

PROJECT FINAL REPORT

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EXECUTIVE SUMMARY

Actinides play an important role for the safety assessment of the nuclear fuel cycle. It is therefore of major interest to understand their very specific properties and to be able to assess and control their behaviour under all relevant conditions from mining to waste geological disposal.

Safety issues related to nuclear energy, such as accidental radionuclide release from a power plant or waste form degradation and discharge of radiotoxic constituents during storage and final disposal are always connected with fuel and fuel components and thus also with actinides and their properties. It is thus of cardinal importance to keep and increase our knowledge on actinide sciences. Moreover, to maintain its high level of expertise in actinide sciences, Europe must also educate the next generation of scientists and engineers who will contribute to develop safe actinide management strategies.

Actinides study requires specific tools and facilities that are only available in a limited number in Europe. Actually, only a few academic and research organisations have the capabilities to work on these elements under safe conditions. It is therefore of strategic importance to coordinate the existing actinide infrastructures available in Europe, and to strengthen the community of European scientists working on actinides.

The establishment of a network of excellence for actinide science – ACTINET-6 – was a first step in this direction, achieved with the support of the European Commission under the 6th Framework Programme. This network gathered major laboratories involved in nuclear research and a wide range of academic research organisations and universities. Its members established a set of communication tools and common procedures to open the facilities to scientists from outside, to share resources and information. Moreover, they launched joint research projects taking advantage of the availability, within the network, of a pool of facilities.

In the continuation of the ACTINET-6 Network of Excellence, the ACTINET-I3 Integrated Infrastructure Initiative, has gathered the main European research centres in actinide sciences in order to maintain the networking between existing European infrastructures in actinide sciences, to significantly promote scientific knowledge in actinide science by offering access to laboratory facilities with advanced cutting edge experimental and spectroscopic capabilities, to combine state-of-the art experimental with theoretical first-principle methods on a quantum mechanical level to tackle the actinide challenge, and to benefit from the synergy between the different scientific and technical communities like large research centers and universities. 59 Joint Research Projects (JRPs) were performed in the five Pooled Facilities (CEA-ATALANTE and DPC, ITU, KIT-INE and ANKA, HZDR-ROBL, PSI-SSL) corresponding to about 1500 days of access. The JRPs addressed the three topics: actinide chemistry for separation, actinides in the geological environment, and actinide materials. These JRPs were supported by ACTINET-I3 after selection by the Scientific Advisory Committee and the Executive Committee. More than 70 young reserachers were then allowed to conduct their projects in the Pooles Facilities.

In parallel, four Joint Research Activies (JRA) were carried out between consortium members in order to improve the performance of infrastructures by developing new relevant instrumentations and/or data of common interest. Further, these activities were complemented by a virtual infrastructure providing a limited support in theory and modelling, with a focus on the complementarities between theory and experiments. The first JRA worked at the understanding of the selectivity in actinide separation, in close collobarion with the ACSEPT project. The second and third ones aimt at developing databases on EXAFS spectra and on actinide materials for fuel respectively. The fourth one was dedicated to the development of a method combining experimental and theoretical approaches to exploit EXAFS data.

ACTINET-I3 has also been a key tool to increase the skills of Europe in nuclear sciences by promoting training and education actions. Three Actinet summer schools, two ThUL schools and two plenary meetings were organised to promote the network and trained young scientists. In addition, ACTINET-I3 sponsored International conferences Migration 2011, Atalante 2012 and ATAS 2012 by supporting travel grants attributed to students by the Conference boards. ACTINET-I3 was also presented through poster (Migration 2011) and lectures (invited or contributed) in international conferences (ICAPP 2012, MRS 2012) and was invited to contribute the 2011 J-ACTINET summer school (5 representatives)

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PART I: FINAL PUBLISHABLE SUMMARY REPORT

1 DESCRIPTION OF PROJECT CONTEXT AND OBJECTIVES

Actinides play a central role in the nuclear energy generation systems: uranium and plutonium are introduced as a fuel in the reactors, and the other actinides are produced by the nuclear reactions. They are all present in spent fuels, and they can be considered either as waste or as potential resources to be processed and recycled.

It is therefore of major interest, from both resource management and waste management, to understand the very specific properties of these elements, and to be able to assess and control their behaviour in a wide variety of environments, ranging from geological systems (mining, deep underground repository...), fabrication processes (fuels, transmutation targets...), nuclear reactor irradiation, spent fuel processing (hydro- and pyro-chemistry), etc.

Indeed, the realization that actinides – like other resources on earth – are only available in finite quantities while the demand on non-fossil energies is foreseen to increase dramatically in the forthcoming decades, leads to a renewed increasing interest for the physics and chemistry underlying actinide management in the nuclear fuel cycle.

In order to keep a leading position in the field of nuclear energy – both in terms of safety and efficient use of natural resources – Europe needs to reinforce its expertise and to prepare the next generation of scientists and engineers who will contribute to develop actinide management strategies based on sound scientific bases.

However, because most actinides are radioactive, their study requires specific tools and facilities that are only available in a limited number of laboratories in Europe. In particular, only a few academic and research organisations have the capabilities to work on these elements. It is therefore strategic to coordinate the existing Actinide Infrastructures available in Europe, and to strengthen the community of European scientists working on actinides.

The establishment of a network of actinide scientists – ACTINET – was a first step in this direction, achieved with the support of the European Commission under the 6th Framework Programme (Network Of Excellence ACTINET-6). This network gathered major laboratories involved in nuclear research and a wide range of academic research organisations and universities. Its members established a set of communication tools and common procedures to share resources and information. Moreover, they launched joint research projects taking advantage of the availability, within the network, of a pool of facilities.

As a second step, ACTINET-I3, as an Integrated Infrastructure Initiative, has the objective to reinforce the networking between existing European infrastructures in actinide sciences, and to facilitate their efficient use by the European scientific community.

In accordance with the guidelines of the EC funding scheme I3, the concept of the ACTINET-I3 has been:

- (i) To establish a network of Actinide facilities across the EU to integrate and to structure better the way these Actinide infrastructures operate and to foster their joint development in terms of capacity and performance. To progress toward the establishment of a European Research Area in the field of actinide sciences through a web based collaborative platform and other communication tools and initiatives;
- (ii) To support and manage jointly an access to appropriate research infrastructures for training and associated research projects making use of the proposed research facilities by supporting Transnational Access to these facilities through the organization of periodic calls for Joint Research Projects (JRP)
- (iii) To conduct on a limited scale a set of Joint Research Activities (JRA) involving member organisations, with an objective to improve the performance of infrastructures by developing new relevant instrumentations and/or data of common interest. Further, these activities were complemented by a virtual infrastructure providing a limited support in theory and modelling, with a focus on the complementarities between theory and experiments.

It was therefore a major objective of the project to develop and reinforce a structure to manage a set of resources pooled for the benefit of the European Community of actinide science. The ACTINET-I3 pooled facilities have laboratories that have allowed users:

- to handle radioactive materials at various levels of activity (hot cells, alpha-glove boxes);
- to work in specific conditions (inert gas, high temperature,...),
- to access analytical tools (elementary and isotopic analysis, liquid, solid and interface analysis etc.),
- to use specific methods (laser spectroscopy, synchrotron radiation...),
- to access expertise in modelling and simulation, education and means to support experimental work in actinide science.

Beyond collaboration among researchers, the challenge was also to organize a structural framework for the sustainable development of the European Research Area, through a policy of research infrastructures in Europe. Two main lines of actions were considered:

- i) benefit from the complementarities of existing tools by implementing appropriate rules for their use, by ensuring their management at European level, and by granting access to a wider set of users, from academic researchers to industrial partners,
- ii) stimulate the complementarities of the national tools by designing and implementing coherent European policies for their evolution and their future development.

Last but not least, the students and young researchers were the main beneficiaries of the access to ACTINET-I3 facilities. This has played a major role in the training of the next generation of actinide scientists and engineers.

2 DESCRIPTION OF THE MAIN S&T RESULTS/FOREGROUNDS

2.1 Networking between pooled facilities and users

2.1.1 Description of the publicity concerning the new opportunities for access

The majority of this activity deals with providing JRP users the best possible access and networking to actinide facilities and infrastructures to solve their scientific problems.

The selection of the JRPs to be funded was organized through calls for proposals (March 2010, October 2010 March 2011, September 2011 and January 2012). At the end of each call, all the proposals were sent to the Scientific Advisory Committee (SAC) for advice. A list of ranking criteria, established by the Executive Committee (ExCom) was delivered to the SAC prior the first evaluation.

These criteria were:

- The originality of the subject, taking into account the state of the art (is it really new or already done?)
- The skills of the teams (both visitor and pooled facility) to carry out the JRP.
- The subject must fit at least with one of the ACTINET-I3 topics.
- The relevance of the choice of the Pooled Facility to carry out the JRP
- All the results must be publishable

Each JRP was therefore ranked between A and C according the following table

A:	Scientifically excellent to good
	Well-formulated proposal
	Well within the scope of ACTINET
B:	Scientifically good to satisfactory
	With some weakness in the proposal
	Within the scope of ACTINET
C:	Proposal is scientifically not acceptable or does not fulfil one or both of the following criteria:
	The scope of ACTINET
	Scientific quality of the proposal

The members of the SAC were Rudy Konings (Chairman), Jan Olov Liljenzin, Ingmar Grenthe, Tobias Reich, Yannick Guérin (Calls 1&2) and Carole Valot (Call 3)

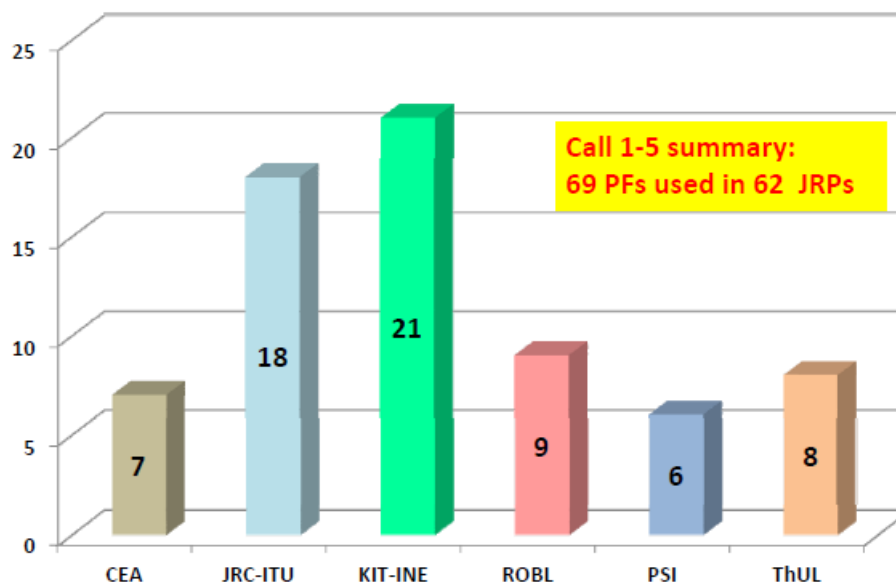
After advice of the SAC, the ExCom proceeded in the JRP selection for funding. All the JRPs ranked A et B were funded. For those ranked B, some conditions were requested or the funding was reduced compare to the initial cost evaluation.

