



Fluoride Salt Properties and Chemistry

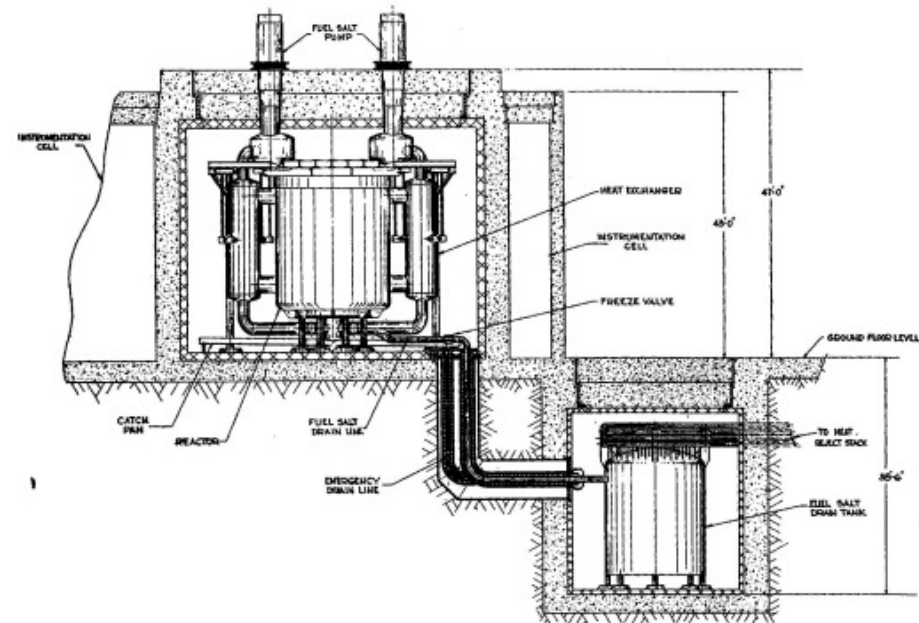
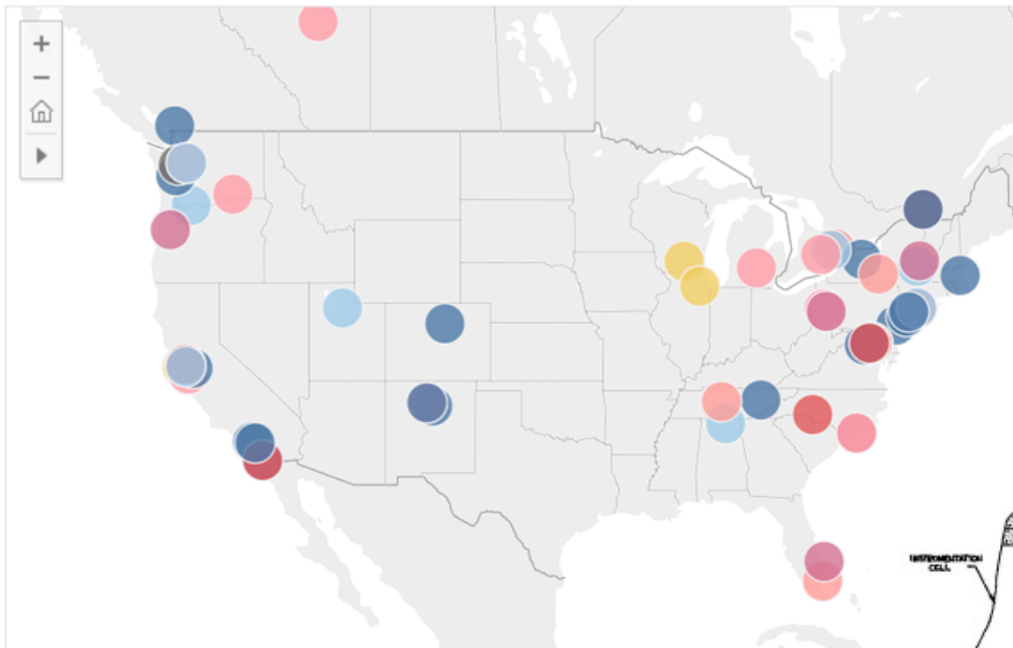
Advanced Non-Light Water Reactors – Materials and Component Integrity Workshop

