

Monday (07 October 2024)

Conference Program

10:30	Registration	
12:00	Lunch	
14:00	Welcome	
Session 1	Spectromicroscopy	
14:20	Application of synchrotron-based microbeam techniques for studying the reactive transport of actinides in clay rock <u>T. Reich (Plenary)</u> (Germany)	S1-T1
15:00	Chemical tomography of Np and Pu diffusion in Opalinus Clay <u>M. Breckheimer, S. Amayri, D. Ferreira Sanchez, D. Grolimund, M. G. Makowska, T. Reich</u> (Germany)	S1-T2
15:20	Chemical imaging and applications using high energy resolution fluorescence detection for the actinides <u>S. M. Webb, N. P. Edwards</u> (USA)	S1-T3
15:40	Quantifying F-Orbital Overlap with Ligand K-edge XAS <u>S. G. Minasian, J. A. Branson, C. H. Booth, Michael A. Boreen, J. Arnold, J. Autschbach, E. R. Batista, J. A. Bradley, A. S. Ditter, O. S. Gunther, J. Kasper, S. A. Kozimor, W. W. Lukens, D. R. Russo, D.-C. Sergentu, D. K. Shuh, Patrick W. Smith, P. Yang</u> (USA)	S1-T4
16:00	Coffee break	
Session 2	Spectromicroscopy / Radiotoxicology	
16:20	AI-assisted lab-on-a-chip experiments: Setting new frontiers in radio-geochemistry <u>J. Poonoosamy, A. Kaspor, C. Schreinemachers, N. I. Prasianakis, E. Curti, G. Deissmann, P. Kowalski, S. V. Churakov, D. Bosbach (Keynote)</u> (Germany)	S2-T1
16:50	Uranium and Plutonium interaction with calcium-binding sites of proteins <u>S. Sauge-Merle, L. Daronnat, R. Pardoux, M.-R. Beccia, E. Faux, N. Brémond, N. Boubals, P. Guilbaud, T. Dumas, D. Lemaire, P. Moisy, D. Moreno Martinez, V. Hoffeltz, J. Pansier, C. Berthon, P. Lorenzo Solari, J. Aupiais, L. Berthon, C. Berthomieu (Keynote)</u> (France)	S2-T2
17:20	Spectromicroscopic characterization of lanthanide-contaminated mammalian cells <u>B. Schacherl, A. Selvam, J. A. Branson, T. Arino, D. M. Jorgens, M. Kang, J. Wang, A. Ditter, R. J. Abergel, S. G. Minasian</u> (USA)	S2-T3
17:40	Impact of Eu(III) on rat kidney cells in the absence and presence of the decorporation agents DTPA and 3,4,3-LI(1,2-HOPO) <u>C. Senwitz, A. Heller, B. Drobot, M. Vogel, T. Stumpf</u> (Germany)	S2-T4
18:00	Combining in vitro cell culture and luminescence spectroscopy: A powerful tool for studying An(III) impact on and speciation in cells <u>A. Heller, C. Senwitz, B. Drobot, T. Stumpf, S. Taut, M. Acker</u> (Germany)	S2-T5
18:20	End of day 1	

Tuesday (08 October 2024)

Session 3 Speciation beyond X-rays

09:00	Speciation of lanthanides and actinides by time-resolved laser fluorescence spectroscopy - Developments from the 1990s to the present day (in honor of J. I. Kim) <u>P. J. Panak (Plenary)</u> (Germany)	S3-T1
09:40	Are actinyl good paramagnetic probe for structural studies by NMR spectroscopy? <u>C. Berthon, H. Bolvin</u> (France)	S3-T2
10:00	Influence of chelating agents on lanthanide and actinide speciation in artificial bodyfluids <u>A. Barkleit, S. Friedrich, D. Butscher, J. Kretzschmar, B. Drobot, R. Steudtner, T. Stumpf</u> (Germany)	S3-T3
10:20	Investigation of gluconate complexation with trivalent Eu, Pu and Am using CE-ICP-MS <u>J. Lohmann, S. Zenker, N. Blum, A. Wiebe, M. Kumke, T. Reich</u> (Germany)	S3-T4
10:40	Coffee break	

