Molten Salt Reactor PROGRAM

Los Alamos NATIONAL LABORATORY

LANL Experimental Support to MSTDB Development

Marisa Monreal & Hannah Patenaude

Inorganic, Isotope, and Actinide Chemistry – Chemistry Division

Los Alamos National Laboratory

Molten Salt Reactor Campaign Annual Review, April 22-24, 2026

LA-UR-26-23013

Argonne NATIONAL LABORATORY · INL Idaho National Laboratory · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY · OAK RIDGE National Laboratory · Pacific Northwest NATIONAL LABORATORY · Sandia National Laboratories · U.S. DEPARTMENT of ENERGY Office of Nuclear Energy

LANL Actinide-Molten Salt Chemistry & Properties Research

Salt systems:

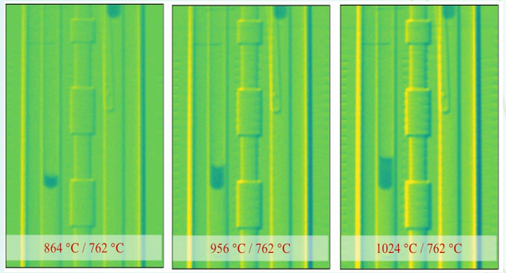
- Actinides: thorium, uranium, plutonium
- Chlorides & fluorides, including FLiBe

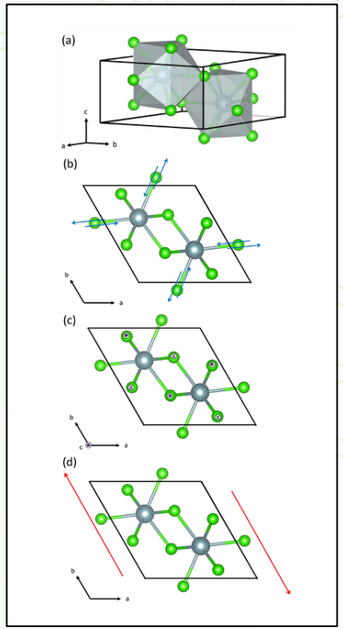
Research:

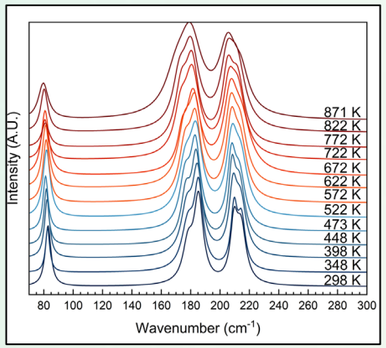
- Chemistry & thermophysical properties
- Both experiment and modeling
- Studies across length scales – local structure, macroscale properties

Benefitting communities:

- Pyroprocessing/recovery & purification of actinide materials, nuclear energy, fundamental actinide science, global security/non- and counter-proliferation







Los Alamos NATIONAL LABORATORY

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

LANL Actinide-Molten Salt Chemistry and Properties Research

Researchers:
- Graduate students, post-docs, scientists, engineers
- Chemistry, materials science, earth and environmental science, theoretical/mod-sim

Collaborations:
- National Laboratories, universities, industry, NEAMS, SciDAC

Sponsors/Projects:
- MSR Campaign, AFC, LDRD, Technology Commercialization Fund (TCF), Industrial partners, IRP, NEUP, NA-22

Scientists & Engineers
Scott Parker
Karla Erickson
Harris Mason
Sven Vogel
Kristen Pace
Alex Long
David Andersson
Matt Jackson
Ping Yang
Gaoxue Wang
Travis Carver

Research Technologists
Clare Hatfield
Marvin Davis

Post-docs & Students
Hannah Patenaude (PD)
Bryn Merrill (S)
Sam Lee (PD)
Lexi Carney (PD)
Dylan Tharp Eralie (PD)

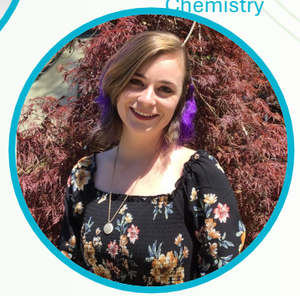
LANL MSR Campaign WPM:

Marisa Monreal
Chemistry

Primary Experimental Support:

Hannah Patenaude
Chemistry

Scott Parker
Sigma



Bryn Merrill
Earth & Environmental Sciences

Sven Vogel

Kristen Pace

Alex Long

David Andersson

Materials Science & Technology

Matt Jackson

Karla Erickson

Harris Mason

Clare Hatfield

Marvin Davis

Sam Lee

Dylan Tharp Eralie

Lexi Carney

Chemistry

Los Alamos NATIONAL LABORATORY

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

LANL Actinide-Molten Salt Chemistry and Properties Research

Properties	Experimental Techniques
Density	Neutron Radiography, Conventional (Push-rod) Dilatometry
Viscosity	Dynamic Neutron Radiography, Rotational Viscometry
Melting Point/Phase Diagram, Heat Capacity	Differential Scanning Calorimetry (DSC)
Corrosion	Electrochemistry
Heat of Dissolution, Enthalpy of Mixing, Heat Capacity	Drop Calorimetry
Local Structure	Pair Distribution Function (PDF) Analysis, Raman Spectroscopy, Electrochemistry
Synthesis & Characterization	Inorganic halide synthesis, SEM, Melting Point (DSC), pXRD, SS-NMR Spectroscopy

Experimental efforts & strategy:

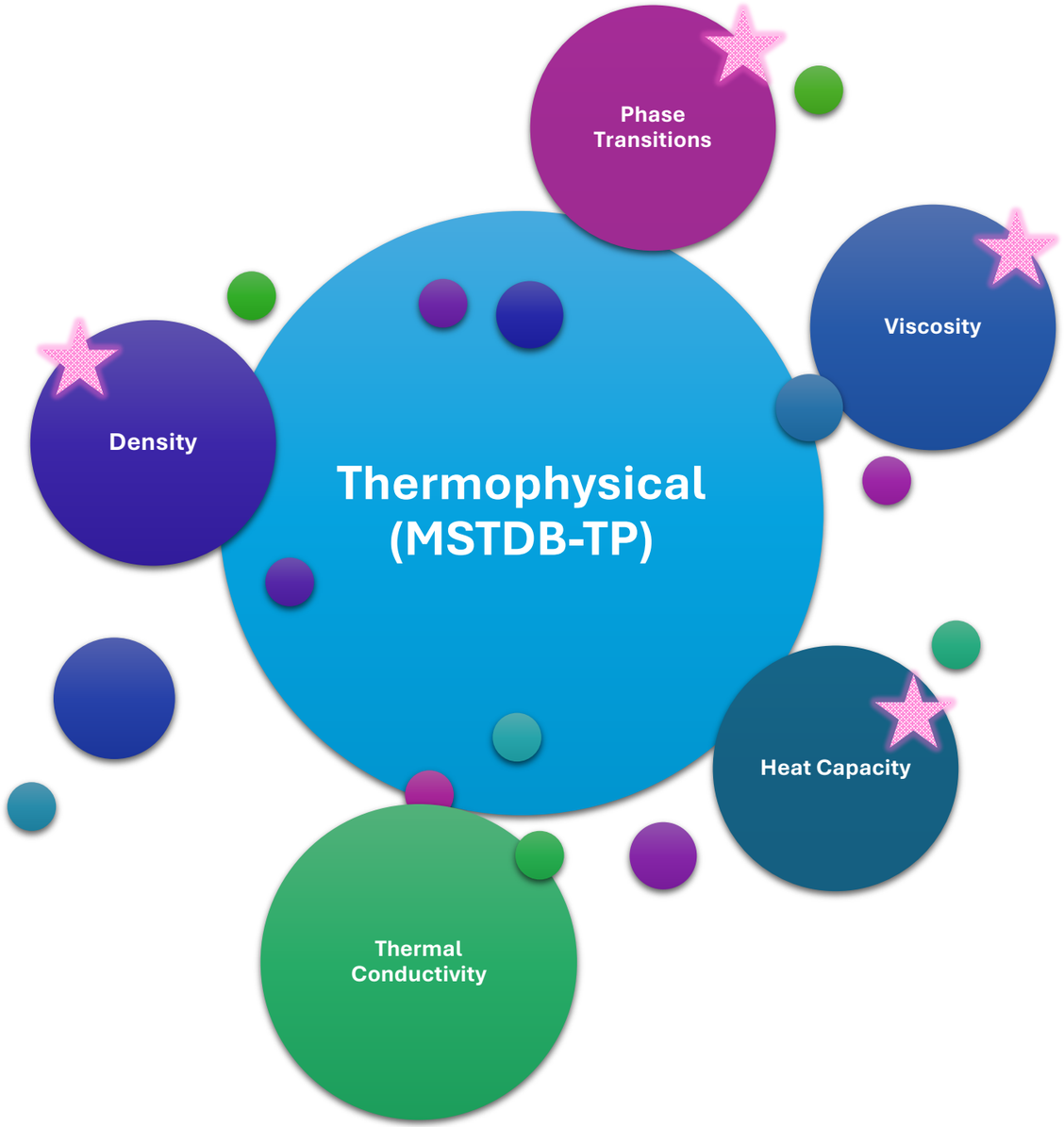
- Method development, uncertainty reduction
- Lower and higher throughput methods
- Non-rad → dU , Th → Pu
- Iterate with mod-sim

