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Actinides and Neutron Scattering at the Spallation Neutron Source and High Flux Isotope Reactor

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OAK RIDGE National Laboratory

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Neutron Scattering Division

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ABBREVIATIONS

DOE	US Department of Energy
DOS	density of states
EOS	equation of state
HFIR	High Flux Isotope Reactor
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
ND	nuclear data
ORNL	Oak Ridge National Laboratory
QIS	quantum information science
RQ	reportable quantity
SAC	sample activation calculator
SNS	Spallation Neutron Source
SRNL	Savannah River National Laboratory
SSRL	Stanford Synchrotron Radiation Light Source

1. INTRODUCTION: SCIENTIFIC IMPORTANCE

The importance of actinides for science, technology, and medicine is widely recognized and does not require a lengthy introduction. However, the fundamental understanding of actinides and their chemical and physical properties lags behind the knowledge of most other elements in the periodic table. Most actinides ($89 \leq Z \leq 103$) are man-made and were produced in particle accelerators or nuclear reactors in the second half of the 20th century. Although trends in bonding and electronic structure are well-characterized and documented across the periodic table, fundamental questions remain regarding the chemistry and physics of the actinides. This lack of knowledge is largely because most isotopes of actinides are intensely radioactive, which greatly increases the difficultly in handling them.

The production, extraction, separation, and purification of actinides are a series of complex operations typically left to the US Department of Energy's (DOE's) national laboratories system. Although much of the current expertise in the science and technology of actinides resides in national laboratories, the role of universities and other research institutions in advancing understanding is also critical. Access to research facilities dedicated to the advancement of actinide science and technology is essential not only to further progress in basic science but also to support the vast array of present and future applications relying on the use of actinides and their compounds. Glenn Seaborg himself was keenly aware of this need as well as the practical limitations encountered at universities by actinide researchers. The creation of Seaborg Institutes, honoring his name, throughout the DOE complex to train the next generation of actinide scientists and engineers helps maintain and develop US proficiency in an increasingly important area of research and development.

Regrettably, neutron scattering remains woefully inaccessible to actinide researchers. The use of synchrotron light sources has permitted great advances in the understanding of lanthanide and actinide compounds. Unfortunately, this understanding is not enough. Neutrons offer several advantages over x-rays largely because of their ability to penetrate matter and probe the bulk of a sample rather than the surface (with x-rays and visible light, for example). The exchange of momentum between neutrons and materials is essential to obtain a complete view of properties such as specific heat, thermal conductivity, or entropy. Such data are needed to develop equations of state or validate electronic structure computer codes. Additionally, numerous gaps exist in neutron cross section databases pertaining to actinides; these databases are vital for the users of radiation transport codes used in nuclear safety, reactor design, and nuclear medicine, to cite a few applications. Other properties of neutrons are also essential in actinide research. For example, neutrons offer contrast between light elements in the periodic table and have sensitivity to hydrogen and deuterium, which is a distinct advantage over x-rays.

The most intense neutron sources in the US are run by the US DOE: the 85 MW High Flux Isotope Reactor (HFIR) reactor and the 2 MW pulsed Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL). However, access to these facilities for actinides research (in large part through programs supported by the DOE) remains elusive. A handful of experiments related to actinides were approved on a case-by-case basis and even then, only after a lengthy process, which is neither practical nor beneficial. In contrast, other DOE facilities (light sources such as the Stanford Synchrotron Radiation Light Source [SSRL], Advanced Light Source, Advanced Photon Source, and now the National Synchrotron Light Source II) have worked out an approach for access that is streamlined and efficient without sacrificing safety and security. Notably, the Los Alamos Neutron Science Center facility at Los Alamos National Laboratory (LANL) ran actinide experiments at various beamlines while the user program was still operational. The remaining two beamlines dedicated to materials research are not sufficient to serve the needs of a wide community of scientists and engineers desperate for access to neutrons to support their work. Lack of access to neutron beamlines and the various techniques offered at HFIR and SNS, such as small-angle neutron scattering, single crystal or powder diffraction, total

scattering, pair distribution function analysis, inelastic scattering, transmission measurements, and quasielastic neutron scattering, are already leading to loss of expertise and scientific leadership as well as affecting actinide-related research projects funded by the DOE and other US Government agencies.

The DOE Accelerator Safety Orders (Spallation Neutron Source Final Safety Assessment Document for Proton Facilities, 102030103- ES0018; Spallation Neutron Source Final Safety Assessment Document for Neutron Facilities, 102030102- ES0016; SNS Accelerator Safety Envelope (ASE): for Full Power Operations of the Front End, Linac, Ring, Transport Lines, Beam Dumps and Target, SNS 102030103-ES0016) under which SNS operates do not explicitly exclude actinides; therefore, actinides currently represent an unevaluated hazard. The accelerator safety order requires researchers to perform this hazard evaluation, but it does not have any explicit limit on actinides—only a requirement that the hazard be managed. Researchers would need to characterize the hazards and determine which controls are appropriate. This requirement is complicated by the fact that the relative hazard of actinides can vary dramatically depending on the isotope. General procedures for the shipping, storage, and handling of samples containing actinides need to be developed without degenerating into the case-by-case situation mentioned here. Similar considerations apply to HFIR. Another factor comes into play with some actinides—namely, criticality safety, which would likely result in explicit limits on quantities and restrictions on storage. Accelerator facilities are subject to DOE Order 420.1, Chapter III, "Criticality Safety." As such, researchers would need to ensure that the quantity of fissile material is below a quantity at which criticality is a risk. A typical limit for SNS would be limited to 700 g of ^{235}U equivalent. ORNL's Standards Based Management System provides some guidance. Finally, security considerations for some isotopes will need to be considered. Many of these issues have already been addressed at other DOE facilities, and access plans are in place that could serve as a basis to develop a similar approach at SNS or HFIR. At the same time, it is important to recognize that irradiation with neutrons presents unique hazards such as activation and the production of fission products, which pose unique radiation protection and waste disposal problems. It should be emphasized that thanks to the high neutron flux available at SNS and HFIR, smaller quantities of actinides can be used while still producing significant results in a reasonable amount of time.