Session 4 Actinide electronic structure / Radioecology

11:00	An entropic approach to multiconfigurational ground states <u>M. Beaux (Keynote)</u> (USA)	S4-T1
11:30	Unravelling the actinides 5f enigma with X-Ray emission spectroscopy <u>J. G. Tobin</u> (USA)	S4-T2
11:50	Speciation and imaging in radioecology <u>J. Aupiais, M. R. Beccia, C. Den Auwer, A. Jeanson, M. Maloubier, M. Monfort, C. Moulin, B. Reeves, P. L. Solari, R. Stefanelli, D. Suhard</u> (France)	S4-T3
12:10	In vivo speciation and molecular mechanisms of the uptake of radioactive metal ions by <i>A. nodosum</i> <u>M. Zerbini, P. L. Solari, F. Orange, A. Jeanson, C. Leblanc, M. Metian, C. Den Auwer, M. R. Beccia</u> (France)	S4-T4
12:30	Lunch break	

Tuesday (08 October 2024)

Session 5 Actinide complex stability / Synchrotron facility reports

14:00	Theoretical studies of the coordination structures, stabilities and electronic spectra of Cm ³⁺ species at the mineral-water interface <i>J. Su, Z.-Q. Chu, R.-Y. Zhu (Keynote) (China)</i>	S5-T1
14:30	Molecular electrochemistry of actinides: Redox and reactivity of Uranium, Neptunium, and Plutonium complexes <i>J. Blakemore (Keynote) (USA)</i>	S5-T2
15:00	Coffee break	
15:20	Probing actinide chemistry and structure with X-rays at the SOLEIL synchrotron: MARS and the other beamlines <i>M. O. J. Y. Hunault, T. G. Burrow, P. Piau, W. Breton, D. Menut, P.-L. Solari (France)</i>	S5-T3
15:40	Combining multiple chemical and physical imaging techniques for comprehensive insight into radioactive specimens at the microXAS beamline and future microXAS 2.0. <i>M. Makowska, D. Grolimund, D. Ferreira Sanchez, B. Meyer, M. Birri, A. Diaz, R. Bruetsch, J. Bertsch, C. Schneider, G. Kuri, L. I. Duarte, S. Bhattacharya, O. Yetik, M. Pouchon (Switzerland)</i>	S5-T4
16:00	Soft X-ray emission and resonant inelastic X-ray scattering for actinide research <i>L. Weinhardt, C. Wansorra, R. Steininger, H. Ramanantoanina, T. S. Neill, R. S. K. Ekanayake, A. Seibert, T. Gouder, N. Palina, J. Rothe, D. Hauschild, T. Vitova, C. Heske (Germany/USA)</i>	S5-T5
16:20	Synchrotron based hard X-ray spectroscopy for radionuclide research at the KIT light source <i>K. Dardenne, J. Göttlicher, T. Prüssmann, J. Rothe, R. Steininger, T. Vitova (Germany)</i>	S5-T6
16:40	Transfer to KARA	
17:00	Introduction to KARA <i>B. Härer (Germany)</i>	
17:45	Poster session with refreshments	
20:00	End of day 2	

Tuesday (08 October 2024)