Dr. Matthew J Memmott – Brigham Young University

December 11th 2019

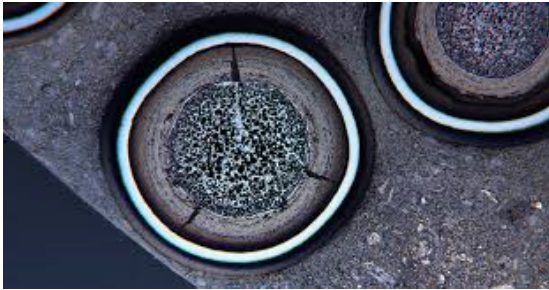
Molten Salt Reactor

Advanced Nuclear Industry: The Next Generation

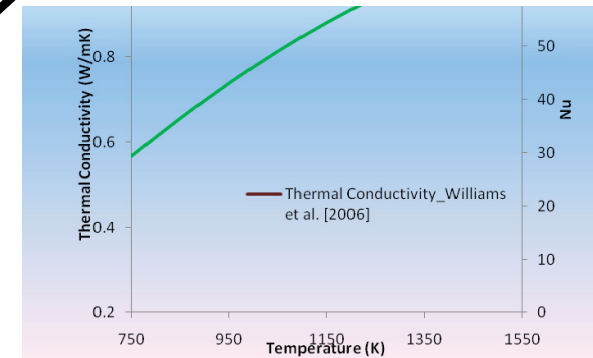


Licensing

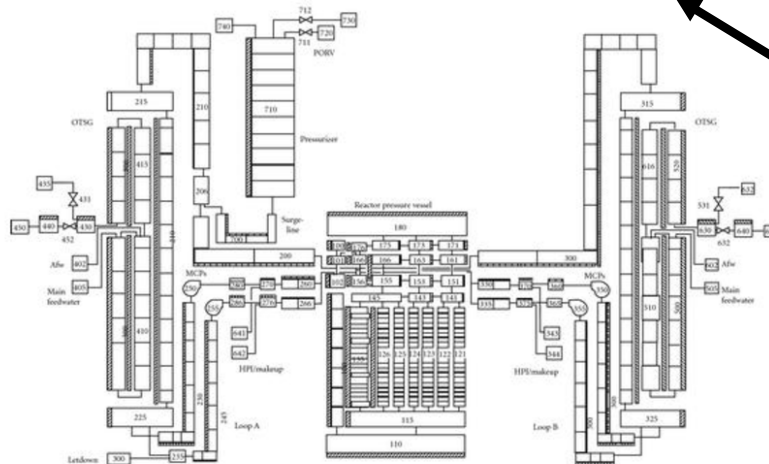
Source Term