The first goal of this report is to impress on the reader the critical importance of neutron scattering techniques (and access to SNS and HFIR) to a vast community of scientists and engineers working on numerous aspects of actinide research—basic or applied. The next section of this report documents some of those needs and collates many outstanding questions in actinide research. Some of these questions have been awaiting an answer for decades and have delayed progress and negatively affected the work of countless workers. They are concrete, down-to-earth problems described in a few sentences as opposed to general, overarching statements. A second goal of the present document is to investigate in more detail the reasons limiting the use of actinides at SNS and HFIR with the aim to develop a plan to facilitate neutron access by actinide researchers. A starting point is the current experience at x-ray sources as well as experience at the Los Alamos Neutron Science Center facility. The ideal outcome would be to define a safety envelope regarding quantities, physical parameters (such as temperature, pressure, or magnetic field), toxicity and radiological hazards, and more, within which a proposal for beam time could be considered by the Science Review Committee. Other practical considerations such as shipping, storage, handling, and security could be approached in the same spirit of defining boundaries within a particular proposal that could be executed rapidly and reliably.

2. SAFETY AND SECURITY

2.1 INTRODUCTION

Actinides are all radioactive by nature. This characteristic adds an additional complication when trying to safely study these elements. However, ORNL, along with other national laboratories, has highly trained

personnel with specialized facilities to make this work possible. Currently, across the nation, there are a handful of user facilities that regularly analyze actinide-containing samples. A few examples include the SSRL, National Synchrotron Light Source II, Advanced Photon Source, and Advanced Light Source. ORNL held a workshop titled "Actinides at SNS" to gather insight for safely running actinide-containing samples at user facilities. This workshop included scientist and engineers from around the country that have both an interest in running actinide samples at SNS and experience running actinide samples at other facilities mentioned here (See Appendixes B and C). This section focuses on the safety of taking actinide-containing samples to SNS.

2.2 SNS

Standing up actinide capabilities at a user facility requires rigorous sample screening, radiation protection, sample storage, security plans, and shipping planning. Starting with sample screening, SNS already has a process to screen for hazardous materials before they are brought to the beamline. The addition of transuranic samples to this list would be needed. After this sample gets flagged, the user would then need to meet specified sample requirements such as an approved sample holder, and in some cases, leak checks of the sample holder prior to shipment may be required.

Next, radiation protection would need a standard procedure for how to handle these samples. This procedure would include regular smear checks of the sample to check for removable contamination and an intelligent alpha/beta continuous air monitor running to detect any airborne radiation in the area. Notably, researchers do not intend to handle or manipulate any samples outside of their secondary containment. All sample loading must be done at the home institution. The storage of these samples would depend on both the dose rates and the security plan. Currently, SNS has a storage room where samples can be taken after measurements are complete. This process is commonly done across the DOE complex when samples are sent off-site. This plan would call out what security measure would need to take place for the sample and for the data collected.

Lastly, concerning shipping samples to and from ORNL, across the DOE complex, personnel are trained and qualified to ship radioactive material. ORNL has a team that focuses on shipments coming to and from ORNL. The biggest risk identified for shipping is the return of material once it has been measured at SNS. Other sites address this issue by requiring the users to have the appropriate paperwork filled out for the return shipment prior to receiving the samples. However, this solution could be complicated by the fact that these samples will become activated and dose rates will change. This risk could be mitigated by making the users sign an agreement to ship. Another concern related to the activation of samples is the ability to ship it back to the home institution because of dose rates or fission products that are produced. To address this issue, this report suggests that modeling and simulation be done for sample activation prior to running the samples at SNS.

In fact, SNS successfully ran a transuranic sample of Pu back in 2013. A tremendous amount of planning and foresight went into this experiment being run safely. However, this was a one-time exception that was made by DOE to run these samples at SNS. Building on the success of these experiments, the authors believe that it would be possible to do this work routinely. The biggest hurdle that needs to be overcome for SNS to regularly run actinide samples would be changing the facility use agreement. Currently, the biggest limitation of taking actinide samples to SNS is the limited quantities that are allowed. Changing the facility use agreement permanently, in conjunction with the discussed considerations, would allow for samples to be routinely run at SNS.

2.3 HFIR

In contrast with SNS, HFIR is allowed to take certain quantities of transuranic complexes. However, depending on whether the researcher is using the Cold Guide Hall (Building 7972) or is running experiments under the reactor (HFIR beamlines HB-1, HB-2, HB-3) the material limits are very different. Material limits in Building 7972 are 20 times Reportable Quantity (RQ)values (sum of fractions based). Because of these limits, microcurie or millicurie quantities (isotope-dependent) would be doable at this time.

However, because HFIR is a Hazard Category 1 nuclear facility, limits for HB-1, HB-2, and HB-3 are much higher. In recent years, neutron diffraction and magnetism experiments have been performed on 40–50 mg of ^{237}Np-containing samples. These samples were prepared at the neighboring Hazard Category 2 nuclear facility (the Radiochemical Engineering Development Center), then hand carried to HFIR for insertion into the wide-angle neutron diffractometer (WAND) on HB-2. Once the sample was done running, it was packaged up and transported back to the Radiochemical Engineering Development Center. These experiments were proof-of-principle experiments to prove that researchers could safely run transuranic samples at HFIR. All samples run on HFIR in recent years have been below accountable quantities. To run accountable quantities of transuranic samples, additional controls would need to be put in place. In coming years, more samples of transuranic material are planned to be analyzed at HFIR.

3. SUMMARY OF BREAKOUT SESSIONS

3.1 BREAKOUT SESSION 1: SCIENTIFIC IMPACT AND SAMPLE ENVIRONMENTS

At the Actinides at SNS and HFIR workshop (see Appendix C, Figure 1), the participants were broken into three different groups to discuss a variety of different topics. Each group consisted of a handful of scientists and at least one beamline scientist to help facilitate the discussion. Scientific impact was discussed and is largely summarized in Appendix A. Many scientists were interested in better learning which beamlines were appropriate for various measurements or sample types. Someone suggested to stand up a working group that would help guide and advocate for this actinide science effort moving forward.

Much time was spent on sample types and environments. Because neutron scattering experiments require relatively large sample sizes, participants were interested to test the smallest size of samples that could be run on certain instruments. In all, the session summarized that new sample containment methods could be designed and then approved. The ability to do in situ reactions was of high interest as well as cooled experiments for magnetism. The session largely agreed that the first actinide experiments run should be simple to demonstrate that researchers can do this method safely. Researchers need to characterize and understand the properties so they can predict and control these properties.

The programs that would support the expansion of actinide science at SNS and HFIR (DOE Basic Energy Sciences–funded facilities) are related to weapons programs or are programmatic in outlook. Involvement from the National Nuclear Security Administration and other applied programs within DOE would have to be supportive. Current examples of programmatic or weapons-related work includes DOE Isotope Program's interest in heavier actinides such as ^{242}Cm and ^{249}Bk, nonproliferation forensic work at ORNL, or Savannah River National Laboratory's (SRNL's) recent engagement in materials characterization and nuclear waste management. Nonetheless, a great deal of interest exists in more fundamental science questions, as discussed in Appendix A of this report, and funded by the Office of Science or other DOE entities such as the Office of Nuclear Energy or Office of Energy Efficiency and Renewable Energy.