A Pooled Facility (PF) Brochure was also prepared made available through the ACTINET-I3 website. In addition, a presentation of the PFs, their available equipment and NA3 activities, as well as cross cutting activities in which the PFs are involved, was also formally made at the Plenary Meeting in Marcoule in Feb. 2011 and again at the Plenary Meeting in Avignon in Jan 2013.

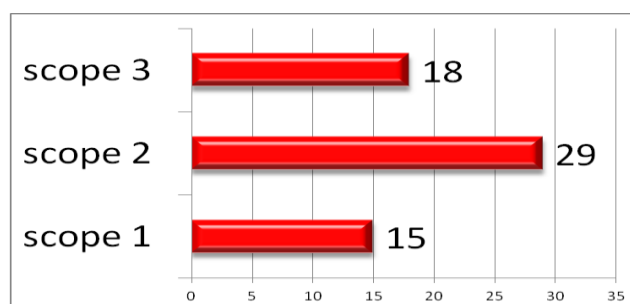
Over the five calls for proposal ACTINET-I3, there were 91 Joint Research Projects (JRPs) submitted. Among them, 62 JRPs were selected for funding and 59 were performed (three were cancelled mainly because of a change in the position of the foreseen student), hosted at 69 stays at PFs. The number of PFs involved is larger than the number of JRPs simply because a number of JRPs (7 in total) requested the use of more than one PF. This often involved using a PF for sample preparation and another PF for a specific type of characterization, not available at the PF where the sample was prepared.

For each JRP, a final activity report was delivered.

Call	Number of submitted JRPs	Number of selected JRPs
1	20	11
2	8	7
3	22	17
4	21	11
5	20	13



The distribution between the three different scopes, scope 1= separations, scope 2= environmental actinide chemistry and scope 3= irradiated materials is shown below. The larger number of JRPs in scope 2 is also reflected in the relatively large number of JRPs performed at KIT-INE, whose expertise lies mainly in this area. The distribution between the three scopes is better than it was in the FP6 ACTINET-6 program, however. This is considered as an improvement.



Another task consisted in defining instrument upgrades. Each PF made equipment available or improved on existing designs, in order to meet the users' needs. In addition, a number of improvements and additions to the available instrumentation and infrastructure were identified. The following summarizes this information provided by all PF responsible persons, with additional comments added from the discussion during the telephone conference:

- Single crystal diffraction and powder diffraction with tunable wavelengths (anomalous dispersion) for actinide materials is missing. Requires a diffractometer, a variable wavelength source (usually a synchrotron), appropriate detectors (e.g., area CCD).
- Optimization of low-energy (P and S K-edge and actinide M edge) measurements at the INE-Beamline (the only PF beamline with this capability). Requires positioning motors and a mirror system for higher harmonic rejection.
- From the ROBL user community, there is substantial interest in having a hard-x-ray STXM for actinides with a resolution in the 10 micron range (i.e. one order of magnitude larger than what can be achieved at PSI), but with excellent stability for low concentration EXAFS (and also XRF and XRD). The recent ROBL optics upgrade is a prerequisite for this, but requires an additional Pb hutch, focussing optics, a table, stages, control units, detector, etc. The investment would be in the range of 1 to 1.5 Mio EUR Even

more important would be accessing the expertise at the INE-BL at ANKA and micro-XAS at PSI to develop the best possible design.

- Need for optimization of EXAFS cells for investigations of actinide containing solutions (e.g., Np, Pu, Am), potentially including hyphenated techniques such as electrolysis and taking into account all the related safety issues was expressed. However, it was noted that there are electrochemical cells, cells for high temperature and pressure, and inert gas cells for liquids already available. Obviously more exchange of information between PFs would be helpful.
- Development of an irradiation cell dedicated to alpha, electron and gamma beam (such as cyclotron or gamma irradiation source) for radioactive solutions (Pu, Np) taking into account all the safety issues, would be nice.
- Development of harmonised methods for the preparation, the characterisation, the stabilisation of actinide solutions (Np, Pu and Am) in the lab, taking into account all the radiolytic effects, analytical measurements' and safety issues. This suggestion caused some hefty discussion, as the wording "harmonized" carried some negative connotations. The main argument was that any development of harmonised methods is in total discord with the very spirit of ACTINET. In ACTINET facilities are pooled to create a virtual (super) facility with the added value of providing a truly broad range of instrumentation, methods and expertise to the community. The word 'harmonize' sounds like 'unify' and was interpreted as potentially reducing this added value of pooling the facilities. A counter argument was expressed that stabilization methods could avoid degradation of samples (from radiolysis, for example) before arrival at a beamline. The MicroXAS and INE-Beamline are on the same site as the PSI and the INE and ITU laboratories, have less problems as transport can be done within minutes, so that this is not an important issue for them.
- PSI suggested that the community would benefit from availability of improved detectors allowing new types of measurements, but also speeding up data acquisition and improving data quality significantly. Examples include
 - An improved area detector (e.g., Pilatus 300K instead of Pilatus 100K), which would enhance the present 2D microXRD imaging capabilities.
 - A large area SDD of the latest generation (enhanced thickness of diode) for improved spectroscopy
 - HR-XES crystal spectrometer allowing new types of measurements (compare, e.g., existing device at INE)
- HR-XES capability is missing and could be developed and managed by a small collaborative project within the network. Requires development of high-yield, high-energy XES spectrometers for actinides. It was noted that INE is building a new multi-crystal HR-XES spectrometer and has a single crystal instrument with dynamical bender already. Another one (only for PFY-XAFS) is available at the MARS beamline and, hence, limited to studies under the exemption limit. Both these activities are nationally funded.
- Methods for reducing, avoiding, circumventing radiation damage during synchrotron measurements with high flux density are needed. Other than cryo-cooling, it is not clear what this would entail, however.
- Training in data processing, analysis, and interpretation should be offered. The idea of having internships reinstated (they were available in the first ACTINET) to support this was discussed and held as especially desirable by all PF responsible persons, but not by the project coordinator.
- There was no specific request to upgrade/improve our equipments at ITU in ACTINET i3.

2.2 Transnational Access to the Pooled Facility: CEA

7 JRPs were hosted at CEA. The 8 researchers hosted were all students (graduates, PhD, Post-Doc) from 7 different research Laboratories (from 6 Universities). All of them are out of the ACTINET-I3 Consortium. All the 7 JRPs involved the handling of minor actinides.

JRP n°	Title	Scope	SAC mark	Visitors number	Country	Organisation	Access quantity	Publication
C1-17	Exploring chemic. difference between trivalent Ln and An by MS-techniques	1	B	2	Portugal	UCQR Portugal	115	1
C3.02	Covalency and CCl studies through reduction and metal-metal interact. in TRU-molecules	1	A	1	UK	Univ. Edinburgh	10	

C3-08	Aqueous An Cation Magnetic Susceptibility as function of oxidation state	1	B	1	USA	Washingt. State Univ.	60	1
C4-08	Using ESI-MS to Understand Actinide Speciation in Separations Systems	1	B	1	USA	Washington State Uni	40	
C4-20	Character. of An carbide interface (UC) during the chemical dissolution in aqueous solution	1	B	1	Russia	Lomonosov Univ	60	
C5-09	Investigations on newly synthesized complexing agents for An selective stripping	1	A	1	Italy	Politecnico di Milano	60	
C5-13	Understanding molecular speciation in SANEX and GANEX separations of An from Ln	1	B	1	UK	Univ Manchester	60	

2.3 Transnational Access to the Pooled Facility: ITU

15 JRPs were performed at ITU from 8 different applicants (7 universities and CEA). 3 publications have already been published.

JRP n°	Title	Scope	SAC mark	Visitors number	Country	Organisation	Access quantity	Publication
AC1-JRP19	A thermodynamic study of mixed oxide solid solution. Part I (Th,U)O ₂	3	B	1	Cz	Charles University, Prague	4 days	
AC1-JRP20	Helium behaviour in glass waste forms, impact of high actinide loading factor?	3	B	2	F	CEA	60days	1
AC2-JRP04	Comparison of laboratory sorption measurements and in situ partitioning data for U	1	C	1	Ro	National Institute of Public Health	10 days	
AC2-JRP05	Redox and magnetism studies of discrete plutonium containing molecular species, from monometallic complexes to multimetallic molecular arrays	2	B	1	UK	University of Manchester	91 days	
AC2-JRP06	In-situ synchrotron studies of the structure, chemistry and stability of U-Ce and U-Pu oxide thin films	3	A	1	UK	Imperial College	60 days	
AC3-JRP01	Interaction of sodium with advanced oxide fuels	3	B	1	UK	University of Cambridge	59 days	1
AC3-JRP02	Covalency and CCl studies through reduction and metal-metal interactions in transuranic molecules	1	B	1	UK	University of Edinburgh	10 days	
AC3-JRP05	Sputter deposition of U-Fe films	3	A	2	Po	Charles University, Prague	17 days	
AC3-JRP19	Effect of alpha decay of actinides on the structure of nuclear waste glasses	3	A	0	F	CEA	21 days	
AC4-JRP07	Effect of the radioactivity on the glass leaching solid analyses	3	A	2	F	CEA	17 days	
AC4-JRP10	TEM studies on UCoGe	3	A	1	P	Istituto Tecnologico e nucleare	5 days	
AC4-JRP18	investigation of the incorporation of neptunium during secondary mineral formation on spent nuclear fuel	3	B	1	UK	University of Cambridge	27 days	
AC5-JRP02	interaction of advanced oxide fuels for Gen-IV SFR with Na	3	B	1	UK	University of Cambridge	50 days	
AC5-JRP19	enhancement of 5f magnetism under very high pressure UGa ₂	2	A	2	P	Charles University, Prague	20 days	

2.4 Transnational Access to the Pooled Facility: KIT

21 Joint Research Projects (JRPs) were performed at KIT over the duration of ACTINETi3 from 14 different applicants. 4 publications have already been written.

