2020 LLNL Nuclear Science and Security Summer Internship Program

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Auspices
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2020 LLNL Nuclear Science and Security Summer Internship Program

The Lawrence Livermore National Laboratory (LLNL) Nuclear Science and Security Summer Internship Program (NS³IP) is designed to give graduate students an opportunity to come to LLNL for 8–10 weeks of hands-on research. Students conduct research under the supervision of a staff scientist, attend a weekly lecture series, interact with other students, and present their work in poster format at the end of the program. Students also have the opportunity to meet staff scientists one-on-one, participate in LLNL facility tours (e.g., the National Ignition Facility and Center for Accelerator Mass Spectrometry), and gain a better understanding of the various science programs at LLNL. Due to the travel and access restrictions imposed by the COVID-19 pandemic, the 2020 NS³IP was organized as an “all-virtual” internship program. With LLNL’s extensive institutional support, students accessed the laboratory’s cyberinfrastructure through a secure virtual desktop environment and all seminars, mentor interactions, summer presentations, and laboratory tours were performed remotely. While this virtual internship format did not allow for hands-on laboratory research projects, both the interns and their mentors constructed creative research projects that maximized student exposure to nuclear science research that is relevant to DTRA and LLNL interests in nuclear security.

Currently titled the Nuclear Science and Security Summer Internship Program, this program began over 20 years ago as the Actinide Sciences Summer Program. The program is run by the Glenn T. Seaborg Institute in the Physical and Life Sciences Directorate at LLNL. The goal of the NS³IP is to facilitate the training of next generation nuclear scientists and engineers to solve critical national security problems in the field of nuclear science and nuclear security. Students are selected from the fields of physics, chemistry, geology, mathematics, nuclear engineering, chemical engineering and environmental sciences. Students engage in research projects in the disciplines of actinide chemistry, radiochemistry, isotopic analysis, computation, radiation detection, and nuclear engineering. This Internship Program is supported by the Defense Threat Reduction Agency (DTRA) which enables the Department of Defense and the U.S. Government to prepare for and combat weapons of mass destruction and improvised threats and to ensure nuclear deterrence. The internship program is intended to strengthen the “pipeline” for future scientific disciplines critical to DTRA and DOE.

The NS³IP is highly competitive, with over 150 applications received in 2020 for the 7-8 available slots. Additional students funded through paid internships and fellowships from NNSA and DOE are invited to participate in the summer lecture series. All students participate in the LLNL summer event that showcases summer internship projects. In past years, the showcase took the form of a poster session. This year, the showcase took the form of an online Student SLAM! event that emulated the short presentation format pioneered by the TED talk series. The NS³IP hosted students from 5 universities (see Table 1) across the United States (Figure 1). The NS³IP students conducted research on such diverse topics as field portable resonance ionization mass spectrometry, nuclear battery development, pre- and post-detonation mass spectrometry, and nuclear signatures development (see Table 2 for research topics). Continued research collaboration between the graduate student, faculty advisor, and LLNL mentors is strongly encouraged. In many cases, NS³IP research evolves into a significant component of the students’ graduate theses. For example, two graduates of the 2019 NS³IP (Michael Klosterman and Meena Said) returned in 2020 and are continuing their
collaboration with LLNL staff and incorporating their summer projects into their PhD research. Meena Said recently applied for a post-doctoral fellowship at LLNL to continue her career in nuclear science.

In addition to hands-on training, students attend a weekly lecture series on topics applicable to the field of nuclear science (Table 3). Speakers are selected to represent the breadth of expertise that is required for nuclear science research. Speakers discuss the importance of their work in the context of national and international nuclear security efforts.

Graduate and undergraduate students on fellowships such as the Nuclear Safeguards internship program and Nuclear Science and Security Consortium, are invited to join our summer internship activities. This year, the Seaborg institute hosted 5 students from Washington State University, Georgia Tech, UC Berkeley, Ohio State University and Oregon State University through nuclear science fellowships and programmatic funding. Our summer program is providing a nuclear science pipeline of top-quality students from universities across the United States. Since 2002, 25% have returned to conduct their graduate research at LLNL. In total:

- 41 interns continued their graduate work at LLNL
- 26 became postdoctoral fellows at LLNL
- 16 became postdoctoral fellows at other national labs
- 16 were hired as career scientists at LLNL
- 19 were hired as career scientists at other national labs
- 21 were hired at other government institutions
- 22 were hired at universities
- 45 transitioned to the private sector

