



ANS Conference

Plutonium Futures



The Science 2014

Official Program

Am	144.91	Sm	156.90	Eu	151.96
Neptunium	237				
Np	144.91	Pu	194	Americium	151.96
			244.06		151.96
				Cerium	196.97



September 7-12, 2014
Renaissance Hotel
Las Vegas, NV

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To access the Plutonium Futures 2014 proceedings, please visit this website:
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PLUTONIUM FUTURES THE SCIENCE 2014



September 7 - 12, 2014
Las Vegas, NV ♦ Renaissance Las Vegas Hotel

Plutonium Futures — The Science 2014 is a topical conference that provides an international forum for presentation and discussion of current research on physical and chemical properties and environmental interactions of plutonium and other closely related actinide elements.

Topical Areas

- ◆ Condensed matter physics
- ◆ Surface science and corrosion
- ◆ Metallurgy and materials science
- ◆ Compounds, complexes and coordination chemistry
- ◆ Detection and analysis
- ◆ Nuclear fuel cycle
- ◆ Environmental behavior and chemistry
- ◆ Solutions and gas-phase chemistry

Meeting Officials



General Chair:

Kerri Blobaum

Lawrence Livermore National Laboratory



Program Chair:

Scott McCall

Lawrence Livermore National Laboratory



Honorary Chair:

David L. Clark

Los Alamos National Laboratory

Meeting Information and Special Events



MEETING INFORMATION

Plutonium Futures — The Science 2014 Meeting is held September 7-12, 2014, in Las Vegas, NV.

NOTE:

Additional tickets can be purchased at the ANS Registration Desk for the Monday, National Atomic Testing Museum Reception and the Wednesday Conference Banquet.

NOTICE FOR SPEAKERS:

All Speakers and Session Chairs must sign in at the ANS Registration Desk located outside the Renaissance Ballroom, during registration hours.

SPECIAL EVENTS

Welcome Reception at the National Atomic Testing Museum

Monday, September 8, 2014

6:00 p.m. – 9:00 p.m.

Location: 755 E. Flamingo Rd.,
Las Vegas, NV

Buses to the museum depart from the Renaissance Hotel front drive.

The National Atomic Testing Museum showcases its collection of more than 12,000 unique artifacts in educational and inspiring exhibits. There is something for everyone to experience in dynamic displays presenting the history of the development and testing of one of man's most significant inventions, a nuclear bomb.

Additional tickets can be purchased at the ANS Registration Desk for \$85.00 each.

MEETING REGISTRATION

Meeting and Speaker Registration will be located at the ANS Registration Desk located outside the entrance of the Renaissance Ballroom of the Renaissance Las Vegas, Sunday, September 7, 2014 – Thursday, September 11, 2014. Meeting registration is required for all attendees, and speakers. Badges are required for admission to all plenaries, technical sessions and events.

REGISTRATION HOURS

Sunday, September 7, 2014
12:00 p.m. – 5:00 p.m.
Monday, September 8, 2014
7:00 a.m. – 8:00 p.m.
Tuesday, September 9, 2014
7:00 a.m. – 7:00 p.m.
Wednesday, September 10, 2014
7:00 a.m. – 5:00 p.m.
Thursday, September 11, 2014
7:00 a.m. – 5:00 p.m.

Conference Banquet

Wednesday, September 10, 2014

5:30 p.m. – 8:30 p.m.

Location: Renaissance
Ballroom



Banquet speaker:

Edward Bruce Held

Bruce Held is the Associate Deputy Secretary of Energy and is responsible for operational and policy matters across the DOE/NNSA enterprise in support of President Obama's nuclear security agenda. Mr. Held has had a distinguished career as a clandestine operations officer for the Central Intelligence Agency (CIA) during which he served as Chief of Station in Asia, Latin America, and Africa. He later worked as Special Assistant to George Tenet, Director of Central Intelligence. After retirement, Mr. Held became Chief of Counterintelligence at Sandia National Laboratories. In December 2009, Secretary of Energy Steven Chu asked Mr. Held to return to federal service and serve as Director of DOE's Office of Intelligence and Counterintelligence. In that capacity, he led all DOE intelligence and counterintelligence activities, as well as over thirty intelligence and counterintelligence offices nationwide, and served as a member of the Executive Committee of the U.S. Intelligence Community.

Mr. Held holds an M.S. in Monetary Theory from the London School of Economics and a B.S. in Economics from the University of Minnesota. He is the author of two books on the impact of espionage in American history: A Spy's Guide to Santa Fe and Albuquerque and A Spy's Guide to the Kennedy Assassination.

He and his wife of 34 years, Lani, have a daughter and two sons.

Additional tickets can be purchased at the ANS Registration Desk for \$120.00 each.

TECHNICAL TOUR

Nevada National Security Site

Friday, September 12, 2014

7:00 a.m. – 4:40 p.m.

The tour departs from the Renaissance Hotel front drive.

Nevada Nuclear Security Site, formerly known as the "Nevada Test Site," provides a unique and indispensable extension of the national laboratories' experimental capabilities in support of the Stockpile Stewardship Program.

The tour will primarily be a bus tour, as the site is very large. The site is approximately 1.5 hours from the hotel. Visitors will have the opportunity to see several well-known sights, including Mercury camp, the Sedan crater, and the Device Assembly Facility (DAF). A tour guide on the buses will provide briefings during the drive.

Participants are prohibited from bringing cameras, cell phones, Bluetooth enabled devices, computers, recording devices, weapons, explosives, animals, ammunition, controlled substances, binoculars, alcoholic beverages, chemical irritants, and GPS devices on the tour. NNSN will provide a mechanism for emergency communication, in case someone on the tour needs to be contacted.

The number of visitors on the tour is limited. US citizens must register 10 days prior to the event, and foreign nationals must register 45 days in advance.

Photo identification is required for the tour. Foreign citizens must present a valid Alien Registration Card or passport.

Sponsored by:



ANS Materials Science and Technology Division

SUNDAY, SEPTEMBER 7, 2014

- 12:00 p.m.- 5:00 p.m. Registration
1:00 p.m.- 4:30 p.m. Tutorial Session

MONDAY, SEPTEMBER 8, 2014

- 7:00 a.m.- 8:00 p.m. Registration
8:00 a.m.-10:20 a.m. Conference Opening and Monday Plenaries
10:40 a.m.-12:20 p.m. Technical Sessions
Condensed Matter Physics—I
Environmental Science—I
12:20 p.m.- 1:10 p.m. Lunch Break
1:10 p.m.- 5:10 p.m. Technical Sessions
Condensed Matter Physics—II
Environmental Science—II
Condensed Matter Physics—III
Environmental Science—III
6:00 p.m.- 9:00 p.m. Welcome Reception at the National Atomic Testing Museum

TUESDAY, SEPTEMBER 9, 2014

- 7:00 a.m.- 7:00 p.m. Registration
8:00 a.m.-10:00 a.m. Tuesday Plenaries
10:20 a.m.-12:00 p.m. Technical Sessions
Metallurgy and Materials Science—I
Solutions and Gas-Phase Chemistry—I
12:00 p.m.- 1:00 p.m. Lunch Break
1:00 p.m.- 5:00 p.m. Technical Sessions
Metallurgy and Materials Science—II
Solutions and Gas-Phase Chemistry—II
Metallurgy and Materials Science—III
Solutions and Gas-Phase Chemistry—III
7:00 p.m.-10:00 p.m. Poster Session

WEDNESDAY, SEPTEMBER 10, 2014

- 7:00 a.m.- 5:00 p.m. Registration
8:00 a.m.-10:00 a.m. Wednesday Plenaries
10:20 a.m.-12:00 p.m. Technical Sessions
Compounds, Complexes and Coordination Chemistry—I
Nuclear Fuel Cycle—I
12:00 p.m.- 1:00 p.m. Lunch Break
1:00 p.m.- 5:20 p.m. Technical Sessions
Compounds, Complexes and Coordination Chemistry—II
Nuclear Fuel Cycle—II
Compounds, Complexes and Coordination Chemistry—III
Nuclear Fuel Cycle—III
5:30 p.m.- 8:30 p.m. Conference Banquet

THURSDAY, SEPTEMBER 11, 2014

- 7:00 a.m.- 5:00 p.m. Registration
8:00 a.m.- 9:00 a.m. Thursday Plenary
9:00 a.m.-12:00 p.m. Technical Sessions
Detection and Analysis—I
Surface Science and Corrosion—I
Detection and Analysis—II
Surface Science and Corrosion—II
12:00 p.m.- 1:00 p.m. Lunch Break
1:00 p.m.- 5:00 p.m. Technical Sessions
Detection and Analysis—III
Surface Science and Corrosion—III
Joint Metallurgy and Materials Science/Condensed Matter Physics—I
Nuclear Fuel Cycle—IV
Joint Metallurgy and Materials Science/Condensed Matter Physics—II
5:00 p.m.- 5:30 p.m. Closing Remarks

FRIDAY, SEPTEMBER 12, 2014

- 7:00 a.m.- 4:40 p.m. Nevada National Security Site Tour

Sunday Tutorial/Monday, September 8, 2014

TUTORIAL SESSION

Capital Room – 1:00-4:30 p.m.

Brian Powell, *Clemson University*: An Overview of Biogeochemical Reactions Controlling Pu Environmental Mobility
This tutorial will provide an overview of the primary chemical, physical, and biological (biogeochemical) interactions that control the mobility of plutonium in the environment. The environmental mobility of Pu is profoundly influenced by sorption, complexation, and solubility which are in turn influenced by the oxidation state of plutonium. Thus, understanding and quantifying the redox speciation of Pu under environmental conditions is vital for the evaluation of the human and environmental health risks posed by disposal of Pu bearing wastes. The specific focus of this tutorial will be on 1) characterizing and quantifying oxidation/reduction reactions in aqueous systems and at solid: water interfaces and 2) identification of solubility controlling phases. Where possible, comparisons will be drawn between field measurements under natural conditions and laboratory based experiments using pure minerals and soils.

