Fluoride Salt Properties and Chemistry

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

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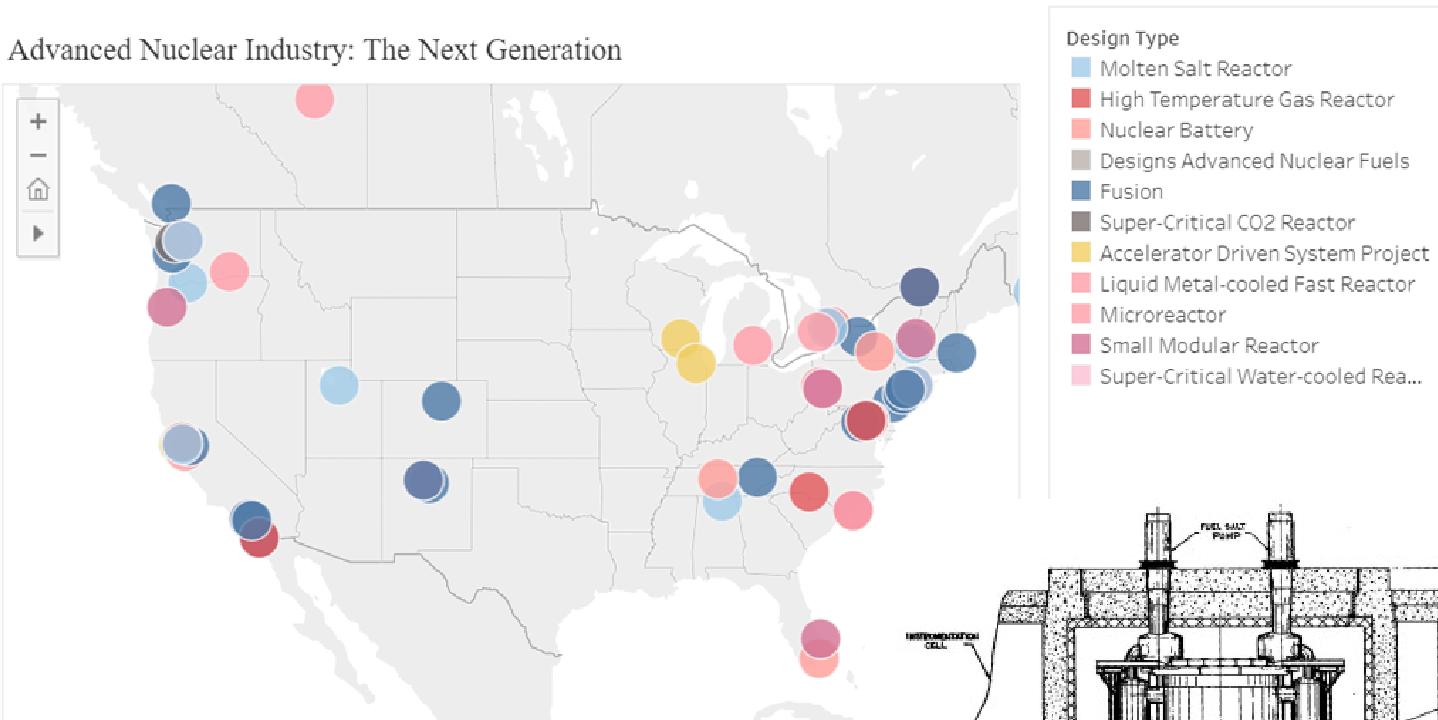
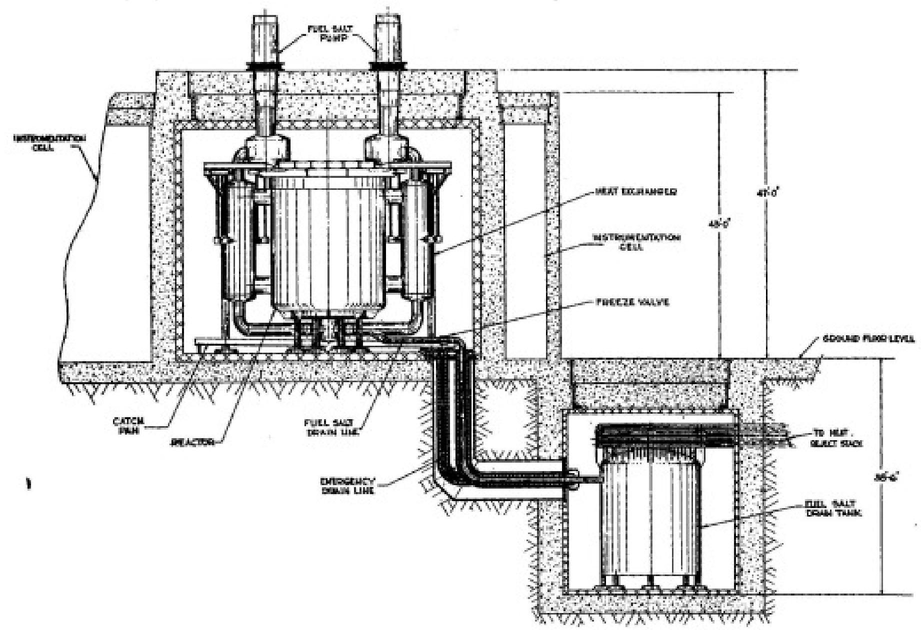
Molten Salt Reactor

