

### 3<sup>rd</sup> International Workshop on Advanced Techniques in Actinide Spectroscopy

#### SCIENTIFIC PROGRAM

Monday, November 7, 2016		
Time	Topic/Participants	Location
8:30 a.m.	Registration and Badging (FNVA badging starts at 8:30 am in the ETB Badging Office)	EMSL Lobby/ETB Badging Office
10:00 a.m.	<b>Welcome and Opening Remarks</b> Allison Campbell, Associate Laboratory Director, Pacific Northwest National Laboratory  Opening Chair: Zheming Wang, Pacific Northwest National Laboratory	EMSL Auditorium  EMSL Auditorium
10:30 a.m.	<b>Actinide Spectroscopy and Quantum Calculations Applied to Understand Uranyl Peroxide Nanoclusters</b> (Keynote, INVITED) <i>Peter Burns, University of Notre Dame</i>	EMSL Auditorium
11:30 a.m.	<b>A Multiple-Technique Round-Robin Test in Actinide Spectroscopy</b> <i>Harald Foerstendorf, Helmholtz-Zentrum Dresden-Rossendorf</i>	EMSL Auditorium
12:00 p.m.	Lunch	EMSL Auditorium
<b>Session 1</b>	<b>COMPUTATIONAL CHEMISTRY</b> (Chair: Ping Yang, Los Alamos National Laboratory)	
1:00 p.m.	<b>Theoretical Studies of Orbital Mixing in Actinide-Ligand Bonds via Core-Level K-edge XAS</b> (INVITED) <i>Enrique Batista, Los Alamos National Laboratory</i>	EMSL Auditorium
1:30 p.m.	<b>Quantum Chemical Modeling of Actinide Hydrolysis Complexes</b> <i>Sven Kruger, Technical University of Munich</i>	EMSL Auditorium
1:50 p.m.	<b>Quantum Chemical Modeling of U(VI) and Np(V) Adsorption on the Solvated (110) Edge Surface of Montmorillonite</b> <i>Alena Kremleva, (Presented by Sven Krueger) Technical University of Munich</i>	EMSL Auditorium
2:10 p.m.	<b>Fragment Molecular Orbital (FMO) Method for Studying Actinide Interaction with DNAs and Proteins</b> <i>Satoru Tsushima, Helmholtz-Zentrum Dresden-Rossendorf</i>	EMSL Auditorium
2:30 p.m.	Intermission	EMSL 1075/1077

Registration and intermission includes light refreshments.

EMSL is located at PNNL

**3<sup>rd</sup> International Workshop on  
Advanced Techniques in Actinide Spectroscopy**

<b>Session 2</b>	<b>FLUORESCENCE</b> (Chair: Harald Foerstendorf, Helmholtz-Zentrum Dresden – Rossendorf)	
2:50 p.m.	<b>Luminescence Spectroscopy of An/Ln in Environmental Systems</b> (INVITED) <i>Robin Steudtner, Helmholtz-Zentrum Dresden-Rossendorf</i>	EMSL Auditorium
3:10 p.m.	<b>Luminescence Lifetime Measurements of Trivalent f-elements in Mixed Solvent Systems</b> <i>Heather Felmy, Washington State University</i>	EMSL Auditorium
3:30 p.m.	<b>Spectroscopic Investigation for the Structure of Actinides Sorption on the Solid/Liquid Inter-surface</b> <i>Wangsuo Wu, Lanzhou University</i>	EMSL Auditorium
3:50 p.m.	<b>TRLFS and ATR-IR Studies on Eu(III) and Am(III) Adsorption on SiO<sub>2</sub> Particles in the Presence of a Small Organic Ligand</b> <i>Hee-Kyung Kim, Korea Atomic Energy Institute</i>	EMSL Auditorium
4:10 p.m.	<b>Spatially-Resolved Sorption Studies of Eu(III) on Granite Surface with Time-Resolved Laser Fluorescence Microscopy (TRLFM)</b> <i>Konrad Zesewitz, Helmholtz-Zentrum Dresden-Rossendorf</i>	EMSL Auditorium
4:30 p.m.	<b>Retardation and Release of Uranium on Phlogopite Mica at the Absence and Presence of Humic Acid: A Batch and TRLFS Study</b> <i>Duoqiang Pan, Lanzhou University</i>	EMSL Auditorium
5:30 – 7:30 p.m.	<b>Poster Session</b>	EMSL 1075/1077

Intermission includes light refreshments.

