

MOBILITY MISSION REPORT

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MISSION TITLE

Attendance at the ATAS-AnXAS 2022 - Joint Workshop, October 17-21, 2022, Grenoble, France

DESCRIPTION


Concerned organisations

- Research entities
- Technical support organisations

Concerned infrastructures or facilities

- Other relevant infrastructure or facility to be specified: European Synchrotron Radiation Facility (ESRF, Grenoble, France), as venue of the workshop as well as a scientific infrastructure.

Concerned phases

- Phase 1: Site evaluation and site selection
 - Phase 2: Site characterisation
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Themes and topics

The following themes and topics (among others) were presented and discussed during the workshop and/or are related to the presented work.

- Theme 3: Engineered barrier system (EBS) properties, function and long-term performance
 - Spent Fuel and high-level waste disposal canisters
 - Clay-based backfills, plugs and seals
- Theme 4: Geoscience to understand rock properties, radionuclide transport and long-term geological evolution
 - Perturbations (gas, temperature and chemistry)
 - Aqueous pathways and radionuclide migration
- Theme 7: Performance assessment, safety case development, and safety analyses
 - Integration of safety-related information
 - Performance assessment and system models
 - Treatment of uncertainties

Keywords

Workshop attendance; scientific exchange; radionuclide migration; reactive transport; chemical imaging and tomography.

EXECUTIVE SUMMARY

The safety case for a deep geological repository (DGR) for high-level radioactive waste (HLW) requires a detailed knowledge about retention and transport processes. Argillaceous rock is considered as a potential host rock, with Opalinus Clay (OPA) as a reference material for a natural clay rock. This natural material is characterized by a multiscale structural and compositional heterogeneity.

In previous studies applying synchrotron-based multimodal chemical imaging on compacted OPA samples in sorption and diffusion experiments with Np and Pu, a significant role of pyrite (FeS_2) was identified in the retention of the studied radionuclides. Extending these studies in a continued collaboration between Johannes Gutenberg University Mainz (JGU, Mainz, Germany) and the Swiss Light Source (microXAS beamline project, Paul Scherrer Institute, Villigen, Switzerland) sub-mm-sized pyrite composites were isolated from OPA, subjected to sorption experiments with Np and Pu and studied by multimodal chemical tomography, gaining structural, elemental, mineralogical and chemical information in three dimensions.

Results of this study were presented at the ATAS-AnXAS 2022 - Joint Workshop (5th International Workshop on Advanced Techniques in Actinide Spectroscopy (ATAS) & 9th Workshop on Speciation, Techniques and Facilities for Radioactive Materials at Synchrotron Light Sources (AnXAS)), jointly organized by the European Synchrotron Radiation Facility (ESRF, Grenoble, France), also serving as the venue of the workshop, and Helmholtz-Zentrum Dresden-Rossendorf (HZDR, Dresden-Rossendorf, Germany). The workshop covered topics concerning research on actinides and radioactive materials with spectroscopy and synchrotron-based techniques, also comprising topical sessions on radioactive waste disposal, actinides-related bio-geochemistry and nuclear materials. The workshop provided an opportunity for presenting the work and results of our

collaboration, scientific exchange and learning about new studies and techniques related to actinides and radioactive waste disposal.

1. MISSION BACKGROUND

1.1. R&D background

In previous studies [1-3] synchrotron-based multimodal chemical imaging was applied to sorption and diffusion studies of actinide species with Opalinus Clay (OPA) from the Mont Terri rock laboratory (St-Ursanne, Switzerland). Pyrite, contained in OPA as micro-scaled mineralogical heterogeneities, was identified to play a significant role concerning the observed redox transformations to reduced, less mobile actinide species. To further elucidate the role of these pyrite heterogeneities in reactive transport, sub-mm-sized particles of pyrite were extracted from OPA, subjected to sorption experiments with Np(V) and Pu(VI) and investigated by multimodal chemical tomography, combining structural, elemental, mineralogical and chemical volume information. Results so far indicate an enhanced geochemical reactivity depending on the morphology of these pyrite particles, namely the framboidal morphology, contributing to a better understanding of the reactive transport of actinide species in Opalinus Clay.

1.2. Mission objectives

The scope of the ATAS-AnXAS 2022 - Joint Workshop [4] comprises topics concerning fundamental and applied research on actinides and radioactive materials with advanced spectroscopic and synchrotron-based techniques. The scientific programme also includes a session on nuclear materials and their storage and geological disposal.