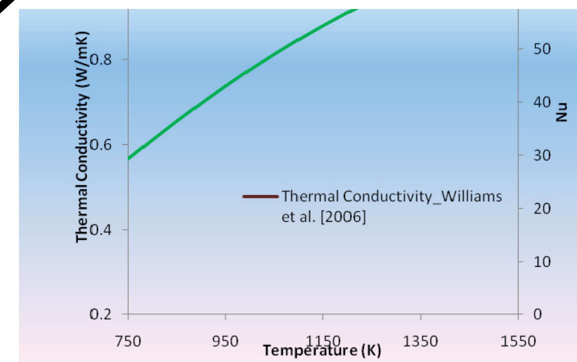




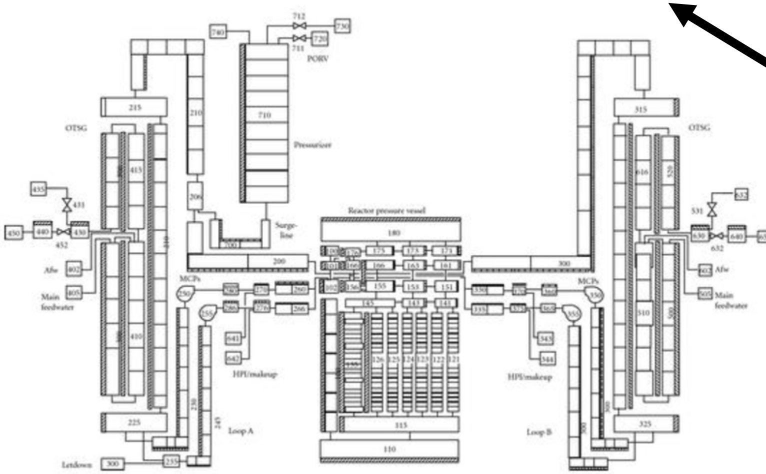
Licensing

Source Term

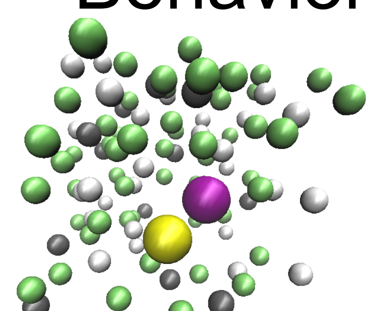
Thermophysical Properties



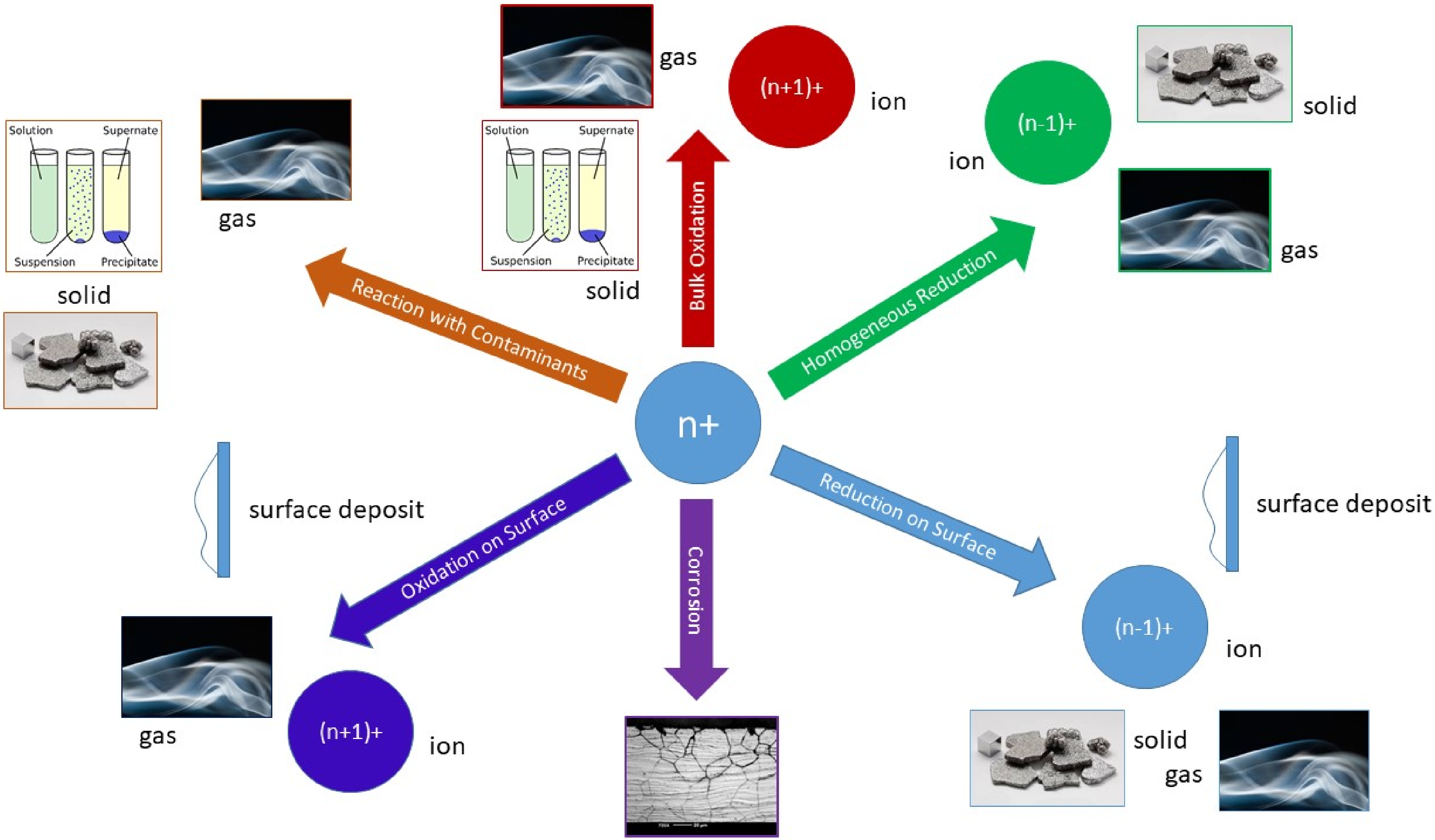
Transport (System Models)