Figure 1. A picture of the Actinides at SNS and HFIR workshop participants.

The neutron scattering techniques of interest cover a wide range, including the following:

- Inelastic neutron scattering involves research into the dynamics of the materials, measuring the phonon density of states or phonon dispersion curves; vibrational spectroscopy; and hydrogen dynamics. These techniques have a major effect on the equation of state determination, electronic structure code validation, thermodynamic properties, magnetic structure and dynamics, and other physical and chemical property determinations.

- Neutron pair distribution function analysis is a technique complementary to x-ray scattering's extended x-ray absorption fine structure method. It measures the local structure of materials and provides a comprehensive view of the short- and medium-range order in materials (nano, disordered materials, amorphous, liquids). Access to medium-range order is denied with extended x-ray absorption fine structure but occurs naturally when using neutrons as a probe. This technique will produce novel results investigating phase transformations kinetics, amorphization/crystallization, structural disorder, and actinide materials aging under self-irradiation.

- Diffraction (powder or single-crystal) is a fundamental technique used by researchers in all areas of science and engineering to obtain structural information at the atomic and molecular levels, which can be exploited in many ways. Neutrons offer multiple advantages over x-ray diffraction, including sensitivity to hydrogen; enhanced contrast among the light elements in the periodic table and the possibility of studying these elements in the presence of actinides; penetration through matter, which enables the use of bulky sample environment equipment such as pressure cells and bulk averaging; and the possibility of isotopic substitution (e.g., hydrogen vs. deuterium).

- Other techniques such as small-angle neutron scattering offer the possibility of observing defect structures in the bulk of a material. Transmission measurements to close the gaps in cross section databases would benefit countless workers in areas such as nuclear energy, nonproliferation, or nuclear medicine, to mention only a few. Imaging and small-angle neutron scattering complements structural studies by providing structural information on microstructure beyond the atomic or molecular level.

SNS and HFIR offer access to these techniques and the corresponding neutron advantages. The x-ray counterparts, when they exist, frequently come with limitations. The joint use of neutrons and x-rays, however, is not to be neglected. Unfortunately, access to neutrons for actinides work has been limited or prohibited worldwide for a long time, which has hindered progress in actinide science.

The list of contributors to this report appears in Appendix B at the end of this report. The list represents a new and eager community of neutron users for whom access to neutron scattering is a priority. The community of potential users requiring the use of neutrons for actinide research is much larger, and reach-out efforts for community building will play an essential role in ensuring that the present effort bears fruits. The Seaborg Institutes at various national laboratories, with their goal of educating and training the next generation of actinide researchers, will play an essential role in this respect.

3.2 BREAKOUT SESSION 2: SHIPPING, STORAGE, SAFETY, RADIATION PROTECTION, HANDLING, AND OTHER PRACTICAL CONSIDERATIONS

The major issues facing the use of actinides at SNS and HFIR are due to the current basis for operation as well as a lack of infrastructure necessary for the handling of small amounts of actinides for research purposes. Although depleted uranium and thorium have been used somewhat routinely, other actinides require approvals and the development of new procedures on a case-by-case basis. This time-consuming and costly approach is perhaps the largest obstacle that the actinides community faces in terms of access to neutron scattering facilities.

Based on the experience at synchrotrons, it is obvious that procedures must be developed, documented, approved, and implemented to

- store actinides safely and securely and track inventories;
- handle shipping and receiving of actinide-containing samples, including irradiated samples;
- review beam time proposals with actinide-based samples;

- ensure safety and security (e.g., total ionizing dose devices) at a beamline during an experiment (sample and data);
- digest lessons learned at synchrotrons and other facilities handling actinides for research purposes;
- address and mitigate potential hazards (radiation, toxicity) and accident scenarios;
- train personnel involved in the handling of actinides at SNS and HFIR; and
- define a safety envelope of acceptable radionuclides, quantities, and experimental conditions and modify the facility use agreement to reflect the new operating conditions.

Implementation will require SNS and HFIR to identify and create Material Balance Areas for storage and accountability transactions. The possibility should be considered that an irradiated sample may have to be stored for an extended time because of activation and US Department of Transportation limitations for transportation of radioactive materials. The SSRL experience suggests that ensuring a path exists to return an activated sample before neutron irradiation is essential. Laboratory space for storage and handling (e.g., in case of a containment breach) must be identified.

Sample containment before, during, and after irradiation represents a central safety issue. Sample holders for double encapsulation will have to be developed and tested. LANL has experience with this process already [1], and SNS/HFIR is already evaluating the LANL sample holders (vanadium and aluminum) that were used successfully for double encapsulation of actinide samples at the Lujan Center over the past decade. Engineering drawings are available with a detailed report describing finite-element calculations and the results of mechanical testing (i.e., deformation, pressure). The development of a database of approved sample holders would be helpful to users.

Nuclear transmutation upon neutron irradiation (including the formation of fission products) is specific to the use of neutrons as opposed to the situation at synchrotrons where sample activation does not occur. A sample emerging from a neutron scattering experiment may have different radiological properties compared to the preirradiation material. Evaluating this process and determining the nature and quantities of radionuclides formed during the experiment should be part of the safety evaluation for a given experiment. The Sample Activation Calculator (SAC) calculator used routinely at HFIR and SNS to determine nuclides inventory in a sample postirradiation is a tool that could be expanded to cover actinides more thoroughly [2].

Shepherding the process from beam time proposal submission, safety evaluation, sample transfer in and out of the facility, and execution of an experiment will require the formation of a working group of subject matter experts (perhaps including members external to ORNL) to evaluate each proposed experiment.

Although a lot of high-visibility scientific work is to be performed, as outlined in Appendix A, the working groups for the second breakout session had a general feeling that a graded approach based initially on the safe and successful completion of simpler, low-risk experiments might be prudent and preferable. Experience over time would then lead to a stepwise, progressive expansion of the operation conditions envelope to more ambitious experiments.