Poster Presentations

- P-1 Development and application of a microfluidic set-up for in-situ studies of formation kinetics of La- and U-complexes using high resolution spectroscopic methods
E. Reynolds, R. S. K. Ekanayake, B. Schacherl, C. Kim, X. Gaona, H. Kaufmann-Heimeshoff, R. Steininger, J. Göttlicher, T. Prüssmann, H. Geckeis, T. Vitova (Germany)
- P-2 Relativistic quantum chemical investigation of actinide covalency measured by electron paramagnetic resonance spectroscopy
M. S. Oakley, L. Birnoschi, E. J. L. McInnes, N. F. Chilton (UK)
- P-3 Experimental characterization and theoretical modelling of X-ray absorption spectra of Protactinium(V) complexes
T. Shaaban, C. Le Naour, H. Oher, T. Aubert, P. L. Solari, T. Burrow, M. Hunault, A. S. P. Gomes, F. Réal, V. Vallet, M. Maloubier (France)
- P-4 Developing Uranium L3 HERFD-XANES and RIXS to investigate Uranium biogeochemical processes
C. Waters, T. S. Neill, K. Morris, N. M. Alcock, M. L. Baker, J. F. W. Mosselmans, K. Ignatyev, S. Shaw (UK)
- P-5 Using experimental actinide chemistry to solve technical challenges in spent fuel and nuclear material management within the nuclear decommissioning authority group
E. M. B. MacCormick, C. R. T. Smylie, R. Bernard, H. M. Steele, R. M. Orr, E. K. Gibson, J. H. Farnaby (UK)
- P-6 Solubility, speciation and thermodynamics of PuCO₃OH(cr) in carbonate containing NaCl solutions
P. Müller, D. Fellhauer, D. Schild, K. Dardenne, J. Rothe, M. Altmaier, X. Gaona, H. Geckeis (Germany)
- P-7 Solubility, redox speciation and sorption of Sn in cement systems
N. Huber, X. Gaona, K. Dardenne, T. Prüssmann, M. Altmaier, H. Geckeis (Germany)
- P-8 Spectroelectrochemical coupling to study Tc speciation in solution
N. Mayordomo, A. Bureika, J. Kretzschmar, K. Müller (Germany)
- P-9 Deciphering crystal-field excitations with HR-RIXS
M. S. Huzan, N. M. Alcock, M. A. Dunstan, K. S. Pedersen, M. L. Baker (UK)
- P-10 Determination of actinide central-field covalency with 3d4f resonant inelastic X-ray scattering (RIXS)
N. M. Alcock, M. S. Huzan, T. G. Burrow, M. L. Baker (UK)
- P-11 Spectroscopic investigations on the behavior of irradiated light water reactor fuels during prolonged dry interim storage and final disposal
K. Dardenne, M. Herm, T. König, Y. Lin, V. Metz, T. Pruessmann, J. Rothe, D. Schild, A. Walschburger, H. Geckeis (Germany)
- P-12 Monitoring the formation of ternary surface complexes and surface precipitates of U(VI) on zirconia by vibrational spectroscopy
H. Foerstendorf, I. Jessat, K. Heim, N. Jordan (Germany)
- P-13 Investigation of Thorium-based generator concepts – improvements, labeling and speciation
K. Maurer, B. Schacherl, M. Schäfer, Y. Remde, Ha. Taş, F. Geyer, A. Fried, S. Happel, M. Benešová-Schäfer, T. Vitova, H. Geckeis (Germany)

Tuesday (08 October 2024)

- P-14 A compact X-ray emission spectrometer at the SUL-X beamline of the KIT synchrotron radiation source: Implications for lanthanide and actinide research
J. Goettlicher, T. Spangenberg, T. Pruessmann, B. Schacherl, R. S. K. Ekanayake, E. M. Reynolds, H. Kaufmann-Heimeshoff, C. Y. Reitz, H. Ramanantoanina, T. Vitova, R. Steininger (Germany)
- P-15 On the Sr coordination, Sr K-edge absorption spectra, and solubility product constants of Sr-bearing calcite
A. S. Kim, A. S. Son, B. S. P. Hyun, A. K. D. Kwon (Korea)
- P-16 Ab-initio Pourbaix diagrams for U-H-O system
A. S. Son, B. S. P. Hyun, A. K. D. Kwon (Korea)
- P-17 The actinide chamber at the X-SPEC beamline
R. S. K. Ekanayake, N. Palina, H. Ramanantoanina, M. Blankenship, C. Vollmer, C. Wansorra, R. Steininger, D. Hauschild, C. Heske, L. Weinhardt, T. Vitova (Germany)
- P-18 Soft and hard x-ray spectroscopy with a novel calorimetric superconducting quantum sensor
M. Blankenship, K. Bitsch, R. Steininger, C. Wansorra, D. Hauschild, N. Arldt, C. Sandrell, F. Adam, M. Müller, T. Vitova, S. Kempf, L. Weinhardt, C. Heske (Germany)
- P-19 Spectroscopic study of the Pu(III)-ISA complex in weak acidic conditions
S. Cho, U. H. Yoon, H. Cho, K. Jeong, H.-K. Kim, H.-R. Cho (Korea)
- P-20 Complexation of U(VI) with N-donor ligands studied by high energy resolution X-ray spectroscopy and computations
C. Reitz, X. Zhang, C. Vollmer, K. Dardenne, T. Prüßmann, T. Sittel, P. Panak, T. Vitova (Germany)
- P-21 Electroanalytical and spectroscopic investigations of redox chemistry in heterobimetallic Uranyl crown ether complexes
A. Ervin, R. Golwankar, M. Makos, E. Mikeska, H. Kaufmann-Heimeshoff, T. Vitova, V.-A. Glezakou, J. Blakemore (USA)
- P-22 Complexation of Cm(III) with silicates at variable ionic strengths and pH values
S. Özyagan, T. Sittel, P. J. Panak (Germany)