A big factor in the success of this program is the dedication of the staff scientists (predominantly DTRA funded) who volunteer to mentor the summer students. Four of our 2020 mentors are, in fact, alumni of the Seaborg Institute summer internship programs. The mentors develop summer projects for their students, oversee necessary safety training, and dedicate time to helping the interns and students maximize their productivity and scientific potential. This internship program would not be possible without the mentors’ dedication. The PowerPoint presentations summarizing the 2020 NS3IP student research projects were presented at the virtual summer student SLAM! event and are included at the end of this report. The recorded video presentations will be available on the Seaborg Institute website (www.seabort.llnl.gov).
Figure 1. The Seaborg Institute summer interns come from universities from across the United States. Universities associated with the 2020 Nuclear Science and Security Summer Internship program are highlighted with a red outline.
Table 1. 2020 Nuclear Science and Security Summer Internship Program Students

<table>
<thead>
<tr>
<th>Student</th>
<th>Major</th>
<th>University</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mike Klosterman</td>
<td>Environmental Engineering</td>
<td>University of Utah</td>
<td>Graduate</td>
</tr>
<tr>
<td>James Totten¹</td>
<td>Nuclear Engineering</td>
<td>University of Florida</td>
<td>Graduate</td>
</tr>
<tr>
<td>Dan Sullivan¹</td>
<td>Geology/Geochemistry</td>
<td>Arizona State University</td>
<td>Graduate</td>
</tr>
<tr>
<td>Sarah Azhar¹</td>
<td>Mechanical Engineering</td>
<td>Georgia Tech</td>
<td>Undergraduate</td>
</tr>
<tr>
<td>Meena Said</td>
<td>Earth Sciences</td>
<td>University of Notre Dame</td>
<td>Graduate</td>
</tr>
<tr>
<td>Neil Taylor</td>
<td>Nuclear Engineering</td>
<td>Ohio State University</td>
<td>Graduate</td>
</tr>
<tr>
<td>Christopher Brais</td>
<td>Analytical Chemistry</td>
<td>State University of New York, Buffalo</td>
<td>Graduate</td>
</tr>
<tr>
<td>Frederick Delawie²</td>
<td>Aerospace Engineering</td>
<td>University of Maryland</td>
<td>Undergraduate</td>
</tr>
<tr>
<td>Nicholas Parham³</td>
<td>Operations Research</td>
<td>USAFA, CO CS-31 Grim Reapers</td>
<td>Undergraduate</td>
</tr>
</tbody>
</table>

¹ Could not participate due to virtual format; will be considered for 2021.
² Funded at 50% by DTRA.
³ Supported through a collaboration with the MARA program.
<table>
<thead>
<tr>
<th>Student</th>
<th>Mentor</th>
<th>Project Poster Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mike Klosterman</td>
<td>Mike Singleton</td>
<td>Oxygen Isotope Signatures in Uranium Oxides</td>
</tr>
<tr>
<td>James Totten(^1)</td>
<td>Chad Durrant</td>
<td>Using Laser Driven Hydrothermal Processing (LDHP) to Accelerate Dissolution of Geological Samples</td>
</tr>
<tr>
<td>Dan Sullivan(^1)</td>
<td>Greg Brennecka</td>
<td>Re and Hg Osotopics in Yellowcake</td>
</tr>
<tr>
<td>Sarah Azhar(^1)</td>
<td>Tashi Parsons-Davis and Keenan Thomas</td>
<td>Gamma Coincidence Data Processing</td>
</tr>
<tr>
<td>Meena Said</td>
<td>Naomi Marks</td>
<td>Uranium Fuel Pellet Signature Characterization</td>
</tr>
<tr>
<td>Neil Taylor</td>
<td>Joshua Jarrell</td>
<td>Nuclear Battery Development</td>
</tr>
<tr>
<td>Christopher Brais</td>
<td>Mike Savina</td>
<td>Automated Laser Operation, Beam Steering, and Power Control for Mobile RIMS Instrument</td>
</tr>
<tr>
<td>Frederick Delawie(^2)</td>
<td>Joshua Jarrell</td>
<td>Atomic Battery Case Design</td>
</tr>
<tr>
<td>Nicholas Parham(^3)</td>
<td>Mavrik Zavarin</td>
<td>Surface Complexation Database Converter Tool</td>
</tr>
</tbody>
</table>

\(^1\) Could not participate due to virtual format; will be considered for 2021.
\(^2\) Funded at 50% by DTRA.
\(^3\) Supported through a collaboration with the MARA program.
Table 3. 2020 Nuclear Science and Security Summer Internship Program Seminar Schedule