4. CONCLUSION AND OUTLOOK

This report attempts to build a robust case for the access to neutron beamlines at SNS and HFIR by the larger actinides research community. Its final version was completed in a workshop organized at SNS and HFIR on June 12–13, 2024, followed by a review by the broader group (email list) that helped develop the science case. The workshop went beyond the science case to examine safety and logistics issues in light of previous experience at other neutron and x-ray scattering DOE facilities. If the science case presented is deemed strong enough to pursue the inclusion of the actinide research community into the community of users at SNS and HFIR, this report suggests that the next few steps revolve around the development of a detailed plan for the access and use of the ORNL neutron scattering facilities similar to the facility user agreement currently in place. The actinide community envisions a local committee appointed by the Neutron Sciences Directorate director and/or the associate laboratory director for the Neutron Sciences Directorate and comprising subject matter experts in neutron scattering (e.g., beamline scientists and scientific associates), sample environment (engineers, scientists, and technicians), general safety matters (health and safety professionals), radiation protection (radiological control technicians and radiological engineers), logistics (including shipping/receiving, storage, building management), and security. Other ORNL personnel and external subject matter experts will be included to capture existing knowledge, processes, and current practices as well as to guide the local team.

The main tasks assigned to the committee would include the following:

- Defining an initial safety envelope of permissible experiments in terms of isotopes, sample mass, activities, temperature, pressure, humidity, magnetic field, and more, as well as admissible sample holders and sample handling
- Developing a process for shipping, receiving, and storage, including verification and radiological controls
- Creating storage space and an inventory tracking system
- Developing a universal process to handle, store, and ship irradiated actinide samples
- Developing a streamlined process for instrument readiness, sample movement within the facility, performing the experiment, and securing a sample and beamline for the duration of the run
- Making recommendations on a new or extended procedure to accept and review actinide-related proposals and process actinide users and experiments
- Examining security requirements related to sample storage and handling, as well as data access and curation (Note: Classified experiments will not be considered at this stage.)
- Evaluating possible accident scenarios and their consequences
- Assessing safety hazards for each step (from receiving to performing the experiment and disposition of the sample[s]) and providing risk mitigation strategies
- Investigating the administrative tasks needed to implement these action items
- Producing a final report documenting the proposed approach for each case

The overarching goal would be to obtain a clearly defined process within an agreed-upon safety envelope that would avoid the current approach, which examines each actinide beam time proposal on a case-by-case basis. Once a beam time proposal has been reviewed by the (external) Science Review Committee and has been granted beam time by the Beam Allocation Committee, the proposal would undergo the normal safety evaluation (taking additional actinide-related restrictions in place at the time). If the proposed work falls within the defined safety and security envelope, it would be allowed to proceed according to the standard procedure that this community hopes to develop upon consideration of the issues listed here.

The deliverable would be a report outlining the new safety envelope and standard process for experimental neutron work at SNS and HFIR. This report would undergo a final review internally by Neutron Sciences Directorate management, ORNL management, and the DOE ORNL Site Office, as well as an independent, external review committee of subject matter experts.

5. REFERENCES

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APPENDIX A. COLLECTIVE

Lawrence Berkeley National Laboratory

The central mission of the Glenn T. Seaborg Center at Lawrence Berkeley National Laboratory (LBNL) combines scientific motivations to uncover fundamental heavy-element chemical interactions in complex systems with the need to educate and train future generations of scientists with proficiencies in actinide chemistry. For several decades, the center has combined its strengths in inorganic chemistry and radiochemistry with x-ray spectroscopic techniques to reveal foundational bonding, reactivity, and physical properties of the actinide and transactinide elements.

In doing these studies, LBNL has become an expert in the sample preparation, containment, measurement, and data analyses of radioactive compounds at US Department of Energy (DOE) user facilities. For example, in collaboration with the Radiation Protection Groups at LBNL as well as the Advanced Lightsource (LBNL) and Stanford Synchrotron Radiation Lightsource, LBNL has successfully performed countless x-ray absorption and x-ray diffraction experiments at synchrotron beamlines with highly radioactive elements, such as plutonium, americium, and berkelium.

Alongside scientific advancements, the experiments proposed herein can also aid in training the next generation of undergraduates, graduates, and postdocs through the Oak Ridge National Laboratory (ORNL) Neutron Scattering School and hands-on experience at the Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) instruments. Collectively, routine work with minimal overhead at this DOE facility can open an innovative avenue to answer overarching questions in actinide science with neutrons. The group at LBNL can support and participate in this endeavor by drawing on their experience in sample handling, holder development, radiation protection organization, and beamline experience from previous x-ray studies.

Given this expertise and experience, the LBNL group sees an exciting opportunity to expand studies to SNS and HFIR to further investigate outstanding problems in actinide science. Access to neutrons can support missions at LBNL to probe fundamental actinide coordination with implications in a variety of applications ranging from nuclear forensics to molten salt reactors. The wide range of instruments at SNS and HFIR opens a new frontier for this program.

Phase transitions in actinide compounds: The LBNL group can leverage the TOPAZ instrument to perform single-crystal x-ray diffraction measurements at a range of temperatures (5–450 K) to reveal temperature-induced phase transitions in actinide compounds.

Protonation state of oxygen ligands: The light or heavy element contrast afforded by neutron diffraction at TOPAZ is critical for determining atomic positions and displacement parameters of light elements (such as hydrogen) next to heavy metals. This technique could be especially useful for understanding the protonation states of oxygen ligands on the surface of actinide clusters with ramifications in actinide processing campaigns and environmental migration. Because the ligands can exist as oxo-, hydroxo-, and aquo- groups, which are otherwise difficult to identify with traditional single-crystal x-ray diffraction methods, neutron diffraction offers a solution to better understand actinide cluster composition.

Cation–cation interactions and disorder in actinide oxides: In addition to single-crystal measurements, powder diffraction measurements with the POWGEN and SNAP instruments could be useful to probe structural features of actinide oxides, the characterization of which is critical to nuclear fuel cycles and the diagnostic tracking of nuclear materials. For example, bonding in the Np_2O_5 framework is unusual because all neptunyl ions in the structure are involved in cation–cation interactions. The Np_2O_5 forms readily under hydrothermal conditions, but recent crystallographic studies show possible structures

inconsistent with pure Np_2O_5. This precipitation of Np_2O_5 is of great importance to environmental considerations associated with long-term nuclear fuel storage. Additionally, samples of plutonium oxides can exhibit a wide range of colors (e.g., tan, khaki, olive green, yellow) despite having nearly identical diffraction patterns. As such, investigating plutonium oxides by powder x-ray diffraction can give a false sense of similarity between samples that have metal atoms in chemically equivalent occupancies but oxygen atoms in different (or disordered) occupations in the lattice structure. Powder diffraction measurements with the POWGEN and SNAP instruments would provide short- and long-range structural insights for high-purity plutonium oxides of nonfissile plutonium isotope samples and thus yield valuable benchmarks for investigations of plutonium process signatures.

Molten salt diffusion in molten salt reactors: Other opportunities lie in the MARS and VISION instruments for radiography and vibrational studies, respectively, to investigate broad questions in molten salt diffusion and nuclear forensics (with radiography) and actinide bonding, as well as structure–property relationships (with vibrational spectrometry) across temperatures and pressures.