Thermodynamic Behavior

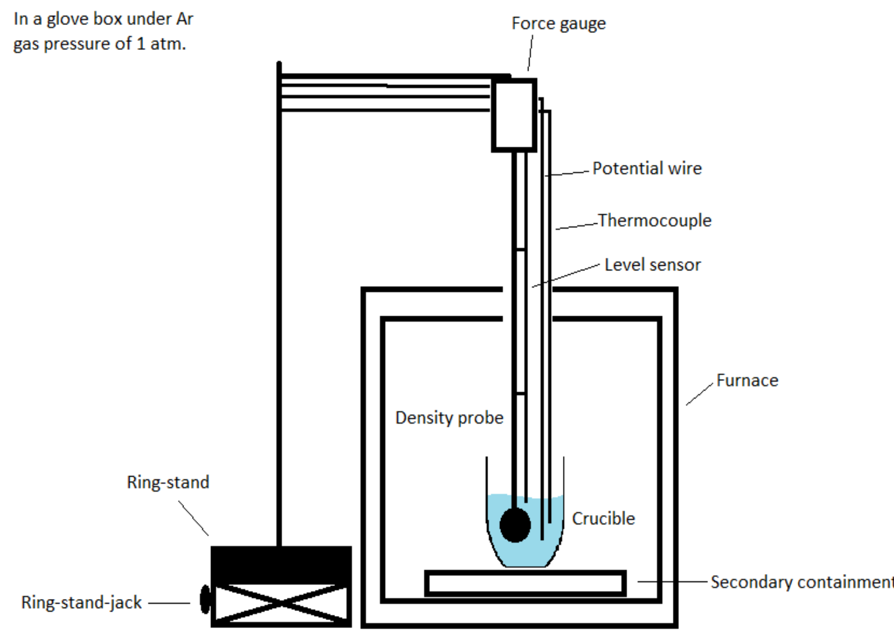


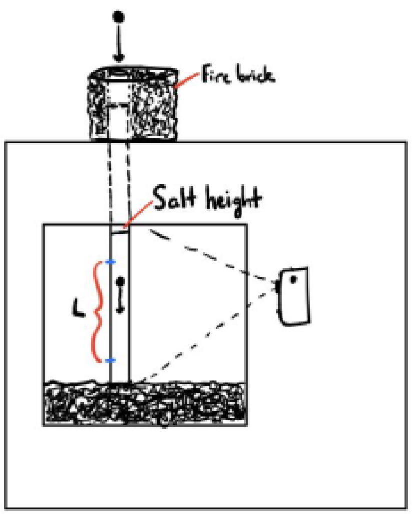
Fission Product Transport



Thermophysical Properties

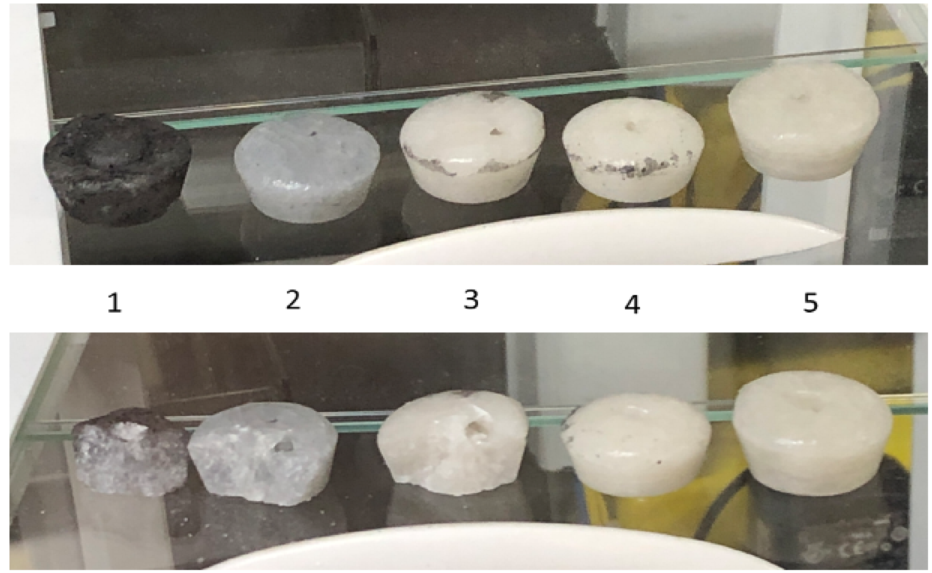
- Salt is challenging!
  - Anaerobic
  - Anhydrous
  - Wall creep
  - Be toxicity
  - High temperature
  - Prone to impurity retention
- Need ρ, k, Cp, μ, γ, etc.

