

A new NMR facility for solid state actinide research at the Institute for Transuranium Elements

*Original*

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# Plutonium Futures – The Science 2010



**Keystone, Colorado, USA, September 19-23, 2010**

## *Supporting safe and secure plutonium research as part of the global energy mix*

Plutonium Futures—The Science is a series of conferences providing an international forum for discussion of current research on the physical and chemical properties of plutonium and other actinide elements. In bringing people together from diverse disciplines, the conference aims to enhance the dialogue among scientists and engineers on the fundamental properties of plutonium and their technological consequences.

## Conference Scope

- Condensed matter physics
- Materials science
- Surface, interfaces, colloids, corrosion
- Plutonium and actinide chemistry
- Fuel cycle issues
- Detection and speciation analyses
- Roundtable discussions  
Global security
- Special tutorial session

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Lawrence Livermore  
National Laboratory

In cooperation with  
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Los Alamos National Laboratory



**OFFICIAL PROGRAM**

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UPDATED: 9/10/2010

Welcome to

# Plutonium Futures— The Science 2010

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September 19-23, 2010

Keystone, CO

Keystone Resort and Conference Center

*Supporting safe and secure plutonium research as part of the global energy mix*

Plutonium Futures—The Science is a series of conferences providing an international forum for discussion of current research on the physical and chemical properties of plutonium and other actinide elements. In bringing people together from diverse disciplines, the conference aims to enhance the dialogue among scientists and engineers on the fundamental properties of plutonium and their technological consequences.

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## CONFERENCE OFFICIALS

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**Honorary Co-Chair:**

Dr. Michael Anastasio,  
*Director,  
Los Alamos National Laboratory*

**Honorary Co-Chair:**

Dr. Siegfried S. Hecker,  
*Senior Fellow, Professor (Research),  
Stanford University*

**Honorary Co-Chair:**

Dr. Gerard H. Lander,  
*Senior Scientist,  
Institut Laue-Langevin, Grenoble, France*

**General Co-Chair:**

Dr. David L. Clark,  
*Laboratory Fellow, Institute Offices,  
Los Alamos National Laboratory*

**General Co-Chair:**

Dr. Michael J. Fluss,  
*Senior Scientist, Condensed Matter and  
Materials Division  
Lawrence Livermore National Laboratory*

**General Co-Chair:**

Dr. Gordon D. Jarvinen,  
*Acting Director, Seaborg Institute,  
Stockpile Manufacturing and Support Directorate,  
Los Alamos National Laboratory*

**Technical Program Co-Chair:**

Dr. David E. Hobart,  
*Project Manager, Chemistry Division  
Los Alamos National Laboratory*

**Technical Program Co-Chair:**

Ms. Susan M. Ramsay,  
*Professional Staff Assistant, Seaborg Institute,  
Stockpile Manufacturing and Support Directorate,  
Los Alamos National Laboratory*

# Conference Schedule

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## SUNDAY, SEPTEMBER 19, 2010

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1:00 PM – 5:00 PM	TUTORIAL SESSION
3:00 PM – 7:00 PM	CONFERENCE REGISTRATION
6:00 PM – 8:00 PM	OPENING RECEPTION

## MONDAY, SEPTEMBER 20, 2010

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7:30 AM – 4:30 PM	CONFERENCE REGISTRATION
8:00 AM – 9:40 AM	PLENARY SESSION—1
9:40 AM – 9:50 AM	BREAK
9:50 AM – 12:15 PM	TECHNICAL SESSIONS <i>Coordination Chemistry</i> <i>Condensed-Matter Physics—I</i>
12:15 PM – 1:30 PM	LUNCH BREAK
1:30 PM – 2:50 PM	PLENARY SESSION—2
2:50 PM – 3:00 PM	BREAK
3:00 PM – 5:25 PM	TECHNICAL SESSIONS <i>Environmental Chemistry</i> <i>Materials Science—I</i>
7:30 PM – 9:30 PM	POSTER SESSION—1 <i>Detection and Analysis</i> <i>Environmental Chemistry</i> <i>Coordination Chemistry</i> <i>Solution and Gas Phase Chemistry</i> <i>Compounds and Complexes</i>

## TUESDAY, SEPTEMBER 21, 2010

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7:30 AM – 4:30 PM	CONFERENCE REGISTRATION
8:00 AM – 9:20 AM	PLENARY SESSION—3
9:20 AM – 9:30 AM	BREAK
9:30 AM – 11:55 AM	TECHNICAL SESSIONS <i>Fuel Cycle—I</i> <i>Condensed Matter Physics—II</i>
11:55 AM – 1:20 PM	LUNCH BREAK
1:20 PM – 2:40 PM	PLENARY SESSION—4
2:40 PM – 2:50 PM	BREAK
2:50 PM – 5:15 PM	TECHNICAL SESSIONS <i>Fuel Cycle—II</i> <i>Material Sciences—II</i>
7:00 PM – 9:00 PM	GLOBAL SECURITY—ROUNDTABLE: “SECURITY IMPLICATIONS OF A GLOBAL EXPANSION OF NUCLEAR POWER”

## WEDNESDAY, SEPTEMBER 22, 2010

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7:30 AM – 4:30 PM	CONFERENCE REGISTRATION
8:00 AM – 9:20 AM	PLENARY SESSION—5
9:20 AM – 9:30 AM	BREAK
9:30 AM – 11:55 AM	TECHNICAL SESSIONS <i>Detection and Analysis—I</i> <i>Surface Science and Corrosion</i>
11:55 AM – 1:20 PM	LUNCH BREAK
1:20 PM – 2:40 PM	PLENARY SESSION—6
2:40 PM – 2:50 PM	BREAK
2:50 PM – 4:50 PM	TECHNICAL SESSIONS <i>Detection and Analysis—II</i> <i>Condensed Matter Physics—III</i>
5:00 PM – 7:00 PM	POSTER SESSION—2 <i>Surface Science and Corrosion</i> <i>Materials Science</i> <i>Condensed Matter Physics</i> <i>Fuel Cycle</i> <i>Radiolysis and Radiation Damage</i>
7:30 PM – 9:00 PM	BANQUET

## THURSDAY, SEPTEMBER 23, 2010

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7:30 AM – 3:00 PM	CONFERENCE REGISTRATION
8:00 AM – 9:20 AM	PLENARY SESSION—7
9:20 AM – 9:30 AM	BREAK
9:30 AM – 11:55 AM	TECHNICAL SESSIONS <i>Compounds and Complexes</i> <i>Radiolysis and Radiation Damage</i>
11:55 AM – 1:20 PM	LUNCH BREAK
1:20 PM – 4:10 PM	TECHNICAL SESSIONS <i>Solutions and Gas Phase Chemistry</i> <i>Material Sciences—III</i>
4:10 PM – 4:20 PM	BREAK
4:20 PM – 4:40 PM	CLOSING

## Conference Information

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### Accommodations/Hotel Information

The Keystone Resort and Conference Center is the location for the Plutonium Futures — The Science 2010 Conference, where all meeting activities and technical sessions will take place. Keystone Resort is located in Colorado's Rocky Mountains, is over 3000 acres and spreads across three mountain peaks.

### Meeting Registration

Registration is required for all attendees and presenters. Badges are required for admission to all events. The Full Meeting Registration fee includes one copy of the printed summary book with a CD of the summaries and one ticket each to the Opening Reception and the Banquet.

*NOTE: Additional tickets can be purchased at the ANS Registration Desk for the Opening Reception and the Banquet.*

### Registration Hours:

The Meeting Registration Desk and Message Center will be located in the Lakeside Gallery Area of the Keystone Resort and Conference Center.

You may register, purchase tickets for events, or pick up your registration packet during the following hours:

SUNDAY, SEPTEMBER 19, 2010  
3:00 P.M. – 7:00 P.M.  
MONDAY, SEPTEMBER 20, 2010  
7:30 A.M. – 4:30 P.M.  
TUESDAY, SEPTEMBER 21, 2010  
7:30 A.M. – 4:30 P.M.  
WEDNESDAY, SEPTEMBER 22, 2010  
7:30 A.M. – 4:30 P.M.  
THURSDAY, SEPTEMBER 23, 2010  
7:30 A.M. – 3:00 P.M.