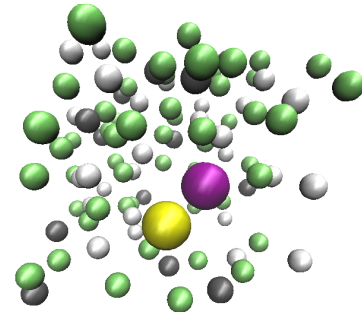
Thermophysical Properties



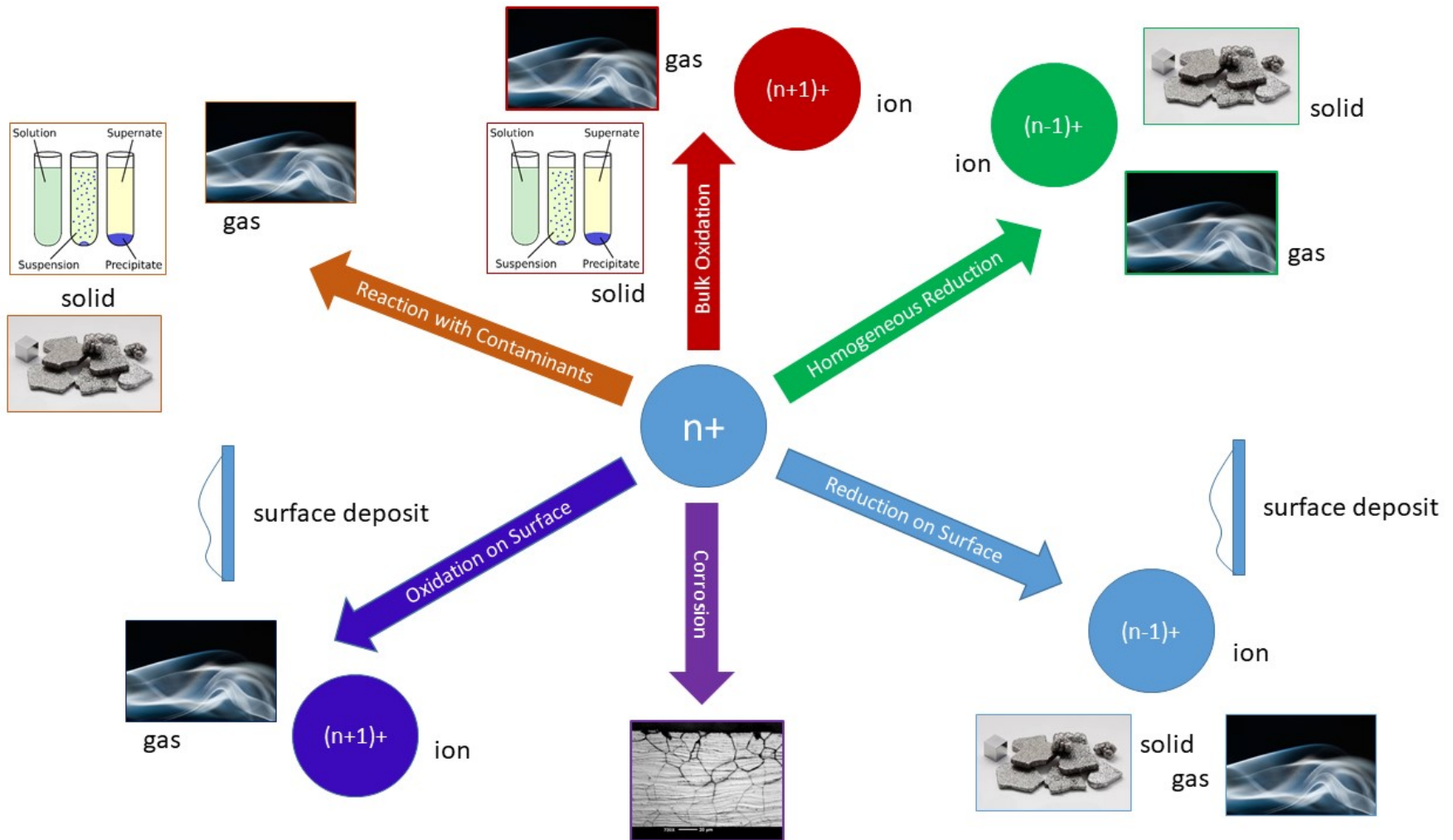
Transport
(System Models)



Thermodynamic Behavior



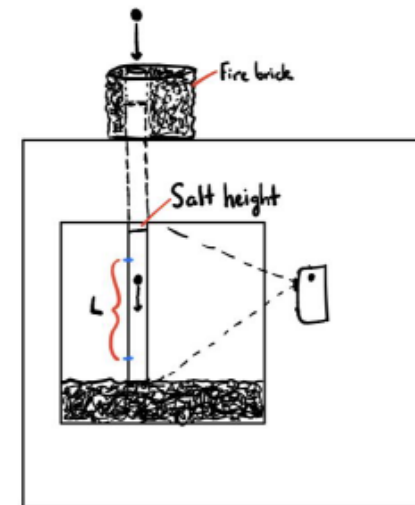
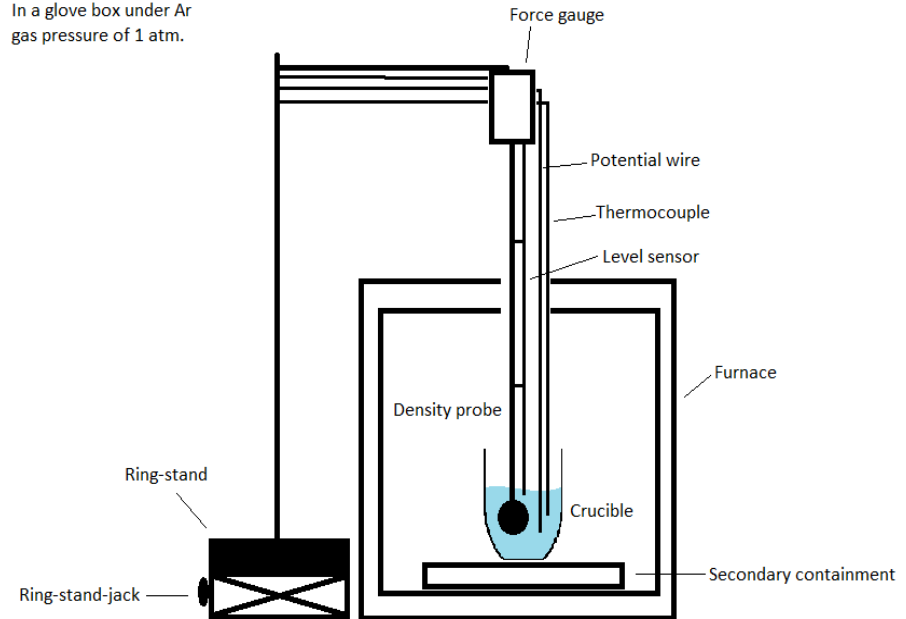
Fission Product Transport