Albert Migliori, *Los Alamos National Laboratory*: Pu—Some Interesting Aspects of Thermodynamics and Electronic Structure

Andreas Kronenburg, *International Atomic Energy Agency*: Nuclear Fuels in the Eyes of a Radiochemist

Based on a lecture series concerning the nuclear fuel cycle established for nuclear engineering students, this lecture will give an overview of current and advanced fuel types, particularly considering fuel behavior during irradiation and options for subsequent fuel reprocessing. An emphasis will be given on UO_2 - ThO_2 and PuO_2 - ThO_2 mixed oxide fuels (including coated particles) and ternary Pu-U alloys as well as PuO_2 space batteries. In order to show the wide range of current research topics, nuclear forensics issues will be briefly discussed.

MONDAY CONFERENCE OPENING SESSION

Renaissance I – 8:00 a.m.

William Goldstein, Director of Lawrence Livermore National Laboratory

MONDAY PLENARIES

Session Chair: Kerri Blobaum (*LLNL*)

8:20 a.m.

Plutonium and Americium Geochemistry at Hanford, A. R. Felmy, K. J. Cantrell, E. C. Buck (*PNNL*), S. D. Conradson (*LANL*), plenary

9:20 a.m.

Consequences of Electronic Correlations in Plutonium-Based Intermetallics, J. D. Thompson, E. D. Bauer, G. Koutroulakis, J. N. Mitchell, A. M. Mounce, P. H. Tobash, H. Yasuoka (*LANL*), plenary

BREAK 10:20 – 10:40 a.m.

Renaissance Foyer

CONDENSED MATTER PHYSICS—I

Session Chair: Roberto Caciuffo (*ITU*)

Renaissance 2 – 10:40 a.m.

10:40 a.m.

A Plutonium-Based Single-Molecule Magnet, N. Magnani, E. Colineau, J.-C. Griveau, C. Apostolidis, O. Walter, R. Caciuffo (*EC, JRC, Inst for Transuranium Elements*), invited

11:20 a.m.

Quantum Criticality in PuMX_5 ($M=\text{Co}, \text{Rh}; X=\text{Ga}, \text{In}$)

Superconductors, Eric D. Bauer, B. Ramshaw, M. Wartenbe, G. Koutroulakis, A. M. Mounce (*LANL*), H. Yasuoka (*JAEA*), P.H. Tobash, R. A. McDonald, J. N. Mitchell, J. D. Thompson (*LANL*), invited

12:00 p.m.

Spin-Fluctuation Induced Nodal s-wave Pairing in the Pu-115 Superconductors, Matthias J. Graf, Tanmoy Das, Jian-Xin Zhu (*LANL*)

ENVIRONMENTAL SCIENCE—I

Session Chair: Brian Powell (*Clemson*)

Renaissance 3 – 10:40 a.m.

10:40 a.m.

Plutonium Speciation in Inorganic Colloidal Suspensions: Experiments and Modeling, A. Yu. Romanchuk, A. V. Egorov (*Moscow State Univ*), Y. V. Zubavichus (*Kurchatov Inst*), S. N. Kalmykov (*Moscow State Univ*), invited

11:20 a.m.

Spectroscopic Evidence of Pu(IV) Favorability on the Surfaces of Hematite and Quartz, Shanna L. Estes (*Clemson Univ*), Amy E. Hixon (*Clemson Univ/Univ of Notre Dame*), Yuji Arai (*Univ of Illinois at Urbana-Champaign*), Brian A. Powell (*Clemson Univ*)

11:40 a.m.

Probing the Stability of Pu on Montmorillonite, James D. Begg, Mavrik Zavarin, Annie B. Kersting (*LLNL*)

12:00 p.m.

Comparison of Plutonium and Neptunium Redox Behavior in Reducing Aqueous Solution, D. Fellhauer, M. Altmaier (*KIT/Inst for Transuranium Elements*), X. Gaona, V. Neck, M. Lagos (*KIT*), T. Wiss (*Inst for Transuranium Elements*), J. Runke (*KIT*), Th. Fanghaenel (*Inst for Transuranium Elements*)

LUNCH BREAK 12:20 – 1:10 p.m.

Renaissance I

CONDENSED MATTER PHYSICS—II

Session Chair: Ladia Havela (*Charles Univ*)

Renaissance 2 – 1:10 p.m.

1:10 p.m.

Observation of ^{239}Pu Resonance: PuO_2 and Beyond, A.M. Mounce (*LANL*), H. Yasuoka (*LANL/JAEA*), G. Koutroulakis, H. Chudo, S. A. Kozamor, S. Richmond, D. K. Veirs, A. I. Smith, E. D. Bauer, J. D. Thompson, G. D. Jarvinen, D. L. Clark (*LANL*), invited

1:50 p.m.

Equilibrium Thermodynamics of Radiation Defects and Helium in the fcc 5f-Metal, Alexey V. Karavaev, Vladimir V. Dremov, Gennady V. Ionov (*RFNC-VNIITF*), Brandon W. Chung (*LLNL*), invited

2:30 p.m.

The Malleability of Uranium: Manipulating the Charge-Density Wave in Epitaxial Films, Ross Stuart Springell (*Univ of Bristol*), Roger Ward (*Univ of Oxford*), Johann Bouchet (*CEA*), James Chivall (*UCL*), Didier Wemeille, Peter Normile (*XmaS*), Sean Ianridge (*ISIS*), Stan Zochowski (*UCL*), Gerry Lander (*ITU*)

2:50 p.m.

Theoretical Phonon Spectra of Strongly Correlated Actinide Compounds, Boris Dorado, Marc Torrent (*CEA*)

ENVIRONMENTAL SCIENCE—II

Session Chair: Annie Kersting (*LLNL*)

Renaissance 3 – 1:10 p.m.

1:10 p.m.

Release of Pu Isotopes into the Environment from the Fukushima Daiichi Nuclear Power Plant Accident: Distribution and Source Identification, Jian Zheng, Keiko Tagami, Tatsuo Aono, Shigeo Uchida (*NIRS*), invited

1:50 p.m.

Plutonium Associations to Natural Chancellor Water Colloids: Implications for Subsurface Transport, Hakim Boukhalfa, Paul W. Reimus, Naomi Wasserman, Bryan Erdmann, Amr I. Abdel-Fattah, Doug S. Ware, Sowmitri Tarimala, Bennie Martinez (*LANL*), invited

2:30 p.m.

AMS of Actinides in Groundwater: Development of a New Procedure for Simultaneous Trace Analysis of U, Np, Pu, Am and Cm Isotopes, F. Quinto, M. Lagos, M. Plaschke, T. Schäfer (*KIT-INE*), P. Steier (*Univ of Vienna*), H. Geckes (*KIT-INE*)

2:50 p.m.

XAS Analysis of Pu Coordination in Minerals and Ligands, Daniel T. Olive, Tashi Parsons-Moss, Deborah Wang, Stephen Jones, Heino Nitsche (*Univ of California, Berkeley/LBNL*)

BREAK 3:10 – 3:30 p.m.

Renaissance Foyer

CONDENSED MATTER PHYSICS—III

Session Chair: Paul Tobash (*LANL*)

Renaissance 2 – 3:30 p.m.

3:30 p.m.

Unveiling the Valence Fluctuations in δ -Pu by Means of High-Energy Inelastic Neutron Spectroscopy, Marc Janoschek, Pinaki Das, Jon M. Lawrence, Frans Trouw (*LANL*), Doug Abernathy, Mark D. Lumsden (*ORNL*), Mike Ramos, Jeremy N. Mitchell (*LANL*), Gerry Lander (*Inst Lave Langevin*), Eric D. Bauer (*LANL*), invited

4:10 p.m.

Theoretical Confirmation of Ga-Stabilized Anti-Ferromagnetism in Plutonium Metal, Per Soderlind, Alex Landa (*LLNL*)

4:30 p.m.

Plutonium Hexaboride is a Correlated Topological Insulator, Kristjan Haule (*Rutgers Univ*), invited

ENVIRONMENTAL SCIENCE—III

Session Chair: Stepan Kalmykov (*Moscow State*)

Renaissance 3 – 3:30 p.m.

3:30 p.m.

Hydroxamate Siderophores in Soil Mineral-Organic Matter Matrix Responsible for Binding $^{239,240}\text{Pu}$ at the Savannah River Site, USA and Fukushima Prefecture, Japan Chen Xu, Saijin Zhang, Yi-Fang Ho, Matthew Athon, Isaac Johnston, Kathleen A. Schwehr (*Texas A&M Univ*), Daniel I. Kaplan (*SRNL*), Nicole DiDonato, Patrick G. Hatcher (*Old Dominion Univ*), Peter H. Santschi (*Texas A&M Univ*), invited

4:10 p.m.

Pu Interaction with Bacterial Isolates from Mont Terri Opalinus Clay, Henry Moll (*Helmholtz-Zentrum Dresden-Rossendorf e.V.*), Laura Luetke (*Leibniz Universität Hannover*), Andrea Cherkouk, Gert Bernhard (*Helmholtz-Zentrum Dresden-Rossendorf e.V.*)

4:30 p.m.

Plutonium Speciation in the WIPP: An Update of the Safety Case for Plutonium Containment, Donald T. Reed, Michael T. Richmann, Juliet S. Swanson, Danielle M. Cleveland, Jean-Francois Lucchini (*LANL*)

4:50 p.m.