Los Alamos NATIONAL LABORATORY

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

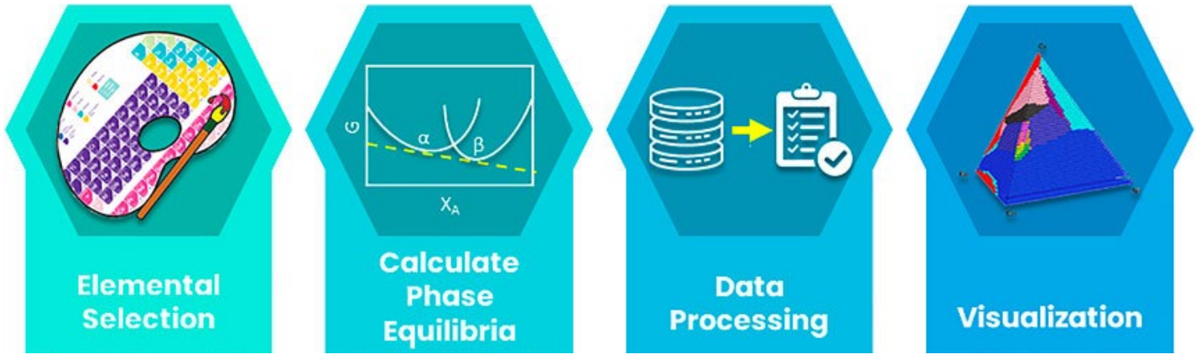
Molten Salt Thermal Properties Database (MSTDB)



Thermochemical (MSTDB-TC)

CALPHAD: CALculation of **PHA**se **D**iagrams

("Computer Coupling of Phase Diagrams & Thermochemistry")



Besmann & Schorne-Pinto, *thermo*, *1*(2), **2021**
Ard et al., *J. Nuc. Mat.*, *563*, **2022**
Ghassemali & Conway, *Front. Mater.*, *9*, **2022**
Termini et al., ORNL/TM-2023/2955, **2023**

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Outline

Thermal Properties

- DSC of UF_4-FLiNaK
- Viscosity

Newly-Commissioned Molten Salt Laboratories

- PluS Lab
- FLAME

Complementary Research Efforts

Los Alamos NATIONAL LABORATORY

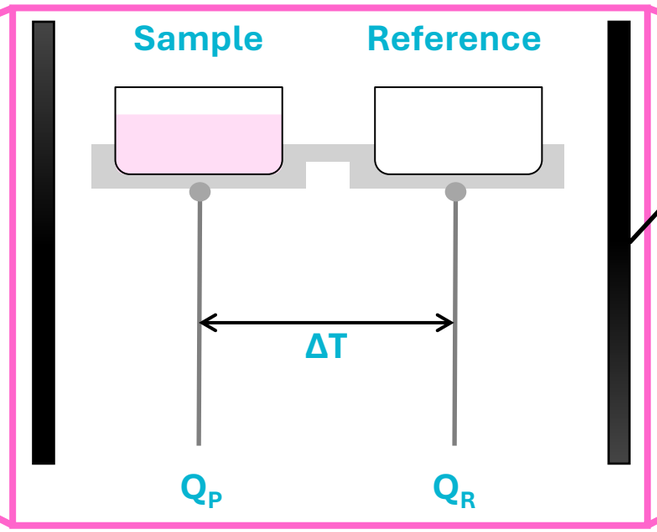
Thermal Properties:
DSC of UF_4-FLiNaK

Molten Salt Reactor PROGRAM

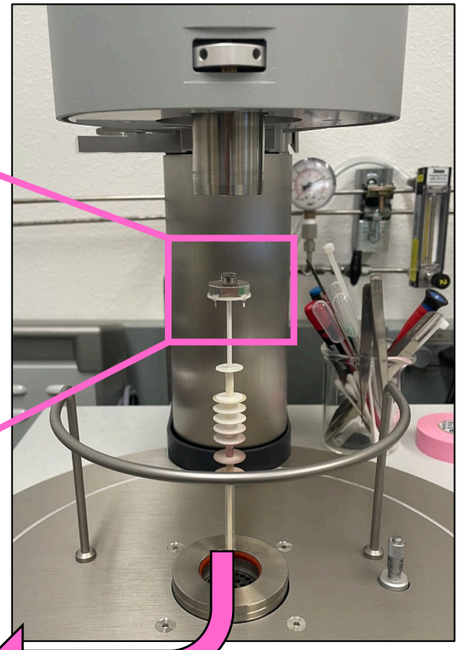
U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Differential Scanning Calorimetry (DSC)

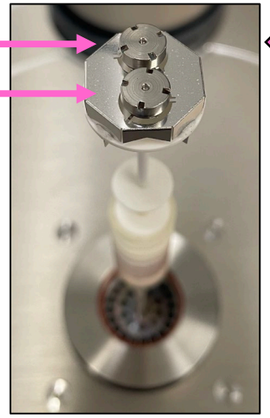
www.netzsch.com



Furnace



Reference
Sample

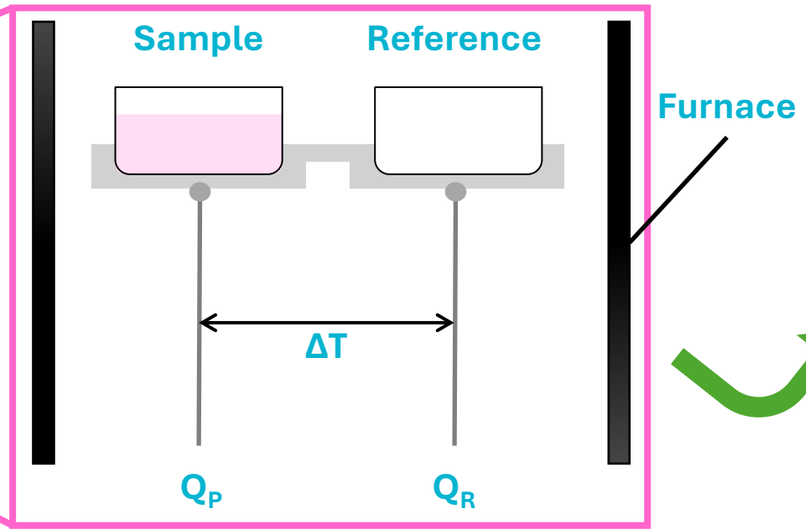


Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

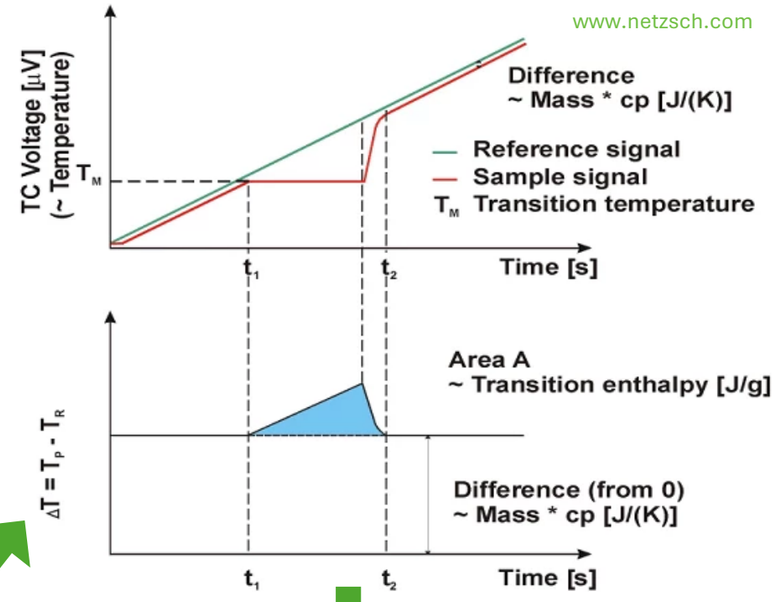
Differential Scanning Calorimetry (DSC)