### Conference Publications

Each full meeting registrant will receive a copy of the printed summary book with a CD of the summaries as part of the full meeting registration fee. Additional copies may be purchased at the meeting registration desk for \$85.00.

### Special Events

#### Opening Reception

SUNDAY, SEPTEMBER 19, 2010  
6:00 P.M. – 8:00 P.M.  
Location: Edgewater

One ticket to the Opening Reception is included with the full meeting registration. *Additional tickets can be purchased at the ANS Registration Desk for \$85.00 each.*

#### Banquet

WEDNESDAY, SEPTEMBER 22, 2010  
7:30 P.M. – 9:00 P.M.  
Location: Keystone Lodge Ballroom

#### *Pulitzer Prize-Winning Author Richard Rhodes to Deliver Banquet Address*

Richard Rhodes is the author or editor of twenty-three books. His fourth and last volume of nuclear history, *The Twilight of the Bombs*, will be published just prior to the Conference. With the completion of this last volume, his quartet of nuclear histories, *The Making of the Nuclear Age*, comprehends the story of the introduction of a historic new technology across more than one hundred years.

One ticket to the Conference Banquet is included with the full meeting registration. *Additional tickets can be purchased at the ANS Registration Desk for \$85.00 each.*

## Tutorial Session

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### Plutonium Futures – The Science 2010

#### TUTORIAL

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A tradition at the conference has been a half-day Tutorial session held on Sunday afternoon. The Tutorial is intended for students and scientists new to the area of plutonium research, and is intended to provide some background material on topics of relevance for the conference. At Keystone, we have arranged the following Tutorial.

#### TUTORIAL SESSION

Sunday, September 19, 2010 • 1:00 PM – 5:00 PM • Location: Suns Room

1:00 PM – 2:00 PM	“Intended Consequences of President Carter’s Comprehensive Policy to Stop Proliferation” A. David Rossin ( <i>Former Assistant Secretary of Energy and Former American Nuclear Society President, Retired</i> )
2:00 PM – 3:00 PM	“Nuclear Fuel Cycle” Gordon Jarvinen ( <i>Los Alamos National Laboratory</i> )
3:00 PM – 4:00 PM	“The Challenges of International Safeguard Efforts to Verify the Peaceful Uses of Plutonium” Brian Boyer ( <i>Los Alamos National Laboratory</i> )
4:00 PM – 5:00 PM	“Electronic Structure Theory for Heavy Elements” Nik Kaltsoyannis ( <i>University College, London</i> )

# Technical Sessions: Monday

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MONDAY, SEPTEMBER 20, 2010, 8:00 A.M.

## Plenary Session—1, All invited

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### Keystone Lodge Ballroom

8:00 a.m.

Welcome

8:20 a.m.

Actinide-Specific Sequestering Agents, David K. Shuh (*LBL*), Kenneth N. Raymond (*Univ of California, Berkeley*), Rebecca J. Abergel (*LBL*), Polly Chang (*SRI International*), Eleanor A. Blakely, Patricia Durbin-Heavey (*LBL*)

9:00 a.m.

Unexpected Covalency in the Actinide Dioxides, Richard L. Martin, E. Bauer, A. K. Burrell, T. M. McCleskey, B. L. Scott, Q. Jia, T. Durakiewicz, J. J. Joyce, K. S. Graham, S. Kozimor, S. R. Conradson, L. E. Roy (*LANL*), G. E. Scuseria (*Rice Univ*)

MONDAY, SEPTEMBER 20, 2010, 9:50 A.M.

## Coordination Chemistry

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### Arapahoe

9:50 a.m.

Non-Aqueous Transuranic Coordination Chemistry, Andrew James Gaunt, David D. Schnaars, Mary P. Neu, Brian L. Scott, Iain May, Sean D. Reilly (*LANL*), Trevor W. Hayton (*Univ of California, Santa Barbara*), Nikolas Kaltsoyannis, Kieran I. M. Ingram (*University College London*), Enrique R. Batista (*LANL*), James A. Ibers (*Northwestern Univ*), Dean R. Peterman (*INL*), Stosh A. Kozimor, James M. Boncella, Alejandro E. Enriquez (*LANL*)

10:15 a.m.

On the Relative Roles of the 5f- and 6d-Orbitals in Covalent Bonding, Stosh A. Kozimor, Enrique R. Batista, Kevin S. Boland (*LANL*), Joseph A. Bradley (*Univ of Washington*), David L. Clark, Steven D. Conradson, Richard L. Martin, Stefan G. Minasian (*LANL*), David K. Shuh (*LBL*), Gerald T. Seidler (*Univ of Washington*), Ping Yang (*PNNL*), invited

11:00 a.m.

Quantifying Covalency in Molecular Actinide Complexes from Th to Cm, Nikolas Kaltsoyannis, Matthew J. Tassell (*University College London*)

11:25 a.m.

Periodicity Across the Actinide Series: Coupling Structural and Solution Chemistry, Richard E. Wilson (*ANL*), invited

11:50 a.m.

Synthesis of a Nitrido-Substituted Analogue of the Uranyl Ion,  $[N=U=O]^+$ , Trevor W. Hayton, Skye Fortier, Guang Wu (*Univ of California, Santa Barbara*)

## Condensed-Matter Physics—I

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### Divide

9:50 a.m.

Electronic Structure and Adaptive 5f Character in Plutonium Materials, John Joyce, Tomasz Durakiewicz, Kevin Graham, Eric Bauer, Jian-Xin Zhu, Richard L. Martin, John Wills, Lindsay Roy, Jeremy Mitchell, David P. Moore, John Kennison, T. Mark McCleskey, Anthony Burrell, Eve Bauer, Quanxi Jia (*LANL*), Gustavo E. Scuseria (*Rice Univ*), invited

10:15 a.m.

Pu and its Neighbours - A Photoemission Study of the Electronic Structure of Actinides, Thomas H. Gouder (*European Commission, JRC*), invited

11:00 a.m.

Resonant Inverse Photoelectron Spectroscopy of the Oxides of Uranium and Cerium, James G. Tobin, S. W. Yu, B. W. Chung (*LLNL*), G. D. Waddill (*UMR*), invited

11:25 a.m.

A Minimal Model for the Energetics of Pu, Chris Marianetti (*Columbia Univ*)

11:50 a.m.

Electronic Structure and Correlation Effects in  $PuCoGa_5$ , Jian-Xin Zhu (*LANL*), M. D. Jones (*Univ of Buffalo*), O. Granas (*Uppsala Univ*), A. K. McMahan (*LLNL*), T. Durakiewicz, J. J. Joyce, E. D. Bauer, J. N. Mitchell, J. A. Kennison, R. C. Albers, J. M. Wills (*LANL*)

MONDAY, SEPTEMBER 20, 2010, 1:30 P.M.

## Plenary Session—2, All invited

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### Keystone Lodge Ballroom

1:30 p.m.

Colloid Facilitated Migration of Radionuclides and Evolution of their Speciation at the Mayak Site, Stepan N. Kalmykov (*Moscow State University*), Boris F. Myasoedov, Alexander P. Novikov (*RAS*), Olga N. Batuk (*LANL*)

2:10 p.m.

Multiple Heating Effects on the Cyclic Expansion of Delta-Pu Alloys: A Model of Gas Pore Formation in Molten Eutectics, Lidia F. Timofeeva (*A. A. Bochar High-Technology Research Institute of Inorganic Materials, VNIINM*)

MONDAY, SEPTEMBER 20, 2010, 3:00 P.M.

## Environmental Chemistry

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### Arapahoe

3:00 p.m.

Plutonium Containing Particles in the Environment, Brit Salbu (*Norwegian University of Life Sciences*), Koen Janssens (*University of Antwerp*), Ole Christian Lind (*Norwegian University of Life Sciences*), Wout De Nolf (*University of Antwerp*), invited

3:25 p.m.

Plutonium Oxidation State Distribution in Anoxic Groundwater, Donald T. Reed, Juliet S. Swanson, David Ams, Hnin Khaing (*LANL*), invited

3:50 p.m.