Los Alamos National Laboratory

There is a pressing need to bridge the experimental gap between the microscopic and macroscopic behavior in actinides. Plutonium is the predominant material in the nation's nuclear stockpile and is the most complex element of the periodic table with six allotropes, numerous oxidation states, and complex phase transitions. The total scattering technique is the current state of the art in determining the atomic structure of disordered or amorphous materials, nanoparticles, and liquids. The development of total scattering methods using the pair distribution function analysis has provided researchers with an indispensable, powerful tool to analyze the local structure of materials, probing both short- and medium-range order—a length scale not accessible to Bragg scattering (diffraction), small-angle scattering, or extended x-ray absorption fine structure. Total scattering of x-rays and neutrons provide complementary information for both average and local structure, covering the short-, medium-, and long-range orders.

Local structure in actinide materials—in particular, plutonium and plutonium compounds: Despite significant efforts being made for a better understanding of self-irradiation processes and phase stability or phase transformations both computationally and experimentally, several problems still exist for which the scientific knowledge is incomplete or elusive. Pair distribution function analysis can connect the microscopic and macroscopic, informing future computational efforts of changes taking place at the local structure level. Important information that is absent from the average crystal structure is provided when local structural distortions exist. The intermediate substructures that occur between the solid phase transformations in plutonium are still unknown.

Consequences of aging under self-irradiation for structural and physical properties: Phase stability and phase transformation in binary plutonium alloys are of high importance for the nation's aging stockpile, especially in relation to the effect of decay products on the integrity of the alloys used—most notably, plutonium–gallium alloys—and effects critical for weapons research and nuclear energy applications. Long-term phase stability affects mechanical properties, microstructure, corrosion behavior, and, most importantly, structural integrity. Understanding the mechanisms behind or associated with phase stability and phase transitions is of high importance, especially in relation to the effect of decay products on the integrity of the alloys used, most notably in plutonium–gallium alloys. Total scattering studies of such materials are critical in assessing everything from the number, type, and relative amounts of structural phases present to details within these of the lattice, atomic positions, and atom types present, as well as any defects, disorder, and inhomogeneity at the local atomic level. Without a clear and detailed understanding of how these characteristics evolve at multiple length scales, researchers have little hope of knowing how the nation's nuclear stockpile will age or respond to unexpected stimuli. NOMAD, POWGEN, and VULCAN can provide information not accessible with x-ray diffraction alone.

Kinetics and ordering near phase transitions in actinide alloys: Investigations near phase transitions using time-resolved diffraction and pair distribution function at constant temperature to *examine the evolution of average and local structure with time as a phase boundary is approached can generate isothermal data sets that will provide a kinetic picture of the structural evolution near the phase transition.*

Plutonium equation of state (EOS): Phonons, as dominant contributors to the entropy and thermal pressure in the regions of interest, are important for the development of multiphase EOSs and phase boundaries. EOS models commonly used at Los Alamos National Laboratory are based on determining the densities of states (DOSs) of the electronic excitations and the vibrational modes of the lattice by comparing theoretical results with thermodynamic data or by first-principles calculations using density functional theory. Inelastic neutron scattering offers a novel and direct path, with the measurement of the experimental phonon DOS at different temperatures and pressures. Density functional theory calculations can be employed to help interpret the experimental results, which are further used in lattice vibrations models for EOS calculations. Comparisons with the measured DOS, the density functional theory calculations, and the degree of fit of the resulting EOS to thermodynamic data will enable a more accurate determination of the reliability of the measurements, improve the ability to calculate DOS from first principles, and produce more accurate EOS for actinides.

Los Alamos National Laboratory has a long history of making, measuring, and modeling complex f-electron materials, leading to exploration and an understanding of new states of matter and behavior in plutonium-, neptunium-, and uranium-based materials, including correlated electron behavior, unconventional and topological superconductivity, quantum criticality, and frustrated and quantum magnetism. A focused effort in actinide science at SNS and HFIR would open several avenues for understanding these quantum states of matter in new ways.

Quantum and frustrated magnetism, Kitaev spin liquids: Kitaev spin liquids have attracted a great deal of attention in recent years because they are predicted to host Majorana quasiparticles, which may be used for quantum computation. The Kitaev model on the honeycomb lattice is an exactly solvable model that gives rise to Majorana excitations. A number of uranium-based honeycomb systems (e.g., Li_2US_3) might be realizations of the Kitaev model, providing another route to finding Majorana modes in real materials. Importantly, inelastic neutron scattering experiments are an ideal probe of these nontrivial excitations. More broadly, uranium-based compounds span the range between localized and itinerant f-electron character, which may be used as a *tuning knob* for understanding the role of frustration in generating unusual magnetic states (e.g., vortex magnetic structure in UNi_4B) and physical properties. As a result, the determination of the exchange parameters through neutron spectroscopy is crucial to modeling unconventional magnetic behavior.

Topological superconductivity in uranium compounds: Uranium superconductors are among the most promising candidates to search for Majorana modes in odd-parity superconductors (e.g., UTe_2, UPt_3, UBe_{13}) for quantum computation. Delineating the excitation spectrum in uranium-based superconductors through inelastic neutron scattering and determining any nearby magnetic states by magnetic diffraction at SNS and HFIR would be a significant advancement in the field to understand the nature of the superconducting pairing mechanism.

Quantum criticality in uranium-based quantum critical systems: Quantum criticality is an organizing principle for understanding the behavior of many actinide, lanthanide, and transition metal–bearing materials. Characterizing the dynamic and static critical exponents, both with and without disorder, would help to move the field toward a unified description of quantum criticality. Furthermore, few studies have been done on the spin waves in uranium-based quantum critical systems. Probing the damping of spin

waves in uranium compounds would help in understanding the role of antiferromagnetic fluctuations (and perhaps other interactions) in quantum critical systems.

2D actinide systems with strong correlations: The investigation of 2D van der Waals and other 2D materials is at forefront of the field for discovering new quantum states of matter, such as unconventional superconductivity, metal–insulator transitions, the quantum anomalous Hall effect, and quantum criticality. With the recent interest in exfoliating the heavy fermion antiferromagnet CeSiI, exploring the behavior of uranium-based van der Waals materials in the 2D limit is a promising direction to pursue.

Universal behavior in unconventional superconductors, $PuCoGa_5$: A superconducting spin resonance occurs in many classes of unconventional superconductors, and its energy obeys a scaling relation (ER ≈ 0.65[2*D*]) with the superconducting energy gap *D*. The energy gap of superconducting $PuCoGa_5$ lies in between the heavy fermion superconductors and the high-technetium cuprate and iron arsenide superconductors. Confirmation of the superconducting spin resonance in $PuCoGa_5$ would be proof of universal behavior in unconventional superconductors.