Influence of Extracellular Polymeric Substances on Plutonium Sorption to Bacteria, Mark Antony Boggs, Mavrik Zavarin, Yongqin Jiao, Annie B. Kersting (*LLNL*)

Tuesday, September 9, 2014

TUESDAY PLENARIES

Session Chair: David Clark (*LANL*)

Renaissance I – 8:00-10:00 a.m.

8:00 a.m.

Evaluation of Orbital Mixing in Soft-Donor Dithiophosphinate Extractants Using Sulfur K-Edge X-Ray Absorption Spectroscopy and Time-Dependent Density Functional Theory, Stosh A. Kozimor, Angela C. Olson, Scott R. Daly, Enrique R. Batista, Kevin S. Boland, Andrew Gaunt, Jason M. Keith, Richard L. Martin, Brian L. Scott (*LANL*), plenary

9:00 a.m.

An Overview of Plutonium Incorporation and Radiation Effects in Nuclear Materials, Gregory R. Lumpkin (*ANSTO*), plenary

BREAK 10:00 – 10:20 a.m.

Renaissance Foyer

METALLURGY AND MATERIALS SCIENCE—I

Session Chair: Deniece Korzekwa (*LANL*)

Renaissance 2 – 10:20 a.m.

10:20 a.m.

Plutonium Futures at NNSA, Kathleen B. Alexander (*NNSA*)

11:00 a.m.

Recent Advances in Studying Actinides with Dynamical Mean Field Theory, Sergey Savrasov (*Univ of California, Davis*), invited

11:40 a.m.

Structural Transformations in Actinide Oxides under Extreme Conditions, Cameron Tracy (*Univ of Michigan*), Maik Lang (*Univ of Tennessee*), Fuxiang Zhang (*Univ of Michigan*), Raul I. Palomares (*Univ of Tennessee*), Rodney C. Ewing (*Stanford Univ*)

SOLUTIONS AND GAS-PHASE CHEMISTRY—I

Session Chair: Daniel Rego (*UNLV*)

Renaissance 3 – 10:20 a.m.

10:20 a.m.

Vibrational Properties of Actinyl Complexes, Richard E. Wilson, David D. Schnaars, Stephanie De Sio (*ANL*), invited

11:00 a.m.

Complexation of Actinides by Ramified N-Macrocyclic DOTA, M. Audras, L. Berthon, C. Berthon, N. Zorz, D. Guillaumount, T. Dumas (*CEA*), P.-L. Sikaru (*Synchrotron SOLEIL*), Ch. Hennig (*ESRF*), Ph. Moisy (*CEA*)

11:20 a.m.

Gas-Phase Plutonium Coordination Chemistry Reveals Solution Behavior, J. K. Gibson, Y. Gong, L. Rao, G. Tian (*LBNL*)

11:40 a.m.

Redox Reactions of Pu Ions in Aqueous Nitric Solutions under Ultrasound Irradiation, M. Virot (*ICSM Marcoule*), L. Venault, P. Moisy (*CEA, Marcoule*), S. I. Nikitenko (*ICSM Marcoule*)

LUNCH BREAK 12:00 – 1:00 p.m.

Renaissance I

METALLURGY AND MATERIALS SCIENCE—II

Session Chair: Anna Maria Adamska (*University of Bristol*)

Renaissance 2 – 1:00 p.m.

1:00 p.m.

Plutonium Aging: an Overview of Thermokinetic and Irradiation-Induced Phenomena, Jason R. Jeffries (*LLNL*), invited

1:40 p.m.

Modelling He Migration and Bubble Formation in δ -Pu, Chris Scott (*Loughborough Univ*), Marc Robinson (*Curtin Univ*), Steven D. Kenny (*Loughborough Univ*), Mark T. Storr, Andrew Willetts (*AWE*)

2:00 p.m.

Behavior of Helium in Aged δ -Plutonium: A Combined Experimental and Theoretical Study, Piheng Chen, Xinchun Lai (*China Academy of Engineering Physics*)

2:20 p.m.

Hydrogen Effects in Pu-Ga Alloys: Defects and Thermodynamics, Daniel S. Schwartz, Scott Richmond, Christopher D. Taylor, Alice I. Smith, Alison L. Pugmire (*LANL*), invited

SOLUTIONS AND GAS-PHASE CHEMISTRY—II

Session Chair: John Gibson (*LBNL*)

Renaissance 3 – 1:00 p.m.

1:00 p.m.

Gas-Phase Actinyl Chemistry of N-Heterocyclic Ligands: A Joint Theoretical and Experimental Study, Ping Yang (*PNNL*), Ana F. Lucena (*Universidade de Lisboa*), Yu Gong (*LBNL*), Leonor Maria, Joaquim Marçalo (*Universidade de Lisboa*), John K. Gibson (*LBNL*), invited

1:40 p.m.

Trends in Actinide Ion Solution Speciation, L. Soderholm, S. Skanthakumar, Richard E. Wilson (*ANL*)

2:00 p.m.

Reduction of Plutonium in Acidic Solutions by Porous Carbon Solids, Tashi Parsons-Moss (*Univ of California, Berkeley/LBNL*), Jinxiu Wang (*Fudan Univ*), Stephen Jones, Deborah Wang (*Univ of California, Berkely/LBNL*), Dongyuan Zhao (*Fudan Univ*), Heino Nitsche (*Univ of California,Berkeley/LBNL*)

2:20 p.m.

X-Ray Absorption Fine Structure (XAFS) Determination of Actinide Speciation in Aqueous Media, Jörg Rothe, Horst Geckeis (*KIT-INE*), invited

BREAK 3:00 – 3:20 p.m.

Renaissance Foyer

METALLURGY AND MATERIALS SCIENCE—III

Session Chair: David Geeson (*AWE*)

Renaissance 2 – 3:20 p.m.

3:20 p.m.

New Valuable Insight on the Martensitic Transformation in PuGa 1 at.%, F. Lalire (*CEA Valduc/Université de Lorraine*), B. Ravat, B. Oudot (*CEA Valduc*), B. Appolaire (*LEM*), E. Aeby-Gautier (*Université de Lorraine*), F. Delaunay (*CEA Valduc*)

3:40 p.m.

MD-MEAM Investigation into Surface vs Bulk Structure When Cooling the Model fcc 5f Metal, V. V. Dremov, G. V. Ionov, A. V. Karavaev, Ph. A. Sapozhnikov, M. A. Vorobyova (*RFNC*), B. W. Chung (*LLNL*)

4:00 p.m.

Impacts of Stress Induced Transformation on the Martensitic Reversion Process in a PuGa 1 at. %., B. Oudot, B. Ravat, F. Lalire, F. Delaunay (*CEA Valduc*), invited

4:40 p.m.

Dilatometry and Crystallography of the $\delta \rightarrow \gamma$ Transformation in Plutonium, Jeremy N. Mitchell, Terence E. Mitchell, Daniel S. Schwartz (*LANL*)

SOLUTIONS AND GAS-PHASE CHEMISTRY—III

Session Chair: Horst Geckeis (*KIT*)

Renaissance 3 – 3:20 p.m.

3:20 p.m.

Predictive Modeling of Actinides in Solution Environments, Wibe A. de Jong (*LBNL*), Samuel O. Odoh (*Univ of Minnesota*), Raymond Atta-Fynn (*Univ of Texas at Arlington*), Eric J. Bylaska (*PNNL*), invited

4:00 p.m.

Preparation of Intrinsic Plutonium Colloids by Sonolysis of PuO_2 in Water, V. Morosini, T. Chave, M. Virot (*ICSM*), C. Den Auwer (*Univ of Nice*), T. Dumas (*CEA/DEN/DRCP*), T. Tyliszczak, D. K. Shuh (*LBNL*), P. Moisy (*CEA, Marcoule*), S. I. Nikitenko (*ICSM*)

4:20 p.m.

Solution Speciation of High Oxidation States of Plutonium, Mark R. Antonio, Yung-Jin Hu, S. Skanthakumar, Richard E. Wilson, L. Soderholm (*ANL*), invited

POSTER SESSION

Renaissance I – 7:00-10:00 p.m.

Compounds, Complexes and Coordination Chemistry

CCCC.1: Supercritical Water as a Synthetic Medium for Actinide Borates, Jared T. Stritzinger (*FSU*), Evgeny Alekseev (*FzJ*), Matthew J. Polinski, Justin N. Cross, Thomas Albrecht-Schmitt (*FSU*)

CCCC.2: Extraordinary Cases of Aliovalent Substitution: $\text{Th}(\text{VO}_3)_2(\text{SeO}_3)$ and $\text{Ln}(\text{VO}_3)_2(\text{IO}_3)$ ($\text{Ln} = \text{Ce}, \text{Pr}, \text{Nd}, \text{Sm}$, and Eu), Teresa Eaton, Jian Lin, Thomas E. Albrecht-Schmitt (*FSU*)

CCCC.3: Intrinsic Formation of Neptunium Nanoparticles in Presence and Absence of Silica: Formation of $\text{Np}(\text{IV})$ -Silica Colloids and NpO_2 Nanocrystals, Richard Husar, Rene Huebner (*Helmholtz-Zentrum Dresden-Rossendorf.e.V.*), Christoph Hennig (*Helmholtz-Zentrum Dresden-Rossendorf.e.V./ESRF*), Stephan Weiss, Atsushi Ikeda-Ohno, Harald Zaenker, Thorsten Stumpf (*Helmholtz-Zentrum Dresden-Rossendorf.e.V.*)

CCCC.4: Characterization of Products from Hydrolysis of UF_6 , G. L. Wagner, M. T. Paffett, K. D. Rector, B. L. Scott, M. P. Wilkerson (*LANL*)