Thermophysical Properties

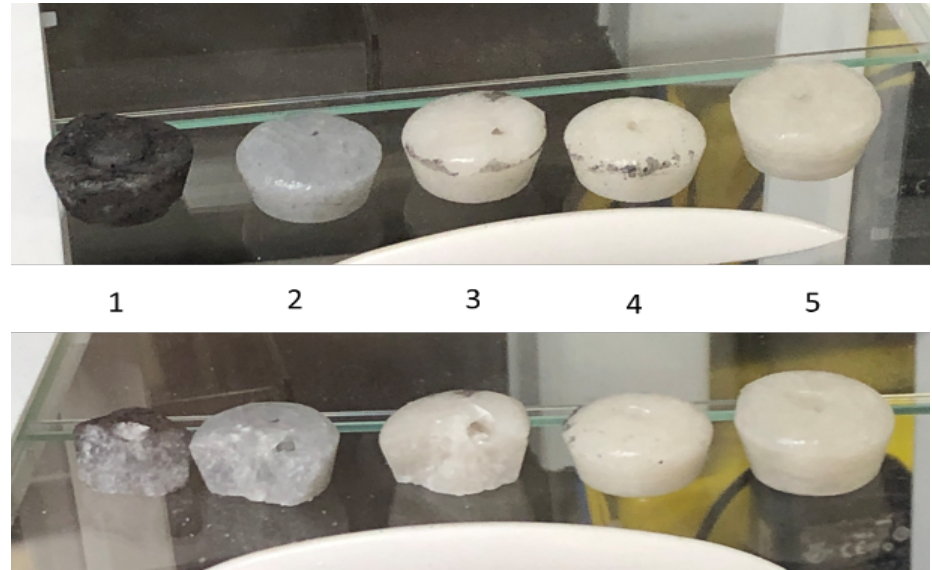
- Salt is challenging!
 - Anaerobic
 - Anhydrous
 - Wall creep
 - Be toxicity
 - High temperature
 - Prone to impurity retention
- Need ρ , k , C_p , μ , γ , etc.

In a glove box under Ar gas pressure of 1 atm.

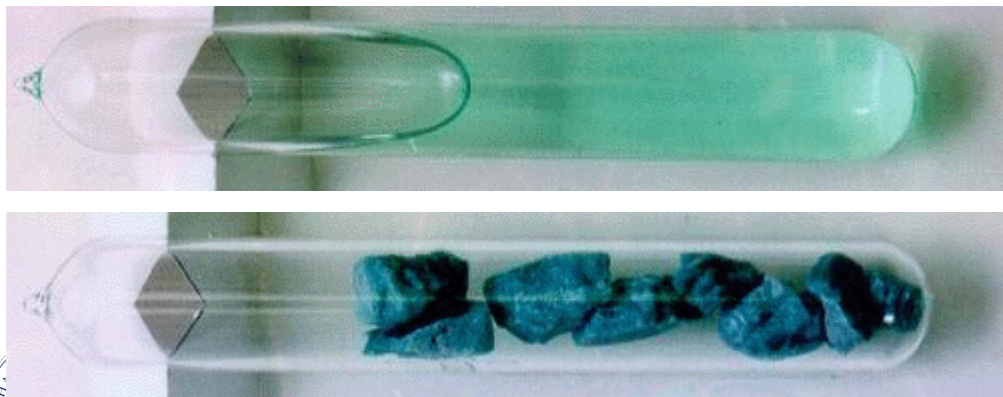


Actinide Bearing Salts

- Purification/standards for clean salt not set
- Clean salt data exists, though limited
- Salt won't remain clean for long!