<table>
<thead>
<tr>
<th>Date</th>
<th>Speaker</th>
<th>Topic</th>
</tr>
</thead>
</table>
| 6/17/20 | Naomi Marks
  
  \textit{Staff Scientist, Chemical & Isotopic Signatures Nuclear and Chemical Sciences Division} | The Fascinating Field of Nuclear Forensics: How A Scientific Subdiscipline Captured My Heart |
| 6/25/20 | John Murphy
  
  \textit{Staff Scientist Materials Engineering Division} | Radioisotope Batteries – An Overview on Historical Developments and Current Work at LLNL |
| 7/2/20  | Dawn Shaughnessy
  
  \textit{Group Leader, Stockpile Radiochemistry Nuclear and Chemical Sciences Division} | Nuclear Science at the National Ignition Facility |
| 7/9/20  | Mike Savina
  
  \textit{Staff Scientist, Chemical & Isotopic Signatures Nuclear and Chemical Sciences Division} | Nuclear Astrophysics for Fun & Profit: Moonlighting in the Nonproliferation Gig Economy |
| 7/16/20 | Gauthier Deblonde
  
  \textit{Staff Scientist, Chemical & Isotopic Signatures Nuclear and Chemical Sciences Division} | Actinide Science: From Nuclear Reactors to Cancer Therapy Drugs |
| 7/23/20 | Mike Singleton
  
  \textit{Staff Scientist, Chemical & Isotopic Signatures Nuclear and Chemical Sciences Division} | Forensic Applications of Light Stable Isotopes |
| 7/30/20 | Jutta Escher
  
  \textit{Staff Scientist, Nuclear Data & Theory Nuclear and Chemical Sciences Division} | Nuclear Reaction Research for Astrophysics and Lab Applications |
2020 NS$^3$IP PowerPoint Presentations from Student SLAM! Event
Oxygen Isotopes as a Forensic Tool for Nuclear Materials

Michael R. Klosterman
PLS/NACS
A.L. Dienhart, E.J. Oerter, L.W. McDonald, M.J. Singleton
Oxygen isotopes in water and atmospheric O$_2$ are predictable worldwide.

We predict the oxygen isotope patterns from process water will be inherited in uranium compounds, providing a new forensic signature.
An experimental model of the fuel cycle to investigate the incorporation of oxygen isotopes

1) Simulate nuclear fuel fabrication

\[ \text{UO}_2^{2+} \text{ (aq.)} \rightarrow \text{UO}_4 \text{ or ADU} \rightarrow \text{UO}_3 \text{ or } \text{U}_3\text{O}_8 \rightarrow \text{UO}_2 \]

Precipitation \hspace{2cm} \textbf{Calcination} \hspace{2cm} \textbf{Reduction}

2) Remove the oxygen from synthetic products for analysis (the hard part)

\[ \text{UO}_2 + 2\text{ClF}_3 \quad 550^\circ\text{C} \quad 4 \text{ hours} \]

\[ \text{UF}_6 + \text{Cl}_2 + \text{O}_2 \quad \text{Purify} \quad \text{Send to MS} \]

Fluorination lab at LLNL (ClF_3) \hspace{2cm} Fluorination system at U of Utah (BrF_5)
Uranium oxides inherit oxygen isotope patterns from calcination atmosphere

Precipitated from H$_2$O with $\delta^{18}$O = -16%

$\text{UO}_4$ ($\delta^{18}$O = +5.3%)

$\text{UO}_3$

$\text{U}_3\text{O}_8$

400°C > 600°C

Calcination with and without humidity

Atmospheric O$_2$ ($\delta^{18}$O = +23.5%)

Dry Air (700°C)

50% RH in Nitrogen (400°C)

50% RH in Nitrogen (600°C)

Water Vapor ($\delta^{18}$O = -20.9%)

Oxygen isotope Composition ($\delta^{18}$O)

0 5 10 15 20 25 30

Calcination Time (hours)

Atmospheric composition, calcination temperature, and calcination time have significant effects on the ultimate signature.
Image Analysis and the Development of Nuclear Forensic Signatures

Meena Said
PLS Directorate, NACS Division
Mentor: Naomi Marks
“A picture is worth a thousand words.”
Scanning Electron Microscopy for Nuclear Forensics Research

- Qualitative image analysis
- Qualitative (Lexicon) → Quantitative (Machine Learning)
  - Discerning characteristics within sample
  - Connections among samples
Innovations in Isotope Production & Shielding for Radio-voltaic Batteries