CCCC.5: Expansion of the Rich Structures and Magnetic Properties of Neptunium Selenites, Kariem Diefenbach, Jian Lin, Thomas Albrecht-Schmitt (*FSU*)

CCCC.6: Metal-Controlled Assembly of Uranyl Diphosphonates Towards the Synthesis of Functional Materials, Yilin Wang, Kariem Diefenbach, Thomas Albrecht-Schmitt (*FSU*)

CCCC.7: Applications of Chlorine Chemistry in Pyrochemical Separations, J. Matt Jackson, Keith W. Fife (*LANL*)

CCCC.8: Microstructure and Its Influence on Americium Chemistry in $(U_{0.54}Pu_{0.45}Am_{0.01})O_{2-x}$ Mixed Oxide, R. Vauchy, P. M. Martin, A.-C. Robisson, L. Aufore, R. Bes, R. C. Belin, T. Truphemus (*CEA, Cadarache*), A. C. Scheinost (*Helmholtz-Zentrum Dresden-Rossendorf*), F. Hodaj (*SIMAP, Grenoble INP*)

CCCC.9: Solubility and Spectroscopic Studies of Np(VI/VII) Under Hyperalkaline and Oxidizing Conditions, X. Gaona, D. Fellhauer, J. Rothe, K. Dardenne, M. Altmaier (*KIT*)

CCCC.10: Do Uranium (VI) and Thorium (IV) Interact with the Squeleton Osteopontin Protein?, G. Creff (*ICN-UMR*), S. Safi (*UMR CNRS*), P. L. Solari (*SOLEIL Synchrotron*), C. Vidaud (*DSV/IBEB/SBTN*), C. Den Auwer (*ICN-UMR*)

CCCC.11: Catalysis with Cerium Organometallic Complexes, Andrew D. Sutton, Marianne P. Wilkerson (*LANL*)

CCCC.12: In situ XAFS Observation Uranyl-Amide Complexes under Light Irradiation, Shinichi Suzuki, Tohru Kobayashi, Hideraki Shiwaku, Tsuyoshi Yaita (*JAEA*)

CCCC.13: Aluminum K-Edge X-Ray Absorption Spectroscopy of F-Element and Aluminum Molecules and Materials, Stefan G. Minasian (*LBNL*), Alison B. Altman, John Arnold (*LBNL/Univ of California, Berkeley*), Eric D. Bauer (*LANL*), Corwin H. Booth, Das Pemmaraju, David G. Prendergast, David K. Shuh, Tolek Tyliszczak (*LBNL*)

Condensed Matter Physics

CMP.1: Magnetic Properties and Phase Stability of α - γ - and ϵ -Ce: LDA+DMFT Study, A. O. Shorikov, S. V. Streltsov (*RAS/Ural Federal Univ*), M. A. Korotin (*RAS*), V. I. Anisimov (*RAS/Ural Federal Univ*)

CMP.2: Pressure-Induced Structural Phase Transition in CeNi, A. V. Mirmelstein, V. N. Matvienko, O. Kerbel (*RFNC-VNIITF*), A. Podlesnyak, A. I. Kolesnikov, António M. dos Santos, B. Saparov, A. S. Sefat (*ORNL*), J.G. Tobin (*LLNL*)

CMP.3: Ab Initio Investigation of the Uranium-Oxygen System, N. A. Brincat, S. C. Parker, M. Molinari (*Univ of Bath*), G. C. Allen (*Univ of Bristol*), M. T. Storr (*AWE*)

CMP.4: Investigating the Itinerant and Localized Crossover of the 5f Electrons in Plutonium Alloys and Compounds, Paul H. Tobash, Eric D. Bauer, Jianxin Zhu, Daniel S. Schwartz, Jeremy N. Mitchell (*LANL*)

CMP.5: Electronic Structure and Chemical Bond Nature in Americium Dioxide, Yu. A. Teterin, A. Yu. Teterin, K. E. Ivanov (*Kurchatov Inst*), M. V. Ryzhkov (*RAS*), K. I. Maslakov, S. N. Kalmykov, V. G. Petrov, D. A. Enina (*Moscow State Univ*)

CMP.6: Electronic Structure and Chemical Bond in $Cs_2PuO_2Cl_4$, Yu. A. Teterin, A. Yu. Teterin, K. E. Ivanov (*Kurchatov Inst*), M. V. Ryzhkov (*RAS*), K. I. Maslakov (*Moscow State Univ*), D. N. Suglobov (*V.G. Khlopin Radium Inst*)

CMP.7: Doped U Hydrides—Structure and Magnetism, Ladislav Havela, Ilya Tkach, Mykhaylo Paukov, Daria Drozdenko, Peter Minarik, Zdenek Matej (*Charles Univ*)

CMP.8: Vibrational Properties of the Actinides from ab-initio Molecular Dynamics, Johann Bouchet, François Bottin, Boris Dorado (*CEA*)

CMP.9: Electronic Structure of Polycrystalline δ -Pu Metal: A Review of Photoemission Spectra Interpretations, Miles F. Beaux, Tomasz Durakiewicz, Kevin S. Graham, Jeremy N. Mitchell, Scott Richmond, Eric D. Bauer, David P. Moore, Franz J. Freibert, Paul H. Tobash, John A. Kennison, John J. Joyce (*LANL*)

CMP.10: Electronic Structure of Pu Materials from ARPES, John Joyce, Tomasz Durakiewicz, Kevin Graham (*LANL*)

CMP.11: Ab initio Modeling of Magnetic and Electronic Properties of (U, Pu)N, A. V. Lukoyanov, V. I. Anisimov (*RAS*)

CMP.12: The Structure and Transport of H Defects in UO_2 , J. M. Flitcroft, S. C. Parker (*Univ of Bath*), M. Storr (*AWE*), M. Molinari (*Univ of Bath*)

Detection and Analysis

D&A.1: Destructive Analysis of Plutonium-Beryllium Sources, N. Xu, K. Kuhn, D. Gallimore, A. Martinez, M. Schappert, D. Montoya, L. Tandon (*LANL*)

D&A.2: Directional Detection of ^{239}Pu , Paul P. Guss, Thomas G. Stampahar (*DOE*), Alexander Barzilov, Amber Guckes (*UNLV*)

D&A.3: Detection of Reprocessing of Weapons Grade Plutonium, Anna C. Hayes, Gerard Jungman (*LANL*)

D&A.4: Laser Ablation of $(U,\text{Pu})O_2$ Simulated Used Nuclear Fuel, Keri Campbell (*UNLV*), Elizabeth J. Judge, James E. Barefield II (*LANL*), Ken Czerwinski (*UNLV*)

D&A.5: Evaluation of Polymer Ligand Extractants for the Rapid Extraction and Sample Preparation of Plutonium for Field Screening of Samples, Dominic S. Peterson, Jung H. Rim, Claudine E. Armenta (*LANL*)

D&A.6: Update of the Rewrite of “The Plutonium Handbook,” David L. Clark (*LANL*), David Geeson (*AWE*), Robert J. Hanrahan Jr. (*Nat'l. Nuclear Security Administration*), David E. Hobart (*LANL*)

Environmental Science

ES.1: Dissolution of High-Fired and Solution Precipitated PuO_2 in the Presence of Montmorillonite at 25 and 80°C, Pihong Zhao, Annie B. Kersting, Zurong Dai, Mavrik Zavarin (*LLNL*)

ES.2: TALISMAN—A European Commission FP7 Project Promoting Transnational Access to Large Infrastructures for a Safe Management of Actinides, M. Altmaier (*KIT-INE*), S. Bourg (*CEA*), P. Collings (*NNL*), N. Dacheux (*CNRS*), B. Duplantier (*LGI Consulting*), Ch. Ekberg (*Chalmers*), D. Grolimund (*PSI*), L. Natrajan (*Univ of Manchester*), Ch. Poinsot (*CEA*), Ph. Raison (*EC-JRC-ITU*), Th. Schaefer (*KIT-INE*), A. Scheinost (*HZDR*), B. Schimmelpfennig (*KIT-INE*)

ES.3: Application of a Sequential Extraction Procedure for Analysis of Actinides in Various Soil and Sediment Samples, Sherry A. Faye, Athena M. Gallardo, Ralf Sudowe (*UNLV*)

ES.4: Colloid-Facilitated Transport of Tetravalent Actinides on Hematite ($\alpha\text{-Fe}_2\text{O}_3$) Colloids in the Presence of Suwanee River Fulvic Acid, Hilary P. Emerson, Katherine A. Hickok, Brian A. Powell (*Clemson Univ*)

ES.5: Colloid-Facilitated Transport of Actinides- Implications for Repository Performance Assessment, Timothy M. Dittrich, Paul W. Reimus (*LANL*)

ES.6: Raman Spectroscopy as a Forensic Tool to Distinguish Between Uranium Minerals, R. J. P. Driscoll (*Univ of Bath*), G. C. Allen (*Univ of Bristol*), S. C. Parker, D. Wolverton, M. Molinari (*Univ of Bath*), I. Khan, D. Geeson (*AWE*)

ES.7: Plutonium Speciation in the WIPP: An Update of the Safety Case for Plutonium Containment, Donald T. Reed (*LANL*), Jean- Francois Lucchini, Michael Richmann, Danielle Cleveland, Juliet Swanson (*LANL*)

ES.8: Plutonium and Other Radionuclides Removal by Graphene Oxide, S. N. Kalmykov, A. Yu. Romanchuk (*Moscow State Univ*), A. Slesarev, J. Tour (*Rice Univ*)

ES.9: Behavior of U(VI) in a Simple Prey (Yeast)-Predator (Paramecium) Food Chain, Naofumi Kozai, Toshihiko Ohnuki, Masashi Koka, Takahiro Satoh, Tomihiro Kamiya, Esaka Fumitaka (*JAEA*)