Subsurface Mobile Plutonium Speciation: Sampling Artifacts for Groundwater Colloids, Daniel I. Kaplan (*SRNL*), Ken O. Buesseler (*Woods Hole Oceanographic Institution*), invited

4:35 p.m.

Plutonium Redox Behavior in Aqueous Solutions and on Nanocrystalline Iron Phases, David Fellhauer (*European Commission, JRC*), Regina Kirsch (*FZD*), Marcus Altmaier, Volker Neck (*KIT*), Andreas Scheinost (*FZD*), Thierry Wiss (*European Commission, JRC*), Laurent Charlet (*LGIT - UJF*), Thomas Fanghaenel (*European Commission, JRC*)

## Technical Sessions: Monday

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### 5:00 p.m.

Plutonium Sorption at the Muscovite-Electrolyte Interface Studied by X-Ray Reflectivity, Moritz Schmidt, Paul Fenter, Richard Wilson, Sang Soo Lee, Lynda Soderholm (*ANL*)

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### Materials Science—I

#### Divide

### 3:00 p.m.

Structural and Phase Transformations, Spall and Shear Fractures in the Sphere of Unalloyed Plutonium under Explosive Loading, Evgeny A. Kozlov (*RFNC—E.I.Zababakhin Research Institute of Technical Physics*), Lidia F. Timofeva (*Bochvar Research Institute of Nonorganic Materials*)

### 3:25 p.m.

MARS: A Synchrotron Beamline for the Characterization of Radioactive Matter. Application to Diamond Anvil Cell Measurements, Marc Souilah (*CEA*), Bruno Sitaud (*Synchrotron SOLEIL*), Philippe Faure (*CEA*)

### 3:50 p.m.

New Investigation of the Pressure and Temperature Phase Diagram of a Delta Plutonium Alloy, Philippe Faure, François Delaunay (*CEA*)

### 4:35 p.m.

Kinetics of Dislocations During Plastic Deformation of  $\delta$ -Plutonium, Victor Alexeevich Pushkov (*RFNC—VNIIEF*)

### 5:00 p.m.

Stability of the Brannerite Structure with Actinides at High Pressures, Fuxiang Zhang, Maik Lang, Rodney C. Ewing (*Univ of Michigan*)

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## MONDAY, SEPTEMBER 20, 2010, 7:30–9:30 P.M.

### Poster Session—I

#### Ten Mile/Lakeside Gallery

##### Detection and Analysis

The Features of OH Radicals Formation in Laser-Induced Excitation of Samarium Hydroxide and Multi-step Chemiluminescence Excitation for Trace Analysis in Solutions., Igor Nikolaevich Izosimov, Nikolay Gorshkov, Vladimir Mikhalev, Nikolay Firsin (*V.G.Khlopin Radium Inst*), Voldemar Tarita, Igor Shantir, Natal'ia Zybina (*A.M. Nikiforov All-Russian Center of Emergency and Radiation Medicine EMERCOM*)

Diffuse Reflectance Spectroscopy of Plutonium Metal, Alloys, and Compounds, David E. Hobart, Dominic S. Peterson, Stosh A. Kozimor, Kevin S. Boland, Marianne P. Wilkerson, Jeremy N. Mitchell (*LANL*)

Announcing the Publication of Volume Six of The Chemistry of the Actinide and Transactinide Elements, Lester R. Morss (*ANL (retired)*), Norman M. Edelstein (*LBNL*), Jean Fuger (*Univ of Liege*)

Chemistry and Metallurgy Research Replacement (CMRR) Project in Support of Analytical Chemistry and Material Characterization Capabilities at Los Alamos National Laboratory, Amy S. Wong, Timothy O. Nelson, Denise L. Thronas, Steven M. Dinehart, Mardoceo Vialpando (*LANL*)

System for Angle Resolve Photoemission Spectroscopy of Plutonium Materials, Kevin Shawn Graham, John J. Joyce, Tomasz Durakiewicz (*LANL*)

Rapid Prototyping of Containment for Plutonium Samples for the Purposes of X-Ray Fluorescence and X-Ray Diffraction Studies Outside a Glovebox, Chris Puxley (*AWE*)

Pre-Concentration and Analysis of Plutonium from Solutions Using Polymer Ligand Films, Dominic S. Peterson, Edward R. Gonzales, Crystal L. Tulley, Jaclyn A. Herrera, Claudine E. Armenta (*LANL*)

Actinide Analytical Chemistry Capabilities at Los Alamos National Laboratory—Plutonium Center of Excellence, Amy S. Wong (*LANL*)

Near-infrared Photoluminescence and Ligand K-Edge X-Ray Absorption Spectroscopies of  $\text{AnO}_2\text{Cl}_4^{2-}$  (An: U, Np, Pu), Marianne P. Wilkerson, Enrique R. Batista, John M. Berg, Kevin S. Boland, David L. Clark, Steven D. Conradson, Stosh A. Kozimor, Richard L. Martin, Brian L. Scott, Gregory L. Wagner (*LANL*), Ping Yang (*PNNL*)

TRU Waste Reduction by Using Gas Pressurized Extraction Chromatography for Pu Removal, Ning Xu, Alexander Martinez, David L. Gallimore (*LANL*)

#### Environmental Chemistry

Chemistry of An(III,IV)/Ln(III) Eigencolloids: Complexation Reactions with Inorganic and Organic Ligands, Javier Gaona (*KIT*), Mireia Grive, Vanessa Montoya, Elisenda Colas (*Amphos 21*), Marcus Altmaier (*Karlsruhe Institute of Technology*), Lara Duro (*Amphos 21*)

Micro-XRF/XAS/XRD Investigations on Actinide Containing Waste Materials, Rainer Daehn (*Scherrer Inst*), Dmitry Popov (*Advanced Photon Source*), Javier Gaona, Erich Wieland (*Scherrer Inst*)

Actinide Sorption by Cementitious Materials: The Case of Neptunium, Jan Tits, Xavier Gaona, Rainer Daehn, Erich Wieland (*Scherrer Inst*)

The Transformations of Uranium Oxides under Repository Conditions, Tatiana V. Kazakovskaya, Vyacheslav Shapovalov (*RFNC—VNIIEF*), Elena Zakharova (*RAS*)

THEREDA - Thermodynamic Data for Waste Management Assessment, Marcus Altmaier, Christiane Bube (*KIT*), Vinzenz Brendler (*FZD*), Christian Michael Marquardt (*KIT*), Helge Moog (*Gesellschaft fuer Anlagen- und Reaktorsicherheit*), Anke Richter (*FZD*), Tina Scharge (*Gesellschaft fuer Anlagen- und Reaktorsicherheit*), Wolfgang Voigt (*TU Bergakademie Freiberg*), Stefan Wilhelm (*AF-Colenco Ltd.*), Georgia Wollmann (*TU Bergakademie Freiberg*)

Characterization of U and Pu Oxide Particles Formed During the Accident at the Chernobyl NPP by Various Spectroscopic and Microscopic Techniques, Olga N. Batuk (*LANL*), Irina E. Vlasova (*Moscow State University*), Alison L. Costello (*LANL*), Stepan N. Kalmykov (*Moscow State University*), Steven D. Conradson, Marianne P. Wilkerson, David L. Clark (*LANL*)

Plutonium in the WIPP Environment: Its Detection, Distribution and Behavior, Punam Thakur, T. B. Kirchner, J. L. Conca (*Carlsbad Environmental Monitoring & Research Center*)

Plutonium Behavior in the Sedimentary Rocks, Irina E. Vlasova (*Moscow State University*), Elena Zakharova, Anna Volkova (*Frumkin IPCE*), Stepan Kalmykov (*Moscow State Univ*)

Neptunium-237 Concentrations in Groundwater from Nevada Test Site Wells, Ruth Maria Tinnacher, Pihong Zhao, Ross W. Williams, Mavrik Zavarin, Annie B. Kersting (*LLNL*)



## Technical Sessions: Monday

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Understanding Uranyl Adsorption at the Water-Mineral Interface: A Theoretical Approach, Ping Yang, Eric J. Bylaska, Wibe A. De Jong (*PNNL*)