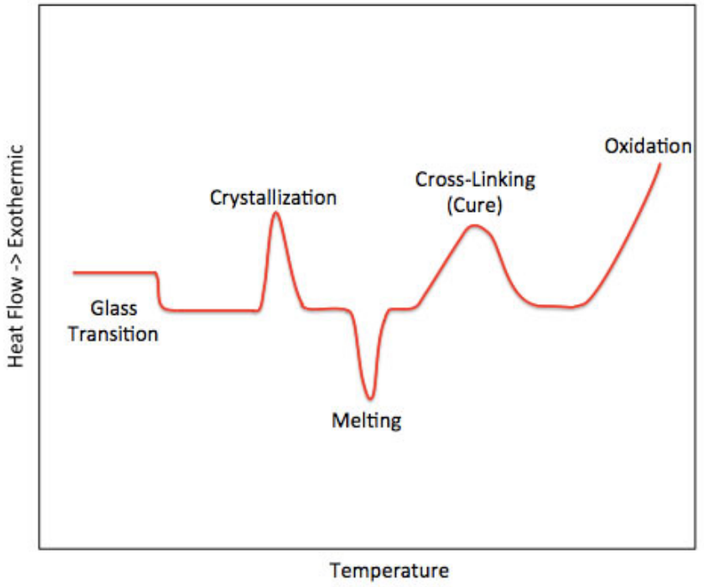
www.netzsch.com



- Phase Transitions
- Enthalpy of Fusion (ΔH_{fus})
- Heat Capacity (C_p)
- Purity & Composition Confirmation

www.netzsch.com

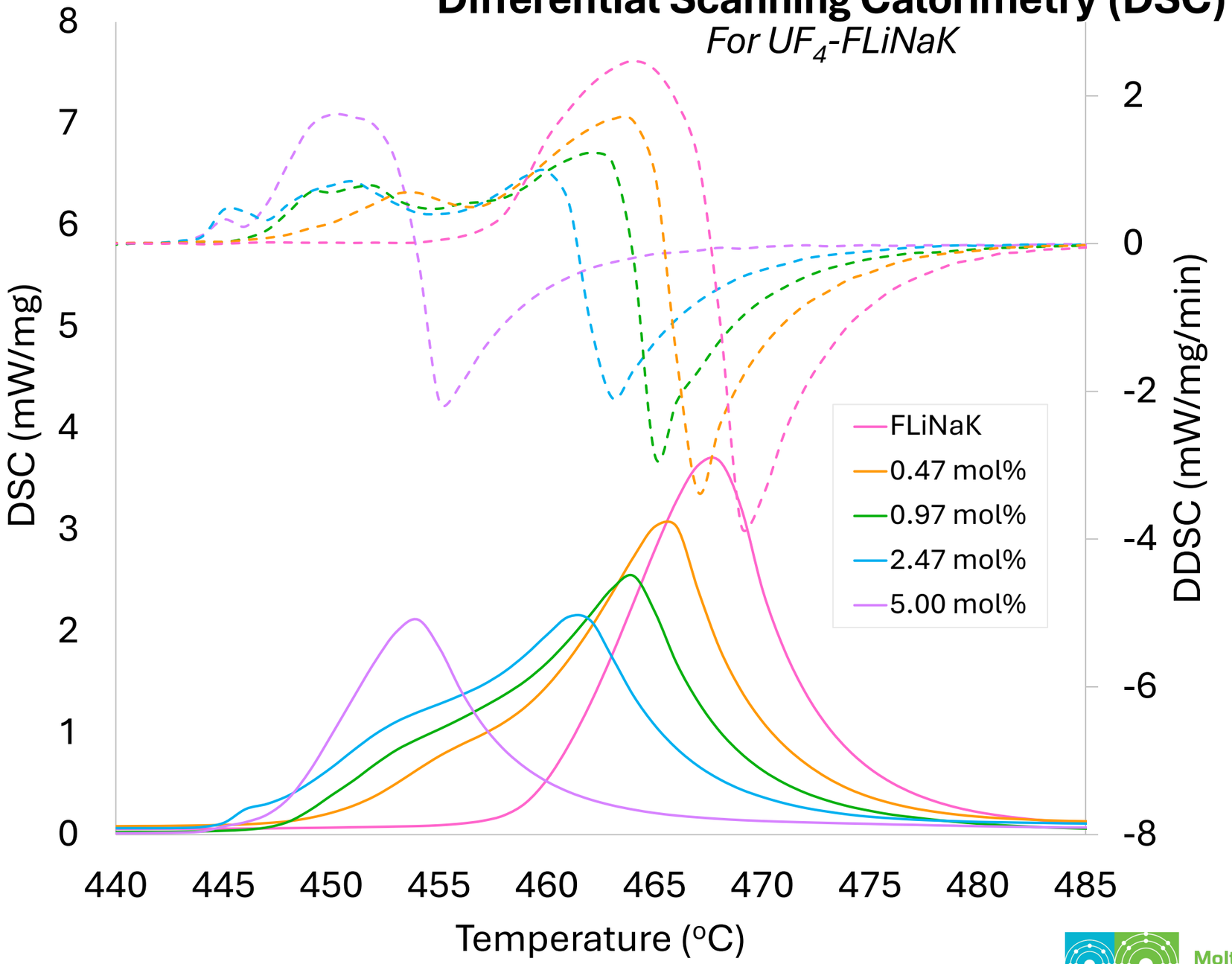




www.creative-proteomics.com

Differential Scanning Calorimetry (DSC)

For UF_4-FLiNaK



UF_4 from novel synthesis pathways

UF_4 (mol%)	Melting Point (onset, °C)	ΔH_{fus} (J/g)
0.00	459.8	398.1
0.51	456.7	381.1
0.97	453.9	363.7
2.47	450.4	315.4
5.00	447.4	201.2

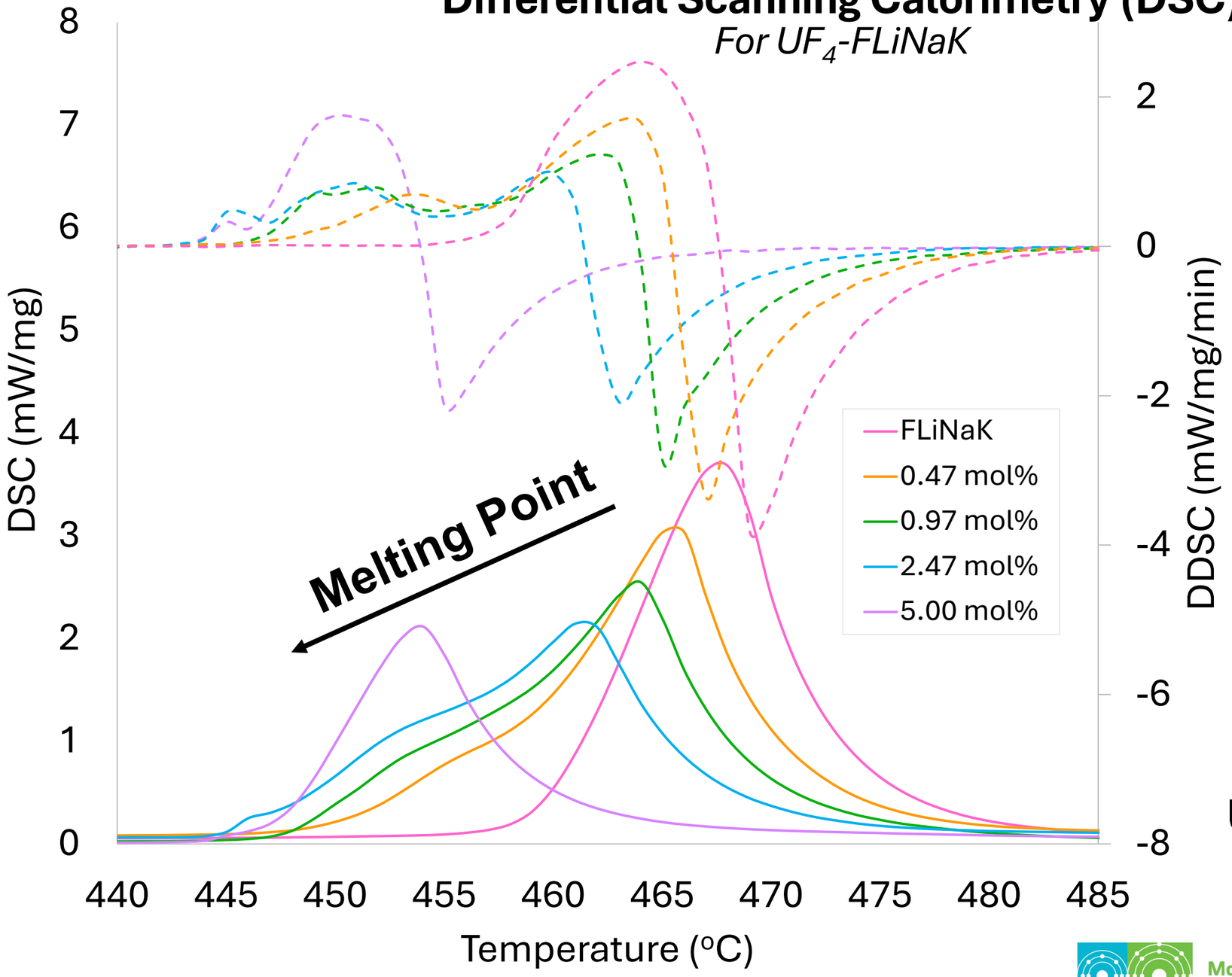
Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Patenaude et al., *in preparation*.

