academic context.

Benefit for the candidate

- **Skill Development:** Upon completion of the thesis, you will have acquired a **recognized expertise** in the field of **nuclear materials**, **recycling,** and **radiochemistry**, opening numerous **professional opportunities in both academic research and industrial R&D**.
- **Working Environment:** The thesis will be supervised by ICSM researchers from the LIME group (N. Clavier, N. Dacheux, and L. Claparède) and by a CEA researcher from the ISEC/DMRC/LSEM team (L. Muller). The **shared supervision** of the thesis will ensure scientific monitoring of all aspects of the subject. Both teams welcome several doctoral students in a dynamic working environment conducive to the production of original results.
- **State-of-the-Art Laboratory**: You will have the opportunity to work in laboratories equipped with a rich array of advanced instruments, and allowing **experiments with radioelements** such as uranium, thorium, and plutonium.

How to apply

Please send a cover letter, a detailed CV, and references to Nicolas Clavier (nicolas.clavier@icsm.fr) and Nicolas Dacheux (nicolas.dacheux@umontpellier.fr).