Wednesday (09 October 2024)

Session 6 Design of radiopharmaceutical and separation agents

- 09:00 Targeted radionuclide therapy: the promise and challenges of short-lived alpha-emitting actinides
A. Rigby, A. G. Cosby, J. J. Woods, J. N. Wacker, T. Arino, J. V. Alvarenga Vasquez, K. E. Martin, R. K. Strong, R. J. Abergel (Plenary) (USA) **S6-T1**
- 09:40 Computational ligand design for targeted alpha therapy
C. Li, I. Carbo-Bague, C. F. Ramogida, G. Schreckenbach (Canada) **S6-T2**
- 10:00 Interaction of Ac³⁺-based radiopharmaceutical with Somatostatin receptor revealed by molecular dynamics simulations
S. Tsushima (Germany) **S6-T3**
- 10:20 Polypyridyl extractant design for actinide separation
X. Zhang, S. L. Adelman, B. T. Arko, C. R. De Silva, J. Su, S. A. Kozimor, V. Mocko, J. C. Shafer, B. W. Stein, G. Schreckenbach, E. R. Batista, P. Yang (USA/Canada) **S6-T4**
- 10:40 Coffee break

Session 7 Data analysis and method development

- 11:00 Using our artificial intelligence tools for analysis of materials characterization data pertaining to nuclear systems: Corrosion and radiation damage
J. Terry (Keynote) (USA) **S7-T1**
- 11:30 Fully automated procedure for XANES and EXAFS processing based on IgorPro
S. Mangold (Germany) **S7-T2**
- 11:50 Exploring f-electron systems through HERFD and RIXS
K. O. Kvashnina (France/Germany) **S7-T3**
- 12:10 New high-resolution X-ray spectroscopic tools for investigating 5f electrons in actinide compounds
H. Kaufmann-Heimeshoff, B. Schacherl, M. Tagliavini, J. Göttlicher, M. Mazzanti, K. Popa, O. Walter, T. Prüssmann, C. Vollmer, A. Beck, R. S. K. Ekanayake, J. A. Branson, T. Neill, D. Fellhauer, C. Reitz, D. Schild, D. Brager, C. Cahill, C. Windorff, T. Sittel, H. Ramanantonina, M. Haverkort, T. Vitova (Germany) **S7-T4**
- 12:30 Lunch break

Wednesday (09 October 2024)