Differential Scanning Calorimetry (DSC)

For UF_4-FLiNaK



UF_4 from novel synthesis pathways

UF_4 (mol%)	Melting Point (onset, °C)	ΔH_{fus} (J/g)
0.00	459.8	398.1
0.51	456.7	381.1
0.97	453.9	363.7
2.47	450.4	315.4
5.00	447.4	201.2

UF_4 ↑ Melting Point ↓ ΔH_{fus} ↓

Molten Salt Reactor PROGRAM

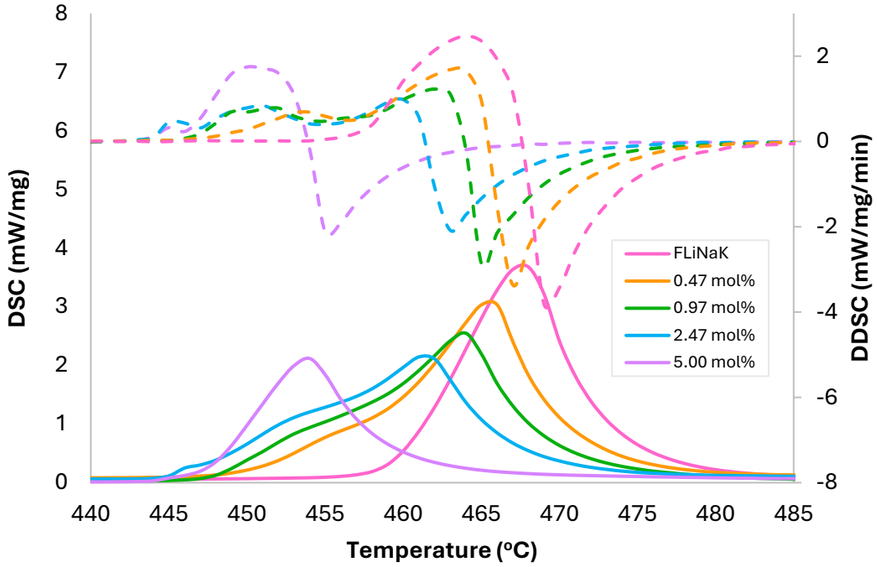
U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

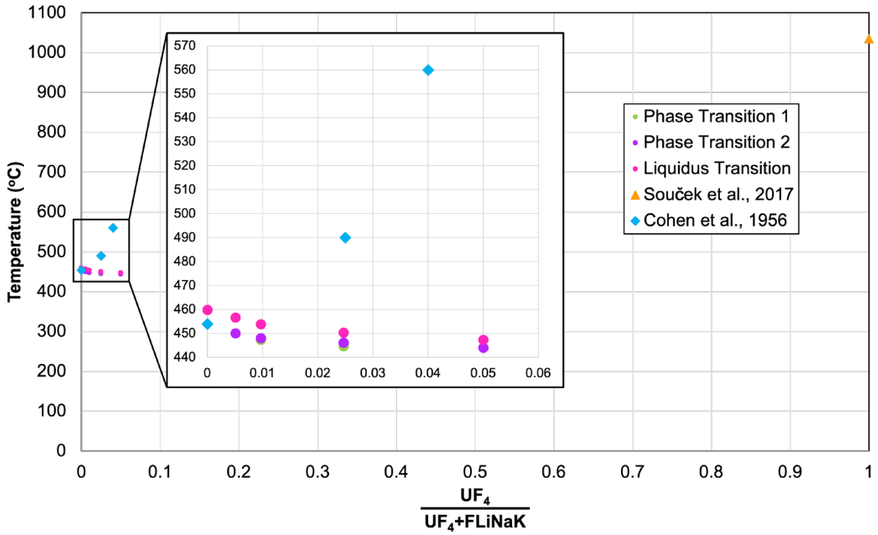
Patenaude et al., *in preparation*.

Differential Scanning Calorimetry (DSC)

For UF_4-FLiNaK

- Primary confirmation for **salt purity**
  - Significant resource for An synthesis
- Exploration of **local eutectic composition**
  - Novel phase diagram mapping
- Testing and development of **robust crucibles**
  - Inconel (Netzsch)
  - Ni liners/custom crucibles
- Pursuit of **$C_{p,s}$** and **$C_{p,l}$**
- Expansion to **additional fluoride systems**
  - Multi-component systems (e.g., FLiBe, UF_4-NaF-KF, UF_4-RbF-NaF)
  - Pure AnF species (e.g., UF_4, UF_3, ThF_4, PuF_3)
- Applicability to **other thermal techniques** (e.g., drop calorimetry)





Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Los Alamos NATIONAL LABORATORY

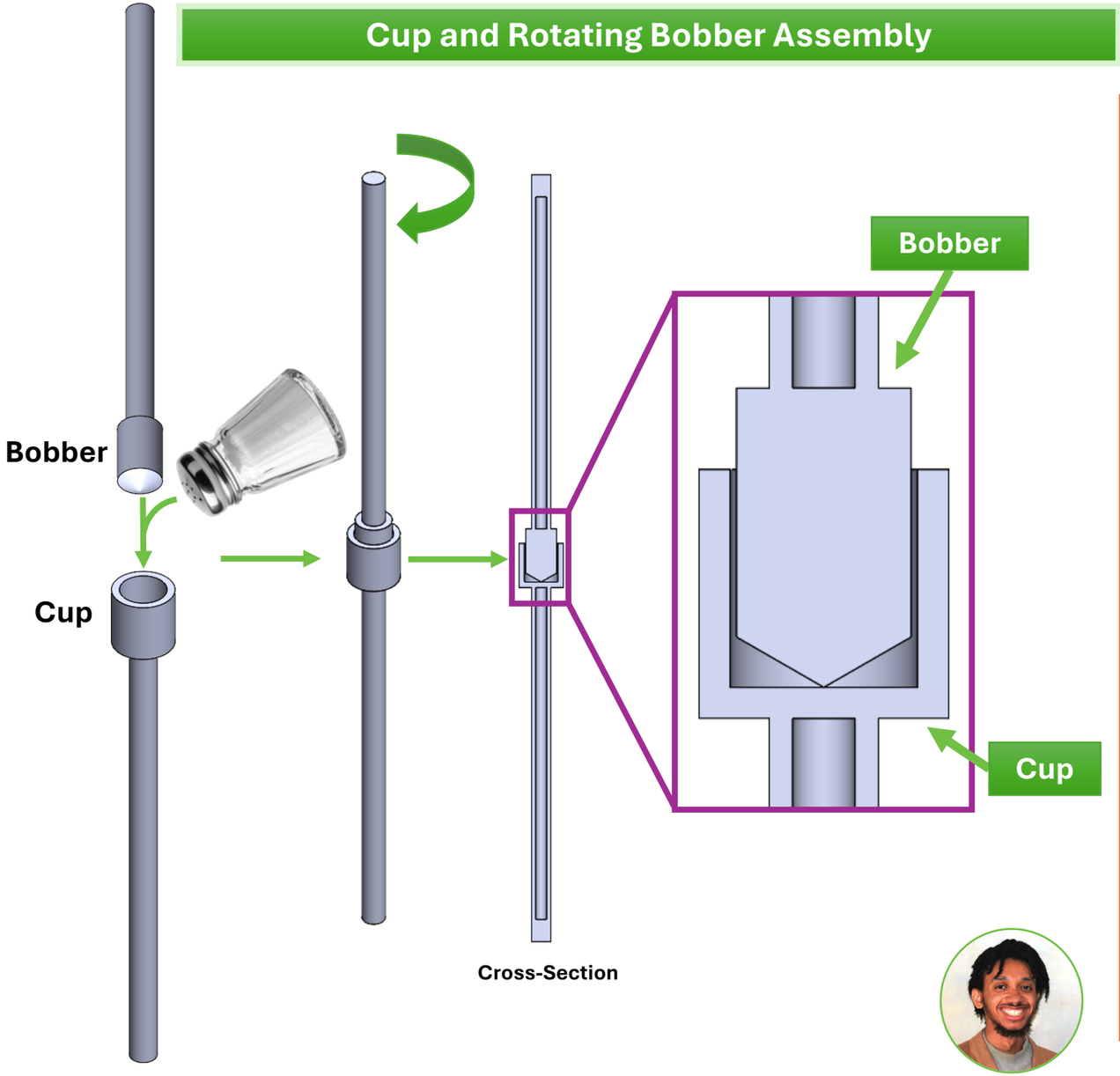
Thermal Properties:
Viscosity

Molten Salt Reactor PROGRAM

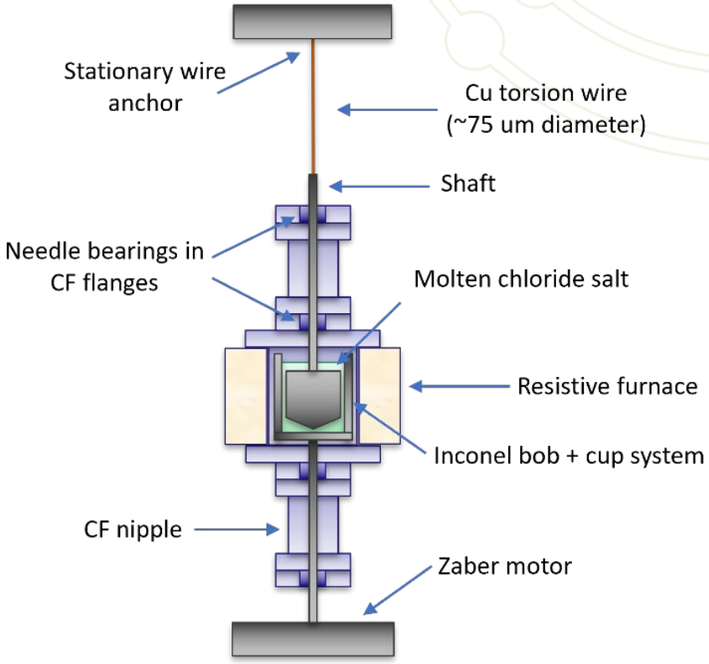
U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Viscosity: Rotational Viscometry