Plutonium Speciation and Solubility in the WIPP, Donald T. Reed, Marian Borkowski, Jean-Francois Lucchini, Michael K. Richmann (*LANL*)

Pu Sorption to Goethite at Micromolar to Attomolar Concentrations, Pihong Zhao, M. Zavarin, S. Tumey, R. Williams, Z. Dai, R. Kips, A. B. Kersting (*LLNL*)

Overview of the Results Obtained from Studies on Mixed Uranium and Plutonium Particles Realised to an Arctic Marine Environment from a Nuclear Bomb Accident, Mats Eriksson (*IAEA*)

### Coordination Chemistry

Structural and Electronic Trends Observed in Actinide Metal–Metal Bonds, Stefan George Minasian, Jamin L. Krinsky, John Arnold (*Univ of California, Berkeley*)

A Spectroscopic Technique to Explore Covalency in Actinide–Oxygen Bonds, Stefan George Minasian, Stosh A. Kozimor (*LANL*), David K. Shuh (*LBL*)

Adventures in Uranium-Element Multiple Bonding: Uranium Mono-, Bis- and Tris(imido) Complexes, James Matthew Boncella, Liam P. Spencer, Robert E. Jilek, David S. Kuiper, Brian L. Scott (*LANL*)

Oxo Functionalization and Reduction of Pentavalent Uranyl, David D. Schnaars, Guang Wu (*Univ of California, Santa Barbara*), Andrew J. Gaunt (*LANL*), Trevor W. Hayton (*Univ of California, Santa Barbara*)

Adjustment of the Paramagnetic Content of the Actinide Carbonate Trimers. Structural Characterization by <sup>13</sup>C-NMR, Raman, and Visible Spectroscopy, Bruce McNamara, Sergei Sinkov, Lucas Sweet, Lanee Snow, Herman Cho, Shane Peper (*PNNL*)

Unexpected Covalency from Actinide 5f Orbital Interactions (An = Th, U, Np, Pu) Determined from Chlorine K-Edge X-Ray Absorption Spectroscopy and Electronic Structure Theory, David Lewis Clark, E. R. Batista, K. S. Boland (*LANL*), J. S. Bradley (*Univ of Washington*), S. D. Conradson (*LANL*), N. Kaltsoyannis (*University College London*), S. A. Kozimor, R. L. Martin (*LANL*), G. T. Seidler (*Univ of Washington*), M. J. Tassell (*University College London*), M. P. Wilkerson (*LANL*), P. Yang (*PNNL*)

Covalency Trends for d- and f-Element Metallocene Dichlorides Determined from Chlorine K-Edge X-Ray Absorption Spectroscopy and Time Dependent–Density Functional Theory, David Lewis Clark, Stosh A. Kozimor (*LANL*), Ping Yang (*PNNL*), Enrique Batista, Kevin Boland, Carol Burns, Steven Conradson, Richard Martin, Marianne Wilkerson, Laura Wolfsberg (*LANL*)

Convenient Materials of UCl<sub>3</sub> for Preparing Trivalent Uranium Complexes, Suguru Ohta, Tomoo Yamamura, Kenji Shirasaki, Isamu Satoh, Tatsuo Shikama (*Tohoku Univ*)

### Solutions and Gas Phase Chemistry

Aqueous Speciation and Solubility of Np(V/VI) in Hyperalkaline Systems, Javier Gaona, Marcus Altmaier (*KIT*), Vladimir Petrov (*Moscow State University*), David Fellhauer (*Institute for Transuranium Elements*), Jan Tits, Erich Wieland (*Paul Scherrer Institut*), Kathy Dardenne (*Karlsruhe Institute of Technology*), Thomas Fanghaenel (*Institute for Transuranium Elements*)

Polymerization Processes of Pu(V) in Chloride Solutions, Michael Steppert, Clemens Walther, Jörg Rothe, Mirek Icker (*KIT*)

Recent Results in Aqueous Nitrate Dissolution at Los Alamos, Mary Ann Stroud, Judy Roybal, Marvin K. Romero, Aquilino Valdez, Yvonne Martinez, Lia Brodnax, Tom Ricketts (*LANL*)

Np(V) Reduction by Humic Acids—Impact of Sulfur Functionalities of Humic Acids, Katja Schmeide, Susanne Sachs, Gert Bernhard (*FZD*)

Reduction Kinetics of Np(V) in Non-Complexing Aqueous Systems at pH 5 - 10, David Fellhauer (*European Commission, JRC*), Marcus Altmaier, Volker Neck, Joerg Runke (*KIT*), Thomas Fanghaenel (*European Commission, JRC*)

Rapid and Selective Electrocatalytic Reduction of NpO<sub>2</sub><sup>+</sup> to Np<sup>4+</sup> by Electrolysis at a Platinized Electrode, Yoshihiro Kitatsuji, Takaumi Kimura (*JAEA*), Sorin Kihara (*Kyoto Inst for Interesting Chemistry*)

Speciation Studies of Tetravalent Protactinium in Aqueous Solution, Nidhu lal Banik, Christian Marquardt, Clemens Walther, Jörg Rothe, Melissa Denecke, Reinhard Klenze (*KIT*)

UV-Vis and EXAFS Spectroscopy of the Plutonium (IV) Nitrate System, Nicholas A. Smith, Ken Czerwinski (*UNLV*)

Structure of Trivalent f-Element Ions Gd<sup>3+</sup> and Bk<sup>3+</sup> in Aqueous Solutions. Association and Hydration Study versus pH, Habib Latrous (*Faculté des sciences de Tunis*), Rafik Besbes (*Institut préparatoire aux études d'ingénieurs de Sfax*), Ouerfelli Noureddine (*Faculté des Sciences de Tunis*)

NMR Studies of the Complexation of Gluconic Acid with Ca<sup>2+</sup>, La<sup>3+</sup> and Th<sup>4+</sup> in Aqueous Solutions, Zhicheng Zhang, K. A. Fitzgerald, G. Helms, S. B. Clark (*Washington State Univ*)

Aqueous An(III-VII) Solvation and Solvent Exchange Mechanisms, Aurora Clark, Alex Samuels, ArunKumar Subramanian (*Washington State Univ*)

Age Determination of <sup>244</sup>Cm Solutions by Alpha and Mass Spectrometry, Hiromu Kurosaki (*Washington State Univ*), James R. Cadieux (*SRNL*), Sue B. Clark (*Washington State Univ*)

### Compounds and Complexes

Crystal Structures and Physico-Chemical Properties of Actinide Carboxyphosphonates, Pius Ojo Adelani, Thomas Edward Albrecht-Schmitt, Allen G. Oliver (*Univ of Notre Dame*)

Actinide Valences in Zirconia and Pyrochlore-Structured Titanates, Yingjie Zhang, Eric R. Vance (*ANSTO*)

Thermodynamic Characterization of Hydroxypyridonate Lanthanide and Actinide Complexes, Manuel Sturzbecher-Hoehne, Clara Hg Pak Leung, Anthony D'Aléo, David K. Shuh (*LBL*), Kenneth N. Raymond (*Univ of California, Berkeley*), Rebecca J. Abergel (*LBL*)

Cubic and Rhombohedral Heterobimetallic Networks Constructed from Uranium, Transition Metals, and Phosphonoacetate, Andrea N. Alsobrook (*Univ of Notre Dame*), Evgeny V. Alekseev, Wulf Depmeier (*Univ of Kiel*), Thomas E. Albrecht-Schmitt (*Univ of Notre Dame*)

Comparisons of Pu(IV) and Ce(IV) Diphosphonates, Juan Diwu, Anna-Gay D. Nelson, Thomas E. Albrecht-Schmitt (*Univ of Notre Dame*)

## Technical Sessions: Monday/Tuesday

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New Insights into Actinide (U, Np, Pu) Borate Materials Relevant to Nuclear Waste Storage, Shuao Wang (*Univ of Notre Dame*), Evgeny V. Alekseev (*Univ of Kiel*), Thomas E. Albrecht-Schmitt (*Univ of Notre Dame*)

Measuring O K-Edge Absorption Spectra Reliably Enough for Quantitative Analysis of Light-Atom Bond Covalency, Joseph A. Bradley (*Univ of Washington*), Stosh A. Kosimor (*LANL*), Gerald T. Seidler (*Univ of Washington*)

Metallic Sodium Assisted Syntheses of Actinide Nitrides, Daniel Bernard Rego, Thomas Hartmann (*UNLV*), Steven D. Conradson (*LANL*), Sean Mulcahy, Kenneth R. Czerwinski (*UNLV*)

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### TUESDAY, SEPTEMBER 21, 2010, 8:00 A.M.