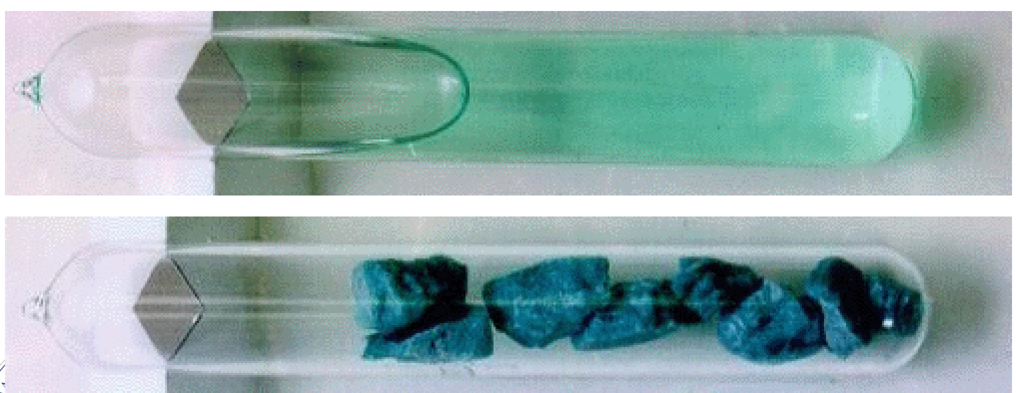




Actinide Bearing Salts

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

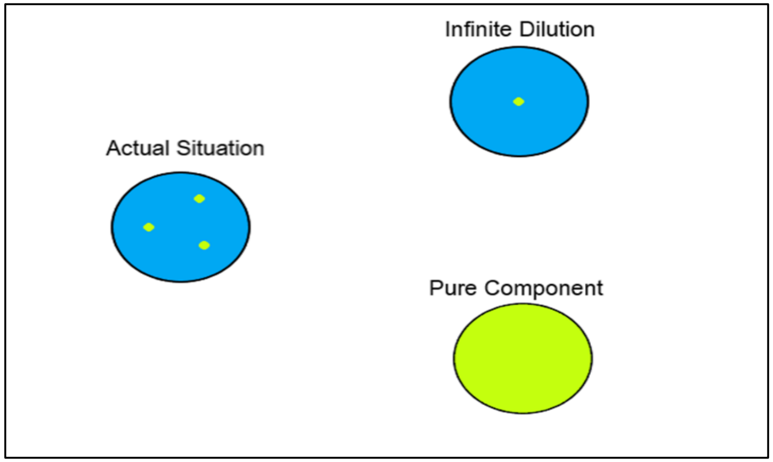


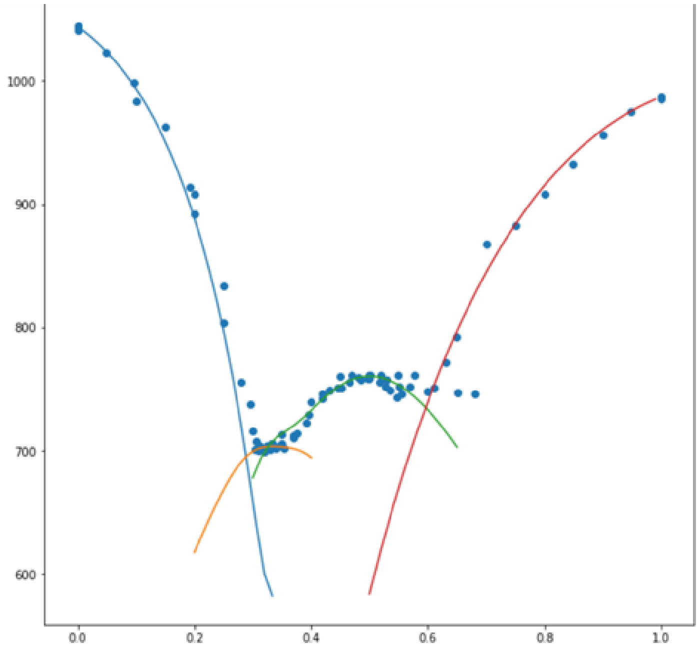


- Actinide salt
- Fission product salt
- Millions of experiments for all combinations