JRP n°	Title	Scope	SAC mark	Visitors number	Country	Organisation	Access quantity	Public -ation
C1-05	Spectroscopic investigation of redox reactions of Pu with Fe minerals	2	B	1	DE	HZDR	18 days	
C1-07	Cm3+/Eu3+ interaction during second. phase formation in affection/diffusion controlled...	2	B	2	FR	BRGM	16 days	
C1-10	Solubility studies of Np(V) and Np(VI) under alkaline pH and controll redox conditions	2	A	2	CH	PSI	21 days	2 in C5-10 (follow-up)
C1-18*	In-situ RIXS studies of the possibil. of existence of Pu(V) ind Pu-dioxide	2	A	1	SE	Uppsala Sweden	10 days	
C2-03	Trivalent actinides binding to magnetite	2	B	2	DK	Univ Copenhagen	6	
C2-06	In.situ Synchrotr. Stud. of U-Ce and U-Pu oxide thin films	2	B	1	UK	Imp. College London	7	
C2-08	Vibrational spectroscopic studies of hydrated Ln(III) and An(III) ions	2	A	2	SE	Stockholm Uni	28	
C3-04	Speciation of U incorporated in bone-like collagen-apatite	1	B	4	FR	ICSM Marcoule	17	
C3-06	Interaction of Nd(III)/Cm(III) and Np(IV) with gluconic acid: solubility, sorption TRLFS study...	2	A	1	ES	CIEMAT	36	1
C3-07	Sorption of trivalent actinides on quartz and silica at high salt concentrations	2	A	2	UK	Lomonosv Univ.	78	1 under preparation
C3-15	Role of Mn in Np cycling...	2	B	1	UK	Uni Manchester	5	
C3-20	Local probes of fundam. struct. in nucl. fuel mater.s: Pu subtitit. a. evolut. dur. irradiation...	3	B	1	UK	Uni Cambridge	1	
C3-21	Actinide-complexation and extraction properties of solid-supported BTP and BTPhen ligands.	1	A	1	UK	Uni Reading	11	
C4-06	Local structure and charge distribution in U1-yAmyO2-x (0.15 < y < 0.50)	3	B	4	FR	CEA Marcoule	12	
C4-15	In-Situ RIXS studies of the possibilities of the Pu(V) existence in Pu dioxide: Continuation	2	A	1	SE	Uppsala Sweden	4	
C4-18	Investigation of incorporation of Np during secondary mineral formation on SF	2	A	1	UK	UniCambridge	2	
C5-01	EXAFS/XANES investigations of PuCrO3 saturated mixed oxide (U,Pu)O2	3	A	3	FR	CEA-Cadarache	39	
C5-06	Np biogeochemistry in a geological disposal facility chemically disturbed zone	2	B	5	UK	Uni Manchester	16	
C5-10	Np(V) solubility and solid phase transformations in NaCl, NaClO4 and MgCl2 solutions...	1	B	1	UK	Lomonosov Univ.	46	2
C5-12	Understanding molecular speciation in SANEX and GANEX separations of An from Ln	1	B	1	UK	UniManchester	49	
C5-20	Coprecipitation of plutonium with magnetite, siderite/chukanovite, and mackinawite:	2	B	1	DE	HZDR-ROBL	20	

2.5 Transnational Access to the Pooled Facility: HZDR

A total of 20 proposals have been submitted to ROBL-HZDR in 5 calls; 11 of these have been accepted as JRPs. Seven of these have been successfully completed at ROBL-HZDR. During the ACTINET-I3 period, ROBL and the ESRF performed major upgrades, causing an extended shutdown period of 9 months (Aug. 2011 – April 2012). Because of this shutdown, 2 JRPs were transferred in mutual agreement to the INE-BL and performed there. Two other experiments (04-14, 05-03) could not be performed before February 2013. The results of these JRPs have been published in 4 rank-A journal articles and presented at several conferences (Actinides, Actinide-XAFS, Plutonium Future, MRI, Migration, Goldschmidt, etc.). Seven more

publications are in preparation or submitted.

JRP n°	Title	Scope	SAC mark	Visitors number	Country	Organisation	Access quantity	Publication
01-04	XAS study of dense U _{1-y} AmyO _{2-x} (y=0.10; 0.15) obtained by conventional powder metallurgy	3	A	4	F	CEA	12	2
01-05	Spectroscopic investigation of redox reactions of plutonium with iron minerals	2	B	1	F	Univ. Grenoble, KIT, HZDR	27 (12 in P2)	1 +1 in prep.)
01-12	EXAFS/XANES investigation of uranium plutonium mixed oxides	3	B	5	F	CEA	18	1 in prep.
02-01	EXAFS study on the influence of humic acid on the sorption of Pu on natural clay	2	B	4	D	Univ. Mainz	12	1 in prep.
02-07	EXAFS/XANES investigation for study of uranium-plutonium-oxygen system for mixed oxide nuclear fuel	3	A	4	F	CEA	9	1 in prep.
04-04	Investigation of Thorium(IV) and Uranium(IV) Silicates: colloid formation - alteration - solid state character	2	B	1	D	FZ-Juelich, HZDR	6	1 in prep.
05-20	Coprecipitation of plutonium with magnetite, siderite/chukanovite, and mackinawite: Structure and solubility	2	A	2	D	HZDR, KIT	15	1 in prep.

2.6 Transnational Access to the Pooled Facility: PSI

In the framework of ACTINET-I3, a total of 9 proposals have been submitted requesting access to the microXAS X-ray microprobe facility hosted by the Swiss Light Source at Paul Scherrer Institute. transnational access was granted to 6 of these submissions. Over the duration of ACTINET-I3, a steady increase in user inquiries and number of finally submitted proposals could be established. This positive trend can be attributed to the only recent opening of the facility (shortly before the start of ACTINET-I3), but also to the permanent networking activities conducted within the framework of ACTINET-I3. The microXAS Beamline Project was approached by several additional requested related to radioactive microprobe analysis, but these were outside the core scope of ACTINET and were not encouraged to submit to ACTINET-I3. A total of 12 scientists were actively involved in experimental work at the beamline facility. Notably, 9 out of the 12 were Young Scientists (PhD student or postdoctoral student level). Accordingly, results elaborated contribute considerably to several doctoral theses. Overall, 5 different European universities or research institutions were involved, all of them being from outside of the ACTINET-I3 core consortium. Further, all of them represent new users to the microXAS beamline facility. Obviously, for both, microXAS and its new users, ACTINET-I3 had a very positive, symbiotic effect. These very stimulating interactions are further documented in a number of fruitful scientific discussions and technical feasibility evaluations resulting in several major upgrades of the experimental facility.

JRP n°	Title	Scope	SAC mark	Visitors number	Country	Organisation	Access quantity	Publication
AC1-JRP11	u-XRF and u-XAFS study of Pu sorption on Opalinus Clay	2	A	4	Germany	University of Mainz	5	ABC 404, 2151 (2012). Image on cover page! For more see AC5-JRP09
AC3-12	Micro-XRF/XRD/XAFS study of Np(V) sorption and diffusion in Opalinus Clay	2	A	4	Germany	University of Mainz	6	see AC5-JRP09

AC4-JRP03	Characterisation of actinide materials in environmental hot particles - depleted uranium munitions residues.	3 (moved to 2)	B	4	UK	University of Sheffield, University of MAnchester	10	1 pub submitted 2 pub in prep 1 conference contribution submitted
AC4-JRP09	Micro-XRF/XRD/XAFS and LA-ICP-MS study of Pu(V)/(III) sorption and diffusion in Opalinus Clay	2	A	4	Germany	University of Mainz	6	see AC5-JRP09
AC4-JRP12	Post Irradiation Investigation of Actinide Targets for the Production of Exotic Isotope Ion Beams	3	B	2	Spain, CH, F	CSIC Spain, CERN	4	2 publ. near submission, 2 publ. in preparation
AC5-JRP09	Micro-XRF, micro-XRD, and micro-XAFS studies on the influence of dissolved Fe(II) on the sorption and diffusion of Pu in natural clay.	2	B	4	Germany	University of Mainz	6	Conf: 21 oral 3 posters 1 proceeding Papers: 1 published 2 near submissions

2.7 Joint Research Activity “Separation science”

2.7.1 Compilation of the status of knowledge

BT(B)P are the most useful extracting or complexing agents for the separation of trivalent actinides from the chemically similar lanthanides: they have very good selectivity and remain effective in nitric acid solutions of relevant concentration. The status of knowledge on BT(B)P is compiled and published in a Chemical Reviews article (Panak, P. J.; Geist, A., Complexation and extraction of trivalent actinides and lanthanides by triazinyipyridine *N*-donor ligands. Chem. Rev. 2013, 113 (2), 1199–1236).

Extraction data for BTP and BTBP have been compared to complex stability constants. Structures of the complexes formed between BT(B)P and trivalent actinides or lanthanides were investigated. Thermodynamic data were collected.

The final complexes (1:3 for BTP; 1:2 for BTBP) identified in solution and in the solid state are representing the complexes that are extracted from an aqueous into an organic phase. The selectivity observed in biphasic extraction experiments correlates directly to differences in the respective stability constants of the 1:3 (BTP) or 1:2 (BTBP) complexes. The unique properties of BT(B)P are explained by the fact that they are able to form strong complexes with trivalent actinides.

2.7.2 Complexation of An(III) and Ln(III) by polynitrogen ligands in organic phases and Relationship between the electronics of the nitrogen ligands and their selectivity between 4f and 5f elements

BT(B)P are the most useful extracting or complexing agents for the separation of trivalent actinides from the chemically similar lanthanides: they have very good selectivity and remain effective in nitric acid solutions of relevant concentration.