Together with involved colleagues from JGU (S. Amayri, T. Reich) and the Swiss Light Source (D. Ferreira Sanchez, D. Grolimund; microXAS Beamline project, PSI, Switzerland) I submitted an abstract about our collaborative and WP FUTuRE related work titled “Chemical tomography of pyrite composites extracted from Opalinus Clay and reacted with Np and Pu” which got accepted for an oral presentation. On this occasion I would like to present our recent study continuing the collaborative work between JGU and microXAS.

With presenting our results at this workshop I hope to get critical feedback and initiate scientific exchange on our recent work but also for future studies. With my interest in X-ray- and synchrotron-based techniques I also hope to learn more about technological progress and advanced techniques, maybe applicable to problems related to reactive transport and radioactive waste in general.

1.3. Mission request

Attending the ATAS-AnXAS 2022 - Joint Workshop, October 17-21, 2022, Grenoble, France.

1.4. Mission composition

Host organisation

The ATAS-AnXAS 2022 - Joint Workshop [4] is jointly organized by the European Synchrotron Radiation Facility (ESRF, Grenoble, France) and Helmholtz-Zentrum Dresden-Rossendorf (HZDR, Dresden-Rossendorf, Germany).

Host facility

European Synchrotron Radiation Facility (ESRF, Grenoble, France).

Mission dates

16 October 2022 - 21 October 2022

2. MAJOR PRACTICES, TECHNIQUES, METHODS, TOOLS OR SYSTEMS OPERATED OR STUDIED

The scope of the workshop was centred around advanced spectroscopic and synchrotron-based techniques as well as related theory for actinide speciation, but no practices, techniques, methods, tools or systems were operated or practically studied during the mission at the workshop.

2.1. Practice, technique, method, tool or system operated or studied during the mission

N/A

Description

N/A

Usage

N/A

Benefits

N/A

Limitations

N/A

Applicability

N/A

2.2. Practice, technique, method, tool or system operated or studied during the mission

N/A

Description

N/A

Usage

N/A

Benefits

N/A

Limitations

N/A

Applicability

N/A

2.3. Practice, technique, method, tool or system operated or studied during the mission

N/A

Description

N/A

Usage

N/A

Benefits

N/A

Limitations

N/A

Applicability

N/A

2.4. Practice, technique, method, tool or system operated or studied during the mission

N/A

Description

N/A

Usage

N/A

Benefits

N/A

Limitations

N/A

Applicability

N/A

3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

Attendance of the ATAS-AnXAS 2022 - Joint Workshop proved to be a valuable experience in several aspects. Scientifically, by gaining feedback on our presented work, especially with an attention on anaerobic experimental conditions as well as an emphasis on the chemical speciation of the immobilized actinides in the presented study.

Several presentations were concerned with studying actinide speciation with the emerging high energy resolution X-ray absorption near-edge structure (HR-XANES) spectroscopy, covering both experimental and theoretical aspects, showing the potential of this technique with an improved probing of the valence state and coordination environment as well as applying these techniques in RWM-related experiments, studying, e.g., the Np speciation at low concentrations of 1 ppm in sorption and diffusion experiments [5].

Another new probe for chemical speciation was presented as an extended modality of the microXAS beamline (SLS, PSI), described as X-ray absorption spectroscopy - contrast microscopy, which represents a spectromicroscopical approach for a spatially resolved species distribution, most probably applicable to our future studies. A presented recent method development for the derivation of improved μ XRF-based actinide speciation maps, compensated for local concentration variations of the probed element [6], may also find an application in current and future work.

Attending the workshop was also personally a valuable experience by gaining experience presenting at an international workshop as well as initiating scientific exchange.

The workshop was very well organized and allowed to focus on the presentations and scientific exchange. The synchrotron facility reports as well as a visit to selected and X-ray absorption spectroscopy (XAS) related beamlines at the ESRF were also valuable by learning about current and future experimental capabilities, some also related to RWM activities.

3.2. Relevant findings and conclusions for home organisation

N/A

3.3. Relevant findings and conclusions for host organisation

N/A

3.4. Relevant findings and conclusions for other organisations

N/A

4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

4.1. Generic potentials

N/A

4.2. Potentials for home organisation

N/A

4.3. Potentials for host organisation

N/A

APPENDICES

Mission journal

16/10/2022 (afternoon) - Travel from Frankfurt (Germany) to Grenoble (France).