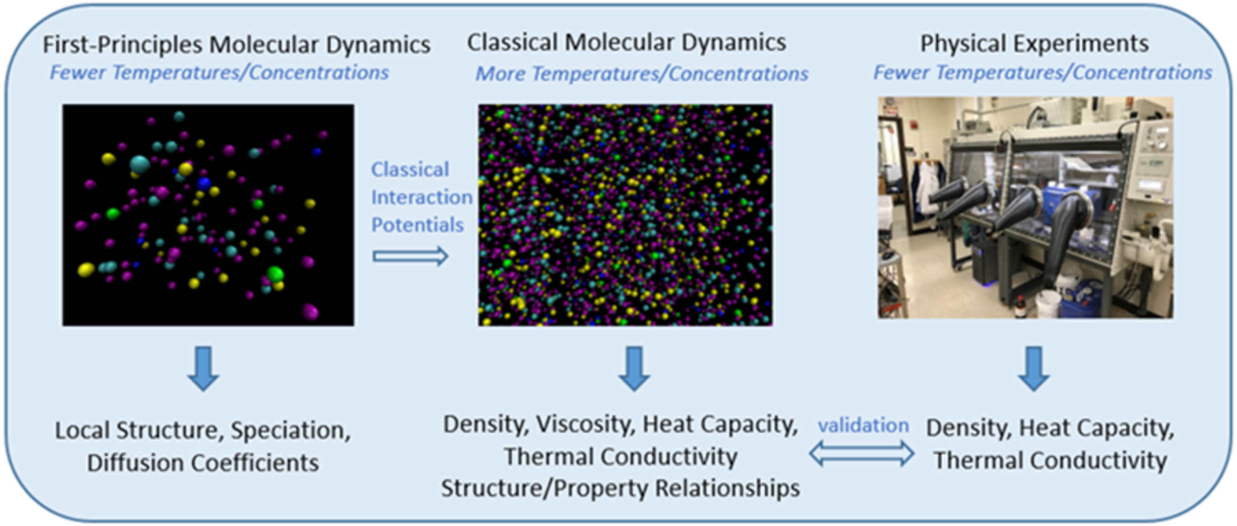
Thermodynamic Analysis

- 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

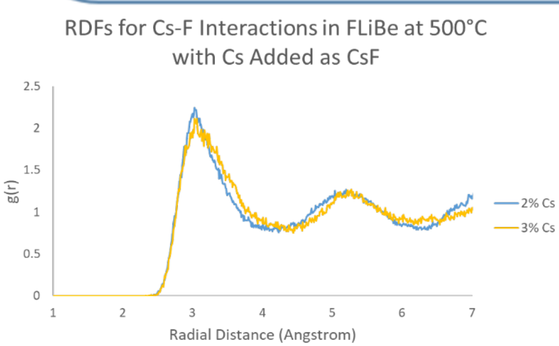


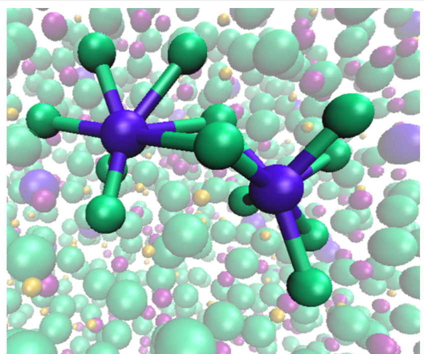


Atomistic Modeling

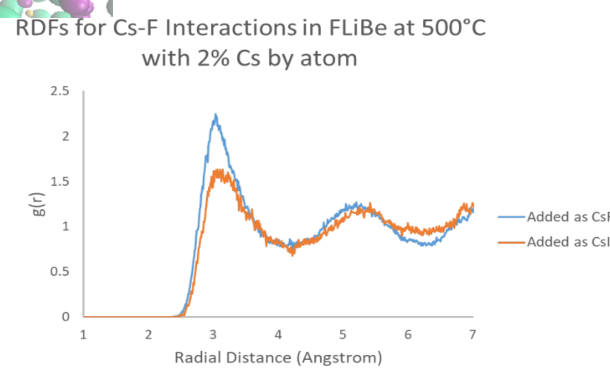


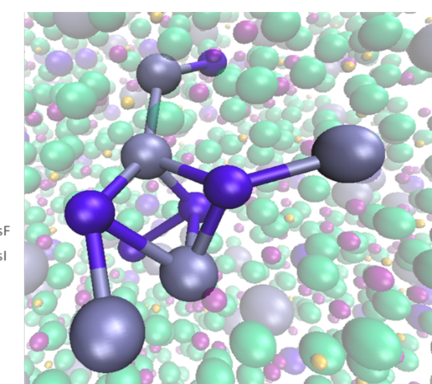
Thermophsyical Property Modeling