To better understand these unique properties, new *N*-donor ligands derived from the BT(B)P structure were synthesized and their extraction and complexation performance towards actinides(III) and lanthanides(III) was studied.

Complexes formed between several Ln(III) (Ln = Nd, Sm, Dy, Ho, Tm) and n-Pr-BTP were investigated by EXAFS. Combined with earlier data for Ln(III) (Ln = Gd, Eu, Lu) and An(III) (An = U, Pu, Am, Cm) a wide range of ionic radii is now covered. TRLFS investigations on the complexation of Cm(III) and Eu(III) with C5-hemi-BTP and C2-BDP in water/alcohol solution were also performed. An NMR study on An(III)-BTP and Ln(III)-BTP complexes is in progress. The role of the anion is of central interest.

From the data available it is concluded that (biphasic) extraction selectivity is governed by (monophasic) complexation selectivity. High selectivity ($SF_{Am(III),Cm(III)/Eu(III)} > 100$) is only achieved if the metal ions are

fully coordinated by N atoms; significant coordination by O atoms lowers selectivity.

2.8 Joint Research Activity “Actinide Reference X-ray Absorption Spectroscopy Database”

2.8.1 XAS Database structure and query masks

A database structure has been created running on Oracle RDBMS 11g, which allows easy adaption to XAFS as well as other spectroscopy data. In order to allow a complete storage of spectra as well as of relevant meta-data, a two-step structure has been established, based on spectra and samples.

A hierarchical permission concept has been implemented, from anonymous login with the most restricted rights via AcXAS-User, AcXAS-Contributor, AcXAS-Editor to AcXAS-Administrator.

Interaction with the user takes place using standard web procedures, html- formatted web-pages generated by the database server (Oracle Application Server) for displaying information as well as CGI compatible form requests for sending data from the client to the server. A data entry and a data query mask has been established.

2.8.2 Data entry

The publications of the three participating beamlines at KIT-INE, PSI-LES and HZDR-IRC were screened for suited reference data. About 150 data were identified and listed in tables.

Thirty of these data sets were selected for an initial data entry, and entry masks and the data base structure was tested and refined.

Users from the group as well as external experts were invited to test the data base with initial data. These tests lead to further improvements of the data base.

2.8.3 Publication and Maintenance

The database containing reference data, data entry and data query masks have been published under <http://www.hzdr.de/Acxas>.

The database has been updated and complemented by additional data sets. As of 31. Jan. 2013, it contains a total of 82 completed and published reference data sets.

2.8.4 Pattern search option

One of the goals of AcXAS was its use as a pattern search database, i.e. to be able to compare experimental spectra with the references spectra in AcXAS for congruency or similarity.

For this, a consistent and automatic EXAFS data extraction module based on IFEFFIT, a freely available code developed at the University of Washington, was implemented

A pattern search module has been established by employing cross-correlation analysis. A special query to compare 2 spectra was implemented.

2.8.5 Database extension to TRIFS

The AcXAS database was adapted to be used also for EELS spectra. It required mainly supplementary variable entries, while the basic structure and query masks could be maintained. Test spectra of NpO₂ were successfully entered.

2.9 Joint Research Activity “Actinide materials”

2.9.1 Experimental investigation of the U-Si-C system

2.9.1.1 Measurement of solid/liquid transition temperatures in UC-SiC

The samples were prepared at CEA Saclay by arc melting under pure argon from pure silicon, uranium and graphite pieces: 4 samples $(UC)_{1-x}(SiC)_x$ with $x=0.1, 0.2, 0.3$ and 0.4 and 5 samples $(UC_{1.04})_{1-x}(SiC)_x$ with $x=0.1, 0.2, 0.3, 0.4$ and 0.5 . The microstructure of the arc-melted samples was analyzed in CEA Marcoule using SEM, EPMA and X-ray diffraction analysis. In some cases, small pieces of graphite were found in some samples. The microstructure of the samples was relatively homogeneous.

The samples were transported to ITU for thermal analysis tests. The samples were heated in an autoclave using a Nd:YAG 4.5 kW cw laser ($\lambda=1064.5$ nm). The melted zone of the sample is of about 8 mm in diameter and less than 100 μm in thickness. Prior to the melting, a preliminary heat treatment of the sample surface was applied at low power ($T\sim 1750$ K) for about 2 minutes to homogenise the sample and to minimize the thermomechanical stresses in the material. Then successive shots were performed at high power to melt the sample. The temperature of the sample versus time was determined using a pyrometer ($\lambda=655$ nm). The analysis of the thermograms of the samples mainly shows at least two thermal arrests. During cooling, the first thermal arrest corresponds to the liquidus temperature, i.e; the formation of UC_{1+x} (or SiC) depending on the composition.

A first comparison between calculations using our preliminary database on U-Si-C with the measured liquidus temperatures shows a qualitative agreement. The calculations systematically overestimate the liquidus temperatures. Thus the modelling has been modified in order to better represent the current liquidus temperatures.

A second arrest was detected around 2100 K. This transition was more difficult to identify. The characterization of the microstructure of the zone melted by the laser coupled with thermodynamic calculations allowed to interpret this second transition. Very thin eutectic regions were highlighted. The characteristic distance between the lamella in these eutectic regions (about 50 nm) is consistent with the cooling rate applied in the current study. According to our results, it may correspond to the solidus related to the following reaction: $\text{Liquid} + UC(1) = SiC + UC(2)$. The UC(1) and UC(2) phases correspond to two uranium carbide phases UC_{1+x} with two different U/C ratios present in the miscibility gap of the U-C system.

The present experimental work was successfully achieved despite of delays in the sample transport. The first experimental results on the phase transitions in the UC-SiC system were obtained. It improves the knowledge on the U-Si-C ternary system and will allow to assess the margin to the melting for the GFR fuel materials.

2.9.1.2 Measurement of uranium carbides using calorimetry

Two different routes were developed to measure the enthalpy of formation of metal carbides using solution calorimetry. The principle of this method is to dissolve the carbides and the pure elements (metal and carbon) in a solvent. The enthalpy of formation of the carbide is then given by the difference between the dissolution enthalpy of the carbide and the dissolution enthalpies of the pure elements. As pure carbon is impossible to dissolve in any solvent, a secondary reference had to be used. For that, several carbides with a well-known enthalpy of formation were tested ().

The first method consisted in dissolving the materials in nitric acid HNO_3 7N in a calorimeter working at room temperature. Many preliminary tests were performed on different carbides (TiC, VC, ZrC, Mo_2C , WC) to determine the duration required to reach the complete dissolution of the materials. As expected the dissolution of carbides is slow. Among the tested compounds, TiC, VC and Mo_2C are good candidates with reasonable times of dissolution (from 22 to 109 hours). The enthalpy of dissolution for these compounds was successfully measured.

The second alternative route was to use a different calorimeter which allows to dissolve the materials at high temperature, here, 1226 K. The experimental conditions were optimized to find and prepare the solvent, a (Mn,Cu) alloy with the composition (Mn_{0.4}Cu_{0.6}). The alloy was prepared by mechanical mixing of Mn and Cu powders and its melting in a Al_2O_3 crucible in the calorimeter.

The dissolution tests on different carbides were successfully achieved. The time of dissolution is shorter, from 1.2 to 2.5 hours. The enthalpy of dissolution of TiC, Mo_2C and WC was measured.

UC and UC_2 carbides were prepared by arc-melting from U and C in CEA Saclay. The characterization in

CEA Marcoule was performed in order to check the purity level and the homogeneity of the samples. The EPMA analysis showed that the uranium monocarbide has an overall composition corresponding to $UC_{1.1}$.

The measurements on these uranium carbides required to modify the safety procedure in the lab in order to be able to handle radioactive samples. Thus the calorimetric tests could not yet be performed on these samples.

The development of such calorimetric methods is of great interest for measurement of enthalpy of formation for all carbide phases, which is quite a challenging task. It will provide in a near future thermodynamic data on UC and UC_2 compounds which will allow us to improve the thermodynamic modelling of the U-C and U-Si-C systems.

2.9.2 JRA3-WP2: Thermodynamic modelling of U-C-Si, and U-C-W systems

The binary sub-systems U-C, Si-C and U-Si were assessed by respectively Dupin et al [09Dup,11Gue], Grobner [96Gro] and Berche et al [09Ber]. In the preliminary assessment of the U-Si-C system, available in the Fuelbase database, the ternary compounds $U_3C_2Si_2$ and $U_{20}C_3Si_{16}$ were introduced and solubility of carbon in U_3Si_2 was taken into account according to the phase diagram data from the literature [12Gue]. No experimental data were available in the UC-SiC system. A comparison between calculations with this version and the experimental data measured in WP1.1 showed that the calculated liquidus temperatures were overestimated. Thus all ternary parameters including the Gibbs energy functions for the ternary compounds and ternary interaction parameters in the liquid phase were assessed to fit the new experimental data.

A very good agreement was obtained. The current version of the database was used to help the interpretation of the microstructure of the quenched zones in the samples.

The present experimental and modeling work was successfully achieved despite of delays in the sample transport. The first experimental results on the phase transitions in the UC-SiC system were obtained. It improves the knowledge on the U-Si-C ternary system and will allow the assessment of the margin to the melting for the GFR fuel materials.

[12Gue] C. Guéneau, N. Dupin, B. Sundman, « Thermodynamic modelling of the U-Pu-Si-C system », F-BRIDGE Report D152 (March 2012)

[11Gue] C. Guéneau et al, « Thermodynamic modelling of advanced oxide and carbide nuclear fuels : description of the U-Pu-O-C systems », J. Nucl. Mater. 419 (2011) 145

[09Ber] A. Berche, C. Rado, O. Rapaud, C. Guéneau, J. Rogez, J. Nucl. Mater. 389 (2009) 101-107

[09Dup] N. Dupin, C. Guéneau, B. Sundman, Fuelbase project report, 2009.

[96Gro] J. Grobner, H.L. Lukas, F. Aldinger, Calphad, 20 (1996) 247-254

2.10 Joint Research Activity “XAS Theoretical chemistry coupling”

The objective of the work was to achieve the structural and electronic description and modelisation of a system of interest from both EXAFS and XANES approaches. Hexacyanoferrate actinide compounds were chosen as the system of interest.