17/10/2022 - 1st day of the workshop - Registration and welcome at the workshop. A detailed e-booklet provides the final programme and abstracts of the contributions [4]. First two sessions related to radioactive waste disposal and actinides-related biogeochemistry.

18/10/2022 - 2nd day of the workshop - Continuation of the workshop with presentations concerning experimental and theoretical topics in aqueous and coordination chemistry, nuclear materials and electronic structure. Current capabilities and recent studies at synchrotron beamlines approved of radioactive samples were presented in facility reports. Concluding the 2nd day with attending the poster session.

19/10/2022 - 3rd day of the workshop - Topics of today's sessions focused on electronic structure, related theory and emerging techniques. Further synchrotron facility reports.

20/10/2022 - 4th day of the workshop - Continuation of topical sessions concerning biogeochemistry, aqueous and coordination chemistry and radioactive waste disposal. Own presentation in the first session. Further synchrotron facility reports. Concluding the 4th and last day of presentations attending the workshop dinner where poster and best young scientist prizes were awarded.

21/10/2022 - 5th and last day of the workshop - Presentation of the ESRF and EBS upgrade. Guided tour visiting three different X-ray absorption spectroscopy (XAS) related beamlines. End of workshop and return travel in the afternoon.

Mission bibliography

[1] Fröhlich, D.R., Amayri, S., Drebert, J., Grolimund, D., Huth, J., Kaplan, U., Krause, J., and Reich T. (2012). Speciation of Np(V) uptake by Opalinus Clay using synchrotron microbeam techniques. *Analytical and Bioanalytical Chemistry*. 404, 2151-2162. <https://doi.org/10.1007/s00216-012-6290-2>

[2] Kaplan, U., Amayri, S., Drebert, J., Rossberg, A., Grolimund, D., and Reich T. (2017). Geochemical Interactions of Plutonium with Opalinus Clay Studied by Spatially Resolved Synchrotron Radiation Techniques. *Environmental Science & Technology*. 51, 7892-7902. <https://doi.org/10.1021/acs.est.6b06528>

[3] Börner, P.J.B. (2017). Sorption and diffusion of Neptunium in Opalinus Clay. PhD thesis. Johannes Gutenberg University Mainz, Germany.

[4] ATAS-AnXAS 2022 Joint Workshop. Workshop website with final programme and abstracts of oral and poster presentations. <https://www.esrf.fr/ATAS-AnXAS>

[5] Schacherl, B., Joseph, C., Lavrova, P., Beck, A., Reitz, C., Pruessmann, T., Fellhauer, D., Lee, J.-Y., Dardenne, K., Rothe, J., Geckeis, H., and Vitova, T. (2022). Paving the way for examination of coupled redox/solid-liquid interface reactions: 1 ppm Np adsorbed on clay studied by Np M₅-edge HR-XANES spectroscopy. *Analytica Chimica Acta*. 1202, 339636. <https://doi.org/10.1016/j.aca.2022.339636>

[6] Ding, H., Dixon Wilkins, M. C., Mottram, L. M., Blackburn, L. R., Grolimund, D., Tappero, R., Nicholas, S. L., Sun, S., Corkhill, C. L., and Hyatt, N. C. (2021). Chemical state mapping of simulant Chernobyl lava-like fuel containing material using micro-focused synchrotron X-ray spectroscopy. *Journal of Synchrotron Radiation*. 28, 1672-1683. <https://doi.org/10.1107/S1600577521007748>

MISSION BENEFICIARY

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PhD student

Klikněte nebo klepněte sem a zadejte text.

Klikněte nebo klepněte sem a zadejte text.

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Workshop committees: organizational, administrative and scientific committees of the ESRF (Grenoble, France), HZDR (Dresden-Rossendorf, Germany) and international research facilities (cf. the e-booklet [4] with a compilation of names and affiliations)

Home organisation experts

- Tobias Reich (PhD supervisor) and Samer Amayri, Department of Chemistry - TRIGA site, Johannes Gutenberg University Mainz, Germany

Other organisations experts

- In the framework of a scientific collaboration, whose work and results were presented at the workshop: Daniel Grolimund and Dario Ferreira Sanchez, microXAS beamline project, Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
18.11.2022	Klikněte nebo klepněte sem a zadejte text.		N/A
	Visa	Visa	N/A