Neil Taylor
Physical & Life Sciences
Frederick Delawie, Dr. John Murphy, and Dr Joshua Jarrell
LLNL-PRES-813252
Radiovoltaic Batteries

- Direct Conversion
  - Simpler
  - Radiation can damage diode

- Indirect Conversion
  - Requires appropriate conversion material
  - Protects diode

Indirect conversion can enable the use of higher power density radioisotopes.
Isotope Production in Nuclear Reactor

- Irradiate material in nuclear reactor for production of battery isotope

![Image of nuclear reactor](https://reactor.osu.edu/info-experiments/reactor-based-experiments)

**Isotope Production in HFIR**

- Weight Percent
- Time (Years)

Unable to achieve desired isotope enrichment production with HFIR
Radiation Shielding Designs

- High Z Shield
- Battery

<table>
<thead>
<tr>
<th>Design</th>
<th>Dose (kRad)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Goal</td>
<td>20</td>
</tr>
<tr>
<td>Design 1</td>
<td>171.7</td>
</tr>
<tr>
<td>Design 2</td>
<td>22.8</td>
</tr>
</tbody>
</table>

- Design 1: Ceramic Scintillator TI-204 (β)
- Design 2: Xe Gas Pu-238 (α)

Alpha-based radiisotope reduces damaging radioactive dose to surroundings
Constant Momentum Acceleration Resonance Ionization Mass Spectrometry

Christopher J. Brais
PLS-NACS-GTSI
Dr. Michael Savina and Prof. Steven J. Ray
Resonance ionization mass spectrometry (RIMS)

- Tunable laser spectroscopy with mass spectrometry

- Why RIMS?
  - ☑ Minimal sample preparation
  - ☑ Highly selective
  - ☑ Highly sensitive
  - ❏ Secondary ions (background noise)
  - ❏ Simultaneous measurements of isobaric species

- Practical example: measure $^{241}\text{Pu}$ & $^{241}\text{Am}$ at the same time
  - Complex laser timing requires:
    - Remote control
    - Ionizing laser
  - $\text{Pu}^+$ and $\text{Am}^+$ are barely resolved

Here, constant momentum acceleration (CMA) shows promise!
Constant Momentum Acceleration (CMA)

- CMA is an alternative method that imparts a different energy to each ion of interest: *small differences in ion birth times result in large differences in energy – easy separation!*
- Simplifies laser timing sequences
- Secondary ions are removed automatically, ‘on-the-fly’
- Requires no new hardware
Workflow for CMA-RIMS development

- Evaluate CMA-RIMS performance using a virtual instrument
  - Generate realistic, ‘virtual’ ion packets
  - Ray tracing software to calculate flight trajectories (SIMION®)
  - Store simulation results in database
  - Query to extract information
    - Mass resolving power
    - Transmission efficiency

- Use results of simulations to develop new and improved RIMS analyses on the existing LION instrument
Atomic Battery Case Design

Frederick Delawie
Engineering/MEPT

Neil Taylor, Dr. Josh Jarrell, Dr. John Murphy
LLNL’s Design

The Lawrence-Livermore Plutonium-Xenon Battery

New design, high efficiency, mW scale
Case Design

- Radiation tolerance
- High pressure
- High purity
- Size limitations
- Longevity

Specialized manufacturing techniques & components can help enable this technology
ML for Surface Complexation Model Development

Jadallah Zouabe
PLS/Seaborg Institute
Nicholas Parham, Haruko Wainwright, Mavrik Zavarin
Motivation/Background

If contamination hurts us and our environment...what do we do about it?

But how??

- Learn about the contamination
- Assess risk and extent of problem
- Design, plan and execute strategy
- Mitigate future risks

Collect experimental data, build model

simulate model, analyze data, fix model

risk assessment, make decision + mitigation
Approach

Modeling is our best friend in understanding what to do, but requires copious amounts of time, is computationally expensive, and requires a lot of money!

**Objective:**
- Reduce modeling complexity and simulation run times.

**Desired End Result:**
- Save time assessing contamination risks, save money and enable our leaders to make decisions faster.
Results/Conclusion

- Single Case: Uranium and Quartz

Value Gained:
- Incredible model predictive ability with environmental data
- Insight into features contributing to uranium quartz surface complexation behavior

What’s Next:
- Sensitivity Analysis
- Start building models for other mineral/contaminant combinations
ACKNOWLEDGEMENTS

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