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Molten Salt Thermal Property Database – Thermophysical Property Overview and Tool Demonstration

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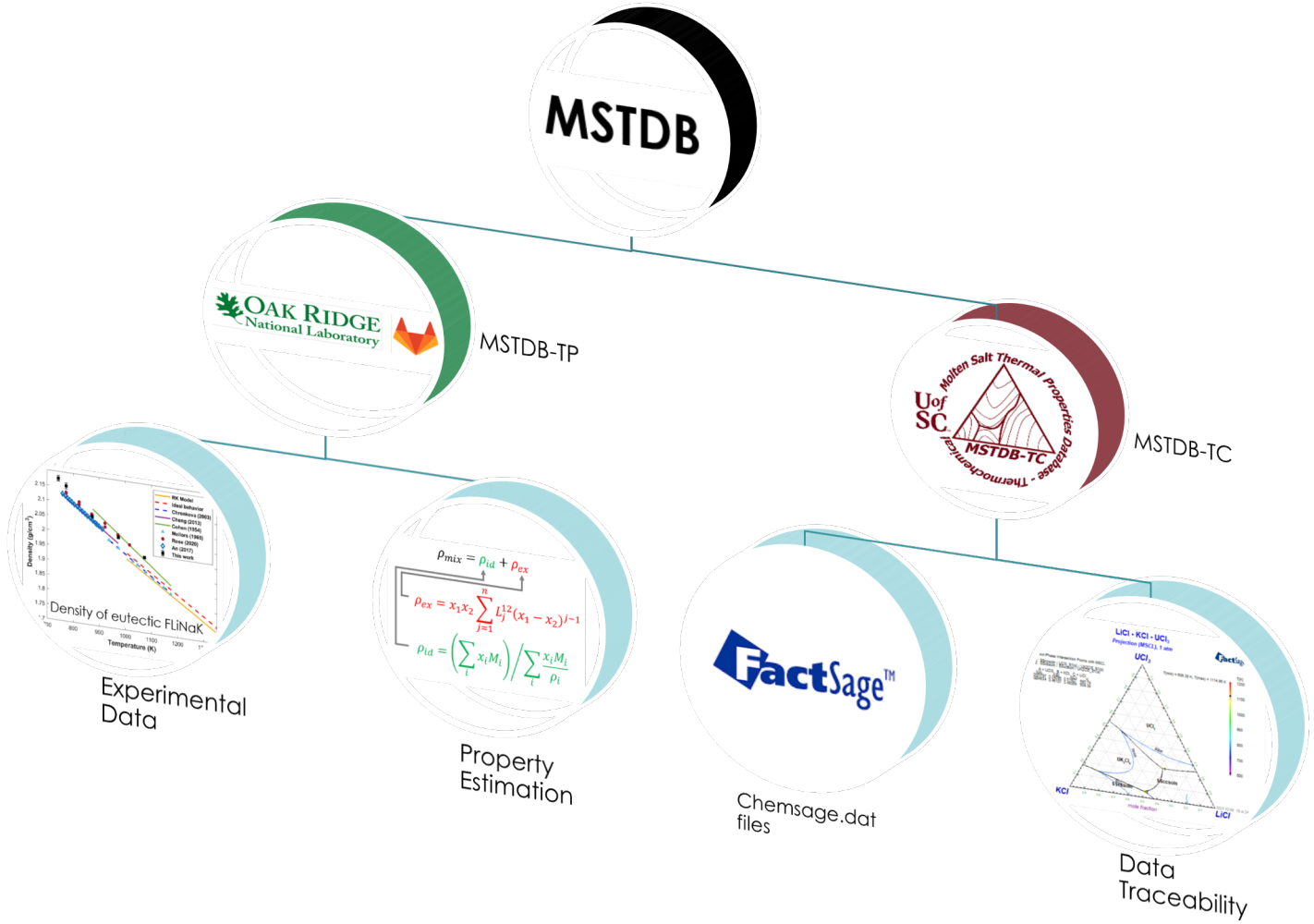
How to get Access

- The databases and associated documents are publicly hosted at: https://code.ornl.gov/neams/mstdb/
- Access instructions:
  - XCAMS account creation
    - Go to https://xcams.ornl.gov
    - Select "I need an account."
    - Read and acknowledge the User Agreement
    - Enter your email address and username following the guidelines on the page.
    - Enter "Personal Information" and "Contact Information" per the guidelines
    - Create an XCAMS password according to the guidelines provided on the page.
    - On the final step, note the activation sequence box at mid-page. Wait until each action item turns green and the box heading reads "Transactions Complete"
    - Log into https://code.ornl.gov using your new XCAMS username and password
  - Request MSTDB membership
    - Send an email to mstdb@ornl.gov with “MSTDB Access Request” as subject
    - Include your XCAMS ID and brief summary of the purpose for your request

What is MSTDB

- Molten salt thermal property database is an effort to characterize thermal properties of molten salts relevant to the nuclear industry
- MSTDB data is split into two categories (thermochemical and thermophysical) because each subsection's data is used in fundamentally different ways
  - TC requires a Gibbs Energy Minimizer to interpret the data (FactSage or Thermochimica)
  - TP data is represented by empirical relations derived from experimental data
- MSTDB-TP is managed by ORNL, and MSTDB-TC is managed by UoSC. Both section's data is hosted on ORNL gitlab servers.