Exploration of 5f electron wavefunction in plutonium: The ground state wavefunction of δ-plutonium has been determined through inelastic neutron scattering at SNS, which is related to the EOS and is key to understanding many of the unusual properties of plutonium. Elucidation of the form factor and excitation spectrum of magnetically ordered plutonium compounds would provide key information about the ground state wavefunction of the plutonium 5f electrons.

Development of the entangled ground state in f-electron materials: The evolution of how the f-electrons hybridize with conduction electrons and the development of a coherent f-electron state has been determined in the mixed valent compound $CePd_3$. Extending this study to uranium mixed-valent compounds would be helpful to understand how the heavy fermion state develops in the more extended (delocalized) 5f electron states.

The instruments at SNS and HFIR, including CNCS, SEQUOIA, and ARCS for inelastic neutron scattering and TOPAZ and HB-2A for magnetic diffraction (and perhaps others), would be particularly useful for exploring these topics in actinide materials.

Oak Ridge National Laboratory

As part of ongoing work for the National Nuclear Security Administration at ORNL, researchers are tasked with understanding the fundamental material chemistry of technogenic actinide materials and generating usable spectroscopic signatures that may be connected to their material production and environmental history. To do this work, researchers engage in fundamental material research related to the formation chemistry of various technogenic phases, collecting and understanding their optical vibrational spectra, and connecting these observations to processing parameters. ORNL has historically leveraged neutron scattering for understanding crystal waters of hydration in uranium complexes because many fuel cycle–relevant materials collect water during exposure to the environment or as part of precipitation reactions. Additionally, fundamental vibrational spectra obtained from inelastic neutron scattering are vital tools in fully understanding the lattice dynamics in these systems, which assist in building models that can be leveraged in lab-scale measurements on real materials.

Materials chemistry of plutonium compounds: For transuranics, ORNL is also tasked with understanding fundamental material chemistry of plutonium compounds. The ongoing collaboration with Savannah River National Laboratory (SRNL) has been focused on the formation dynamics and structure of plutonium metal precursors—specifically, plutonium oxalates, fluorides, oxides, and cesium salts of plutonium. Unsurprisingly, given the difficulty of handling and obtaining significant quantities of

plutonium, many questions remain regarding the fundamental structure of these materials. Neutrons will provide valuable insight because all these compounds readily form crystal hydrates. ORNL would like to pursue lines of research pertaining to the fundamental structural determination of these materials with neutrons.

Phonon DOS: The spectral characterization work performed for uranium compounds is also relevant for plutonium, for which fundamental vibrational spectra knowledge is essentially nonexistent. The phonon DOS measured with neutrons is averaged over the entire Brillouin zone and provides access to force constants and thermodynamic properties such as entropy and specific heat. Such information is critically important to validate computational work on 5f electron systems.

PUREX: Essentially all plutonium existing on Earth has undergone the so-called PUREX process for the separation of plutonium and uranium and other fission products from irradiated fuel, which is the only method for producing significant quantities of plutonium. Despite its importance in plutonium processing, the fundamental, atomic-scale chemistry of the PUREX process is still not completely understood. Efforts are underway across the DOE complex and within academia to model the aqueous/organic phase boundary using molecular dynamics and ab initio methods. Neutrons present a fascinating opportunity to study the PUREX separations process in model systems via quasielastic neutron scattering, which directly probes the diffusion of atoms on the microelectron volt timescale. PUREX is extremely complicated because of the high activity of the solutions (self-irradiation of plutonium and ongoing activity of daughter products). Nevertheless, it is an open area of study and perhaps the most important area of research in plutonium processing.

Fundamental structural chemistry of actinide compounds: ORNL's university collaborators at The University of Notre Dame have been pursuing questions related to conserved structural units across the actinides, including uranium, neptunium, and plutonium compounds. Fundamental coordination chemistry of the actinides is important foundational research at the boundaries of inorganic chemistry, and searching for patterns within their bonding and coordination could lead to important advances in researchers' understanding of actinide coordination chemistry. This research has been primarily focused on oxalate compounds because oxalates tend to support multiple oxidation states of the heavy metal cation; however, they once again tend to accept significant quantities of crystalline water. Neutron diffraction, with its high sensitivity to hydrogen, is an ideal tool to study these systems.

Closing gaps in neutron cross section libraries: Neutron induced cross section measurements are of great value to both science experiment and instrument technology applications at the Neutron Sciences Directorate's sources. Understanding the energy-dependent interactions of neutrons with materials is fundamental to neutron radiography and traditional scattering experiments, as well as an important input to complex safety simulations used to determine radiological and background performance of shielding in instrument designs. Modeling and simulation of any nuclear application using codes such as SCALE , GEANT, or MCNP rely on the quality of the existing evaluated nuclear data libraries such as the Evaluated Nuclear Data File (ENDF/B), the Joint Evaluated Fission and Fusion nuclear data library, or the Japanese Evaluated Nuclear Data Library. In some cases, the cross section evaluations of those libraries were found to be deficient in accurately describing criticality benchmarks, to name just one example. Additionally, those libraries have gaps in neutron-induced cross section data of radioactive isotopes (actinides and fission products) and, in many cases, rely on theoretical calculations or estimations. Modern simulation codes are capable of handling covariance data, but the lack of these data for radioactive isotopes can create large uncertainties in those calculations.

Also, nuclear data (ND) experimental capabilities will expand ORNL's scientific portfolio by providing the ability to perform cross section measurements of radioactive nuclei and to provide additional cross section information that is important to understanding heavy-element nucleosynthesis processes within

unique stellar phenomena. Advanced reactor development projects also need cross section information on long-lived fission products that can potentially be a neutron poison. This new cross section information on radioactive isotopes will support the DOE Isotope Program, radiological shielding calculations, and burnup credit for reactor simulations. Homeland security–focused projects can be supported by providing basic experimental capabilities toward the development of nondestructive assay techniques, nuclear nonproliferation, and novel sensing of special nuclear materials.

Performing ND experiments at SNS aims to develop further the synergies at ORNL by enhancing experiments using the HFIR irradiation system and hot cells for short- to long-lived radioactive sample production. This system, in combination with the high flux of SNS obtained from the thermal water moderator, will enable neutron induced cross section experiments on small radioactive samples in microgram to milligram quantities. The high neutron flux will enable examination of small samples, which is beneficial for radiological protection concerns and mitigates the difficulties encountered in harvesting enough material to perform a good measurement. The SNS facility at ORNL is uniquely suited to provide these measurements because the neutron flux is approximately 10–20 times greater than comparable sources at other US facilities assuming current accelerator conditions. After the Proton Power Upgrade project is complete, the flux is expected to be an additional 40% greater.