Metallurgy and Materials Science

M&MS.1: Unalloyed Uranium Deformation Curves under Static and Dynamic Loading, V. A. Pushkov, M. L. Andreeva, A. V. Yurlov, A. V. Kalmanov, I. V. Shiberin (*RFNC-VNIIEF*)

M&MS.2: Modeling of Stress Generated by the Precipitation of Hydride in the Near Surface of Uranium Metal, S. Blaxland, N. Stevens (*Univ of Manchester*), R. Harker (*AWE*)

M&MS.3: Effects of Annealing on Metallurgical Properties of Aged Plutonium Alloys, Brandon W. Chung, Kenneth E. Lema, Patrick G. Allen (*LLNL*)

M&MS.4: Growth and Characterization of Poly- and Single-Crystal Uranium-Alloy Thin Films, A. M. Adamska, T. B. Scott, R. Springell, A. D. Warren, L. Pico, O. Payton (*Univ of Bristol*)

M&MS.5: Modeling of Helium Bubble Growth in Plutonium, Hui Zheng, Haifeng Liu, Haifeng Song (*Inst of Applied Physics and Computational Mathematics*)

M&MS.6: Local Structural Investigation of the Pu-7at%Ga Using Neutron Total Scattering, Alice I. Smith, Katharine L. Page, Scott Richmond, Joan Siewenie, Tarik A. Saleh, Michael Ramos, Daniel S. Schwartz (*LANL*)

M&MS.7: The Structure of Spherical Shell Out of U-1.5% Mo Alloy After Explosive Loading, D. A. Belyaev, A. S. Aleksandrov, E. A. Kozlov, E. A. Levi, I. L. Svyatov, Yu. N. Zouev (*RFNC-VNIITF*)

M&MS.8: Experimental Study of Shape Memory Effect in $\text{U}_{6.3}\text{Nb}$ Alloy, A. V. Troshev, A. M. Golunov, D. A. Chentsov, A. V. Baluev, A. V. Shestakov (*RFNC-VNIITF*)

M&MS.9: Uranium Dislocation Structure after Different-Rate Deformation and Different-Temperature Annealing, A. E. Shestakov, I. V. Artamonov (*RFNC-VNIITF*)

M&MS.10: H Diffusivity in Ga Stabilised $\delta\text{-Pu}$, Chris Scott, Steven D. Kenny (*Loughborough Univ*), Mark T. Storr (*AWE*), Andrew Willetts (*AWE*)

M&MS.11: Elastic Moduli and Nonlinear Ultrasound Resonance Spectroscopy Studies of Alpha Plutonium Rods, Tarik A. Saleh, Adam M. Farrow, Timothy J. Ulrich, Franz J. Freibert (*LANL*)

M&MS.12: Studies of Fission-Induced Surface Damage in Actinides Using Ultracold Neutrons, Leah Broussard (*LANL*)

M&MS.13: The Synthesis of Pu_6Fe from Plutonium Deuteride and Iron Powders, Scott Richmond, Paul H. Tobash, Dan Schwartz (*LANL*)

M&MS.14: Structure and Properties of a Pu-0.42 wt. % Ga Alloy, D. W. Wheeler, M. B. Matthews, S. M. Ennaceur, R. F. E. Jenkins, P. Roussel (*AWE*)

M&MS.15: Ab Initio Study of Ga-Stabilized $\delta\text{-Pu}$ Bulk and Surfaces, Sarah C. Hernandez (*Univ of Texas at Arlington*), Daniel S. Schwartz (*LANL*), Christopher D. Taylor (*DNV GL*), Asok K. Ray (*Univ of Texas at Arlington*)

M&MS.16: Precision Lapping of Alpha-Pu Surfaces: Technique and Characterization, M. A. Wall, K. J. M. Blobaum (*LLNL*)

M&MS.17: Finite-Element Simulations of the Coining Process in Plutonium at Ambient and Elevated Temperatures, Y. Morris Wang, Mark Wall, Richard Seugling, Kerri Blobaum (*LLNL*)

M&MS.18: On the Equation of State and Elastoplastic and Strength Properties of Beryllium, B. A. Nadykto, I. N. Pavlusha, M. O. Shirshova (*RFNC-VNIIEF*)

M&MS.19: Phase Stability of Plutonium Alloys Following Low Temperature Treatment and Plastic Deformation, S. M. Ennaceur (*AWE*)

M&MS.20: Deformation Processes and Casting Behavior of Unalloyed Pu, Adam M. Farrow, Tarik A. Saleh, D. R. Korzekwa, C. M. Knapp, J. N. Mitchell, T. D. Knapp (*LANL*)

M&MS.21: Grain Boundaries and Interfaces in Delta-Phase Plutonium Alloys, S. M. Valone, S. J. Fensin, R. G. Hoagland (*LANL*)

M&MS.22: Resonant Ultrasound Studies of Naturally Aged Plutonium, A. Migliori, A. Shekhter, B. Ramshaw, J. B. Betts, C. Mielke, F. J. Freibert, M. Ramos, T. A. Saleh (*LANL*)

M&MS.23: Radiogenic-Thermally Coupled Lifetimes in Defects of Aged δ -phase Pu-Ga Alloys, F. J. Freibert, J. N. Mitchell, D. S. Schwartz, A. Migliori (*LANL*)

Tuesday, September 9, 2014

M&MS.24: Thermal Properties of Plutonium Dioxide Produced from the Oxidation of Metal (LA-UR-14-22253), D. M. Wayne, P. C. DeBurgomaster, J. M. Berg (*LANL*)

M&MS.25: Entangled Crystal, Magnetic, and Electronic Structures of PuGa₃, Sven P. Rudin (*LANL*)

M&MS.26: Phase Transformations at a Temperature of Liquid Helium and Density Variations in Plutonium and its Alloys under Prolonged Keeping at T = 4 K, B. A. Nadykto (*RFNC-VNIIEF*)

M&MS.27: Beryllium Strain under Dynamic Loading, V. A. Pushkov, A. V. Yurlov, A. A. Okinchits, T. G. Naydanova (*RFNC-VNIIEF*)

M&MS.28: The Current Status in Developing Ce-La Alloys as Pu-Ga Surrogate Alloys at AWE, Michael Ling (*AWE*)

M&MS.29: New Regimes of Plastic Flow in BCC Metals at Extreme Conditions of Pressure and Strain Rate, Bruce A. Remington (*LLNL*)

M&MS.30: A Renaissance of Plutonium Metal Production at the Gram Scale, R. A. Henderson, N. K. Harward, K. E. Roberts, J. A. McNeese, K. J. M. Blobaum (*LLNL*)

Nuclear Fuel Cycle

NFC.1: Dissolution of Aged PuO₂ to Production of ²⁴¹Am for Use in Space Exploration, Chris J. Maher (*NNL/Univ of Manchester*), S. R. Baker (*ESA*), Mike Carrott, Bob Lewin, Mark Sarsfield (*NNL*), Sven L. M. Schroeder (*Univ of Manchester*), K. Stephenson (*ESA*)

NFC.2: Modeling the PUREX Process for Plutonium Reprocessing at the Savannah River Site, T. Hang, J. A. Pike (*SRNL*)

NFC.3: Stabilisation of Chloride Contaminated Plutonium Oxide for Long Term Storage, Robin Taylor, Kevin Webb, Colin Gregson, Robin Orr, Howard Sims, Chris Mason (*NNL*), Jeff Hobbs, Robert Bernard (*Sellafield Ltd*)

NFC.4: Discovery of Plutonium-Bismuth and Plutonium-Bismuth- Phosphate Containing Phases in a Hanford Waste Tank, J. G. Reynolds, G. A. Cooke, J. K. McCoskey, W. S. Callaway (*Washington River Protection Solutions, LLC*)

NFC.5: Cask Size and Weight Reduction Through the Use of Materials Based on Depleted Uranium Oxides, Tatiana Kazakovskaya, Sergey Ermichev, Vitaly Matveev, Vyacheslav Shapovalov (*RFNC- VNIEF*)

NFC.6: HPLC Method for Determination of Th, U and Pu in Irradiated (Th,Pu)O₂ Using Hydroxycarboxylic Acids as Eluents, Pranaw Kumar, Sumana Paul, P. G. Jaison, D. Alamelu, Suresh K. Aggarwal (*BARC*)

NFC.7: Rapid Separation of Used Nuclear Fuel Using Extraction Chromatography, Audrey Roman, Ralf Sudowe (*UNLV*)

NFC.8: Simulation of the Products Formed at Storage of the Curium Fraction of High Level Waste, Sergey Stefanovsky, Sergey Dmitriev, Alexander Zherebtsov (*RAS*)

NFC.9: Plutonium Complexation by Ligands for Nuclear Fuel Cycle Separations, Sean D. Reilly, Andrew J. Gaunt, Brian L. Scott (*LANL*)

NFC.10: Creating a Wiki Framework to Navigate Nuclear Forensic Information, K. S. Holliday, M. Robel, L. W. Gray (*LLNL*)

NFC.11: Experimental and Calculated Parameters of Spherical Critical Assemblies with a δ-phase Plutonium Metal Core (²³⁹Pu (98%) and Duralumin, Lead and Tungsten Reflectors, A. A. Kaigorodov, S. V. Vorontsov, E. A. Gumennykh, A. A. Devyatkin, M. I. Kuvshinov, A. V. Panin, S. V. Finogeev, V. Kh. Khoruzhiy (*RFNC-VNIIEF*)

NFC.12: Room-Temperature Oxidation of Hypostoichiometric (U_{0.55}Pu_{0.45})O_{2-x} Mixed Oxide Evidenced by X-Ray Diffraction, Romain Vauchy, Anne-Charlotte Robisson, Renaud C. Belin (*CEA DEN, DEC*), F. Hodaj (*SIMAP, UJF/INP-Grenoble*)