#### Plenary Session—3, All invited

##### Keystone Lodge Ballroom

8:00 a.m.

DOE's Fuel Cycle Research and Development Program, Carter (Buzz) D. Savage (*DOE*)

8:40 a.m.

NMR Studies of Transuranium Dioxides, Yo Tokunaga, Tsuyoshi Nishi, Shinsaku Kambe (*JAEA*)

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### TUESDAY, SEPTEMBER 21, 2010, 9:30 A.M.

#### Fuel Cycle—I

##### Arapahoe

9:30 a.m.

Compelling Reasons for Near-Term Deployment of Plutonium Recycle from Used Nuclear Fuels—A System Analysis Study, E. D. Collins, G. D. Del Cul, K. A. Williams (*ORNL*)

9:55 a.m.

Evaluation of Promising Extractants for Actinide Partitioning, Vijay Kumar Manchanda (*BARC*), invited

10:40 a.m.

Plutonium Extraction Chemistry in Diglycolamide Based Solvents for the GANEX Process, Robin J. Taylor (*National Nuclear Lab*), Fiona McLachlan, Mark John Sarsfield (*NNL*)

11:05 a.m.

Plutonium Nuclear Data Research at LANSCE, Fredrik Tovesson, Robert C. Haight, Ronald O. Nelson (*LANL*)

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#### Condensed Matter Physics—II, All invited

##### Divide

9:30 a.m.

Magnetic Fluctuations and Unconventional Superconductivity in Actinide Compounds, Shinsaku Kambe, Yo Tokunaga, Hironori Sakai (*JAEA*)

9:55 a.m.

Optical Pump-Probe Study of the Heavy-Fermion Superconductor PuCoGa<sub>5</sub>, Diyar Talbayev (*Yale Univ*), K. S. Burch (*Univ of Toronto*), Elbert E. M. Chia (*Nanyang Technological Univ*), S. A. Trugman, J.-X. Zhu, E. D. Bauer, J. A. Kennison, J. N. Mitchell, J. D. Thompson, J. L. Sarrao, A. J. Taylor (*LANL*)

10:40 a.m.

Composite Pairing in a Mixed Valent Two Channel Anderson Model, Rebecca Flint, Andriy Nevidomskyy, Piers Coleman (*Rutgers Univ*)

11:05 a.m.

The Electronic Structure of Multiple Phases in Cerium-Plutonium Superlattices, Sven Peter Rudin (*LANL*)

11:30 a.m.

Actinide Theory Examined Through an Experimentalist's Eyes, Kevin T. Moore (*LLNL*)

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### TUESDAY, SEPTEMBER 21, 2010, 1:20 P.M.

#### Plenary Session—4, All invited

##### Keystone Lodge Ballroom

1:20 p.m.

Dominique Warin (*CEA*)

2:00 p.m.

Time-Dependent Processes in Pu Alloys: From Femtoseconds to Teraseconds, Adam J. Schwartz (*LLNL*)

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### TUESDAY, SEPTEMBER 21, 2010, 2:50 P.M.

#### Fuel Cycle—II

##### Arapahoe

2:50 p.m.

Chemistry R & D for Fast Reactor Fuel Cycle, P. R. Vasudeva Rao (*Indira Gandhi Centre for Atomic Resch*), invited

3:15 p.m.

Study of the Carbothermic Reduction Mechanisms of UO<sub>2</sub>, PuO<sub>2</sub> and (U,Pu)O<sub>2</sub> (co-Grinded or Co-Converted), Alan Handschuh, Sylvie Dubois, Christelle Duguay, Stephane Vaudez, Gilles Leturcq, Stephane Granjean (*CEA*), Francis Abraham (*UCCS*)

4:00 p.m.

Possibilities of Closing Nuclear Fuel Cycle with Innovative METMET Fuel, Alexey Savchenko (*A.A. Bocharov Inst of Inorganic Materials (VNIINM)*)

4:25 p.m.

Actinide Partitioning in Carbonate-Peroxide Solutions, George S. Goff, Sean D. Reilly, Wolfgang Runde (*LANL*)

4:50 p.m.

The Solvent Extraction of Plutonium(VI) from Carbonate Solutions, Egor O. Nazarov, Alfiya M. Safiulina (*RAS*), Sergey I. Stepanov (*MUCTR*), Alexander M. Chekmarev (*RAS*)

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#### Material Sciences—II

##### Divide

2:50 p.m.

Direct MD Modeling of Self-Irradiation Effects on Mechanical Properties and Phase Stability of Plutonium, Vladimir V. Dremov (*RFNC*), invited

3:15 p.m.

Phase Ordering and Stacking Fault Energies in Plutonium Metal, Steven M. Valone, Sven Peter Rudin (*LANL*), Michael Baskes (*Univ of California, San Diego*)

## Technical Sessions: Tuesday/Wednesday

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### 4:00 p.m.

An Overview of Isothermal Conditioning in Pu-1.9 at% Ga Alloys, Jason R. Jeffries, Kerri J. M. Blobaum, Mark A. Wall, Adam J. Schwartz (*LLNL*)

### 4:25 p.m.

Evidence for Hydrogen Induced Vacancies in Plutonium Metal, Scott Richmond, Joseph Anderson, Jeff Abes (*LANL*)

### 4:50 p.m.

Measurement and Prediction of Swelling on Plutonium Alloys, Benoit Oudot, B. Ravat, F. Delaunay (*CEA Valduc*)

## TUESDAY, SEPTEMBER 21, 2010, 7:00-9:00 P.M.

### Global Security—Roundtable: “Security Implications of a Global Expansion of Nuclear Power”

Session Chair: Siegfried Hecker (*Stanford University*)

#### Keystone Lodge Ballroom

##### SPEAKERS:

- Claude Guet (*Commissariat à l'énergie atomique (CEA), France*)
- Vijay Manchanda (*Bhabha Atomic Research Center, India*)
- Nikolai N. Ponomarev-Stepnoi (*Kurchatov Institute, Russia*)
- Maegon Barlow (*U.S. Department of Energy*)

## WEDNESDAY, SEPTEMBER 22, 2010, 8:00 A.M.

### Plenary Session—5, All invited

#### Keystone Lodge Ballroom

##### 8:00 a.m.

Safeguarding Against Unconventional Weapons, John Cardinal (*U.S. Federal Bureau of Investigation*)

##### 8:40 a.m.

Ab Initio Studies of Atomic and Molecular Adsorptions on Plutonium Surfaces, Asok Kumar Ray (*Univ of Texas at Arlington*)

## WEDNESDAY, SEPTEMBER 22, 2010, 9:30 A.M.

### Detection and Analysis—I

#### Arapahoe

##### 9:30 a.m.

Plutonium Isotopic Analysis Without Radiochemical Separation, Pam Thompson (*AWE*)

##### 9:55 a.m.

Electrospray Ionization and Gas-Phase Chemistry of F-Element Complexes, John K. Gibson, Travis H. Bray, Philip X. Rutkowski, Daniel Rios, David K. Shuh (*LBNL*), Maria C. Michelini (*Università Della Calabria*), Roy Copping (*LBNL*), Joaquim Marcalo (*Instituto Tecnológico e Nuclear*), invited

##### 10:40 a.m.

Advanced X-Ray Absorption/Emission Spectroscopic Tool for Actinide Speciation, Tonya Vitova, M. A. Denecke, M. Löble, K. Dardenne, J. Rothe, H. Geckeis (*KIT*), K. Kvashnina (*ESRF*), J. Vegelius, S. M. Butorin (*Uppsala Univ*), G. Nocton, M. Mazzanti (*CEA*), A. Seibert, R. Caciuffo (*European Commission, JRC*), R. G. Denning (*Oxford Univ*)