**3<sup>rd</sup> International Workshop on  
Advanced Techniques in Actinide Spectroscopy**

**SCIENTIFIC PROGRAM**

Tuesday, November 8, 2016		
Time	Topic/Participant(s)	Location
7:45 a.m.	Continental Breakfast	EMSL 1075/1077
<b>Session 3</b>	<b>SOLUTION CHEMISTRY</b> (Chair: Robert Baker, University of Dublin)	
8:00 a.m.	<b>Actinide Solution Chemistry and the Processing of Nuclear Materials</b> (INVITED) <i>Sue Clark, Pacific Northwest National Laboratory and Washington State University</i>	EMSL Auditorium
8:30 a.m.	<b>Detection of Actinides and Lanthanides in Solutions by Chemiluminescence Laser Spectroscopy</b> <i>Igor Izosimov, Joint Institute for Nuclear Research</i>	EMSL Auditorium
8:50 a.m.	<b>Complexation of Actinides by Branched N-macrocycle DOTA</b> <i>Thomas Dumas, CEA (Atomic Energy Comm.)</i>	EMSL Auditorium
9:10 a.m.	<b>Electrochemical and Spectroscopic Behavior of Neptunium in Aqueous Nitric Acid</b> <i>Dev Chatterjay, Pacific Northwest National Laboratory</i>	EMSL Auditorium
9:30 a.m.	<b>Efficient Removal of Radionuclides from Aqueous Solutions Using Carbon Nanomaterials</b> <i>Xiangke Wang, North China Electric Power University</i>	EMSL Auditorium
9:50 a.m.	Intermission	EMSL 1075/1077
10:10 a.m.	TOURS: EMSL and RadEMSL	EMSL and 3410 Building
12:00 p.m.	Lunch	EMSL Auditorium
<b>Session 4</b>	<b>NMR and VIBRATIONAL SPECTROSCOPY</b> (Chair: Herman Cho, Pacific Northwest National Laboratory)	
1:00 p.m.	<b>Structure and Ligand Exchange Dynamics in Ternary Uranium(VI)-Peroxide Complexes Studied by NMR Spectroscopy</b> (INVITED) <i>Zoltan Szabo, Royal Inst. of Technology (KTH)</i>	EMSL Auditorium
1:30 p.m.	<b>Probing the Pu<sup>4+</sup> magnetic moment in PuF<sub>4</sub> with <sup>19</sup>F NMR spectroscopy</b> <i>Gigdem Capan, Washington State University, Tri-Cities</i>	EMSL Auditorium
1:50 p.m.	<b><sup>31</sup>P Nuclear Magnetic Resonance as a Probe of Plutonium Incorporation and Radiation Damage in Phosphates</b> <i>Ian Farnan, University of Cambridge</i>	EMSL Auditorium
2:10 p.m.	<b>Raman Scattering Investigations on Actinide Oxides</b> (INVITED) <i>Patrick Simon, National Center for Scientific Research</i>	EMSL Auditorium
2:30 p.m.	<b>Assignment of Unexpected Raman Spectra of Uranyl Triperoxide Complexes</b>	EMSL 1075/1077

Intermission includes light refreshments.

**3<sup>rd</sup> International Workshop on  
Advanced Techniques in Actinide Spectroscopy**

*Mateusz Dembowski, University of Notre Dame*

<b>Session 5</b>	<b>COMPUTATIONAL CHEMISTRY II</b> (Chair: Satoru Tsushima, Helmholtz–Zentrum Dresden–Rossendorf)	
2:50 p.m.	<b>Structures of Plutonium(IV) and Uranium(VI) with <i>N,N</i>-Dialkyl Amides from Crystallography, X-ray Absorption Spectra, and Theoretical Calculations</b> <i>Dominique Guillaumont, Atomic Energy Commission</i>	EMSL Auditorium
3:10 p.m.	<b>Quantum Chemical Investigation of Incorporation of Uranium(V) into Magnetite: Combining Multi-Reference <i>ab initio</i> Methods and Density Functional Theory</b> <i>Robert Polly, Karlsruhe Institute of Technology</i>	EMSL Auditorium
3:30 p.m.	<b>Probing the Structure of Uranium Complexes in Molten Salt by Absorption Spectroscopy and DFT Calculation</b> <i>Tao Su (presented by Hongtao Liu) – Shanghai Institute of Applied Physics</i>	EMSL Auditorium
3:50 p.m.	<b>Unusual Magnetic Properties of Actinide Thiocyanate and Selenocyanate Complexes</b> <i>Robert Baker, Trinity College, Dublin</i>	EMSL Auditorium
4:10 p.m.	<b>Interplay Between Theory and Spectroscopy in Understanding Interfacial Interactions: A Case Study for CeO<sub>2</sub></b> <i>Ping Yang, Los Alamos National Laboratory</i>	EMSL Auditorium

Intermission includes light refreshments.