NFC.13: New Opportunities in Plutonium Research and Development in the UK, Tim Tinsley, Robin Taylor, Fiona Rayment (*NNL*)

NFC.14: Development of an Alternative Electrorefining Process for Metal Pu Residues, Robert Campbell-Kelly, Timothy J. Paget (*AWE*)

Solutions and Gas-Phase Chemistry

S&GPC.1: Modeling Actinide Solubilities in Alkaline to Hyperalkaline Solutions: Part One, Solubility of Am(OH)₃ in KOH Solutions, Yongliang Xiong (*SNL*)

S&GPC.2: Radiation Chemistry of Gases in the Presence of an Oxide Surface, Luke Jones (*Univ of Manchester*)

S&GPC.3: Time Resolved Luminescence and Resonant Non-Radiative Energy Transfer in a Cs₂NpO₂Cl₄Doped Cs₂UO₂Cl₄Matrix, Beau J. Barker, John M. Berg, Marianne P. Wilkerson (*LANL*)

S&GPC.4: Selective Separation of Uranium and Select Fission Elements Utilizing β-Diketones, Daniel Bernard Rego (*UNLV*), Helen Xun (*Gonzaga Univ*), Paul M. Forster, Julie Bertoia, Kenneth R. Czerwinski (*UNLV*)

S&GPC.5: Self-Diffusion of Bk³⁺ in Aqueous Solutions at Neutral pH and pH 2.5. Comparison with the Trivalent f-elements (Eu³⁺, Gd³⁺, Tb³⁺, Tm³⁺), Habib Latrous (*Faculté des sciences de Tunis*)

S&GPC.6: Is Octavalent Pu(VIII) Viable in PuO₄? Wei Huang, W. H. E. Schwarz, Jun Li (*Tsinghua Univ*)

Surface Science and Corrosion

SS&C.1: The Effect of Work-Hardening and Thermal Annealing on the Early Stages of the Uranium-Hydrogen Corrosion Reaction, Antonios Konstadinos Banos, Tom B. Scott (*Univ of Bristol*)

SS&C.2: Observation of $\text{UO}_2\text{-Zr}$ System at the Initial State of Melting, Young-Sang Youn, Jong-Goo Kim, Soon Dal Park, Yeong-Keong Ha, Kyuseok Song (*KAERI*)

SS&C.3: Plutonium Work Function: Effects of Oxidation and Materials Properties, David P. Moore, David L. Pugmire, Thomas J. Venhaus (*LANL*)

SS&C.4: Hydrogen and Oxygen G-Values from Water Adsorbed onto Plutonium Dioxide, D. Kirk Veirs, John M. Berg, Joshua E. Narlesky, Leonardo Trujillo, Edward L. Romero, Kennard V. Wilson, Jr. (*LANL*)

SS&C.5: Gas-Mediated Interior Corrosion of Stainless Steel Containers by Plutonium Oxide with Chloride Impurities, J. M. Berg (*LANL*), J. M. Duffey, J. I. Mickalonis (*SRNL*), J. E. Narlesky, D. K. Veirs (*LANL*)

SS&C.6: To the Mechanism of Moisture-Induced Corrosive Processes in Plutonium, A. A. Karnozov, V. K. Orlov (*VNIINM*)

SS&C.7: Structural Insights into the Oxide Formed During the Room Temperature Corrosion of Plutonium, Alison L. Pugmire (*LANL*), Corwin H. Booth (*LBNL*), Thomas J. Venhaus, David L. Pugmire (*LANL*)

SS&C.8: Analysis of Pu Surfaces with Time-of-Flight SIMS, T. J. Venhaus, D. P. Moore (*LANL*)

SS&C.9: Corrosion of Nuclear Waste: A Surface Study of Single Crystal UO_2 Thin Films, Sophie Rennie, Laura Glaubes, Camilla Stitt (*Univ of Bristol*), Elizabeth Cocklin (*Univ of Liverpool*), Didier Wermielle (*ESRF*), David Morgan (*Cardiff Univ*), William Nuttall (*The Open Univ*), Chris Lucas (*Univ of Liverpool*), Gerry Lander (*EC Joint Research Centre Inst for Transuranium Elements*), Ross Springell (*Univ of Bristol*)

SS&C.10: Evaluating of Initiation Times of the Plutonium-Hydrogen Reaction Based on a Diffusion Barrier Model, J. P. Knowles, A. Willetts, I. M. Findlay, G. W. McGillivray (*AWE*)

SS&C.11: SIMS Analysis of C, H, and O at the Boundary of Uranium-Carbonitride Inclusions, and Its Relevance to Hydride initiation on Uranium Surfaces, Wigbert Siekhaus, Peter Weber (*LLNL*)

SS&C.12: Oxidation Rates of Alpha Versus Delta Plutonium: An X-Ray Photoelectron Spectroscopy Study, A. J. Nelson, J. A. Stanford, W. K. Grant, R. G. Erler, W. J. Siekhaus, W. McLean (*LLNL*)

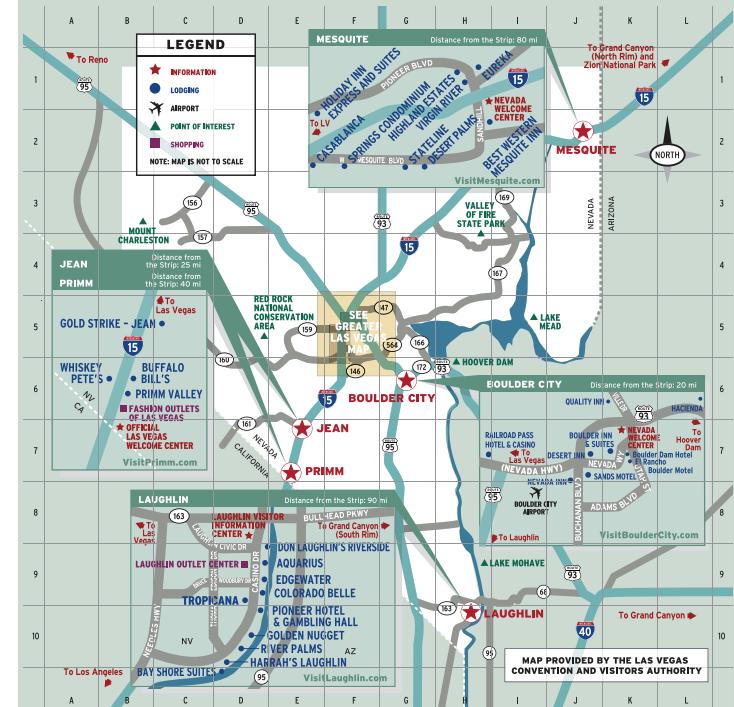
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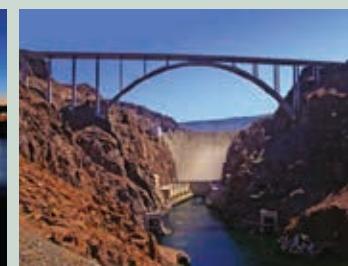
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WEDNESDAY PLENARIES

Session Chair: Patrick Allen (*LLNL*)

Renaissance I – 8:00-10:00 a.m.

8:00 a.m.

Science Based Stockpile Stewardship, Plutonium, and Cargo Cult Science, Victor Reis (*DOE*), plenary

9:00 a.m.

Management of Used Fuel and the Nuclear Fuel Cycle, Peter Lyons (*DOE*), plenary

BREAK 10:00 – 10:20 a.m.

Renaissance Foyer

COMPOUNDS, COMPLEXES AND COORDINATION CHEMISTRY—I

Session Chair: Tatiana Kazakovskaya (*RFNC-VNIIEF*)

Renaissance 2 – 10:20 a.m.

10:20 a.m.

The Future of Actinide Science with Soft X-Ray Synchrotron Radiation, David K. Shuh (*LBNL*), Sergei Butorin (*Uppsala Univ*), Jinghua Guo (*LBNL*), Stosh Kozimor (*LANL*), Stefan G. Minasian, David G. Prendergast, Tolek Tyliszczak (*LBNL*), Tsuyoshi Yaita (*JAEA*)

10:40 a.m.

Unusual Electronic Properties in Plutonium(III) N-Donor Complexes and Materials, Samantha K. Cary, Justin N. Cross, Jared T. Stirzinger, Matthew J. Polinski, Thomas E. Albrecht-Schmitt (*FSU*)

11:00 a.m.

Molecular Np and Pu Coordination Chemistry, Andrew J. Gaunt, Jessie L. Brown, Sean D. Reilly, Brian L. Scott (*LANL*), Nikolas Kaltsosyannis (*UCL*)

11:20 a.m.

Actinide (IV) Hydrolysis and Condensation Products: Polynuclear An(IV) Clusters Isolated from Aqueous Solution, Karah E. Knope, L. Soderholm (*ANL*), invited

NUCLEAR FUEL CYCLE—I

Session Chair: Gordon Jarvinen (*LANL*)

Renaissance 3 – 10:20 a.m.

10:20 a.m.

Plutonium Management in France: Future Possible Scenarios, Bernard Boullis (*CEA*), invited

11:00 a.m.

Actinide Separations by Membrane Based Methods, P. K. Mohapatra (*BARC*), invited

11:40 a.m.

^{241}Am Production for Use in Radioisotope Power Systems, M. J. Sarsfield, K. Bell, C. J. Maher M. J. Carrott, C. Gregson, J. Brown, D. A. Woodhead, S. R. Baker, R. J. Taylor, T. P. Tinsley, T. G. Rice, C. J. Rhodes, M. Clough (*NNL*), K. Stephenson (*ESA*), T. Wiss (*EC-JRC*)

LUNCH BREAK 12:00 – 1:00 p.m.