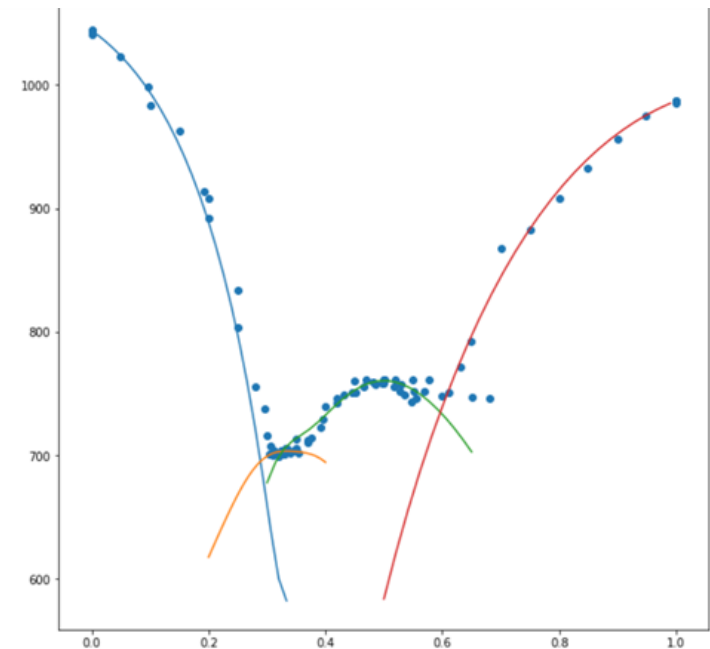
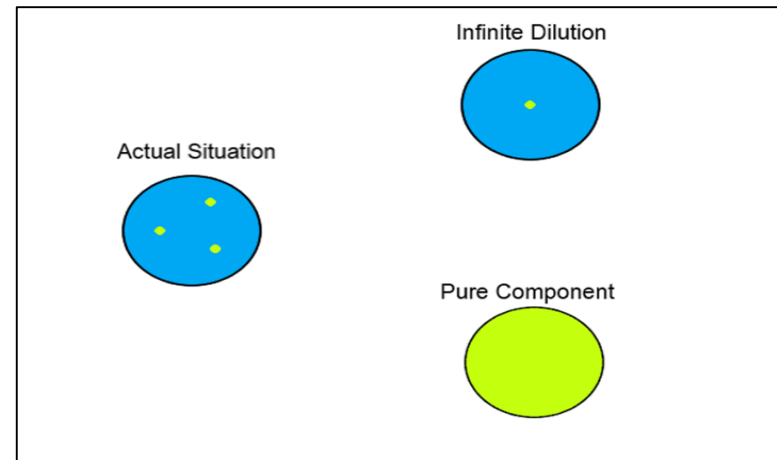


- Actinide salt
- Fission product salt
- Millions of experiments for all combinations



Thermodynamic Analysis

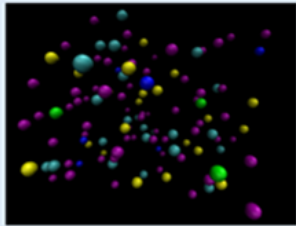
- Equilibrium potentials for actinides (Th, U) or fission products at low concentrations
- Analyze/evaluate thermodynamic data, assess trends/behaviors
- Phase prediction using modified quasi-chemical model



Atomistic Modeling

First-Principles Molecular Dynamics

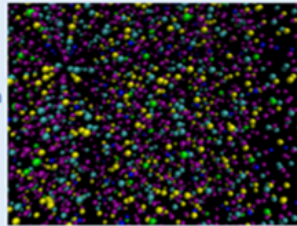
Fewer Temperatures/Concentrations



Local Structure, Speciation,
Diffusion Coefficients

Classical Molecular Dynamics

More Temperatures/Concentrations



Density, Viscosity, Heat Capacity,
Thermal Conductivity
Structure/Property Relationships

Physical Experiments

Fewer Temperatures/Concentrations



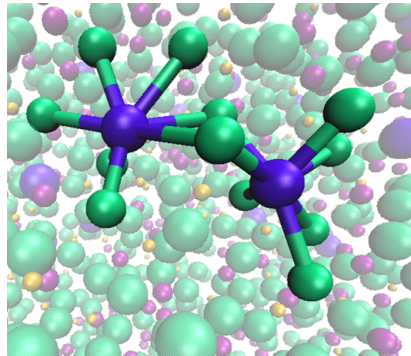
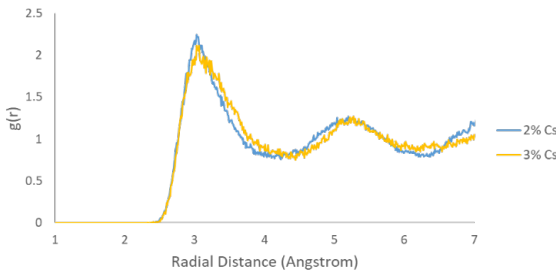
Density, Heat Capacity,
Thermal Conductivity