Session 8 High resolution X-ray spectroscopy: theory and application

- 14:00 Origins of actinyl XAS features: Application to NpO_2^{2+}
P. S. Bagus, C. J. Nelin, B. Schacherl, T. Vitova (Keynote) (USA) **S8-T1**
- 14:30 A practical computational tool for actinide coordination chemistry (LFDFT): study of M4,5-edge core-to-core and valence-band resonant inelastic x-ray scattering
H. Ramanantoanina, C. Celis-Barros, T. Vitova (Keynote) (Germany) **S8-T2**
- 15:00 HERFD-XANES vs conventional XANES. The implications of cutting through the RIXS plane
L. Amidani (France/Germany) **S8-T3**
- 15:20 U M4,5 edge XANES of Uranyl: Potential energy curves of core-excited states and applications to x-ray spectroscopy
R. Polly, P. S. Bagus (Germany) **S8-T4**
- 15:40 New generation HPGe detector technologies for synchrotron applications
P. Quirin, N. Brocard, M. Ginz, G. Ilie, J.-B. Legras, V. Marian, J. Masseron (France) **S8-T5**
- 16:00 Coffee break

Session 9 Nuclear waste forms and debris materials

- 16:20 Real-time tracking of oxidation states of UO_2 nano particulate electrode using HR-XANES at Uranium M4 edge and a microfluidic technique
J. Yao, B. Schacherl, B. K. McNamara, V. Christian, E. S. Ilton, H. Jaeyoung, S. Schenk, E. C. Buck, H. Ramanantoanina, T. Vitova (Keynote) (USA) **S9-T1**
- 16:50 Application of X-ray absorption spectroscopy in support of Pu disposition strategy
L. R. Blackburn, A. A. Friskney, L. T. Townsend, C. L. Corkhill (Keynote) (UK) **S9-T2**
- 17:20 X-ray absorption spectroscopy (XAS) study on Technetium incorporation within iron oxides, waste glass, and grout waste forms
G. Wang, S. A. Saslow, M. R. Asmussen (USA) **S9-T3**
- 17:40 Dissolution behavior of simulated debris in the presence of malonic acid
R. Tonna, Y. Okamoto, T. Kobayashi, T. Sasaki (Japan) **S9-T4**
- 18:00 X-ray analysis for radioactive particulates from Fukushima-Daiichi nuclear power plant using synchrotron radiation at SPring-8
T. Kobayashi, M. Kobata, H. Tanida, S. Fujimori, Y. Takeda, T. Tsuji, T. Fukuda, G. Shibata, I. Kawasaki, R. Doi, Y. Okamoto, T. Okane, T. Yaita, Y. Satou, S. Suzuki, K. Maeda (Japan) **S9-T5**
- 18:20 End of day 3

Thursday (10 October 2024)

Session 10 Quantum theory supporting spectroscopy of 5f-element compounds

09:00	Chemical bonding and electronic structure enabled by 5f-electrons <i>P. Yang (Plenary) (USA)</i>	S10-T1
09:40	Determination of actinide central-field covalency with 3d4f resonant inelastic X-ray scattering <i>M. L. Baker (UK)</i>	S10-T2
10:00	Sensitivity to cis- versus trans- actinide-ligand covalency in M4-edge Resonant Inelastic X-ray Scattering <i>T. G. Burrow, N. M. Alcock, M. S. Huzan, M. O. J. Y. Hunault, M. L. Baker (UK/France)</i>	S10-T3
10:20	Quantum chemical studies of binary and ternary U(VI) hydroxo silicate complexes <i>I. Chiorescu, S. Krüger (Germany)</i>	S10-T4
10:40	Coffee break	

Session 11 Actinide coordination chemistry

11:00	Exploring actinide free radical interactions with electron paramagnetic resonance spectroscopy and density functional theory calculations <i>T. Z. Forbes, H. Rajapaksha, S. J. Kruse, S. K. Scherrer (Keynote) (USA)</i>	S11-T1
11:30	The coordination chemistry of U ⁴⁺ in aqueous solutions: Challenges and insights from spectroscopy and theory <i>G. Raposo-Hernández, R. R. Pappalardo, F. Réal, V. Vallet, E. Sánchez Marcos (France)</i>	S11-T2
11:50	Complexation of Protactinium(V) with chlorides in aqueous solution: Thermodynamic and structural insights <i>M. Maloubier, T. Shaaban, T. Aubert, V. Vallet, F. Réal, B. Siberchicot, C. Le Naour (France)</i>	S11-T3
12:10	Re-evaluation of the Pu(IV)-acetate speciation diagram taking into account polynuclear species <i>G. Chupin, C. Tamain, T. Dumas, P. L. Solari, P. Moisy, D. Guillaumont (France)</i>	S11-T4
12:30	Lunch break	