**3<sup>rd</sup> International Workshop on  
Advanced Techniques in Actinide Spectroscopy**

**SCIENTIFIC PROGRAM**

<b>Wednesday, November 9, 2016</b>		
Time	Topic/Participant(s)	Location
7:45 a.m.	Continental Breakfast	EMSL 1075/1077
<b>Session 6</b>	<b>ENVIRONMENTAL XAS</b> (Chair: Carolyn Pearce, Pacific Northwest National Laboratory)	
8:00 a.m.	<b>XAFS Spectroscopic Studies of Uranium Speciation at Mineral-Water and Sediment-Water Interfaces (INVITED)</b> <i>Jeffrey Catalano, Jeffrey – Washington University St. Louis</i>	EMSL Auditorium
8:30 a.m.	<b>The Effect of Iron Oxides and Montmorillonite Clays on the Transformations of Uranium Under Reducing Conditions</b> <i>Maxim Boyanov, Institute of Chemical Engineering</i>	EMSL Auditorium
8:50 a.m.	<b>Investigations of Plutonium Behavior in Vadose Zone</b> <i>Melody Maloubier, Clemson University</i>	EMSL Auditorium
9:10 a.m.	<b>Actinides Speciation in Seawater and Uptake by Marine Accumulating Organisms</b> <i>Christophe Den Auwer, University Nice Sophia Antipolis</i>	EMSL Auditorium
9:30 a.m.	<b>XAFS Investigations of UVI Reduction by Biotic and Abiotic Green Rusts</b> <i>Ken Kemner, Argonne National Laboratory</i>	EMSL Auditorium
9:50 a.m.	Intermission	EMSL 1075/1077
<b>Session 7</b>	<b>HANFORD</b> (Chair: Zheming Wang, Pacific Northwest National Laboratory)	
10:10 a.m.	<b>Migration at the Hanford Site: Understanding and Models Provided by Microscopic Methods and Important Remaining Challenges (INVITED)</b> <i>John Zachara, Pacific Northwest National Laboratory</i>	EMSL Auditorium
11:10 a.m.	Lunch	EMSL 1075/1077
	<b>TOURS</b>	
12:15 p.m.	Load onto bus	EMSL Parking Lot
12:30 – 4:30 p.m.	B Reactor Tour	B Reactor
4:30 – 6:00 p.m.	LIGO – Laser Interferometer Gravitational-Wave Observatory	Hanford Site
6:00 – 8:00 p.m.	Banquet/Announcements	BSF/CSF Lobby

Intermission includes light refreshments.

**3<sup>rd</sup> International Workshop on  
Advanced Techniques in Actinide Spectroscopy**

**SCIENTIFIC PROGRAM**

Thursday, November 10, 2016		
Time	Topic/Participant(s)	Location
7:45 a.m.	Continental Breakfast	EMSL 1075/1077
<b>Session 8</b>	<b>XAS</b> (Chair: Ken Kemner, Argonne National Laboratory)	
8:00 a.m.	<b>X-ray Absorption Spectroscopy of Actinium and Comparison with Actinide +3</b> <i>Maryline Ferrier, Los Alamos National Laboratory</i>	EMSL Auditorium
8:20 a.m.	<b>Actinide and Lanthanide EXAFS Applications for the Nuclear Fuel Cycle</b> <i>Vanessa Hoffeltz, Pacific Northwest National Laboratory</i>	EMSL Auditorium
8:40 a.m.	<b>Coordination Structure of Uranium Complexes in disordered Systems using X-ray Absorption Fine Structure Spectroscopy</b> <i>Linjuan Zhang, Shanghai Institute of Applied Physics</i>	EMSL Auditorium
9:00 a.m.	<b>XAFS and <math>\mu</math>-XRF Investigation of Highly Radioactive Nuclear Waste Samples at KIT/ANKA</b> <i>Jorg Rothe, Karlsruhe Institute of Technology</i>	EMSL Auditorium
9:20 a.m.	<b>Actinide- and Actinide-Relevant XAS without a Synchrotron</b> <i>Gerald Seidler, University of Washington</i>	EMSL Auditorium
9:40 a.m.	Intermission	EMSL 1075/1077
<b>Session 9</b>	<b>XPS and Other</b> (Chair: Christophe Den Auwer, University Nice Sophia Antipolis)	
10:00 a.m.	<b>XPS Determination of Uranium Oxidation States (INVITED)</b> <i>Eugene Ilton, Pacific Northwest National Laboratory</i>	EMSL Auditorium
10:20 a.m.	<b>Diffuse Reflectance Spectroscopy of Plutonium Fluorides and Other Pu Solids: Evolution of Spectral Signature in Time as a Built-In Chronometer of the Sample Age and Crystallinity</b> <i>Sergey Sinkov, Pacific Northwest National Laboratory</i>	EMSL Auditorium
10:40 a.m.	<b>The optical properties of uranium carbide measured by spectroscopic ellipsometry</b> <i>Wigbert Siekhaus, Lawrence Livermore National Laboratory</i>	EMSL Auditorium
11:00 a.m.	<b>Probing the Electronic Structures of Thorium Oxides Using Anion Photoelectron Velocity Map Imaging</b> <i>Hongtao Liu, Shanghai Institute of Applied Physics</i>	EMSL Auditorium
11:20 a.m.	<b>Investigation of Europium (III) Acetylacetonate Complexes at Air/Water Interface by Sum Frequency Generation Vibrational Spectroscopy</b> <i>Zheming Wang, Pacific Northwest National Laboratory</i>	EMSL Auditorium

Intermission includes light refreshments.

**3<sup>rd</sup> International Workshop on  
Advanced Techniques in Actinide Spectroscopy**

11:55 a.m.      **Adjourn**

Intermission includes light refreshments.