validation

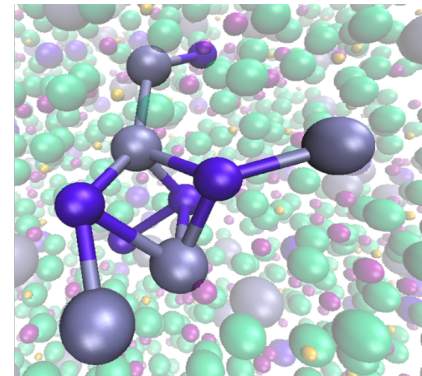
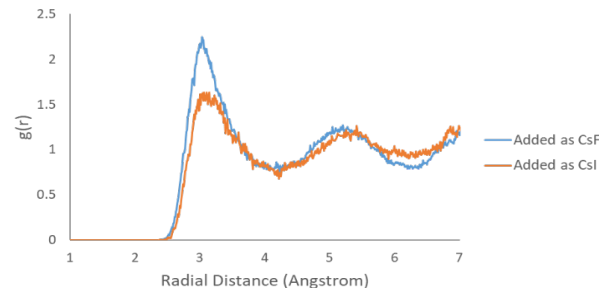


Thermophysical Property Modeling

RDFs for Cs-F Interactions in FLiBe at 500°C
with Cs Added as CsF



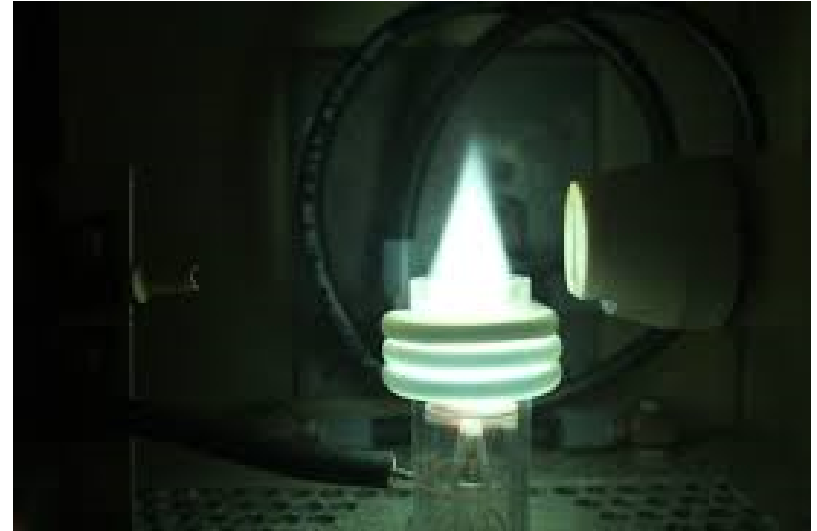
RDFs for Cs-F Interactions in FLiBe at 500°C
with 2% Cs by atom



Ion-Ion Interactions

Salt Property Characterization

- Inductively coupled plasma
 - Common method for composition analysis
 - Can't see Hydrogen
 - Can't see Oxygen
- Need alternative method to fully characterize salts