Providing a high-accuracy cross section measurement station would open new scientific avenues for the user facilities at ORNL. With the high flux of the SNS, experiments that have been very difficult or impossible to perform are now within reach. Several DOE offices have a vital interest in ND for actinides and radioactive isotopes. The need is of a wide variety, ranging from isotope production, homeland security, and nonproliferation to nuclear energy and basic science. The need to support ND for isotope production in nuclear reactors was published in the DOE proposal call DE-FOA-0002440. Many of these reaction and data needs can be satisfied via total cross section and fission cross section experiments.

The DOE Office of Nuclear Energy has emphasized the need for long-lived fission product cross sections for advanced reactors in the epithermal neutron energy range—in particular, neutron capture on ^{85}Kr, $^{89, 90}$Sr, ^{91}Y, ^{95}Nb, $^{88, 93, 95}$Zr, ^{99}Tc, ^{107}Pd, ^{115}Cd, $^{129, 131}$I, ^{125}Sb, $^{134, 135, 136, 137}$Cs, ^{133}Xe, ^{140}Ba, ^{141}Ce, ^{143}Pr, ^{147}Nd, ^{147}Pm, $^{155, 155}$Eu, and ^{151}Sm. In some cases, capture cross sections can also be inferred from resonance parameters obtained via transmission experiments and Hauser–Feshbach statistical model calculations.

Savannah River National Laboratory

Recently, SRNL has broadened its approach to encompass the study of magnetism in actinide materials. This expansion includes the establishment of capabilities for actinide crystal growth and characterization, such as the introduction of single-crystal x-ray diffraction and the Dynacool Physical Property Measurement System at SRNL for the first time. Handling samples beyond uranium and thorium presents challenges because of the highly radioactive and reactive nature of these elements. Only a select few laboratories, including SRNL, possess the necessary capabilities to safely handle and understand the fundamentals of actinide materials.

f-electron behavior: SRNL's collaboration extends to working with neutron staff scientists at HFIR on characterizing actinide oxides that were synthesized at SRNL. The ongoing expansion of actinide neutron studies at both SNS and HFIR holds the potential to provide valuable insights, contributing to the resolution of challenges associated with f-electron behavior in actinide science.

Magnetic ground states: SRNL is always excited to explore the magnetic ground state and local structure of actinide materials, including actinide oxides and halides. If various beamlines at SNS and HFIR can offer actinide measurements in the future, researchers aim to characterize SRNL actinide

materials properties by leveraging the capabilities of SNS and HFIR. For example, the neutron pair distribution function beamline NOMAD can be used to explore local structure and distortion, and neutron spectroscopy provided by ARC can offer insights into the valence-fluctuating ground state and phonon dispersion of actinide materials.

Magnetic structures: Neutron diffraction beamlines such as WAND^2, TOPAZ, and POWGEN can be employed for the examination of magnetic structures in actinide materials. This comprehensive approach using different beamlines allows researchers to gain a better understanding of both local structural characteristics and magnetic properties in bulk actinide materials.

Local structural changes upon self-irradiation: At present, determining the ground state of even simpler actinide binary oxides remains an outstanding challenge because of several factors, including a lack of characterization tools. The self-irradiation in many actinide materials induces changes in the local structure, consequently influencing the magnetic and thermodynamic properties. The availability of SNS and HFIR beamlines to actinide science would play a crucial role in addressing and resolving these issues.

Georgia Institute of Technology

Molecular and extended actinide systems for quantum information science (QIS): The study of actinide-based materials in condensed matter physics is usually associated with strongly correlated electron and heavy fermion physics. However, in recent years, researchers have realized that the magnetism of actinides can serve as a good platform to realize molecular and single-ion qubits. The two fundamental challenges to overcome in qubit design from an as-is chemical system is to (1) increase T2 coherence times and (2) create optically addressable centers. Both lanthanide- and actinide-based systems can offer some advantages on these fronts. For instance, Er^{3+} ions embedded in solid-state matrices of $CaWO_4$ are now a vast topic in applied QIS research, specifically to create quantum repeaters.

Even if actinide systems (both molecular and extended) do not end up as realistic qubit platforms, their study under the QIS framework is important. Researchers anticipate that it will create new fundamental knowledge on the interaction mechanisms between spins and their host lattice because it frames the problem of solid-state magnetism in terms of time-domain relaxation processes and coherence times. To pursue that goal, groups at Georgia Institute of Technology are now funded by the DOE QIS program to combine traditional approaches to solid-state magnetism (i.e., magnetometry, neutron scattering on molecular and extended systems) with more QIS-centric approaches (i.e., pulsed electron paramagnetic resonance, infrared spectroscopy on single-ion and molecular systems) to investigated qubit physics in actinides. The main thrust of this program is to achieve coordination control of spin–phonon coupling in actinide molecular and extended spin qubit candidates. This goal requires the determination of the phonon and magnetic spectra with neutron, magneto-infrared, and magneto-Raman spectroscopies. The spectroscopy instruments at SNS and HFIR, including VISION, CNCS, SEQUOIA, ARCS, and HB-3 for inelastic neutron scattering, will be essential for exploring these topics in actinide materials. The first experiment, which will take place in 2024, is the study of Np^{6+} ions diluted in a solid-state crystalline structure of $Cs_2UO_2Cl_4$.