Metal hexacyanoferrates are well known molecular solids for a large variety of cations, although very little has been described for actinide adducts.

2.10.1 Development of models for Actinide EXAFS

Comparison between actinide(III) and lanthanide(III) thiocyanato complexes is relevant to the problematic of lanthanide versus actinide selective complexation with hard/soft donor ligands. EXAFS and XRD (monocrystal) data of the Lu-thiocyanate complex $[n-(C_4H_9)N]_3[Lu(NCS)_4(NO_3)_2]$ have been recorded. This complex has been synthesized in order to further compare with the americium adduct. For solid-solution comparison, solution of the $[n-(C_4H_9)N]_3[Lu(NCS)_4(NO_3)_2]$ complex in ethanol has been investigated by EXAFS. As a point of comparison, the structure in solution of Lu nitrate ($Lu(NO_3)_3 \cdot 6H_2O$) has also been probed by EXAFS. Molecular dynamic calculations of the Lu-nitrate system in a box of ethanol have also been performed and are being coupled with the fitting of the EXAFS data. The main question here is the ligation geometry of the nitrates (bidentate versus monodentate, outer sphere versus inner sphere) in ethanol compared to water. In addition, new members of actinide(III) and Actinide(IV) hexacyanoferrates were

synthesized with the cations americium (III), californium(III), thorium(IV), uranium(IV), neptunium(IV) and plutonium(IV). They were structurally characterized by infrared and X-ray absorption spectroscopy. Combined EXAFS data at the iron K edge and actinide L-3 edge provided evidence for a three-dimensional model for these new compounds. Structural data in terms of bond lengths were compared to those reported for the parent lanthanide(III) compounds.

Actinide and lanthanide environments appeared to be very similar except for Cf(III), they are arranged in a tricapped trigonal prism polyhedron of coordination number 9 (CN: 9), in which the actinid atom is bonded to six nitrogen atoms and to three water molecules. For the californium adduct, a similar comparison and bond length and angle values derived from EXAFS studies suggest that the californium cation sits in a bicapped trigonal prism (CN: 8) as in (KGdFeII)-Fe-III(CN)(6)center dot 3H(2)O. This arrangement differs from that in the structure of (KGdFeII)-Fe-III(CN)(6)center dot 3.5H(2)O, in which the gadolinium atom is surrounded by 9 atoms. Quantum chemical calculations were also performed on finite-sized clusters.

It was also planned to investigate the structure of Polonium aquo ion from EXAFS and quantum chemical calculations. However because of the impossibility to obtain a weighable amount of 209-Po, no EXAFS experiment could be done and the project was dropped. However, the quantum chemical calculations were performed by our colleagues in Sevilla.

2.10.2 Actinide multiple absorption edge investigation

NEXAFS data of compounds of the series $An(IV)Fe(II)CN_6 \cdot xH_2O$ ($An = Th, Np, Pu$) have been completed at the ALS (Berkeley). These data are still currently under interpretation. Because of their sensitivity to iron 3d orbital, iron $L_{II,III}$ edges are particularly fruitful in order to assess the properties of the cyano bond. At oxidation state +III, iron exhibits one hole in the t_{2g} orbital, leading to the presence of an intense pre-peak as seen in Figure 4 for $\{Fe^{III}CN_6^{3-}\}$. On the contrary, at the +II oxidation state, all the 3d orbital are full and no pre-peak is present. This is the case for $\{Fe^{II}CN_6^{4-}\}$ but also for Nd^{III}/Fe^{II} and Pu^{IV}/Fe^{II} . Complementary cyano K edge have also been recorded. Coupling these data with theoretical chemistry and simulation codes like Feff and FDMNES is currently being complemented. In addition, XAS spectroscopy were performed at multiple absorption edges for actinide(IV) and lanthanide(III) hexacyanoferrates. The iron $L_{2,3}$ -edges, the carbon and nitrogen K-edges together with the actinides $N_{4,5}$ -edges and lanthanides $M_{4,5}$ -edges were investigated. They probe, respectively, unoccupied iron 3d orbitals, nitrogen and carbon 2p orbitals and actinide 5f orbitals.

XAS spectra were then confronted to DFT calculations in order to link experimental and theoretical results and to determine the electronic structure of the compounds. The electronic charges obtained by DFT were used in the FDMNES program in order to simulate experimental edges. Using a phenomenological approach, a clear distinctive behaviour between actinides and lanthanides has been shown as well as amongst the actinide series. From this approach, it was possible to probe actinide-ferrocyanide bonds and their differences with lanthanide-ferrocyanide bonds. More specifically, π interactions with 5f orbitals were underlined by both theoretical and experimental methods and can be involve in the observed distinctive optical behaviour of the actinides compounds.

3 POTENTIAL IMPACT, MAIN DISSEMINATION ACTIVITIES AND EXPLOITATION OF RESULTS

3.1 Potential impact

The major challenges of the nuclear industry – such as the definition, safety assessment, and implementation of waste management strategies, the development and implementation of innovative concepts minimizing environmental impact and improving safety and cost effectiveness – require the development of the expertise in actinide sciences.

To face this challenge, existing institutes cannot run the necessary research programmes and attract the required number of students and young researchers to the fields of actinide science on a national basis.

It is therefore of strategic importance both to the management of the existing European industrial tool, and to the potential development of future concepts, to network the major European institutes in order to reinforce the European excellence in this field.

These networking activities can have impact in three main areas:

- i) Make it easier to conduct heavy programmes in actinide science by increasing the set of possible experiments on active materials available to researchers in the European Community.
- ii) Generate circulation of researchers between these facilities, thus contributing to the spreading of excellence at the European scale,
- iii) Foster training and education activities at the European scale, both through a specific Training Programme, and by providing the opportunity to take advantage of a larger connected scientific community for students and young researchers. In this respect, the very existence of the network, and its support by the European Commission, will make this community much more visible and attractive to students and young researchers.

3.2 Dissemination activities

The first action was to create and put online the public website of the project: www.actinet-i3.eu

Main menu structure:

- Home: latest articles and announcements
- Project: presentation of the project and the consortium
- Facilities: description of each pooled facility
- Calls: call information and documents for submission and report
- Schools: registration information and summary of the Summer and ThUL schools
- Events: registration information and presentations documents of the plenary meetings
- Newsletters: newsletters of the project
- ACTINET Club: registration to the club
- Contact: form to contact the coordinator

In addition, the “ACTINET Club” was created in order to give the opportunities to users deeply involved in ACTINET-I3 to be visible on the website and to receive specific information on ACTINET-I3.

Two newsletters were edited and widely distributed per email and during the plenary meetings. They are available on the website. They were used to announce the project events, schools or calls and to promote the facilities. Articles on JRPs students and successful schools participated in the promotion of the network.

Last but not least, two successful Plenary Meetings were organised in February 2011 and January 2013 at CEA Marcoule France. It gathered around 90 and 60 participants respectively, mainly from Europe but also from abroad (USA, Russia, Japan, Israel...). They were the occasion to widely promote ACTINET-I3 activities and specifically the Transnational Access. All the contributions to the meeting are available online on the public website.

In addition, promotion of ACTINET-I3 work and calls has been done and are still planned in several

workshops and conferences:

- IEMPT (San Francisco, USA) 1-4/11/2010
- FAIRFUELS workshop (Stockholm, Sweden) 9-10/02/2011
- J-ACTINET summer school (5 representatives) September 2011
- Migration 2011, poster, September 18-23 2011
- ICAPP 2012, 24-28 June 2012
- MRS 2012 November 25-30 2012
- E-MRS 2023, Strasbourg, May 2013
- GLOBAL 2013, Salt Lake City, September 2013 (Invited Paper)

3.3 Training and Education

3.3.1 ACTINET Summer school (AnSS)

Three Summer schools were organised on the period. One by CEA in September 2010, one at ITU in June 2011 and one by CEA, in association with NNL and Plutonium Futures Conference in July 2012

2010 Summer School

The first ACTINET-I3 Summer School took place at CEA Marcoule, early September 2010. Around 70 applications were received and 42 were selected, mainly from Europe but also from USA, Japan, Korea, Australia. Focused on actinide chemistry and the associated analytic techniques, the school was very successful, as highlighted by the evaluation from the attendees. In order to increase the exchanges between the students, the school was organised in the hotel where the students lived. A specific session where each student presented him/herself also helped to increase the exchanges.

2011 Summer School

In 2011, 63 young researchers coming from 17 different countries (EU and non EU) and representing 23 nationalities have participated. The excellent gender proportion (47,6 % females, 52,4 % males) is very encouraging for the promotion of female scientists in nuclear science. The lectures, featuring experts from international organisations and JRC-ITU, focussed on three main topics: Basic Actinide Science, The Nuclear Fuel Cycle as well as Nuclear Safeguards, Security and Forensics. While morning lectures were dedicated to academic lectures, the afternoons have been devoted to demonstrations and practical exercises in the laboratories of JRC-ITU and the neighbouring German research centre, Karlsruher Institut für Technologie (KIT). A particularly open and social atmosphere was powered to stimulate opportunities between 'pupils' and 'teachers' to build up new contacts and to strengthen existing links. The Summer School concluded on Friday afternoon with the delivery of a 'certificate of attendance'.

2012 Summer School

The 2012 Actinet Plutonium Futures Summer School was hosted by the UK National Nuclear Laboratory on 10-13 July in Whitehaven, Cumbria. By exploring the physical, chemical and radiological properties of plutonium and the other actinides, the school introduced the Plutonium Futures - Science 2012 Conference that was held in Cambridge the following week. 47 delegates from Europe, Russia and Korea attended the sessions, during which presentations were given by distinguished speakers from NNL, AWE, CEA, SUBATECH and the universities of Manchester, Bristol and Edinburgh. Students were given an introduction to the nuclear fuel cycle, learned about reprocessing and chemical separations, actinide coordination chemistry, condensed matter physics, radiolysis and radiation chemistry, atomistic simulation techniques, the detection of actinide species and the practicalities of storing separated plutonium. In addition to lectures, the school included some more interactive elements held at the University of Manchester's Dalton Cumbrian Facility, including the chemical analysis of irradiated polymers, exploring actinide chemistry using computational methods and developing strategies for the disposition of plutonium. Students also visited the NNL Central Laboratory at Sellafield and watched a live demonstration of the dissolution of a UO₂ pellet and the method of separation of uranium and plutonium from spent nuclear fuel used in the PUREX process.