Thursday (10 October 2024)

Session 12 Spent nuclear fuel and waste conditioning

14:00	The application of neutron and synchrotron methods to the chemical and structural characterization of disordered systems of relevance to radioactive materials challenges <i>D. T. Bowron (Keynote) (UK)</i>	S12-T1
14:30	XAS studies on nuclear fuels: from simulated to spent fuels characterizations <i>V. Klosek, M. Rochedy, W. Tomczak, C. Le Gall, E. Geiger, L. Balice, S. Gobert, F. Audubert, M. O. J. Y Hunault, D. Menut, P. L. Solari (Keynote) (France)</i>	S12-T2
15:00	Multi-scale investigation of fission product speciation in $U_{1-y}Pu_yO_{2-x}$ SIMMOx using synchrotron techniques <i>R. Caprani, P. Martin, D. Prieur, J. Martinez, F. Lebreton, K. Kvashnina, E. F. Bazarkina, N. Clavier (Germany/France)</i>	S12-T3
15:20	Actinide immobilization by incorporation into ceramic phases <i>C. Hennig, V. Svitlyk, S. Weiss, L. Braga Ferreira dos Santos, J. Niessen, S. E. Gilson, J. Marquardt, T. Lender, S. Richter, G. L. Murphy, N. Huittinen (Germany)</i>	S12-T4
15:40	Coffee break	
16:15	Transfer to Speyer	
17:30	Reception and visit of space exhibition hall	
19:15	Conference dinner Historical perspectives on the development of actinide XAS <i>D. L. Clark (Dinner talk) (USA)</i>	
22:00	End of day 4	

Friday (11 October 2024)

Session 13 Radionuclide geochemistry

- 09:00 Incorporation of some f-block elements in ancient and synthetic Fe oxides
E. S. Ilton, S. T. Mergelsberg, E. J. Bylaska (Plenary) (USA) **S13-T1**
- 09:40 Understanding the varying mechanisms of radionuclide immobilization by alternative bentonite materials. Combined sorption, EXAFS and luminescence spectroscopy studies
G. F. Vettese, X. Li, L. Sirén, K. Silenius, M. Siitari-Kauppi, N. Huittinen, L. B. F. dos Santos, S. Shams Aldin Azzam, A. Rossberg, R. Bes, M. Niskanen, T. Peltola, G. T. W. Law (Finland) **S13-T2**
- 10:00 Effect of citrate on aqueous U(VI) speciation and U(VI) retention on Ca-bentonite
C. Sieber, J. Kretzschmar, B. Drobot, K. Schmeide, T. Stumpf (Germany) **S13-T3**
- 10:20 Insights into U(VI) reduction during bio-stimulation of microbes in U mine water
A. M. Newman-Portela, K. Kvashnina, E. Bazarkina, A. Roßberg, F. Bok, A. Kassahun, J. Raff, M. L. Merroun, E. Krawczyk-Bärsch (Germany) **S13-T4**
- 10:40 Coffee break

Session 14 Speciation of actinide materials: from nuclear legacies to fundamental science

- 11:00 Applications of X-ray absorption spectroscopy to the UK's nuclear legacy challenges
T. S. Neill, S. Shaw, C. Waters, E. Howard, R. Margreiter, J. F. W. Mosselmans, L. Abrahamsen-Mills, F. Schofield, C. Foster, K. Ignatyev, K. Morris (Keynote) (UK) **S14-T1**
- 11:30 Investigation of actinide-transition metal bonding
R. Gericke, D. Grödler, P. Kaden, M. Patzschke, R. Polly, K. Kvashnina (Keynote) (Germany) **S14-T2**
- 12:00 Poster and young scientist awards, closing remarks
- 12:30 Lunch break
- 14:00 End of conference