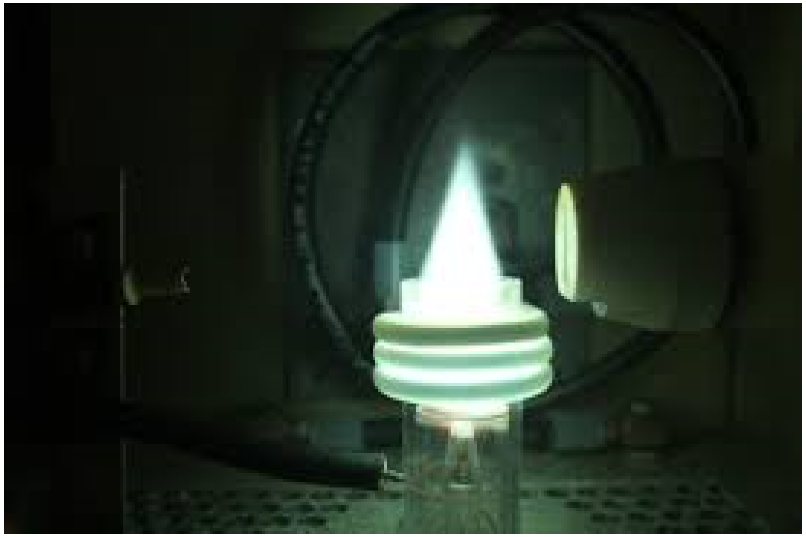
Ion-Ion Interactions





Salt Property Characterization

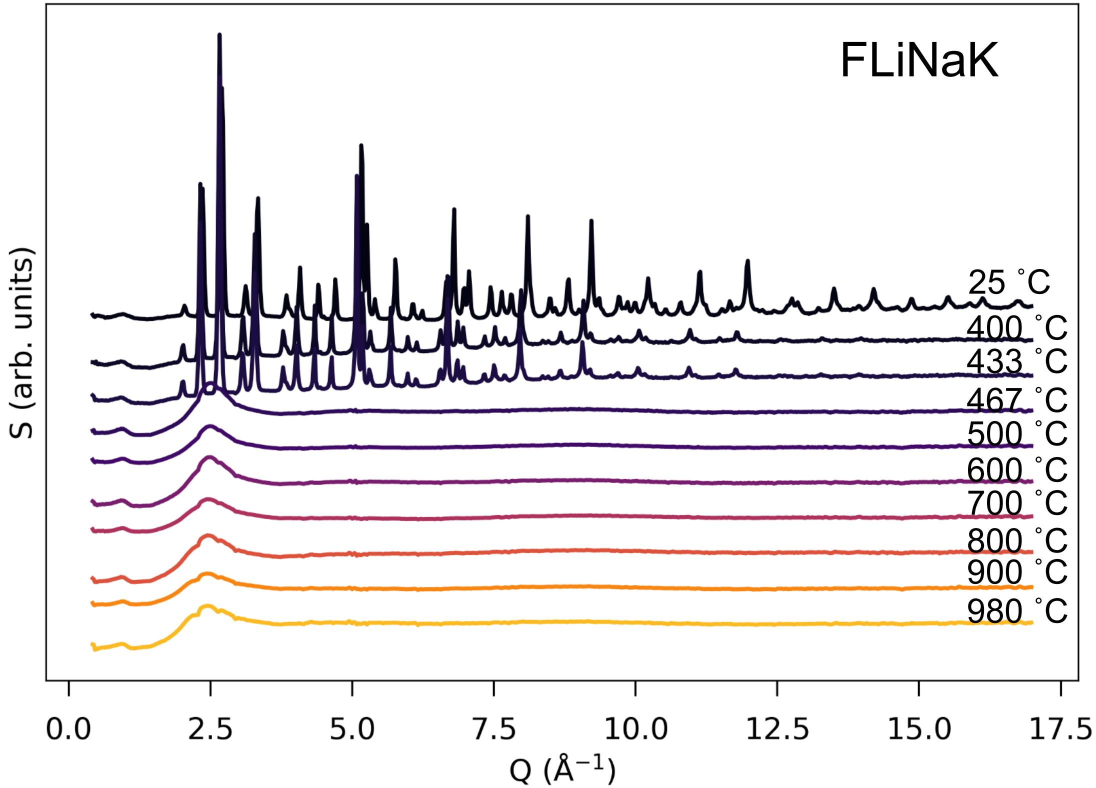
- Inductively coupled plasma
  - Common method for composition analysis
  - Can't see Hydrogen
  - Can't see Oxygen
- Need alternative method to fully characterize salts



Neutron Total Scattering Experiment on FLiNaK

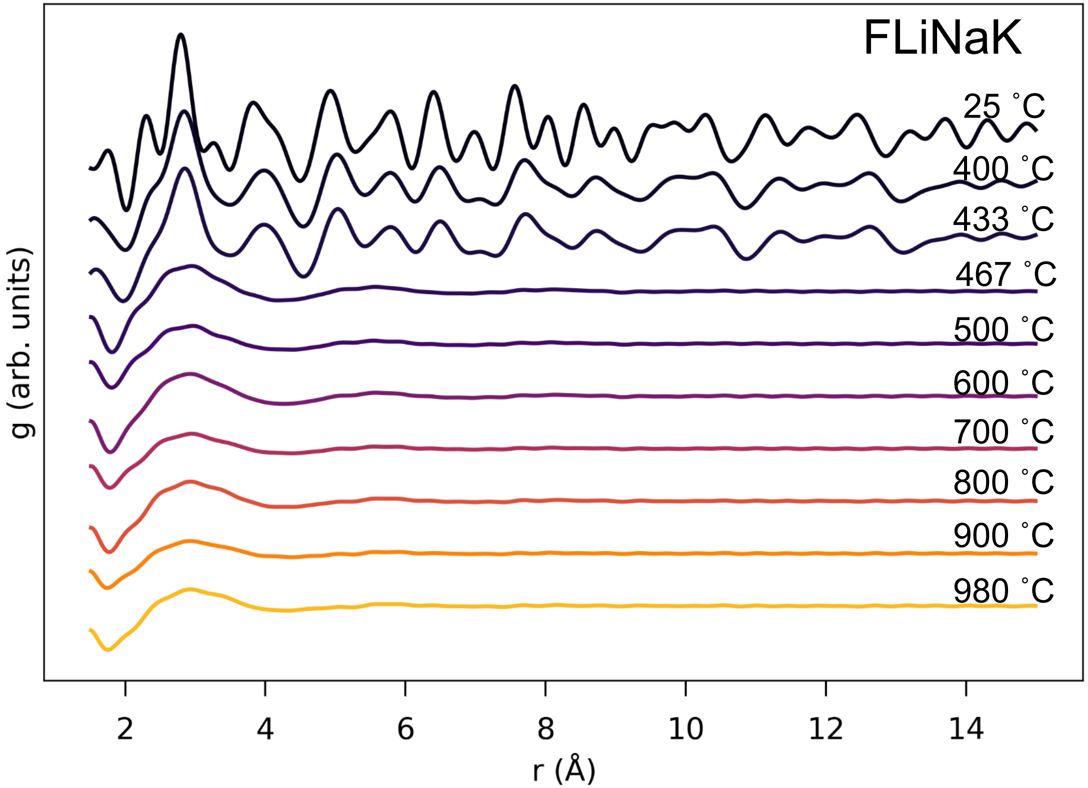
- Experiment conducted at Oak Ridge National Laboratory Spallation Neutron Source (NOMAD instrument) November 17-19, 2019
- Objective: Obtain neutron scattering data to probe the structure of the salts in both the solid and molten states, enabling quantitative comparison with simulations
- Preliminary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