##### 11:05 a.m.

Raman Spectroscopy Characterization of Actinide Oxides (U,Pu)O<sub>2</sub>, Christophe Jegou (*CEA*)

##### 11:30 a.m.

Application of Absorption Spectroscopy to Actinide Process Analysis and Monitoring, Robert Lascola (*SRNL*), Vinay Sharma (*Savannah River Nuclear Solutions*), invited

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## Surface Science and Corrosion

### Divide

##### 9:30 a.m.

New Insights into the Oxidation of Plutonium at Room Temperature, David L. Pugmire, Harry G. Garcia Flores, David P. Moore, Amanda L. Broach (*LANL*), Paul Roussel (*AWE*)

##### 9:55 a.m.

Derivation of Interatomic Potentials for PuO<sub>2</sub> and the Calculation of Lattice and Defect Properties, Mark S. D. Read (*AWE*), invited

##### 10:40 a.m.

Atomic Scale Mechanism of Pu Corrosion, Steven D. Conradson, Alison L. Costello (*LANL*), Francisco J. Espinosa-Faller (*Centro-Marista de Estudios Superiores*), David E. Hobart, Jeremy N. Mitchell, Marianne P. Wilkerson (*LANL*), invited

##### 11:05 a.m.

A Theoretical/Experimental Approach to Understanding the Interactions of H with Pu Metal, Christopher D. Taylor, Dave Moore (*LANL*)

##### 11:30 a.m.

The Role of Pu<sub>2</sub>O<sub>3</sub> and Defects in The PuO<sub>2</sub> Layer in The Plutonium Hydriding Process, Long Ngoc Dinh (*LLNL*)

## WEDNESDAY, SEPTEMBER 22, 2010, 1:20 P.M.

### Plenary Session—6, All invited

#### Keystone Lodge Ballroom

##### 1:20 p.m.

Measurements at the Crime Scene and in the Lab—Challenges and Opportunities, Maria Susanna Wallenius, Verena Kleinrath, Andrey Berlizov, Klaus Mayer, Magnus Hedberg, Zsolt Varga, Thierry Wiss, Evelyn Zuleger (*EC, JRC, ITU*)

##### 2:00 p.m.

Multi-Phase Thermal and Elastic Properties of Pu Metal from First-Principles Theory, Per Soderlind (*LLNL*)

## WEDNESDAY, SEPTEMBER 22, 2010, 2:50 P.M.

### Detection and Analysis—II, All invited

#### Arapahoe

##### 2:50 p.m.

“Overview of the United States Nuclear Reference Materials Program,” Jon Neuhoff (*DOE*)

##### 3:15 p.m.

A New NMR Facility for Solid State Actinide Research at the Institute for Transuranium Elements, O. Pauvert, J. Somers, Roberto Caciuffo, T. Fanghänel (*European Commission, JRC*), G. A. Ummarino (*Politecnico di Torino*), H. Chudo, S. Kambe (*IAEA*)

## Technical Sessions: Wednesday

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### 4:00 p.m.

Characterisation of Uranium Ore Concentrates to Identify Origin, Terry Piper, Katherine Duff (*AWE*)

### 4:25 p.m.

Determining Plutonium Mass in Spent Fuel with Non-Destructive Assay Techniques, Melissa A. Schear, Stephen Tobin (*LANL*)

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## Condensed Matter Physics—III

### Divide

### 2:50 p.m.

Broken Rotational Symmetry in the Hidden Order Phase of  $\text{URu}_2\text{Si}_2$ , T. Shibauchi, H. J. Shi (*Kyoto Univ*), Y. Haga, T. D. Matsuda, E. Yamamoto (*JAEA*), Y. Onuki (*JAEA/Osaka Univ*), H. Ikeda, Y. Matsuda, R. Okazaki (*Kyoto Univ*)

### 3:15 p.m.

Competition of Charge Density Waves and Superconductivity in Uranium, Johann Bouchet (*CEA DAM*), S. Raymond (*CEA Grenoble*), G. Lander (*ILL Grenoble*), M. Krisch (*ESRF Grenoble*), J. C. Lashley, R. C. Albers (*LANL*), M. Le Tacon, G. Garbarino, M. Hoesch (*ESRF Grenoble*), J-P Rueff (*Synchrotron Soleil*)

### 4:00 p.m.

Elastic Moduli, Debye-Waller and Electron Localization in Plutonium, Victor Roberto Fanelli, Albert Migliori, Yoko Suzuki, Jon B. Betts (*LANL*), invited

### 4:25 p.m.

From Low to High Density Metals, Behavior of the Shear Modulus versus Temperature, Marie-Helene Nadal (*CEA*), invited

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## WEDNESDAY, SEPTEMBER 22, 2010, 5:00-7:00 P.M.

### Poster Session—II

#### Ten Mile/Lakeside Gallery

#### Surface Science and Corrosion

Influence of  $\text{PuO}_2$  Surface Layer Condition on Release of Gas Products as a Result of Sorbed Water Radiolysis, Andrey Aleksandrovitch Karnozov, Tatiana Karnozova (*JSC VNIINM*)

On Issue of Confining Stage of Uranium Metal Oxidation in Water Vapour, Andrey Aleksandrovitch Karnozov, T. B. Karnozova, V. K. Orlov (*JSC VNIINM*)

Moisture and Gas Production in Storage Containers of Plutonium Oxide, John M. Berg, Joshua E. Narlesky, D. Kirk Veirs, Laura A. Worl (*LANL*), Jonathan M. Duffey, Philip M. Almond (*SRNL*)

Plutonium Speciation at Solid/Gas and Liquid/Solid Interfaces, John Douglas Farr (*LANL*)

Cleaning Effectiveness Study of FC-43 Used as a Plutonium Density Fluid, Krystyna M. Dziejwinska, Jacek Dziejwinski, Leisa Davenhall, Kelly Hakonson, Daniel Kelly (*LANL*)

Measurement of the Auger Parameter for Cerium in Oxidizing and Reducing Environments, Art J. Nelson, T. W. Trelenberg, D. K. Castro, J. J. Welch, P. G. Allen, W. McLean (*LLNL*)

Transformation of Pu Surface Chemistry: An X-Ray Photoelectron Spectroscopy and Secondary Ion Mass Spectrometry Study, Art J. Nelson, Patrick Allen, William McLean (*LLNL*), Paul Roussel, Peter Morrall, David Geeson (*AWE*)

The Plutonium / Hydrogen Reaction: Hydride Spot Initiation Time, Nucleation Rate and Radial Growth Rate as a Function of Hydrogen Pressure and Oxide Structure, Gordon William McGillivray, Ian M. Findlay, John P. Knowles, Marina J. Dawes (*AWE Aldermaston*)

Hydrogen Generation and Reduced Pressure in Plutonium-Bearing Storage Containers, Philip M. Almond, Jonathan M. Duffey, Nicholas J. Bridges (*SRNL*), Binh V. Nguyen, Lance E. Traver, Matthew J. Arnold, Ronald R. Livingston (*SRS*), Glen F. Kessinger (*SRNL*)

Effect of Moisture Absorption on Plutonium Oxide Storage Container Relative Humidity, Joshua E. Narlesky, John M. Berg, David M. Harradine, Max A. Martinez, Laura A. Worl, D. Kirk Veirs (*LANL*)

Orientation Imaging Microscopy of Plutonium: Grain Structure and Oxidation, David P. Moore, Amanda L. Broach, David L. Pugmire, Harry G. Garcia Flores (*LANL*), Paul Roussel (*AWE Aldermaston*)

Relative Corrosion Resistance of 304 and 316 Stainless Steel to Plutonium Residues, D. Kirk Veirs, Laura A. Worl, Scott Lillard (*LANL*)