Renaissance I

COMPOUNDS, COMPLEXES AND COORDINATION CHEMISTRY—II

Session Chair: Thomas Fanghaenel (*Inst for Transuranium Elements*)

Renaissance 2 – 1:00 p.m.

1:00 p.m.

Interaction of An(III/IV/V and VI) with Borate in Dilute to Concentrated NaCl, CaCl₂ and MgCl₂ Solutions, K. Hinz, M. Altmaier, X. Gaona, Th. Rabung (*KIT-INE*), E. Alekseev (*FZJ*), D. Schild, H. Geckeis (*KIT-INE*)

1:20 p.m.

Divergence Between Pu(III) and Am(III) Oxoanion Materials, Thomas E. Albrecht-Schmitt (*FSU*), invited

2:00 p.m.

Complexation of Nitrate with An(III) and Ln(III) in Na-, Mg- and Ca-Brines: Thermodynamic and Activity Models, M. Herm, X. Gaona, Th. Rabung, D. Fellhauer (*KIT-INE*), C. Crepin (*ENSCM*), K. Dardenne, M. Altmaier, H. Geckeis (*KIT-INE*)

2:20 p.m.

Actinide and Lanthanide Recognition Properties of Oxygen-Nitrogen Hetero Donor Ligand PTA, Toru Kobayashi, Shinichi Suzuki, Hideaki Shiwaku, Tsuyoshi Yaita (*JAEA*)

2:40 p.m.

Ionothermal Flux Syntheses of Isomorphous Molecular f-Element Borate Cluster Complexes, T. Gannon Parker, Thomas E. Albrecht-Schmitt (*FSU*)

NUCLEAR FUEL CYCLE—II

Session Chair: Robin Taylor (*NNL*)

Renaissance 3 – 1:00 p.m.

1:00 p.m.

Mathematical Modelling of the Oxidation of Uranium Carbide Fuel, James Shepherd, Michael Fairweather, Bruce Hanson, Peter Heggs (*Univ of Leeds*)

1:20 p.m.

New Opportunities in Plutonium Research and Development in the UK, Tim Tinsley, Robin Taylor, Fiona E. Rayment (*NNL*)

1:40 p.m.

Potential Applications of Uranyl Peroxide Cage Clusters in the Nuclear Fuel Cycle, Ginger E. Sigmon, Peter C. Burns, Enrica Balboni, Kristi L. Pellegrini, Yi Liu, Brendan T. McGrail, Kathryn M. Peruski, Ernest M. Wylie (*Univ of Notre Dame*), invited

2:20 p.m.

Evaluation of Oxygen Stoichiometry during the Sintering of (U, Pu)O₂ Fuel, S. Vaudez, J. Léchelle, S. Berzati (*CEA*)

BREAK 3:00 – 3:20 p.m.

Renaissance Foyer

COMPOUNDS, COMPLEXES AND COORDINATION CHEMISTRY—III

Session Chair: Marcus Altmaier (*KIT*)

Renaissance 2 – 3:20 p.m.

3:20 p.m.

Impact of a Phosphonate Compound (NTMP) on Plutonium Oxalate Structure and Morphology, Anne-Lise Vitart (*CEA, Marcoule*), Murielle Rivenet (*ENSCL-Lille1*), Bénédicte Arab-Chapelet (*CEA, Marcoule*), Nicolas Clavier, Nicolas Dacheux (*JCSM-UMR*), Isabelle Bisel, Stephane Grandjean (*CEA, Marcoule*), Francis Abraham (*ENSCL-Lille1*)

3:40 p.m.

Actinide Oxalates: Main Structural Features and Comparison with Lanthanide Oxalates, Murielle Rivenet (*UCCS - ENSCL*), Bénédicte Arab-Chapelet, Christelle Tamain, Anne-Lise Vitart, Stephane Grandjean (*CEA, Marcoule*), Francis Abraham (*UCCS - ENSCL*), invited

4:20 p.m.

Structural Characterization of Actinide Single-Crystals with Several Ligands of Interest in the Nuclear Fuel Cycle, C. Tamain, C. Marie, J. Bisson, R. Copping (*CEA, Marcoule*), I. Charushnikova (*Frumkin Inst*), G. Dupouy, M-C. Charbonnel, M. Miguiditchian, B. Arab-Chapelet (*CEA, Marcoule*), M. Rivenet (*UCCS-UMR*), S. Grandjean (*CEA, Marcoule*), F. Abraham (*UCCS- UMR*), D. Dubreuil (*Univ of Nantes*)

4:40 p.m.

Speciation of Actinides and Lanthanides with Extractants Proposed for Use in Next Generation Partitioning of Spent Nuclear Fuel, Clint A. Sharrad (*Univ of Manchester*), invited

NUCLEAR FUEL CYCLE—III

Session Chair: Harve Bernard (*CEA*)

Renaissance 3 – 3:20 p.m.

3:20 p.m.

Cathodic Reduction of Plutonium IV Nitric Acid Solutions in a Plate Electrolyzer, S. Georgette, S. Picart, C. Bouyer, J. Maurin, L. Venault, I. Bisel, S. Grandjean (*CEA*), J. Deseure (*LEPMI, UMR*), F. Lapicque (*LRGP, UPR*)

3:40 p.m.

Experimental and Computational Analysis of Nuclear Physics Properties of Assemblies Containing ²³⁷Np and ²³⁵U(36%) in the Core and a Duralumin Reflector, A. A. Kaigorodov, E. A. Gumennykh, A. A. Devyatkin, I. Yu. Drozdov, N. V. Zavialov, M. I. Kuvshinov, A. V. Panin, S. V. Finogeev, V. Kh. Khoruzhiy (*RFNC-VNIIEF*)



Thursday, September 11, 2014

THURSDAY PLENARY SESSION

Session Chair: David Hobart (*LANL retired*)

Renaissance 1 – 8:00 a.m.

8:00 a.m.

Analytical Techniques for Plutonium in Nuclear Safeguards and Nuclear Security Applications, Klaus Luetzenkirchen, Klaus Mayer (*Inst for Transuranium Elements*), plenary

10:40 a.m.

Overview on Plutonium Particle Analysis, Mats Eriksson (*Swedish Radiation Safety Authority*), invited

11:20 a.m.

Experimental and Theoretical Aspects of Nuclear Magnetic Resonance Spectroscopy of Pu Compounds, H. Cho (*PNNL*), E. Bauer, D. Clark, S. Kozimor, A. Mounce, H. Yasuoka (*LANL*), K. Mueller, J. Sears, N. Washiton (*PNNL*), invited

DETECTION AND ANALYSIS—I

Session Chair: Melissa Denecke (*University of Manchester*)

Renaissance 2 – 9:00 a.m.

9:00 a.m.

Small Scale Plutonium Analysis, Pamela Thompson (*AWE*), invited

9:40 a.m.

Plutonium Detection with Straw Neutron Detectors, Sanjoy Mukhopadhyay, Richard Maurer (*NSTec*), Paul Guss (*Remote Sensing Lab-Nellis*)

SURFACE SCIENCE AND CORROSION—II

Session Chair: David Moore (*LANL*)

Renaissance 3 – 10:20 a.m.

10:20 a.m.

The Microstructure of Plutonium Hydride Reaction Sites, Martin Brierley, John Knowles, Gordon McGillivray (*AWE*)

10:40 a.m.

Plutonium Hydriding: Hydrogen Transport, Chemistry, and Reaction Front Morphology, L. N. Dinh, S. K. McCall C. K. Saw, J. M. Haschke, P. G. Allen, W. McLean II (*LLNL*), invited

11:20 a.m.

The Roles of Pu-Oxide Overlayers in Surface Corrosion of Pu-Metal: A View from Ab Initio Molecular Dynamics, Bo Sun, Hai-Feng Liu, Hai-Feng Song, Ping Zhang (*Inst of Applied Physics and Computational Mathematics*), invited

SURFACE SCIENCE AND CORROSION—I

Session Chair: Art Nelson (*LLNL*)

Renaissance 3 – 9:00 a.m.

9:00 a.m.

The Study of Reaction of δ-Plutonium Surface with Water Vapor, Xinchun Lai, Xiaoguo Fu, Yongqiang Zhong (*China Academy of Engineering Physics*)

9:20 a.m.

The Room Temperature Oxidation/Corrosion of δ-Pu: Historical Perspective vs. Modern Understanding, David L. Pugmire (*LANL*), Harry G. Garcia Flores (*SRNL*), invited

LUNCH BREAK 12:00 – 1:00 p.m.

Renaissance I

DETECTION AND ANALYSIS—III

Session Chair: Kiel Holliday (*LLNL*)

Renaissance 2 – 1:40 p.m.

1:40 p.m.

Application of Focused Ion Beam (FIB) to Nuclear Forensics, Brandon W. Chung, Robert G. Erler (*LLNL*)

2:00 p.m.

High-Selective Chemiluminescence Initiated by Multi-Step Laser-Induced Excitation of Actinide and Lanthanide Ions in Solutions, I. N. Izosimov (*Joint Inst for Nuclear Research*), N. G. Firsin, N. G. Gorshkov, S. N. Nekhoroshkov (*Khlopin Radium Inst*)

2:20 p.m.

Present Status of Pu-238 Determination by Mass Spectrometry and Radiometry, Suresh K. Aggarwal (*BARC*)

2:40 p.m.