3.3.2 School of the Theoretical User Lab (ThuLS)

1st ACTINET Theoretical Userlab Spring School

The ThUL spring school was held at the Karlsruhe Institute of Technology (KIT), Campus North from April 26th to 30th 2012. There were about 30 participants from several European countries as well as from KIT and the European Joint Research Centre ITU. The school consisted of several theoretical and experimental lectures as well as hands-on exercise sessions with different ab initio software packages. The feedback response of the participants was overwhelmingly positive, attesting the organizers a flawless organization and appreciating the high quality of the presented lectures as well as the exercise sessions.

ACTINET-I3 ThUL Winter School 2013 in Actinide Chemistry

The 2nd ThUL spring school was held at the Karlsruhe Institute of Technology (KIT), Campus North from 14th to 18th of January 2013 in Karlsruhe, Germany. 55 participants from 11 countries attended this ThUL school – an overwhelming success. Based on the positive responses from 2012's ThUL School, once again a balanced schedule of theoretical and experimental lectures as well as hands-on exercise sessions with different ab initio software packages was presented by internationally reputed speakers. Invited key lectures were delivered by Prof. Trond Saue (Toulouse, F), Dr. Mathias Krack (PSI, CH), Prof. Michael Bühl (St Andrews, UK), Vincenzo Rondinella (JRC-ITU, GER) and Dr. Andrew Kerridge (London, UK) covering a wide range of topics spanning fundamental relativistic quantum chemistry, to computational chemistry issues of both solid materials and coordination compounds in addition to the calculation of spectroscopic parameters, focussing on NMR. During the poster session, students benefitted from discussions with leading experts, whereas social events fostered the network of researchers in actinide science and enhanced communication and collaboration between the scientific communities. Extremely positive feedback was obtained, accompanied by an unexpected number of requests for a continuation of the school, underlining the significance of the event.

3.4 Exploitation of results

Through these different activities, ACTINET-I3 aimed at gathering the actinide scientific community in Europe and give mainly scientists from universities and academic research to access unique infrastructures in which weighable amounts of actinides can be used. This is of primary importance in order to maintain Europe at the highest level in actinide sciences. Thanks to a wider access to facilities where actinides and specifically transuranics can be handled, researchers from European universities and academic bodies brought their knowledge in the nuclear field and, in parallel, increase their own skills, leading to an enhancement of Europe in actinide sciences.

PART II: USE & DISSEMINATION OF FOREGROUND

I SECTION A (PUBLIC): LIST OF ALL SCIENTIFIC (PEER REVIEWED) PUBLICATIONS & ALL DISSEMINATION ACTIVITIES

JRA1

Panak, P. J.; Geist, A., Complexation and extraction of trivalent actinides and lanthanides by triazinylpyridine *N*-donor ligands. *Chem. Rev.* 2013, 113 (2), 1199–1236

JRA3

C. Guéneau et al, « Thermodynamic modelling of advanced oxide and carbide nuclear fuels : description of the U-Pu-O-C systems », *J. Nucl. Mater.* 419 (2011) 145

JRA4

“Local Structure in Americium and Californium Hexacyanoferrates –Comparison with Their Lanthanide Analogues” G. Dupouy *et al.* *Eur. J. Inorg. Chem.* 2011, 1560.

“Multi-edge X-ray absorption spectroscopy of thorium to plutonium hexacyanoferrate compounds: Part II” T. Dumas *et al.* [submitted to Eur. J. Inorg. Chem.](#)

JRP01-05 “SPECTROSCOPIC INVESTIGATION OF REDOX REACTIONS OF PLUTONIUM WITH IRON MINERALS”

Publications

- Kirsch, R.; Fellhauer, D.; Altmaier, M.; Neck, V.; Rossberg, A.; Fanghänel, T.; Charlet, L.; Scheinost, A. C., Oxidation state and local structure of Pu reacted with magnetite, mackinawite and chukanovite. *Environ. Sci. Technol.* 2011, 45, 7267–7274.

- Kirsch, R.; Fellhauer, D.; Altmaier, M.; Fanghänel, T.; Charlet, L.; Scheinost, A. C, Sorption and redox reactions of plutonium with iron(II)-bearing minerals, [under writing, to be submitted to Geochimica et Cosmochimica Acta.](#)

Presentations at international conferences:

- Kirsch, R., Fellhauer, D., Altmaier, M., Rossberg, A., Fanghänel, Th., Charlet, L., Scheinost, A.C., Plutonium redox reactions with iron oxides under anoxic conditions, Goldschmidt Conference 2011, Prague, Czech Republic, (Oral).

- Fellhauer, D., Kirsch, R., Altmaier, M., Neck, V., Scheinost, A.C., Charlet, L., Wiss, T., Fanghänel, Th., Thermodynamic evaluation of Pu redox processes in homogeneous solutions and heterogeneous Fe mineral suspensions, Migration Conference 2011, Beijing, China (Poster).

- Kirsch, R., Fellhauer, D., Altmaier, M., Rossberg, A., Fanghänel, Th., Charlet, L., Scheinost, A.C., XANES and EXAFS analysis of oxidation state and local structure of plutonium reacted with iron oxides under anoxic conditions, Migration Conference 2011, Beijing, China, (Oral).

- Kirsch, R., Fellhauer, D., Altmaier, M., Fanghänel, Th., Charlet, L., Scheinost, A.C., Plutonium redox chemistry under anoxic conditions in the presence of iron-(II) bearing minerals, Goldschmidt Conference 2012, Montreal, Canada (oral).

JRP01-10 "SOLUBILITY STUDIES OF Np(V) AND Np(VI) UNDER ALKALINE pH AND CONTROLLED REDOX CONDITIONS"

JRP05-10 “Np(V) SOLUBILITY AND SOLID PHASE TRANSFORMATIONS IN NaCl, NaClO₄ AND MgCl₂ SOLUTIONS...”

Publications

- Gaona, X., Tits, J., Dardenne, K., Liu, X., Rothe, J., Denecke, M.A., Wieland, E., Altmaier, M. (2012) Spectroscopic investigations of Np(V/VI) redox speciation in hyperalkaline TMA-(OH, Cl) solutions. *Radiochimica Acta*, 100, 759-770
- Petrov, V.G., Kalmykov, S.N., Altmaier, M. (2011) Solubility and phase transformations of Np(V) hydroxide in solutions with different ionic strengths. *Geochimica et Cosmochimica Acta* (to be submitted)

Posters:

- V.G. Petrov, S.N. Kalmykov, M. Altmaier. Solubility of Np(V) in alkaline saline solutions. 4th Russian School on Radiochemistry and Nuclear Technology. 6-10 September, Ozersk, Russia.
- X. Gaona, M. Altmaier, V. Petrov, D. Fellhauer, J. Tits, E. Wieland, K. Dardenne, Th. Fanghänel. Aqueous speciation and solubility of Np(V/VI) in hyperalkaline systems. Plutonium Futures "The Science", Keystone, Colorado, USA, September 19-23, 2010
- V.G. Petrov, X. Gaona, D. Fellhauer, S.N. Kalmykov, M. Altmaier Solubility and phase transformations of Np(V) hydroxide in NaCl solutions. ReCosy 3rd Annual Workshop. Balaruc-les-Bains (Sète, France), March 21-24, 2011

Orals:

- Gaona, X., Altmaier, M., Petrov, V., Fellhauer, D., Tits, J., Wieland, E., Dardenne, K., Fanghänel, Th. Aqueous speciation and solubility of Np(V/VI) in hyperalkaline systems. Plutonium Futures - The Science 2010, Keystone, CO (USA), Sept.19.-23., 2010
- Gaona, X., Tits, J., Dähn, R., Dardenne, K., Fellhauer, D., Wieland, E., Altmaier, M. Redox chemistry of Np(V/VI) under hyperalkaline conditions: sorption on cementitious materials, aqueous speciation and solid phase formation. Abstract in the Proceedings of the 13th International Conference on the Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere (MIGRATION), Beijing (China), September 18-23, 2011
- Petrov, V., Gaona, X., Fellhauer, D., Dardenne, K., Rothe, J., Kalmykov, S., Altmaier, M. Np(V) solubility and solid phase transformation in dilute to concentrated NaCl solutions. Abstract in the Proceedings of the 13th International Conference on the Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere (MIGRATION), Beijing (China), September 18-23, 2011
- Gaona, X., Fellhauer, D., Dardenne, K., Rothe, J., Altmaier, M. Redox chemistry of Np(V/VI) under hyperalkaline conditions: aqueous speciation, solubility and chemical analogies with Pu. Abstract in the Proceedings of the ABC-Salt II workshop "Actinide Brine Chemistry in a Salt-Based Repository", Karlsruhe (Germany), November 7-8, 2011
- Petrov, V., Gaona, X., Fellhauer, D., Dardenne, K., Kalmykov, S., Altmaier, M. Pentavalent Neptunium Solubility and Solid Phase Transformation at high ionic strengths. Abstract in the Proceedings of the ABC-Salt II workshop "Actinide Brine Chemistry in a Salt-Based Repository", Karlsruhe (Germany), November 7-8, 2011

JRP01-14 "DEVELOPMENT OF AB INITIO BASED FORCE-FIELD MODELS FOR LN AND AN IONS"

JRP03-09 "DEVELOPMENT OF AB INITIO BASED FORCE-FIELD MODELS FOR LANTHANIDE AND ACTINIDE IONS"

JRP05-18 "DEVELOPMENT OF AB INITIO BASED FORCE-FIELD MODELS FOR LANTHANIDE AND ACTINIDE IONS"

Publications

- "Quantum Chemical and Molecular Dynamics Study of the Coordination of Th(IV) in Aqueous Solvent" F. Réal, M. Trumm, V. Vallet, B. Schimmelpfennig, M. Masella, and J.-P. Flament, *J. Phys. Chem. B*, 2010, 114, 15913–15924. <http://dx.doi.org/10.1021/jp108061s>
- "Modeling the hydration of mono-atomic anions from the gas phase to the bulk phase: The case of the halide ions F⁻, Cl⁻, and Br⁻", M. Trumm, Y. O. Guerrero Martinez, F. Réal, B. Schimmelpfennig, M. Masella, and V. Vallet, *J. Chem. Phys.*, 2012, 136, 044509. <http://dx.doi.org/10.1063/1.3678294>
- "Further insights in the ability of classical nonadditive potentials to model actinide ion–water interactions" F. Réal, M. Trumm, B. Schimmelpfennig, M. Masella, and V. Vallet, *J. Comput. Chem.*, 2012.