### Materials Science

Acoustic Measurements of the Elastic Properties and Quality of Plutonium and Uranium Based Oxide Fuels, Tarik A. Saleh, Stephen P. Willson, Erik P. Luther, Douglas J. Safarik, Timothy J. Ulrich, W. Sue Duncan, Darrin D. Byler (*LANL*)

Phase Transformation in  $\delta$ -Pu- Alloys at Low Temperature, Brice Ravat (*CEA*)

Characterization of a Uranium-Niobium Alloy Over a Range of Temperatures and Strain Rates, Carl M. Cady, S.-R. Chen, G. T. Gray, E. K. Cerreta, R. Aikin, D. R. Kozekwa (*LANL*)

Recent Efforts in Quantifying Heterogeneity, Adam M. Farrow, Charles C. Davis, Rollin E. Lakis (*LANL*)

Annealing of Aged Plutonium, Jeremy N. Mitchell, Adam M. Farrow, Franz Freibert, Daniel S. Schwartz (*LANL*)

Phase Transitions of Unalloyed Pu in Shock Waves, Evgeny A. Kozlov (*RFNC- E. I. Zababakhin Research Institute of Technical Physics*), Lidia F. Timofeeva (*Bochvar Research Institute of Nonorganic Materials*)

Evidence of Abrupt Lattice Expansion in Delta-Plutonium Due to Self-Irradiation During the Aging Process, Cheng K. Saw, Mark A. Wall, Brandon W. Chung (*LLNL*)

Compatibility Assessment of Replacement Fluids for Use in Plutonium Processing, Susan O'Connell (*AWE*)

Specific Hydriding Rates of Delta-Plutonium, Camille Kenney (*AWE*)

Modelling Hydrogen Solubility and Diffusion in Plutonium Dioxide, Mark Timothy Storr (*AWE*)

Plutonium Metal Density Reflects Changing Chemical Composition, Roberta N. Mulford (*LANL*)

Burst Transformations and Other Transformation Characteristics of Unalloyed Plutonium, Franz J. Freibert, Jeremy N. Mitchell, Dan S. Schwartz, Taleh S. Saleh (*LANL*)

## Technical Sessions: Wednesday

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Neutron Diffraction Studies on Plutonium Alloys, Tarik A. Saleh, Alice I. Smith, Thomas E. Proffen, Frans R. Trouw, Jeremy N. Mitchell (LANL)

### Condensed Matter Physics

Precision Elastic Moduli of Pure Alpha, Beta, Gamma Polycrystal Plutonium-Three Different Metals, Albert Migliori, Victor R. Fanelli, Yoko Suzuki, J. B. Betts, Jeremy N. Mitchell, Franz Freibert (LANL)

Characterization of Point Defects in UO<sub>2</sub> by Positron Lifetime Spectroscopy: A First-Principles Study, Gerald Jomard, Marc Torrent (CEA, DAM, DIF)

Evolution of Electrical Resistivity and Electronic Structure of Transuranium Metals Under Pressure., Yuri Tsiolkovkin, A. V. Lukoyanov, A. O. Shorikov, A. A. Povzner, L. Yu. Tsiolkovkina, A. A. Dyachenko, V. B. Bystrushkin, M. V. Raybukhina (Ural Federal Univ), M. A. Korotin (RAS), V. V. Dremov (RFNC), V. I. Anisimov (RAS)

Novel Band Renormalization Mechanisms in f-Electron Systems, Tomasz Durakiewicz, John Joyce, Eric D. Bauer, Kevin S. Graham (LANL), Peter S. Riseborough (Temple Univ), Peter M. Oppeneer (Uppsala Univ)

Temperature and Concentration Dependencies of Electrical Resistivity of Am-Pu Alloys at High Temperature, Yuri Tsiolkovkin, A. A. Povzner, L. Yu. Tsiolkovkina (Ural Federal Univ), V. V. Dremov (RFNC), L. R. Kabirova, M. V. Raybukhina, A. O. Shorikov, A. A. Dyachenko, V. B. Bystryshkin, A. V. Lykoyanov, A. N. Filanovich (Ural Federal Univ)

Plutonium Properties in Multiple Intermediate Valence Model, Alexey Mirmelstein, Oleg Kerbel (RFNC-VNIITF), Evgeny Clementyev (RAS)

Atomistic Calculations of Fundamental Physical Properties of Uranium, Benjamin Joseph Good, Chaitanya Deo (Georgia Tech), Michael Baskes (Univ of California, San Diego)

Spin Fluctuations in Delta-Plutonium, Vladimir P. Antropov, Alexander Z. Solontsov (Ames Lab)

Complex Magnetic Order in PuSb<sub>2</sub> Single Crystals, Eric D. Bauer, P. H. Tobash, J. N. Mitchell, J. A. Kennison, J. J. Joyce, T. Durakiewicz, B. L. Scott, J. L. Sarrao, L. A. Morales, J. D. Thompson (LANL)

Physical Properties of the New Intermetallic Compound Pu<sub>2</sub>Ni<sub>3</sub>Si<sub>5</sub>, Paul H. Tobash, Eric D. Bauer, Filip Ronning, Jeremy N. Mitchell, John A. Kennison, Brian L. Scott, Joe D. Thompson (LANL)

Electron Phases of Solids and Compression-Induced Changes in Electron Structure of Actinides, Boris A. Nadykto (RFNC-VNIIEF)

### Fuel Cycle

Plutonium Rock-Like Oxide Fuel (ROXf) System, Their Once-Through Burning and Usage, Ashraf Elsayed Mohamed (West Coast Univ)

Pyrochemical and Electrochemical Separations Studies on Plutonium, Ashraf Elsayed Mohamed (West Coast Univ)

Study of Americium and Plutonium Chemistry in Mixed Oxide Fuel, Philippe Martin, Anne-Charlotte Robisson, Renaud Belin (CEA), Andreas Scheinost (FZD)

Fabrication and Characterization on (U,Am)O<sub>2</sub> Target for GEN(IV) Fast Reactor System, Marika Vespa, Matteo Rini, Jacobus Boshoven, Serge Fourcadaut, Patrick Lajarge, Sarah Stohr, Joseph Somers (EC-JRC-ITU)

Selective Adsorption of Trivalent Actinides to Carbon Materials, Masayuki Watanabe, Makoto Arisaka, Takaumi Kimura (JAEA)

Plutonium Breeding In Micro-Hetero Structures Enhances the Fuel Cycle, Liviu Popa-Simil (LAVM LLC)

Separation of Americium and Curium in Metal Nitrate and Nitric Acid Systems, Narek Gharibyan, Ralf Sudowe (UNLV)

Preparation and Characterization of N-Donor Extraction-Chromatography Resins for Actinide/Lanthanide Separations., Christopher L. Klug, Ralf Sudowe (UNLV)

Potentiometric Study of the Reaction Ln<sup>3+</sup> + e<sup>-</sup> = Ln<sup>2+</sup> (where Ln = Tm, Yb) in Molten Caesium Chloride, Valeri Vladimir Smolenski (RAS), invited

Fission Cross Sections of Plutonium Isotopes and Other Actinides at the Neutron Source GNEIS, Alexander Laptev (LANL), O.A. Shcherbakov, A.S. Vorobyev (PNPI), R.C. Haight (LANL)

Thermal Recovery Evaluation of Thermal Conductivity in Self-Irradiated MOX Pellet, Kyoichi Morimoto, Masato Kato (JAEA), Masahiro Ogasawara (Inspection Development Company)

Burn-Up Effect on MOX Fuel Thermal Conductivity, Yoshihisa Ikusawa, Kyoichi Morimoto, Takayuki Ozawa, Masato Kato (JAEA)

Model Compounds for MOx Fuel Dissolution Studies in Atalante Facility, Gilles Robert Leturcq, Alastair Magnaldo (CEA)

Dissolution Flowsheet for Digestion of PuO<sub>2</sub>-Bearing Residues, G. F. Kessinger (SRNL), R. R. Livingston (SRS), M. G. Bronikowski (SRNL)

Disproportionation of Neptunium(V) in Tributyl Phosphate and N,N-Dihexyloctanamide/n-Dodecane Media, P N. Pathak (BARC), Neelam Kumari, D. R. Prabhu, V. K. Manchanda (BARC)