Cup and Rotating Bobber Assembly



Small-Scale, Low-Viscosity, High-Temperature Design



Marvin Davis

Dylan Tharp Eralie

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Los Alamos NATIONAL LABORATORY

Newly Commissioned Labs

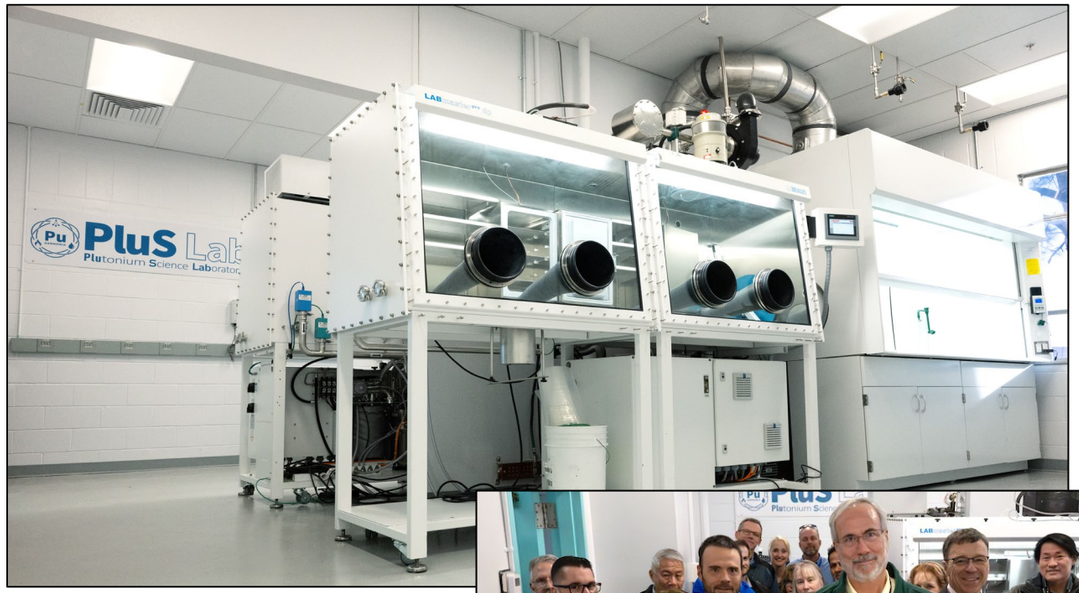
Molten Salt Reactor PROGRAM

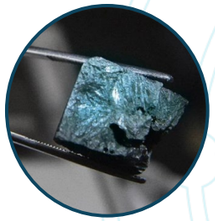
U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Plutonium Science (PluS) Laboratory

The **PluS Lab** will **grow, sustain, and innovate workforce proficiency** to address **current and emerging nonproliferation challenges** through **targeted fundamental plutonium S&T**.

Gram-scale, non-irradiated Pu experiments • Unclassified • Flexible, agile





Molecular Chemistry & Materials Science

Aqueous Systems

Molten Salt Science

Renovation and Commissioning Completed: FY25
Inaugural Pu Experiments: Jan 2026

Plutonium Science (PluS) Laboratory

Molten Salt Science

PluS Lab Leads

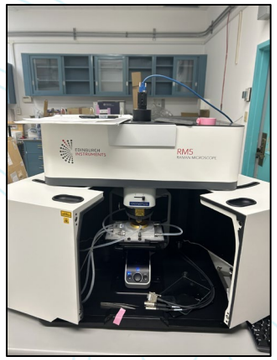
Karla Erickson

Marisa Monreal

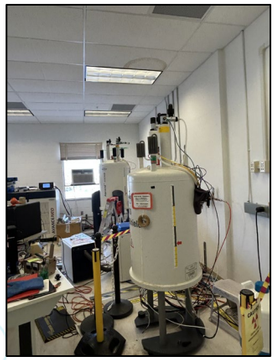
Molecular Chemistry & Materials Science

SEM/EDS

FTIR



Raman



NMR

Clare Hatfield

Sam Lee

Hannah Patenaude

Kristen Pace

PuO_2

- Source comparisons
  - High-fired vs. alpha-metal
- Characterization
  - Raman
  - FTIR
  - SEM
  - UV-Vis. Spectroscopy
    - *Diffuse Reflectance*

$PuCl_3$

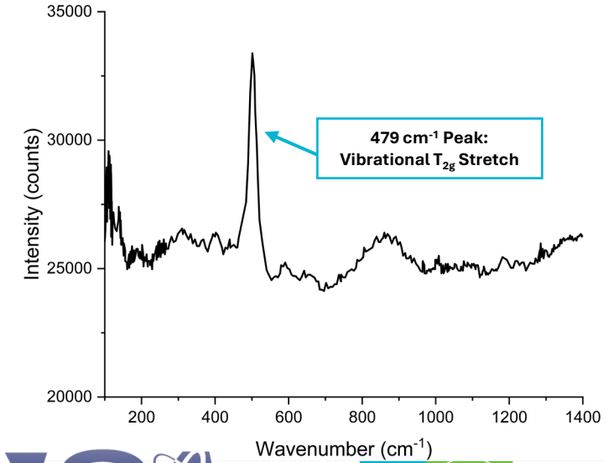
- Molten Salt Studies
  - Electrochemistry
  - Speciation
- Characterization
  - DSC
  - Raman
  - SEM

Aqueous Solutions

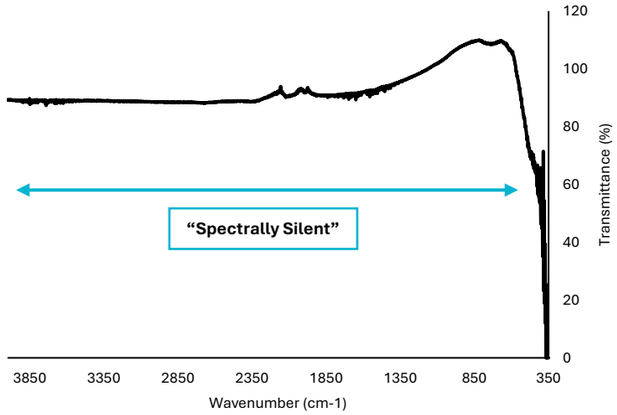
- Separations
- Speciation
- Characterization
  - UV-Vis. Spectroscopy
    - *Absorbance/ Transmission*
  - Electrochemistry

PuO_2 | High-Fired (975 °C)

Raman Spectroscopy



FTIR



National Nuclear Security Administration

NA-22: DNN R&D

Molten Salt Reactor PROGRAM

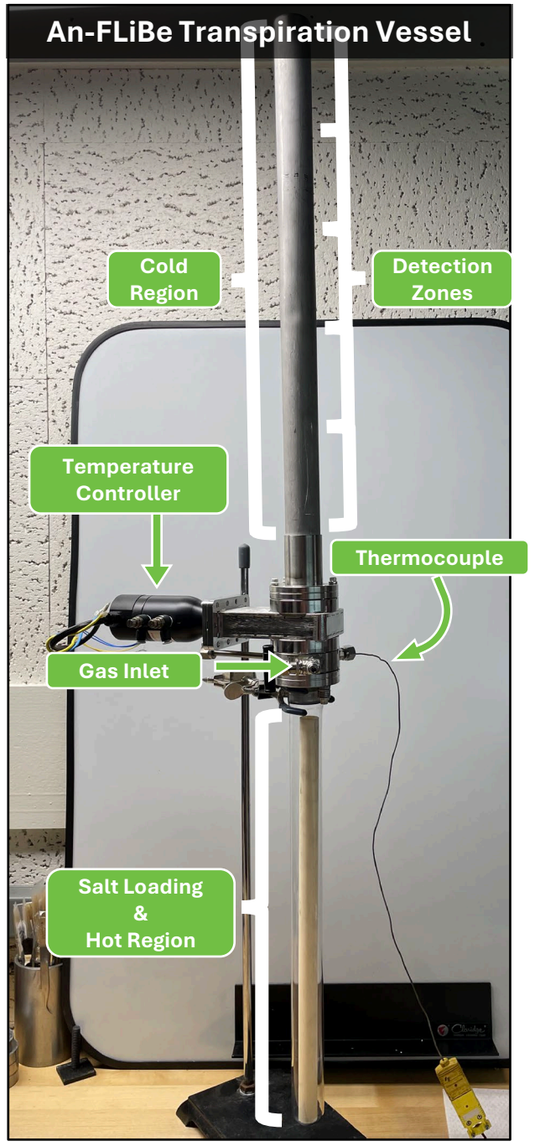
U.S. DEPARTMENT of ENERGY

Office of Nuclear Energy

FLiBe Laboratory for Actinide Molten Salt Experiments (FLAME)