<http://dx.doi.org/10.1002/jcc.23184>

Oral presentations

- "A quantum chemical and long-time molecular dynamics study of the coordination of Th(IV) in aqueous solvent", F. Réal, M. Trumm, V. Vallet, B. Schimmelpfennig, J.-P. Flament, M. Masella, Migration '09 - 12th International Conference on the Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere. Kennewick, USA, 2009.
- "TCPEP Force Field Calculations on Actinide Salts in Aquatic Solvent", M. Trumm, F. Réal, B. Schimmelpfennig, M. Masella, and V. Vallet, Migration '11 - 13th International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere. Beijing, China, 2011.
- "Macroscopic modeling: insights in the ability of classical non-additive potentials to model radionuclides in aqueous solution.", V. Vallet, Symposium of the 14th ICQC conference: Chemistry and Physics of the Heavy Elements. Santa Fe, USA, 2012.
- "Development and application of a polarizable force field for actinides in aqueous solution including cooperative charge-transfer terms.", F. Réal, Les XIIIèmes Journées Nationales de Radiochimie. Nantes, France, 2012.

Posters

- "A quantum chemical and long-time molecular dynamics study of the coordination of Th(IV) in aqueous solvent", F. Réal, M. Trumm, V. Vallet, B. Schimmelpfennig, J.-P. Flament, M. Masella, 13th ICQC. Helsinki, Finland, 2009.
- "Macroscopic modeling: insights in the ability of classical non-additive potentials to model radionuclides in aqueous solution", V. Vallet, F. Réal, Y. O. Guerrero Martínez, M. Trumm, B. Schimmelpfennig, and M. Masella Boulder, USA, 2012. 13th ICQC (International Conference of Quantum Chemistry).
- "Ab initio polarizable force-field models to explore the coordination, dynamics and spectroscopy of trivalent lanthanides in aqueous solvent", F. Réal, V. Vallet, Y. O. Guerrero Martínez, M. Trumm, B. Schimmelpfennig, and M. Masella, Beijing, China, 2011. Migration '11 - 13th International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere.
- "Macroscopic modeling: insights in the ability of classical non-additive potentials to model radionuclides in aqueous solution.", V. Vallet, F. Réal, Y. O. Guerrero Martínez, M. Trumm, B. Schimmelpfennig, and M. Masella, Advanced Techniques in Actinide Spectroscopy (ATAS). Dresden, Germany, 2012.

JRP01-17 "SOLUBILITY STUDIES OF NP(V) AND NP(VI) UNDER ALKALINE pH AND CONTROLLED REDOX CONDITIONS":

Publications

- "The lanthanide and actinide contractions in the gas phase - Experimental evaluation of ionic sizes by mass spectrometry", C. Lourenço, A. F. Lucena, P. X Rutkowski, M. C. Michelini, J. M. Carretas, N. Zorz, L. Berthon, J. K. Gibson, J. Marçalo; **to be submitted to Inorg. Chem. ?**
- "III/IV Oxidation State Stabilities of Lanthanides and Actinides in the Gas Phase", A. F. Lucena, C. Lourenço, J. M. Carretas, P. X Rutkowski, M. C. Michelini, N. Zorz, L. Berthon, J. K. Gibson, J. Marçalo; **to be submitted to Inorg. Chem. ?**
- "Mass Spectrometry Study of the Coordination of New Multidentate N-Donor Ligands by Lanthanide(III) and Americium(III) Ions", B. Monteiro, C. Lourenço, J. M. Carretas, J. Marçalo, N. Zorz, L. Berthon; **to be submitted to Int. J. Mass Spectrom. ?**
- "Relative Affinity of N- and O-donor Bases towards Lanthanide(III) and Americium(III) Ions in the Gas Phase", C. Lourenço, A. F. Lucena, J. M. Carretas, I. Paiva, N. Zorz, L. Berthon, J. Marçalo; **to be submitted to Int. J. Mass Spectrom. ?**

Posters

- "Probing the Lanthanide Contraction by ESI/QITMS", J. M. Carretas, C. Lourenço, J. Marçalo, MS2010 - 4th Portuguese Mass Spectrometry Meeting, Lisboa, December 2010.
- "ESI/QITMS Study of the Coordination of a New Tetradentate N-donor Ligand by Lanthanide(III) Ions", B. Monteiro, C. Lourenço, J. M. Carretas, J. Marçalo, MS2010 - 4th Portuguese Mass Spectrometry Meeting, Lisboa, December 2010.
- "ESI/QITMS Study of the Relative Affinity of N-donor Bases towards Pr(III) Ions in the Gas Phase", C. Lourenço, J. M. Carretas, I. Paiva, J. Marçalo, MS2010 - 4th Portuguese Mass Spectrometry Meeting, Lisboa,

December 2010.

- “Coordination Study of a New Tetradentate N-Donor Ligand by Lanthanide(III) and Americium(III) Ions”, B. Monteiro, C. Lourenço, J. M. Carretas, J. Marçalo, N. Zorz, L. Berthon, XXII National Meeting of the Portuguese Society of Chemistry, Braga, July 2011.
- “III/IV Oxidation State Stabilities of Lanthanides and Actinides in the Gas Phase”, A. F. Lucena, C. Lourenço, J. M. Carretas, P. X Rutkowski, M. C. Michelini, N. Zorz, L. Berthon, J. K. Gibson, J. Marçalo, EUFEN1 - Meeting of COST Action CM1006: European f-Element Network, Tarragona, April 2012.
- “Gas-Phase Studies of the Relative Affinities of N- and O-donor Bases toward Ln(III) and An(III) Ions”, C. Lourenço, A. F. Lucena, J. M. Carretas, B. Monteiro, I. Paiva, J. Marçalo, N. Zorz, L. Berthon, ATALANTE 2012 – Nuclear Chemistry for Sustainable Fuel Cycles, Montpellier, September 2012.

Oral presentation

- “Mass Spectrometry of Rare Earths—From Compound Characterization to Fundamental Gas-Phase Properties”, J. Marçalo, A. F. Lucena, C. Lourenço, B. Monteiro, L. Maria, J. M. Carretas, P. X Rutkowski, J. K. Gibson, XXIV. Terrae Rarae 2011, Karlsruhe, October 2011.

JRP01-19 " A THERMODYNAMIC STUDY OF MIXED OXIDE SOLID SOLUTION. PART I. ((Th,U)O₂):"

Publications

- O.S. Valu, O. Benes, R. J. M. Konings, “The high temperature heat capacity of (Th,Pu)O₂ system” submitted in July 2012 to Journal of Chemical Thermodynamics, **publication to be confirmed**

JRP01-20 “HELIUM BEHAVIOUR IN GLASS WASTE FORMS, IMPACT OF HIGH ACTINIDE LOADING FACTOR?”

Publications

- “Calorimetric Study of Glass Structure Modification Induced by Decay, Journal of the American Ceramic Society”
Authors Emilio Andrea Maugeri, Sylvain Peugeot, Dragos Staicu, Alessandro Zappia, Christophe Jegou, Thierry Wiss
Article first published online: 9 JUN 2012
DOI: 10.1111/j.1551-2916.2012.05304.x

JRP03-01 "INTERACTION OF ADVANCED OXIDE FUELS WITH SODIUM IN OPERATING CONDITIONS FOR SODIUM COOLED FAST REACTORS"

JRP05-02 “INTERACTION OF ADVANCED OXIDE FUELS FOR GEN-IV SODIUM COOLED FAST REACTORS”

Publications

- A.L. Smith, J.Y. Colle, O. Benes, A. Kovacs, P. Raison, R.J.M. Konings, Mass spectrometric study of the vaporization behaviour of α -Na₂NpO₄: Thermodynamic investigation of the enthalpy of formation, The Journal of Chemical Thermodynamics
available online: 26-JAN-2013, DOI 10.1016/j.jct.2012.11.034

Oral presentation

- Plutonium Futures conference, Cambridge, July 2012

JRP03-06 “EXPLORING THE CHEMICAL DIFFERENCES BETWEEN TRIVALENT LANTHANIDES AND ACTINIDES BY MASS SPECTROMETRY TECHNIQUES”:

Publications

- H. Rojo, X. Gaona, Th. Rabung, M. Garcia, T. Missana, M. Altmaier. Complexation of Nd(III)/Cm(III) and

Np(IV) with Gluconate in dilute to concentrated alkaline NaCl and CaCl₂ solutions. Proceedings of the ABC-Salt II Workshop, Actinide Brine Chemistry. Karlsruhe (Germany), 7-8 th November, 2011.

- Rojo, H., Gaona, X., Rabung, T., Garcia, M., Missana, T., Altmaier, M. (2012). Complexation of Nd(III)/Cm(III) with Gluconate in NaCl and CaCl₂ solutions: solubility and TRLFS studies (**under writing**) (**to be submitted to Radiochimica Acta**)

Conferences

- H. Rojo, X. Gaona, Th. Rabung, M. Garcia, T. Missana, M. Altmaier. Complexation of Nd(III)/Cm(III) and Np(IV) with Gluconate. Abstract in the Proceedings of the ABC-Salt II workshop "Actinide Brine Chemistry in a Salt-Based Repository", Karlsruhe (Germany), November 7-8, 2011

- X. Gaona, H. Rojo, C. Adams, M. Böttle, M. Garcia, T. Missana, P. Kaden, M. Altmaier. Effect of Ca in the Np(IV)-gluconate system under hyperalkaline conditions. 3rd International Workshop Mechanisms and modelling of waste/cement interactions", Ghent (Belgium), May 6-8, 2013

- H. Rojo, X. Gaona, Th. Rabung, M. Garcia, T. Missana, M. Altmaier. Complexation of Nd(III)/Cm(III) with gluconate in dilute NaCl and CaCl₂ alkaline solutions: solubility and TRLFS studies. 3rd International Workshop "Mechanisms and modelling of waste/cement interactions", Ghent (Belgium), May 6-8, 2013

JRP03-07: SORPTION OF TRIVALENT ACTINIDES ON QUARTZ AND SILICA AT HIGH SALT CONCENTRATIONS - EXPERIMENTS AND FIRST MODELLING ATTEMPTS

Posters

- Schnurr A., Petrov V., Rabung Th., Lützenkirchen J., Geckeis H. Trivalent metal ion sorption under saline conditions. Migration 2011, PKU, Beijing, China, 2011, 246-248.