Temperature Dependent Scattering Pattern



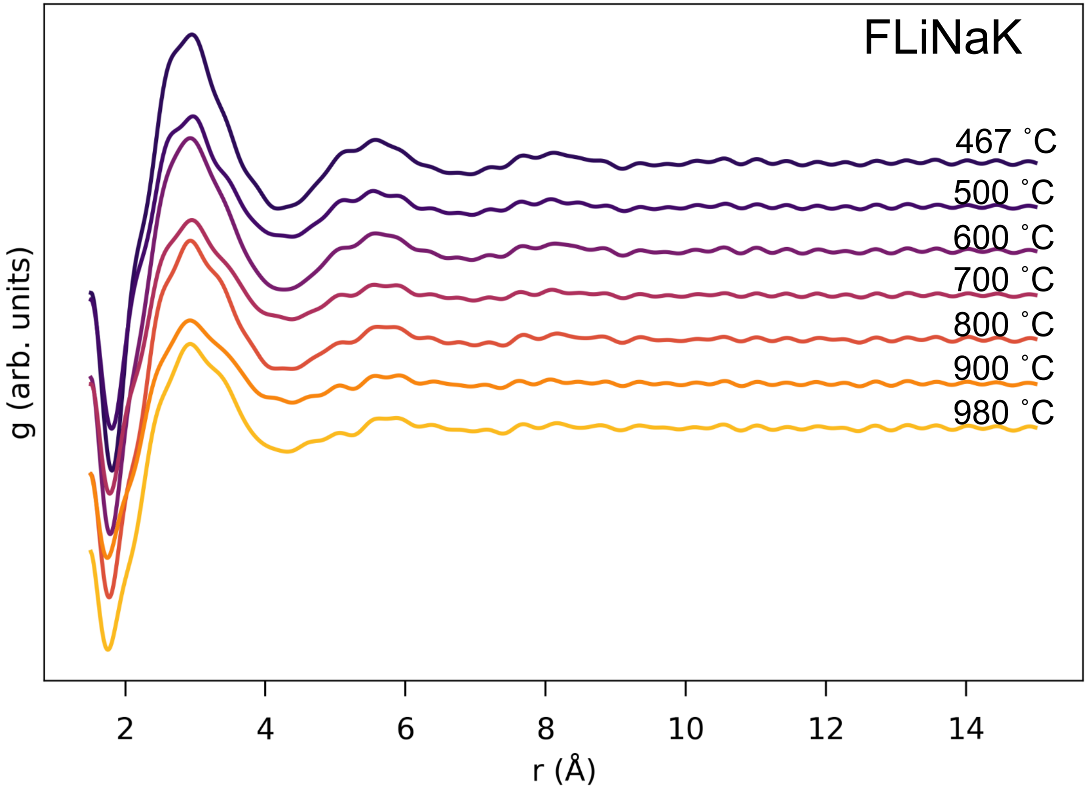
- Sharp peaks in the scattering patterns for 25 ˚C, 400 ˚C, and 433 ˚C indicate long-range structural correlations
- Diffuse features in the scattering patterns for 467 ˚C and higher indicate short-range structural correlations (but no long-range structure)
  - Consistent with the known melting point 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 Å 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 Å
- Broad features persist to 8-9 Å, 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