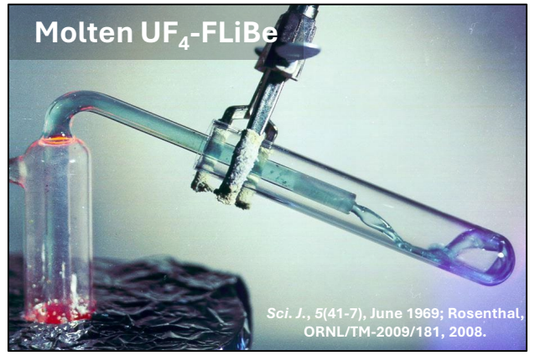
Instrumentation

- TGA
- Cryogen Pumps
- Transpiration Furnace
- SEM/EDS



Analytical Efforts

- Transpiration of An-bearing FLiBe
- Thermal property measurements
- Solid-state characterization
- Corrosion & material compatibility
- Radiography
- Electrochemistry



Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Los Alamos NATIONAL LABORATORY

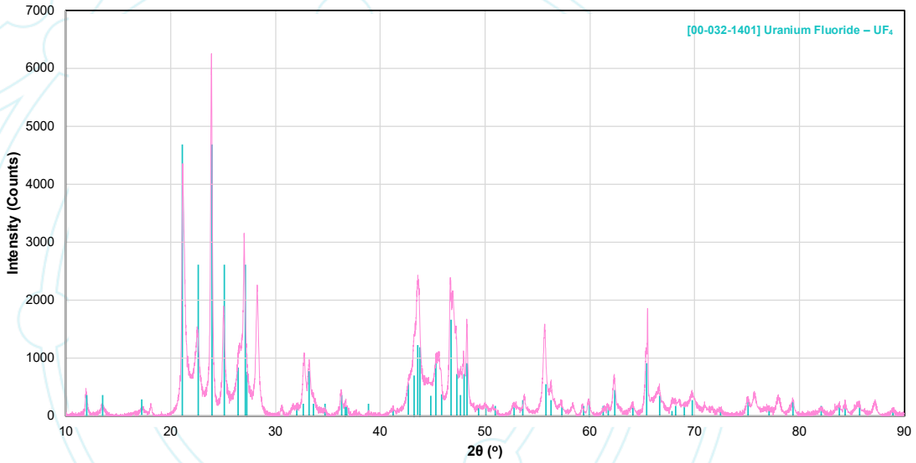
Complementary Research Efforts

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Novel Synthesis – UF_4

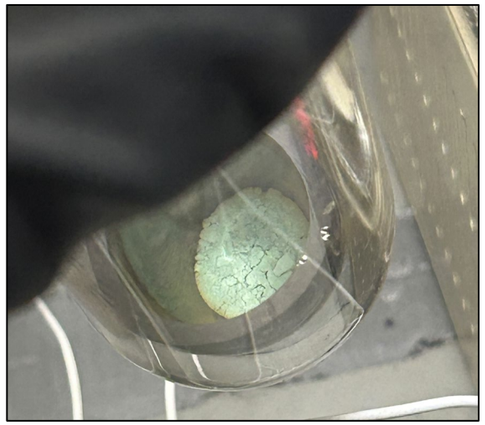
Quartz Vacuum Reactor



Room Temperature, HF-Avoidant Pathway via Mild Main Group Fluoride Reagents

$U^{IV}Cl_4(Py)_n \xrightarrow[-\ [E]\text{-}Cl]{+\ [E]\text{-}F} U^{IV}F_4(Py)_n \xrightarrow[-\ Py]{\Delta,\ vacuum} U^{IV}F_4$ 70-98%

[E]-F = main group fluoride



Gram-Scale UF_4 Synthesis (<1% C Impurity by EA)

PFAS Reagents

UO_2 or U_3O_8 + PFOA, PFOS, other fluorocarbons (PFAS) $\xrightarrow[2.\text{vacuum}]{1.\ \Delta}$ $U^{IV}F_4$ $- CO_2$

Karla Erickson

Sam Lee

Bulk Production – UF_4

Yeamans, 2003

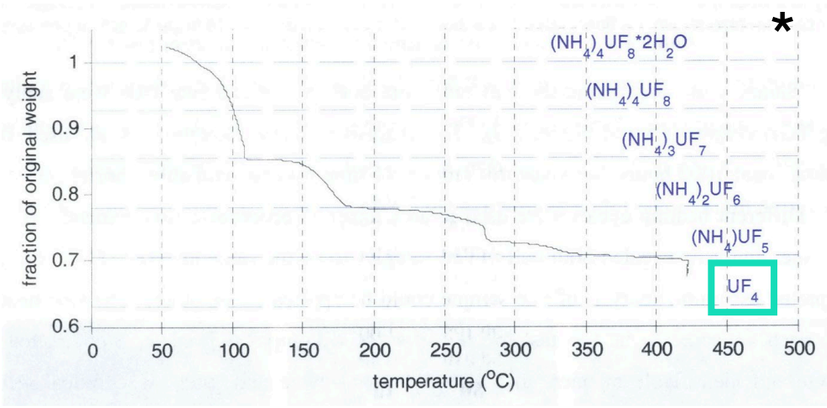
+

$(NH_4)_4UF_8 \cdot 2H_2O$

Δ^*

UF_4

1. **Solid-solid ball mill reaction**
   - Uranium dioxide & ammonium bifluoride
   - STP, air (fume hood)
   - ~10 g batches
   - 1-2 day process
   - Well-studied rxns, mechanisms & kinetics
2. **Step-wise thermal decomp. to UF_4**
3. **Purification check**
   - pXRD
   - DSC (melt point)



Molten Salt Reactor PROGRAM

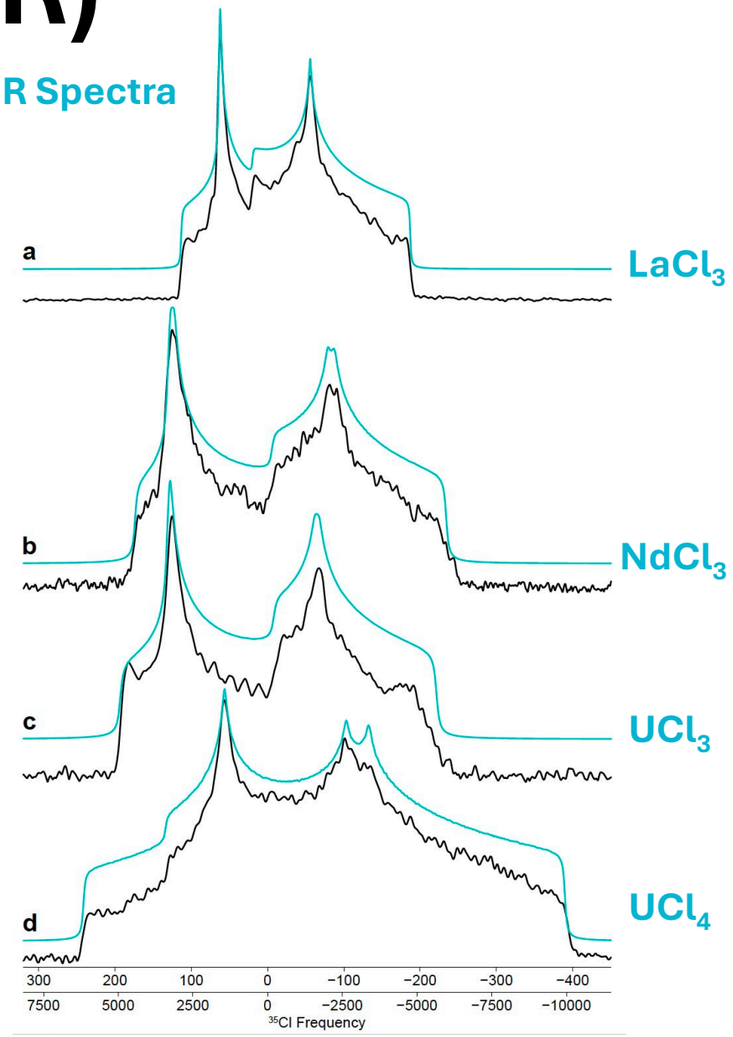
U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Altenhof et al., *Phys. Chem. Chem. Phys.*, [accepted], **2026**.