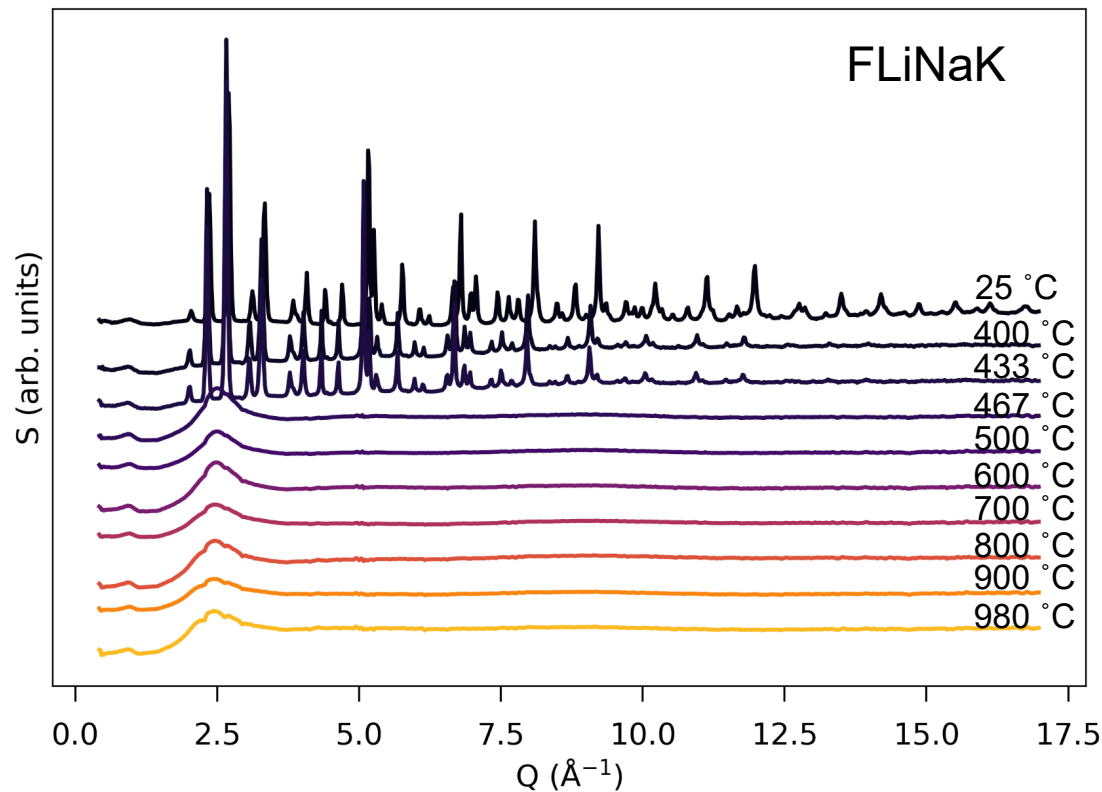


Neutron Total Scattering Experiment on FLiNaK

- Experiment conducted at Oak Ridge National Laboratory Spallation Neutron Source (NOMAD instrument) November 17-19, 2019
- Objective: Obtain neutron scattering data to probe the structure of the salts in both the solid and molten states, enabling quantitative comparison with simulations
- Preliminary analysis is promising