APPENDIX B. INTERESTED USERS AND WORKSHOP ATTENDEES

First Name	Last Name	Affiliation	Attended Workshop
Alice	Smith	Los Alamos National Laboratory	Yes
Eric	Bauer	Los Alamos National Laboratory	Yes
David	Clark	Los Alamos National Laboratory	Yes
Martin	Mourigal	Georgia Institute of Technology	Yes
Henry	La Pierre	Georgia Institute of Technology	Yes
Binod	Rai	Savannah River National Laboratory	Yes
Jennifer	Wacker	Lawrence Berkeley National Laboratory	Yes
Scott	Daly	University of Iowa	Yes
Appie	Peterson	Lawrence Berkeley National Laboratory	Yes
Daniel	Olive	Los Alamos National Laboratory	Yes
Tarik	Saleh	Los Alamos National Laboratory	Yes
David	Moore	Los Alamos National Laboratory	Yes
Franz	Freibert	Los Alamos National Laboratory	Yes
Gary	Lynn	Oak Ridge National Laboratory	Yes
Chris	Chapman	Oak Ridge National Laboratory	Yes
Luke	Daemen	Oak Ridge National Laboratory	Yes
Sam	Schrell	Oak Ridge National Laboratory	Yes
Andrew	Miskowiec	Oak Ridge National Laboratory	Yes
Connor	Parker	Oak Ridge National Laboratory	Yes
Duncan	Moseley	Oak Ridge National Laboratory	Yes
Jisue	Braatz	Oak Ridge National Laboratory	Yes
Luke	Sadergaski	Oak Ridge National Laboratory	Yes
Cristian	Celis-Barros	Oak Ridge National Laboratory	Yes
Frankie	White	Oak Ridge National Laboratory	Yes
Tyler	Spano	Oak Ridge National Laboratory	Yes
Zach	Brubaker	Oak Ridge National Laboratory	Yes
Daniel	Felton	Oak Ridge National Laboratory	Yes
Matthias	Frontzek	Oak Ridge National Laboratory	Yes
Michael	Herr	Oak Ridge National Laboratory	Yes
Stuart	Calder	Oak Ridge National Laboratory	Yes
Matt	Stone	Oak Ridge National Laboratory	Yes
Matthias	Frontzek	Oak Ridge National Laboratory	Yes
Melanie	Kirkham	Oak Ridge National Laboratory	Yes
Michelle	Everett	Oak Ridge National Laboratory	Yes
Adam	Aczel	Oak Ridge National Laboratory	Yes
Natalie	Hogan	Oak Ridge National Laboratory	Yes
Tatum	Price	Oak Ridge National Laboratory	Yes
Raine	Palmer	Oak Ridge National Laboratory	Yes
Richard	Mayes	Oak Ridge National Laboratory	Yes
Luiz	Leal	Oak Ridge National Laboratory	Yes
Dante	Quirinale	Oak Ridge National Laboratory	Yes

First Name	Last Name	Affiliation	Attended Workshop
Todd	Sherline	Oak Ridge National Laboratory	Yes
Brodie	Barth	Oak Ridge National Laboratory	Yes
Jeffrey	Einkauf	Oak Ridge National Laboratory	Yes
Eugene	Mamontov	Oak Ridge National Laboratory	Yes
Sam	Sasser	Oak Ridge National Laboratory	Yes
Bill	Matisiak	Oak Ridge National Laboratory	Yes
Iyad	Al-Qasir	Oak Ridge National Laboratory	No
Jennifer	Niedziela	Oak Ridge National Laboratory	No
Goran	Arbanas	Oak Ridge National Laboratory	No
Kathryn	Peruski	Oak Ridge National Laboratory	No
Martin	Leigh	Oak Ridge National Laboratory	No
Kemal	Ramic	Oak Ridge National Laboratory	No
Klaus	Guber	Oak Ridge National Laboratory	No
Jesse	Brown	Oak Ridge National Laboratory	No
Samuel	Greer	Los Alamos National Laboratory	No
Sandra	Davern	Oak Ridge National Laboratory	No
Van Veelen	Arjen	Los Alamos National Laboratory	No
Stosh	Kozimor	Los Alamos National Laboratory	No
Matthew	Jackson	Los Alamos National Laboratory	No
Matthew	Carpenter	Los Alamos National Laboratory	No
Mark	Corce	Los Alamos National Laboratory	No
Rebecca	Abergel	Lawrence Berkeley National Laboratory	No
Daniel	McNeel	Los Alamos National Laboratory	No
David	Shuh	Lawrence Berkeley National Laboratory	No
Hunter	Henderson	Lawrence Livermore National Laboratory	No
David	Dan	Tennessee Tech University	No
Gauthier	Deblonde	Lawrence Livermore National Laboratory	No
Ryan	Baumbach	University of California Stata Cruz	No
Alyssa	Gaiser	Michigan State University	No
Alexander	Baker	Lawrence Livermore National Laboratory	No

APPENDIX C. WORKSHOP AGENDA

OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE LLC FOR THE US DEPARTMENT OF ENERGY

Actinides and Neutron Scattering at SNS/HFIR

June 12, 2024		**Building 8600 Room C-156**
Time	**Event**	**Lead**
7:00–8:00am	Badging (for non-ORNL attendees) SNS Lobby	Natalie Hogan and Tatum Price
8:10-8:25pm	Welcome and Purpose	S. Schrell (ORNL)
8:25–8:50am	HFIR/SNS overview	G. Lynn (ORNL)
8:50–9:10am	Application of Neutron Scattering to Pu-Ga Alloys	A. Smith (LANL)
9:10–9:20am	Break	All
9:20–9:35am	Science Somewhere Else: Plutonium EXAFS Experiments at User Facilities	D. Olive (LANL)
9:35-9:50am	From X-rays to Neutrons: Expanding Characterization Tools for Actinide Chemistry	J. Wacker (LBL)
9:50-10:15am	Actinides at HFIR	M. Frontzek (ORNL)
10:15-10:25am	Break	All
10:25–10:50am	Determination of the Valence Fluctuating Ground State of δ-Pu by Means of Inelastic Neutron Spectroscopy at SNS	E. Bauer (LANL)
10:50–11:15am	Neutron Scattering for Nuclear Nonproliferation Science	A. Miskowiec (ORNL)
11:15-11:40am	Actinide experiments at SSRL	D. Clark (LANL)

OAK RIDGE National Laboratory

AGENDA

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June 12, 2024		**Building 8600 Room C-156**
Time	**Event**	**Lead**
11:40–12:30am	Lunch	All
12:30-2:30pm	Breakout Session 1: Scientific Impact and Sample Environments (Group 1: C-156; Group 2: C-482; Group 3: J-337)	All
2:30-2:50pm	Summary of Breakout Session 1	All
2:50-3:00pm	Break	All
3:00-3:15pm	Travel to HFIR	All
3:15-4:30pm	HFIR Tour	Tour Guides: Stuart Calder, Matthias Frontzek, Adam Aczel
4:30-4:45pm	Travel to SNS	All
4:45pm	Adjourn	All

Day 2

June 13, 2024		**Building 8600 Room C-156**
Time	**Event**	**Lead**
8:00–8:05am	Welcome	S. Schrell
8:05-10:00am	Breakout Session 2: Shipping, Storage, Safety, Radiation protection, Handling, and other practical considerations (Group 1: C-156; Group 2: C-482; Group 3: J-337)	All
10:00–10:20am	Summary of Breakout Session 2	All
10:20-10:40am	Break	All

OAK RIDGE National Laboratory

AGENDA

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June 13, 2024		**Building 8600 Room C-156**
Time	**Event**	**Lead**
10:45am-12:00pm	Tour of SNS	Tour Guides: Michelle Everett, Matt Stone, Melanie Kirkham
12:00pm	Adjourn	All