Nuclear Magnetic Resonance (NMR)

- Solid-State NMR (SSNMR)
  - Mature technique for An-bearing chloride at LANL
  - Expansion to more challenging systems
    - Pu (chloride and fluoride)
    - Fluorides (e.g., FLiNaK, UF_4, FLiBe, etc.)
- <u>Stretch Goal</u>: more complex experimental improvements
  - Solid sample spinning
  - High-temperature liquid salt measurements

***f*-Block ^{35}Cl NMR Spectra**



Harris Mason
Scientist, NMR Lead

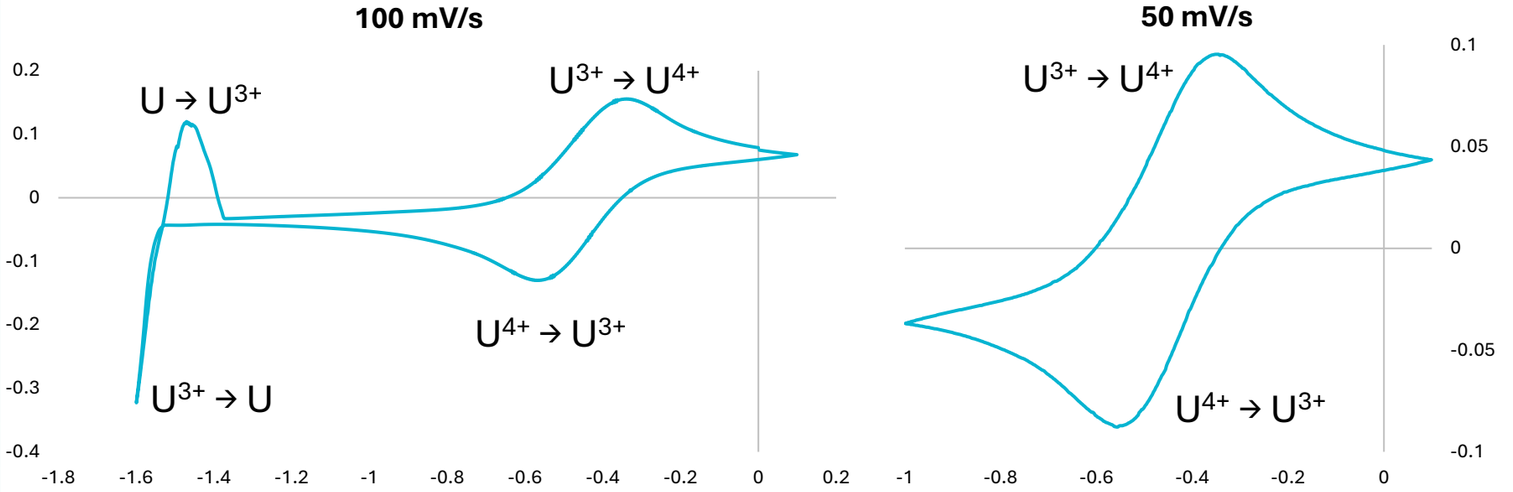
Lexi Carney
Postdoc, SSNMR Expertise

Actinide Molten Salt Electrochemistry

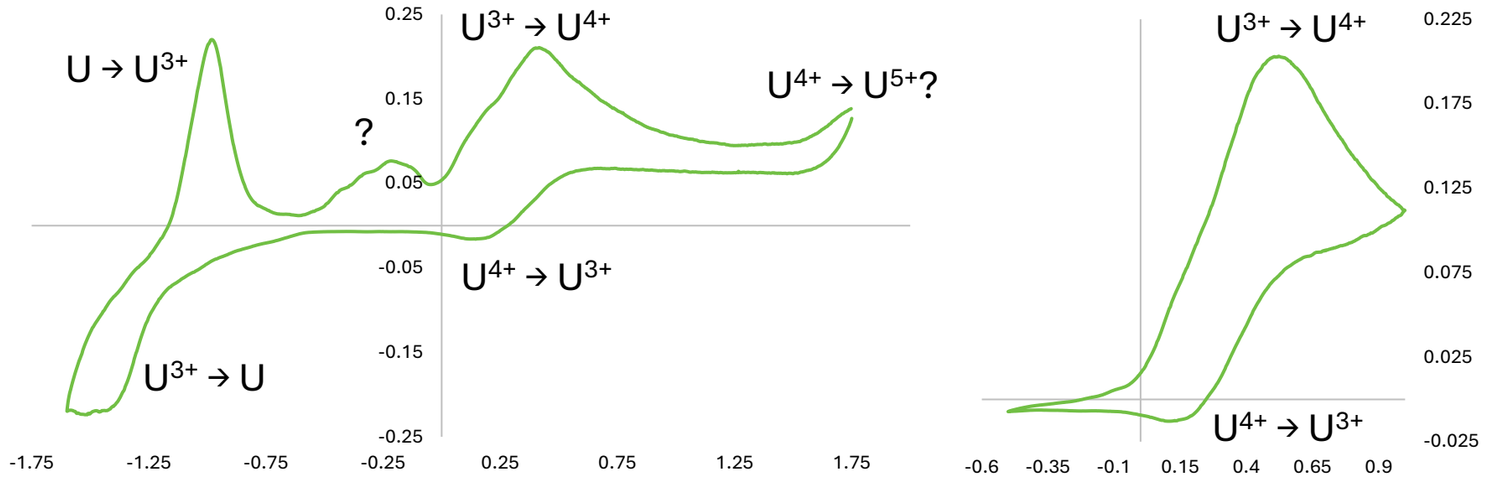
Lead: Hannah Patenaude,
Director's Post-Doctoral Fellow

- **Boron-Doped Diamond** Electrodes
  - Material customization
  - Measurement optimization
    - Geometry, topography, & surface chemistry
- Example Focus Areas:
  - Signal optimization & improved sensitivity
  - Fluoride reference electrodes
  - Cation influence on coordination & redox
  - Plutonium oxidation ($Pu^{4+/3+}$)

UCl_3-LiCl-KCl | 455 °C | vs. Ag/AgCl
1.5 mol% **5 mol%**



UF_4-FLiNaK | 50 mV/s | 665 °C | vs. Ni/NiF_2
0.18 mol% **1 mol%**



Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Los Alamos NATIONAL LABORATORY

FY25-27 Molten Salt LDRD Project: Salt Modeling with GNNs

PI: Gaoxue Wang, Co-PI Marisa Monreal

Published work: DFT-based AIMD on NaCl, UCl_3, NaCl–UCl_3 (and analogous $ThCl_4$, $PuCl_3$)

- VASP (PBE + vdW corrections + Hubbard U corrections)
- **Accurate** densities, heat capacities, mixing energies
- **Limitations:** can only afford small systems (~100 atoms), short times (~50 ps)

Current work: AIMD as high-accuracy training data→fine-tuning Graph Neural Network(GNN) interatomic potentials (IPs)

- **Enables** large systems (~1000s atoms), long-timescales (ns)
- **Access** to full property set: density, Cp, viscosity, diffusivity, corrosion

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Ab initio molecular dynamics (AIMD) simulations of NaCl, UCl_3 and NaCl-UCl_3 molten salts

D.A. Andersson[a,*], B.W. Beeler[b,c]

[a] Materials Science and Technology Division, Los Alamos National Laboratory P.O. Box 1663, Los Alamos, NM 87545, USA
[b] Department of Nuclear Engineering, North Carolina State University, Raleigh, NC, United States
[c] Idaho National Laboratory, Idaho Falls, ID 83415, United States

Journal of Molecular Liquids
Volume 385, 1 September 2023, 122347

Ab-Initio molecular dynamics simulations of binary NaCl-$ThCl_4$ and ternary NaCl-$ThCl_4$-UCl_3 molten salts

Gaoxue Wang[a], Bo Li[a], Ping Yang[a], David A. Andersson[b]

Journal of Nuclear Materials
Volume 591, 1 April 2024, 154902

First-principles investigation of the thermophysical properties of NaCl, $PuCl_3$, and NaCl-$PuCl_3$ Molten salts

Kai Duemmler[a], David Andersson[c], Benjamin Beeler[a,b]

"Advanced Characterization to Enable Prediction of Actinide-Molten Salt Behavior" (#20210113DR)

"Navigating Vast Chemical Space: Empowering Molten Salt Modeling with Universal Graph Neural Networks" (#20250148ER)

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

FY25-27 Molten Salt LDRD Project: Local Structure by nPDF

- PDF experimental data for pure UCl_3 was collected at NOMAD at SNS and compared to simulations and published values
  - Observed: reduction in g(r) with increasing temperature at 3.3 Å, Cl-Cl peak
  - Statistics show *less edge- and face-sharing* and *more corner sharing as temperature increases*
- Experimental data for molten UCl_3-NaCl eutectic, pure $MgCl_2$, and $MgCl_2$-NaCl eutectic also collected
- Recently returned to NOMAD to collect data at additional molten temperatures for pure UCl_3 and UCl_3-NaCl – analysis underway

Additional project experimental work includes:

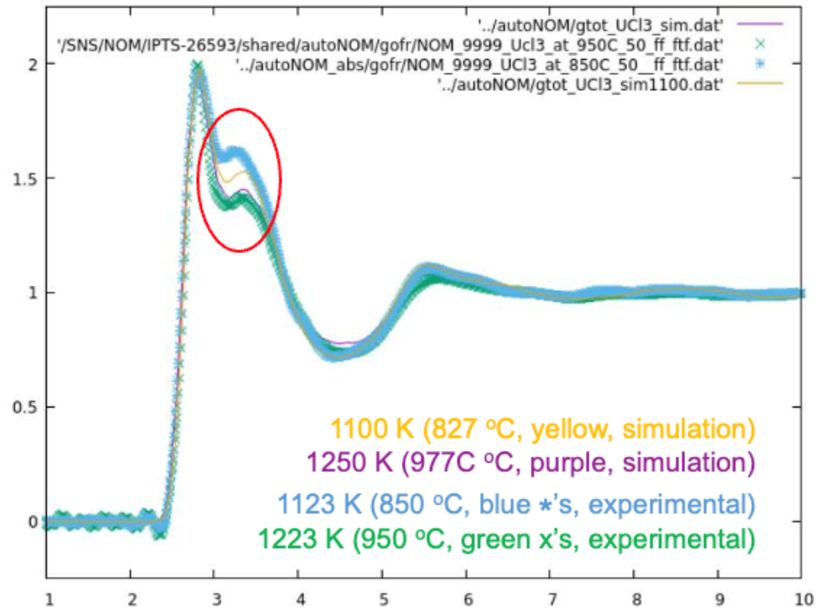
➢ Collecting molten Raman spectra for same salt systems