Quantifying Fissile Content in Spent Fuel Using Cf-252 Interrogation with Prompt Neutron Detection, Jianwei Hu (Univ of Illinois), Stephen Tobin, Stephen Croft (LANL), invited

Diglycolamides: Promising Extractants for Actinides, Prasanta Kumar Mohapatra, Rajesh B. Gujar, Seraj A. Ansari, Vijay K. Manchanda (BARC)

Transformation of Uranium Products from the Pyrometallurgical Processing of Used Nuclear Fuel, Brian Robert Westphal, Ken Marsden, Dee Vaden, J. C. Price, Mike Simpson (INL)

Electronic Structure and the Energetics of Actinide Diffusion in UO<sub>2</sub>, Jianwei Wang, Rodney C. Ewing, Udo Becker (Univ of Michigan)

Thorium Fuel System and Plutonium's Contribution in Sustaining Nuclear Energy, Atnatiwos Zeleke Meshesha (Ethiopian Radiation Protection Authority), invited

Novel Polystyrene—TODGA Nano Composite Material for Am(III) Uptake, Vijay Kumar Manchanda (BARC), A. S. Patole, J. H. Ahn, T. H. Kim (Sungkyunkwan Univ), S. A. Ansari, P. K. Mohapatra (BARC), L. Hyemi (Sungkyunkwan Univ)

Magnetic Property of AnO<sub>2+x</sub> Prepared by Hydrothermal Synthesis, Tomoo Yamamura, Suguru Ohta, Kenji Shirasaki, Isamu Satoh, Tatsuo Shikama (Tohoku Univ)

### Radiolysis and Radiation Damage

Incidental Neutron Irradiation and Color Center Generation in LiF Windows Used in Actinide Shock Physics Experiments, Franz Freibert, James J. Gallegos, Michael Ramos (LANL)

## Technical Sessions: Thursday

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**THURSDAY, SEPTEMBER 23, 2010, 8:00 A.M.**

**Plenary Session—7**, All invited

**Keystone Lodge Ballroom**

**8:00 a.m.**

Actinide Borates, Thomas Edward Albrecht-Schmitt (*Univ of Notre Dame*)

**8:40 a.m.**

Clemens Walther (*KIT*)

**THURSDAY, SEPTEMBER 23, 2010, 9:30 A.M.**

**Compounds and Complexes**

**Arapahoe**

**9:30 a.m.**

Actinide Valences in Monazite and Xenotime, Eric R. Vance, Yingjie Zhang (*ANSTO*)

**9:55 a.m.**

Actinide Electronic Structure and X-ray Scattering: Answering Old Questions and Asking New Ones, Joseph Bradley

**10:40 a.m.**

Structure Determination of Actinide Complexes by Nuclear Magnetic Resonance Spectroscopy, Herman Martin Cho, Wibe de Jong, Andrew R. Felmy, Chuck Z. Soderquist (*PNNL*), invited

**11:05 a.m.**

Novel Methods for Synthesis and Characterization of Actinide Nitrides, Ken Czerwinski (*UNLV*), invited

**11:30 a.m.**

Raman Spectroscopy of Plutonium Dioxide and Related Materials, Mark John Sarsfield, Robin J. Taylor (*National Nuclear Lab*), invited

**Radiolysis and Radiation Damage**

**Divide**

**9:30 a.m.**

Effect of Metal Oxide Impurities on Hydrogen Generation by Alpha-Radiolysis, Jonathan M. Duffey (*SRNL*), Ronald R. Livingston (*Savannah River Nuclear Solutions*), Robert A. Pierce, David M. Missimer, Philip M. Almond (*SRNL*)

**9:55 a.m.**

Gas Evolution From Polypropylene Under the Effect of Alpha-Radiolysis Due to Plutonium Dioxide, Laurent Venault, J. Vermeulen, J. Maurin, Ph. Moisy (*CEA*), S. Bouffard, Y. NGono-Ravache (*GANIL*), A. Dannoux, V. Dauvois, S. Esnouf, V. Martin (*CEA*)

**10:40 a.m.**

Radiation Damage and 5f-Electron Localization of Plutonium Compounds:  $\delta$ -Pu, PuGa<sub>3</sub>, and PuAl<sub>2</sub>, Yu Jiang, Corwin H. Booth (*LBNL*), Eric D. Bauer, Jeremy N. Mitchell, Steven M. Valone (*LANL*), Mark A. Wall, Patrick G. Allen (*LLNL*)

**11:05 a.m.**

Influence of Self-Irradiation on Kinetics of Stress Relaxation at Elastic Precursor Front in Unalloyed Plutonium under Explosive Loading, Evgeny A. Kozlov (*RFNC–E. I.Zababakhin Research Institute of Technical Physics*), invited

**11:30 a.m.**

A Magnetic Study of Radiation Damage in PuCoGa<sub>5</sub>, Scott K. McCall, Michael J. Fluss, Brandon W. Chung, Patrick G. Allen (*LLNL*), Eric D. Bauer, Jeremy N. Mitchell, Luis A. Morales, John L. Sarrao (*LANL*)

**THURSDAY, SEPTEMBER 23, 2010, 1:20 P.M.**

**Solutions and Gas Phase Chemistry**

**Arapahoe**

**1:20 p.m.**

Plutonium Solubility and Solid Phase Stability under Reducing Conditions in MgCl<sub>2</sub> Brines, Marcus Altmaier, Volker Neck (*KIT*), Boris Brendebach (*Gesellschaft fuer Anlagen- und Reaktorsicherheit*), Thomas Fanghaenel (*Institute for Transuranium Elements*)

**1:45 p.m.**

Redox Behaviour of the Pu(IV)/Pu(III) Couple in Nitric Acid – Pu(IV) - Nitrate Complexes Speciation, Xavier Crozes, Philippe Moisy (*CEA*), Gérard Cote (*ENSCP*)

**2:10 p.m.**

A Computational Study of the Reduction of Pu(IV) by Hydroxamic Acids, Helen M. Steele, Robin J. Taylor (*National Nuclear Lab*)

**2:35 p.m.**

New Insight into the Stability of DTPA Complexes of Trivalent Actinides, Thomas Vercouter, Sylvain Topin, Jean Aupiais, Nicolas Baglan (*CEA*), Claire Le Naour, Mickael Mendes, Sébastien Leguay (*CNRS*), Manuel Miguirditchian, Philippe Moisy (*CEA*)

**3:20 p.m.**

Plutonium Peroxycarbonate Solution Studies Underpinning Alkaline Separations Chemistry, Sean D. Reilly, George S. Goff, Iain May, Wolfgang Runde (*LANL*)

**3:45 p.m.**

Closing

**Material Sciences—III**

**Divide**

**1:20 p.m.**

The Impact of Heat Transfer Kinetics on Phase Transformation Kinetics in Plutonium Metals, Boris A. Nadykto (*RFNC–VNIIEF*)

**1:45 p.m.**

Large Volume Change Phase Transformations in Pu and Pu-Ga Alloys, Daniel S. Schwartz, Jeremy N. Mitchell (*LANL*), invited

**2:10 p.m.**

In Situ x-Ray Diffraction Investigation of the Delta to Alpha-Prime Transformation in a Pu-Ga Alloy, Kerri J. M. Blobaum, Jason R. Jeffries, Mark Wall, Adam J. Schwartz (*LLNL*)

**2:35 p.m.**

Fabrication of Unalloyed Plutonium, Franz Freibert, Paula J. Crawford, John W. Gibbs, David A. Korzekwa, Robert M. Aikin, Deniece R. Korzekwa (*LANL*)

**3:20 p.m.**

Elastic and Mechanical Properties of Plutonium and Plutonium Alloys, Tarik A. Saleh, Adam M. Farrow, Franz J. Freibert, Albert Migliori, Jeremy N. Mitchell, Michael E. Bange (*LANL*), invited

**3:45 p.m.**

Evolving Metallurgical Properties of Plutonium from Self-Irradiation, Brandon W. Chung, Kenneth E. Lema, David S. Hiromoto (*LLNL*)

**4:20 p.m.**

Closing