Plutonium Speciation Influence on the ^{22}Na Yield from the $^{19}\text{F}[\alpha, \text{n}]$ Reaction, William M. Kerlin (*UNLV*), John D. Despotopoulos (*UNLV/LLNL*), Dallas D. Reilly (*PNNL*), Ralf Sudowe, Kenneth R. Czerwinski (*UNLV*)

BREAK 10:00 – 10:20 a.m.

Renaissance Foyer

DETECTION AND ANALYSIS—II

Session Chair: Dominic Peterson (*LANL*)

Renaissance 2 – 10:20 a.m.

10:20 a.m.

Advanced X-Ray Imaging of Uranium Distribution in Biological Samples, Manuel Sturzbecher-Hoehne, Abdelmoula Haboub, Kathleen A. Bjornstad, Dahlia D. An, Albert Thompson, Alastair A. MacDowell, Rebecca J. Abergel (*BNL*)

SURFACE SCIENCE AND CORROSION—III

Session Chair: Robert Hanrahan (*NNSA*)

Renaissance 3 – 1:00 p.m.

1:00 p.m.

Oxygen Vacancies in PuO_2 (110) Surfaces via Density Functional Theory, Edward F. Holby (*LANL*)

1:20 p.m.

Adsorption of Water on Plutonium Dioxide Powder, Robin M. Orr, Robin J. Taylor, Howard E. Sims, Kevin J. Webb, David A. Woodhead (*NNL*), Paul M A. Cook, Jeff W. Hobbs (*Sellafield Ltd.*)

1:40 p.m.

The Absorption of CO_2 , H_2O and $\text{CO}_2\text{-H}_2\text{O}$ on Plutonium Dioxide, Xiaolin Wang, Gan Li, Junbo Lv (*China Academy of Engineering Physics*)

2:00 p.m.

Nuclear Waste Viewed in a New Light, C. A. Maid-Stitt, T. B. Scott (*Univ of Bristol*)

JOINT METALLURGY AND MATERIALS SCIENCE/CONDENSED MATTER PHYSICS—I

Session Chair: Franz Freibert (*LANL*)

Renaissance 3 – 2:20 p.m.

2:20 p.m.

Influence of Doping and Ageing on Electrical Resistivity of Plutonium, Pavel V. Ratnikov, Alexander Z. Solontsov (*N.L. Dukhov Research Inst for Automatics*)

2:40 p.m.

Local Structure in Plutonium and Plutonium Intermetallics Damaged by Self-Irradiation, C. H. Booth, Yu Jiang, S. A. Medling, D. Olive, D. L. Wang (*LBNL*), A. L. Pugmire, D. S. Schwartz, J. N. Mitchell, P. H. Tobash, E. D. Bauer (*LANL*), S. K. McCall, M. A. Wall, P. G. Allen (*LLNL*)

BREAK 3:00 – 3:20 p.m.

Renaissance Foyer

NUCLEAR FUEL CYCLE—IV

Session Chair: P. K. Mohapatra (*BARC*)

Renaissance 2 – 3:20 p.m.

3:20 p.m.

Overview of the CEA's R&D Dedicated to the Treatment/Recycling of Pu-Based Fuels (Towards PuMulti-Recycling), Stephane Grandjean, Nathalie Reynier-Tronche, Andrea Salvatores, Nathalie Herlet, Xavier Heres, Jean-Philippe Dancausse, Michel Masson, Christophe Poinsot, Laurent Paret, Dominique Warin, Bernard Boullis (*CEA*), invited

4:00 p.m.

Oxygen Self-Diffusion in Polycrystalline $(\text{U}_{0.55}\text{Pu}_{0.45})\text{O}_2$ Mixed Oxide, Romain Vauchy, Anne-Charlotte Robisson, Philippe Bienvenu, Ingrid Roure (*CEA, DEN, DEC*), Fiqiri Hodaj (*SIMAP, UJF/INP*), Philippe Garcia (*CEA, DEN, DEC*)

4:20 p.m.

Particle Size as a Function of Age in ^{238}Pu Oxide, Roberta N. Mulford (*LANL*)

4:40 p.m.

Diffusion Studies of U-Zr Alloys with HT-9 Stainless Steel at 700 C, Daniel Koury, Ken Czerwinski, Andrew J. Swift (*UNLV*), Morgan Luckey (*Harvey Mud College*)

JOINT METALLURGY AND MATERIALS SCIENCE/CONDENSED MATTER PHYSICS—II

Session Chair: Brandon Chung (*LLNL*)

Renaissance 3 – 3:20 p.m.

3:20 p.m.

Growth and Characterization of Poly- and Single-Crystal Uranium-Alloy Thin Films, A. M. Adamska, T. B. Scott, R. Springell, A. D. Warren, L. Pico, O. Payton (*Univ of Bristol*)

3:40 p.m.

The Phase Stability of Actinide Alloys: An ab Initio Aided CALPHAD Study, A. Perron, P. E. A. Turchi, A. Landa, P. Söderlind (*LLNL*), B. Oudot, B. Ravat, F. Delaunay (*CEA-Centre de Valduc*), invited

4:20 p.m.

Phase Equilibria in the Uranium-Plutonium-Oxygen System, Renaud C. Belin, Michal Strach, Christine Guéneau, Thibaut Truphemus, Romain Vauchy, Jean-Christophe Richaud (*CEA*), Jacques Rogez (*IM2NP, UMR 6122, CNRS*), invited

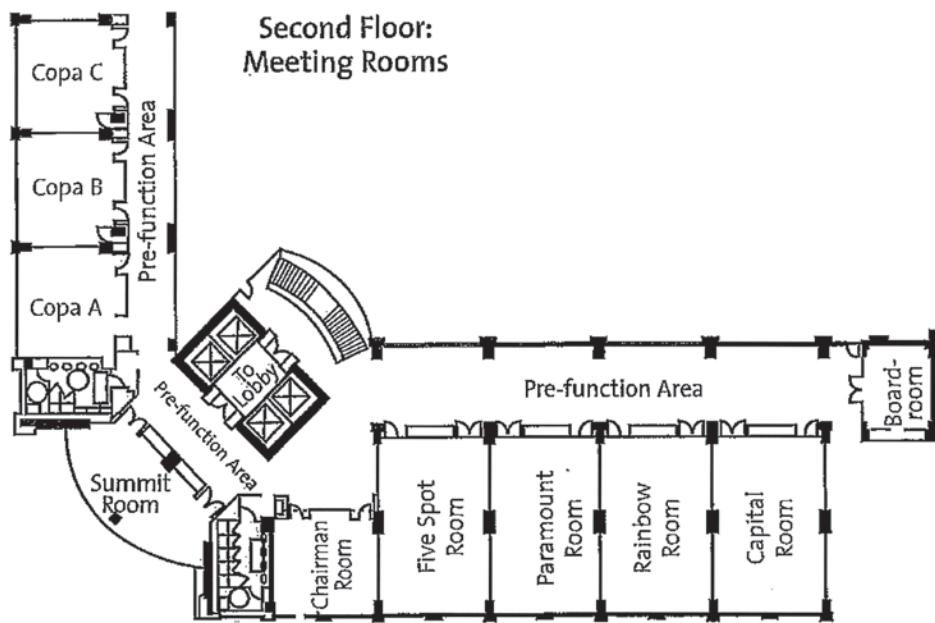
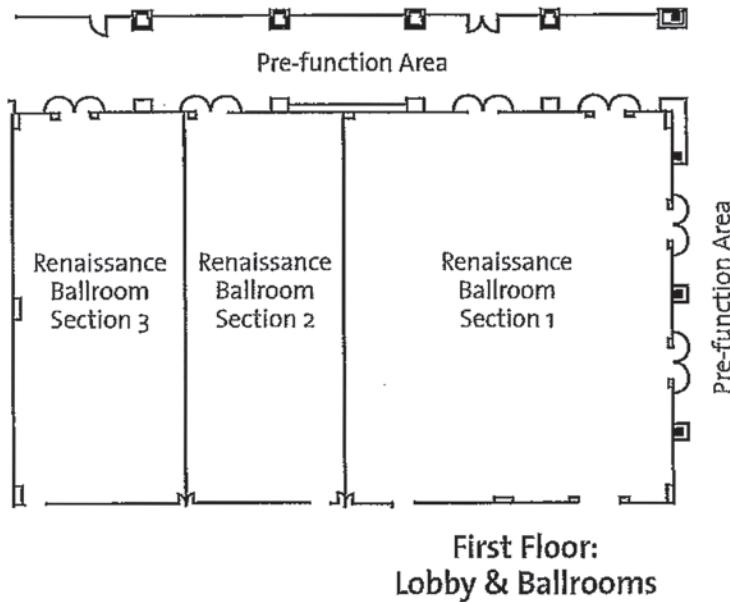
CLOSING REMARKS

Renaissance 1 – 5:00 p.m.

Sigfried Hecker (*Stanford Univ*)

David Clark, Honorary Conference Chair (*LANL*)

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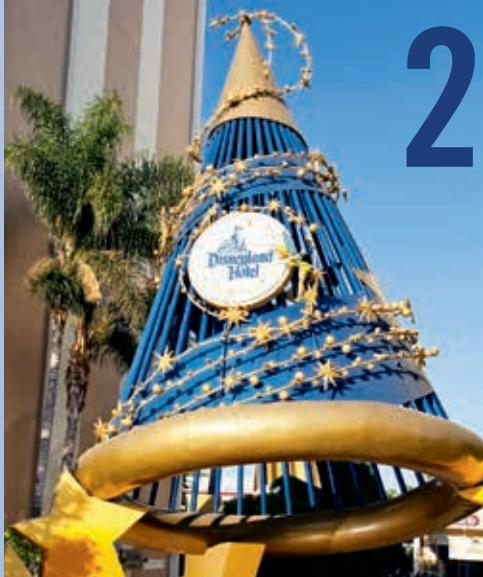


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