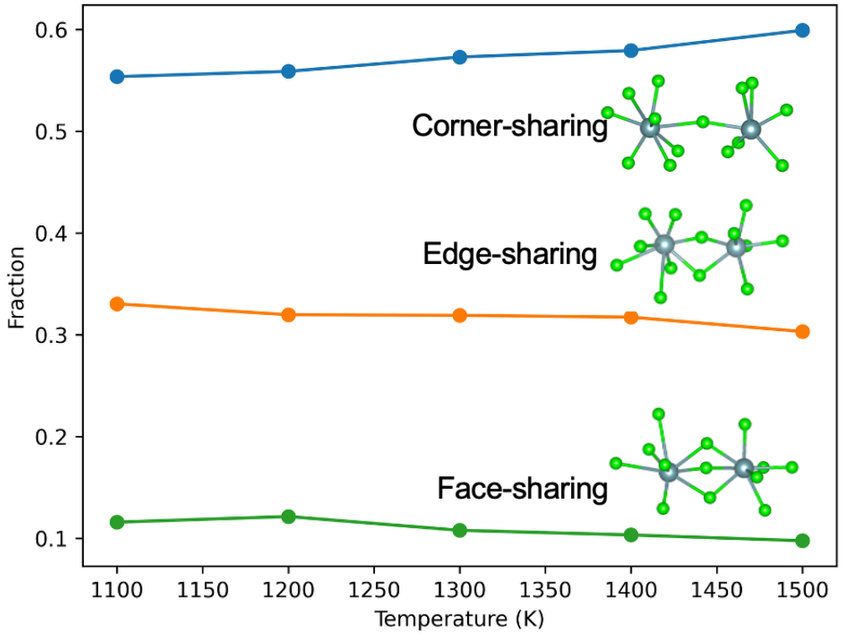
Sven Vogel

Hannah Patenaude

Bryn Merrill

Clare Hatfield





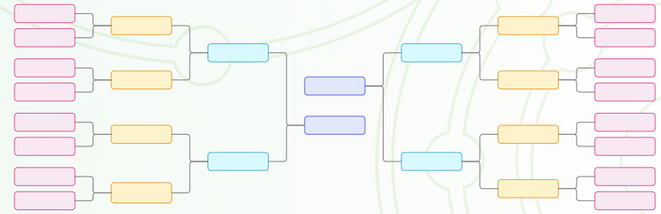
MSR Safeguards Technology Development

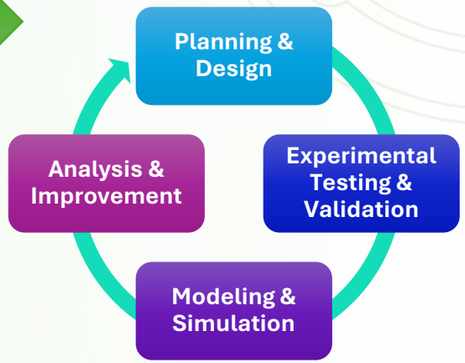
NA-22: Office of Defense Nuclear Nonproliferation (DNN) R&D

Marisa Monreal
LANL PI

Hannah Patenaude
LANL Experimental Lead

- **Safeguards Technology Roadmap**
  - Identification of primary needs
  - Compilation of promising, underexplored techniques
  - Description of molten salt testbeds
- **Low-TRL Measurement Technique Feasibility Studies**
  - Downselection of three techniques for TRL advancement
  - Targeted campaigns at each partnering lab
    1. **ORNL** – Mod/Sim, Molten Salt Loops, USTC, etc.
    2. **INL** – MSTEC, Irradiation, Molten Salt Loops, etc.
    3. **LANL** – MSSL, PluS Lab, FLAME, etc.
- **Safeguards System Development**
  - Downselection of system components based on prioritization metrics
  - Establish design criteria
  - Develop experimental, modeling, and simulation for testing components





OAK RIDGE National Laboratory

INL Idaho National Laboratory

Los Alamos NATIONAL LABORATORY

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Acknowledgements

Scientists & Engineers

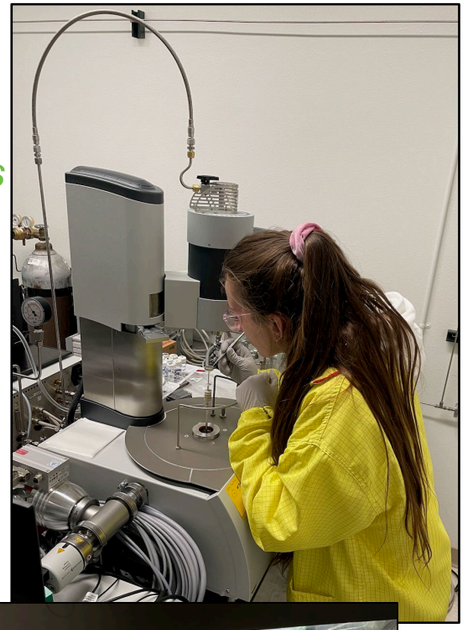
Scott Parker
Karla Erickson
Harris Mason
Sven Vogel
Kristen Pace
Alex Long
David Andersson
Matt Jackson
Ping Yang
Gaoxue Wang
Travis Carver

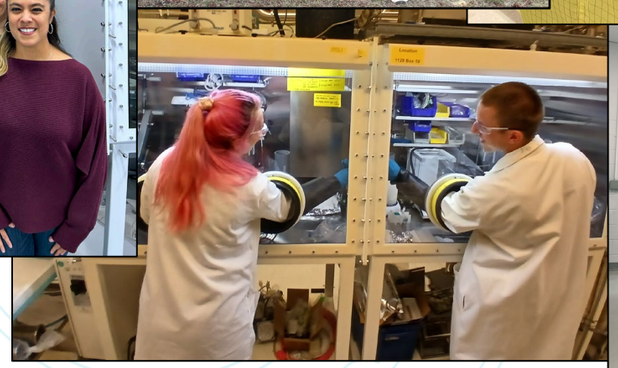
Research Technologists

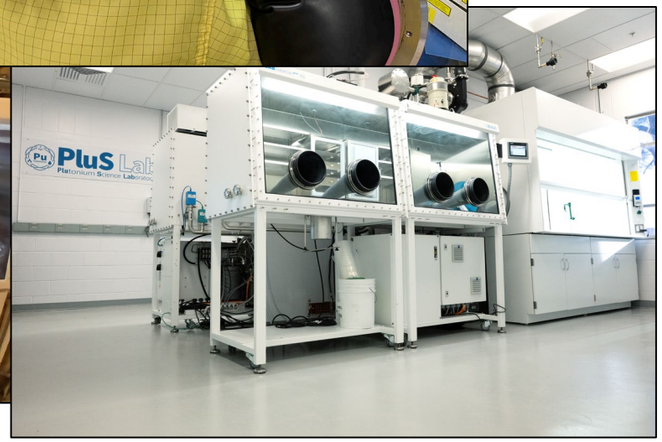
Clare Hatfield
Marvin Davis

Post-docs & Students

Hannah Patenaude (PD)
Bryn Merrill (S)
Sam Lee (PD)
Lexi Carney (PD)
Dylan Tharp Eralie (PD)







Funding

- Molten Salt Reactor Campaign
- Advanced Fuels Campaign
- LANL Laboratory Directed Research and Development (LDRD)
  - #20210113DR
  - #20250148ER
  - #20251145PRD1
- NA-22, NNSA
- Technology Commercialization Fund (TCF) with Kairos Power

Molten Salt Reactor PROGRAM

AFC Advanced Fuels Campaign

LDRD

Kairos Power

NNSA National Nuclear Security Administration

Technology Commercialization Fund | OTT Office of Technology Transitions

University Collaborators & Visiting Students

UNLV

Berkeley UNIVERSITY OF CALIFORNIA

Massachusetts Institute of Technology

Oregon State University

THE UNIVERSITY OF UTAH

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

WASHINGTON STATE UNIVERSITY

Molten Salt Reactor PROGRAM

U.S. DEPARTMENT of ENERGY
Office of Nuclear Energy

Thank you!

mmonreal@lanl.gov

hpatenaude@lanl.gov

Molten Salt Reactor PROGRAM

New April 16, 2026: LANL job ad posted for a **Research Technologist** to join our molten salt research team.
Search **IRC143593** at **https://lanl.jobs/** or scan the QR code.