- Rothmeier M., Petrov V., Rabung Th. Surface charging of (oxyhydr)oxide minerals to high ionic strength. ABC-Salt (II) – Actinide Brine Chemistry in a Salt-Based Repository, 2011, Karlsruhe, Germany

Oral presentation

Petrov V., García D., Kalmykov S., Duro L., Lützenkirchen J. Sorption of An(III) and An(V) onto silica colloids in NaCl solutions of different ionic strengths. 7th Russian Conference on Radiochemistry "Radiochemistry-2012", October 2012, Dimitrovgrad, Russia

Publication **under preparation**

- Sorption of An(III) and Ln(III) under high saline conditions

JRP03-08 "AQUEOUS ACTINIDE CATION MAGNETIC SUSCEPTIBILITY AS A FUNCTION OF OXIDATION STATE":

Publications

- **Submitted in Inorganic Chemistry or Dalton**: Paramagnetism of Aqueous Actinide Cations in Perchloric Acid Media, by authors: Thomas F. Wall, Steve Jan, Kenneth L. Nash, Laetitia Guerin, Philippe Moisy, and Claude Berthon.

JRP03-10 "TOWARDS AN ACCURATE DESCRIPTION OF ENVIRONMENT EFFECTS ON THE ELECTRONIC SPECTRA OF ACTINIDES IN CONDENSED PHASE"

JRP05-08 "TOWARDS AN ACCURATE DESCRIPTION OF ENVIRONMENT EFFECTS ON THE ELECTRONIC SPECTRA OF ACTINIDES"

Publications

- "Towards an efficient ab initio description of environment effects: solvatochromic shifts from coupled-cluster theory embedded in density functional theory", Höfener S, Gomes ASP and Visscher L , **in preparation** (**January 2013**)

- "Towards an efficient ab initio description of environment effects: solvatochromic shifts from coupled-cluster theory embedded in density functional theory", Gomes ASP, Jacob CR, Real F, Vallet V and Visscher L , **in preparation** (**January 2013**)

- "The electronic spectrum of CUONg₄ (Ng = Ne, Ar, Kr, Xe): New insights in the interaction of the CUO molecule with noble gas matrices", Tecmer P, van Lingen H, Gomes ASP and Visscher L, Journal of Chemical Physics, 137, 084308, 2012 (10.1063/1.4742765)

Conferences

- "Towards an efficient ab-initio description of environment effects: Solvatochromic shifts from coupled-cluster theory embedded in density-functional theory", Höfener S, Gomes ASP, Visscher L, 48th Symposium on Theoretical Chemistry (STC 2012), Karlsruhe, Germany, 2012.
- "Modeling the Spectra of Heavy Elements in Condensed Phase Using WFT-in-DFT and DFT-in-DFT Embedding", Gomes ASP, Jacob CR, Real F, Visscher L and Vallet V, 48th Symposium on Theoretical Chemistry (STC 2012), Karlsruhe, Germany, 2012
- "Towards an efficient ab-initio description of environment effects: Solvatochromic shifts from coupled-cluster theory embedded in density-functional theory", Höfener S, Gomes ASP, Visscher L, XIVth International Congress of Quantum Chemistry, Boulder, USA, 2012.
- "Using WFT-in-DFT and DFT-in-DFT Embedding to model actinide spectra in condensed phase", Gomes ASP, Jacob CR, Real F, Visscher L and Vallet V, Simpósio Brasileiro de Química Teórica, Ouro Preto, Brazil, 2011

JRP03-12 "M-XRF/XRD/XAFS STUDY OF Np(V) SORPTION AND DIFFUSION IN OPALINUS CLAY":

Publications

- D.R. Froehlich, S. Amayri, J. Drebert, D. Grolimund, J. Huth, U. Kaplan, J. Krause, T. Reich: Speciation of Np(V) uptake by Opalinus Clay using synchrotron microbeam techniques. Analytical Bioanalytical Chemistry, 10.1007/s00216-012-6290-2

JRP03-13 "FIRST-PRINCIPLES MODELLING OF RADIATION DAMAGE IN U NITRIDE AND U CARBIDE":

Oral presentation

"Study of uranium carbides using first-principles electronic structure calculations", M. Freyss, F-BRIDGE international workshop, 21-23 February 2012, Aix-en-Provence, France.

Poster

"First-principles DFT+U study of point defects in uranium and plutonium carbides", M. Freyss, NUMAT Conference, 22-25 October 2012, Osaka, Japan.

JRP03-15 "ROLE OF MN IN NP CYCLING" JRP05-06 "NP BIOGEOCHEMISTRY IN A GEOLOGICAL DISPOSAL FACILITY CHEMICALLY DISTURBED ZONE"

Conference presentations

- (i) Law, GTW; Thorpe, CL; Shaw, S; Atkins, A; Livens, FR; Peacock, CL; Lloyd, JR; Denecke, MA; Rothe, J; Dardenne, K; Morris, K (2012). Neptunium biogeochemistry and the manganese cycle. Goldschmidt Conference, Montreal, Canada.
- (ii) Brookshaw, DR; Morris, K; Lloyd, JR; Patrick, RAD; Law, GTW; Vaughan, DJ (2012). Enhanced radionuclide capture by bioreduced biotite and chlorite. Goldschmidt Conference, Montreal, Canada.
- (iii) Law, GTW (2012). Novel technologies for the management of radioactive contaminated land (invited). Saudi Environmental Technologies Conference, Riyadh, Saudi Arabia.
- (iv) Law, GTW; Thorpe, CL; Geissler, A; Lloyd, JR; Livens, FR; Denecke, MA; Dardenne, K; Rothe, J; Morris, K (2012). Actinide Bioremediation. Min. Soc. Geomicrobiology Conference, Manchester, UK.
- (v) Thorpe, CL; Law, GTW; Denecke, MA; Shaw, S; Rothe, J; Dardenne, K; Lloyd, J; Livens, FR; Morris, K (2012). Neptunyl reduction in manganese amended sediment systems. Min. Soc. Geomicrobiology Conference, Manchester, UK.

JRP04-03 “CHARACTERISATION OF ACTINIDE MATERIALS IN ENVIRONMENTAL HOT PARTICLES - DEPLETED URANIUM MUNITIONS”:

Publications

Submitted Manuscripts

- Remediation of soils contaminated with particulate depleted uranium by multi stage chemical extraction Daniel E. Crean^{1,2}, Francis R. Livens², Mustafa Sajih², Martin C. Stennett¹, Daniel Grolimund³, 4 Camelia N. Borca³ and Neil C. Hyatt¹ 5 1 J. Haz. Mat., **submitted (Jan 2013)**

Publications near submission

- Microscale characterisation of depleted uranium munitions residues Daniel E Crean, Francis R Livens, Martin C Stennett, Daniel Grolimund, Camelia N Borca and Neil C Hyatt In preparation for submission. Intended journal Environ. Sci. Technol.

- Iron-Uranium Compounds in the Environment – Characterisation of FeU₆ and UFeO₄ Hot Particles Daniel E Crean, Francis R Livens, Martin C Stennett, Daniel Grolimund, Camelia N Borca and Neil C Hyatt In preparation for submission as a short manuscript/letter

Intended Conference Presentations/Abstracts

- Characterisation of depleted uranium munitions residues from a UK firing range - A Micro XAS Study Daniel E Crean, Francis R Livens, Martin C Stennett, Daniel Grolimund, Camelia N Borca and Neil C Hyatt Intended for presentation at Goldschmidt Conference 2013, including publication of abstract.

JRP04-04 "INVESTIGATION OF Th(IV) AND URANIUM (IV) SILICATES: COLLOID FORMATION - ALTERATION - SOLID STATE CHARACTERISTICS"

Publications

- C. Hennig et al. Solid-state properties and colloidal stability of thorium(IV)-silica nanoparticles Geochim. Cosmochim. Acta 103 (2013) 197-212.

<http://dx.doi.org/10.1016/j.gca.2012.10.051>

Poster

- Poster presentation at the EMRS spring meeting 2013 in Strasbourg:

S. Labs, S. Weiss, C. Hennig, H. Curtius, D. Bosbach, Synthesis and structure investigation of USiO₄ - comparison between local structure and bulk. **[not yet approved]**

JRP04-12: POST IRRADIATION INVESTIGATION OF ACTINIDE TARGETS FOR THE PRODUCTION OF EXOTIC ISOTOPE ION BEAMS:

Oral presentations

- EURORIB 2012 - European Radioactive Ion Beam Conference 2012, May 21-25, 2012, Abano Terme (Padova), Italy: Uranium Carbide Target Material Investigations at ISOLDE/CERN

A. Gottberg^{1,2,3}), J.P. Ramos¹), C. Degueldre⁴), C. Borca⁴) , D. Grolimund⁴), I. Günther-Leopold⁴), C. Lau⁵), P. Delahaye⁶), A. Andrichetto⁶) and T. Stora¹)

1) CERN, 2) CSIC, Madrid, Spain, 3) CENBG, Bordeaux, France, 4) PSI, Villigen, Switzerland, 5) IPN, Orsay, France, 7) INFN LNL, Legnaro, Italy

URL: <http://agenda.infn.it/materialDisplay.py?contribId=81&sessionId=8&materialId=slides&confId=3946>

- E-MRS, 2012 Spring Meeting, Strasbourg, May 14-18 2012, Symposium E: Uranium Carbide Material Investigations at CERN and at the Swiss Light Source

A. Gottberg^{1,2,3}), J.P. Ramos¹), C. Degueldre⁴), C. Borca⁴) , D. Grolimund⁴) and T. Stora¹)

1) CERN, 2) CSIC, E-Madrid, 3) CENBG, F-Bordeaux 4) PSI, CH-Villigen

Publications

- **Proceedings to be published in: J. Alloys and Compounds**