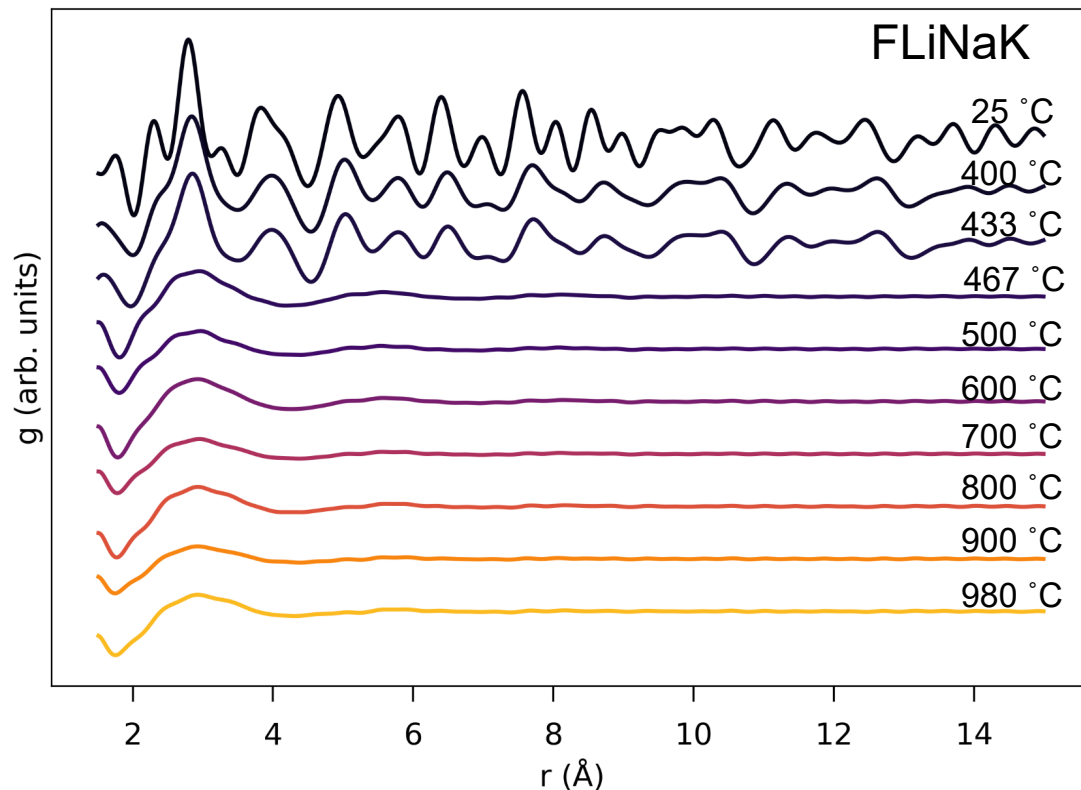


Temperature Dependent Scattering Pattern



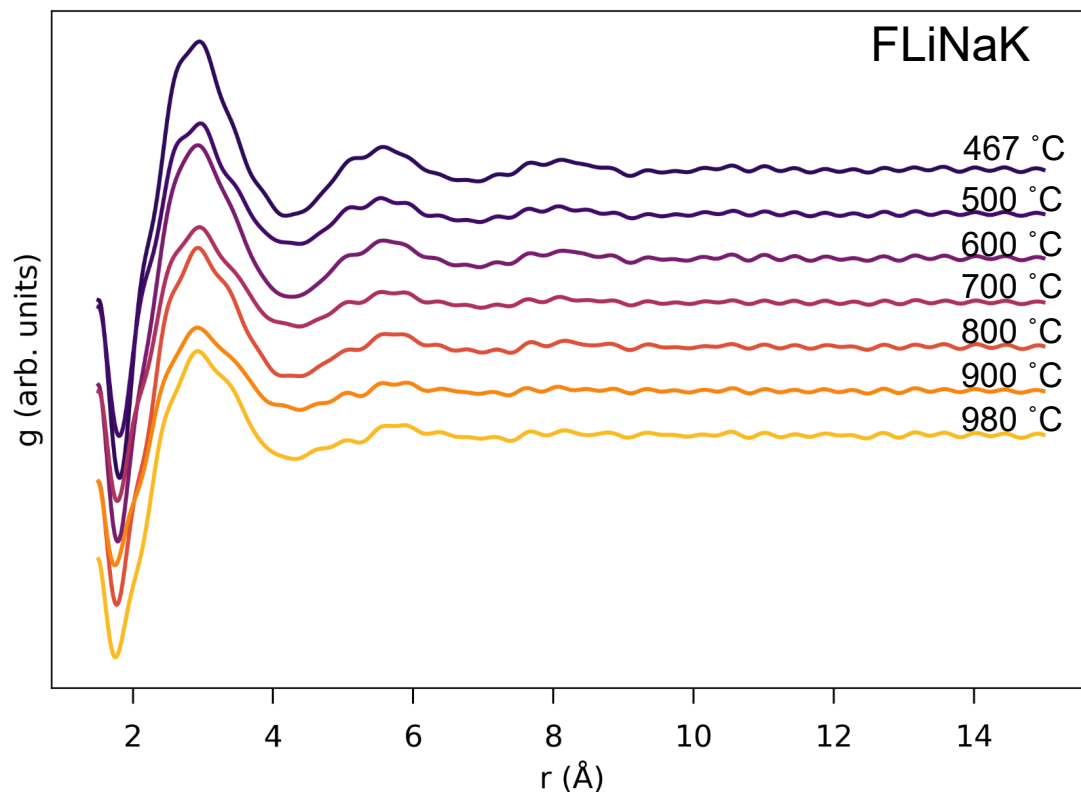
- Sharp peaks in the scattering patterns for 25 °C, 400 °C, and 433 °C indicate long-range structural correlations
- Diffuse features in the scattering patterns for 467 °C and higher indicate short-range structural correlations (but no long-range structure)
 - Consistent with the known melting point of 450 °C
 - Note: Patterns are offset vertically for clarity

Temperature Dependent Pair Distribution Function (PDF)



- The PDF is essentially the Fourier transform of the scattering pattern, yielding structural information in real space rather than reciprocal space
 - Peaks in the PDF indicate the presence of well-defined pairs of atoms separated by that distance
 - Long-lived peaks at low temperature reveal well-defined, long-range correlations in the solid state
 - The peaks are much broader in the molten state due to the amorphous nature of the liquid
- Note: Patterns are offset vertically for clarity

Temperature Dependent Pair Distribution Function (PDF)



- Negative peak at 1.8 \AA originates from Li-F nearest-neighbor pairs (negative due to negative scattering length of Li)
- Na-F and K-F nearest neighbor pairs contribute to the peak centered around 3 \AA
- Broad features persist to 8-9 \AA , indicated non-random correlations on this length scale
- These experimental patterns can be compared quantitatively to MD simulations (work in progress) to extract detailed structural information
- Note: Patterns are offset vertically for clarity

Conclusion

- Salt experiments needed to inform MSR design and licensing processes
- Actinide and FP bearing salts essential for system modeling, but massive in scope
- Thermodynamic assessment informs experiments, reveals correlations
- Trends in ion-ion interactions minimize experimental load
- Improved characterization capability needed: PDF analysis promising