NEAMS
Nuclear Energy Advanced Modeling and Simulation

Molten Salt Reactor PROGRAM

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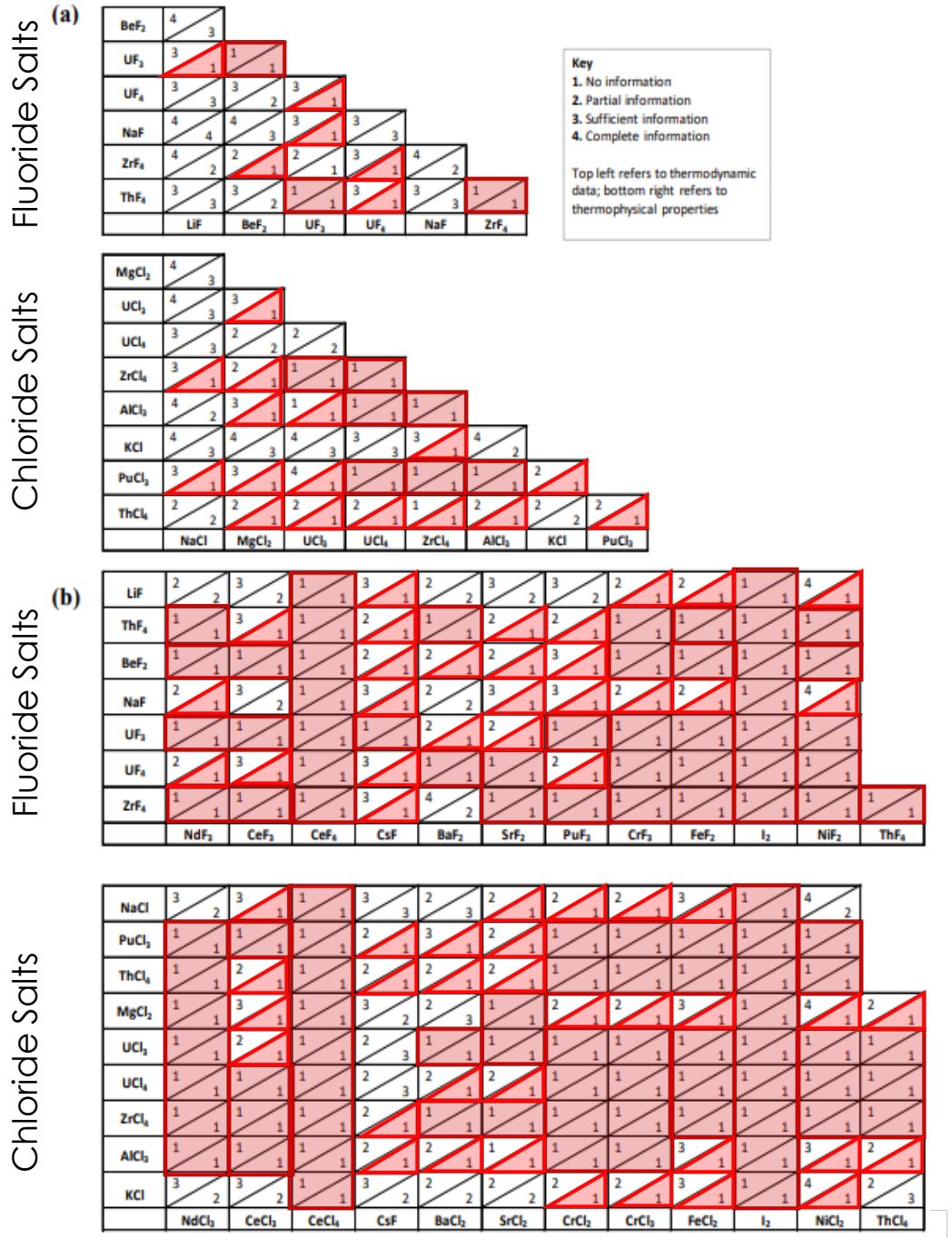
Roadmap for Molten Salt Measurements

- The collection of salts in the MSTDB is informed by a roadmap for MSR systems developed by Dr. Jake McMurray
  - From the roadmap: *"While the building blocks of MSTDB are fundamental in nature, its data facilitates constructing engineering models that allow stakeholders to investigate the behavior of specific compositions of interest and supports broader modeling and simulation of MSRs through coupling to multi-physics, multi-scale mass accountancy tools." [14]*
- The roadmap defines a list of pure compounds and a matrix of binary mixtures which need to be measured/evaluated for thermophysical/thermochemical properties
- National labs are working to fill the gaps with experimental measurements
- Ultimately, this roadmap is large, and requires strategic planning and cooperation to address the gaps present in it.



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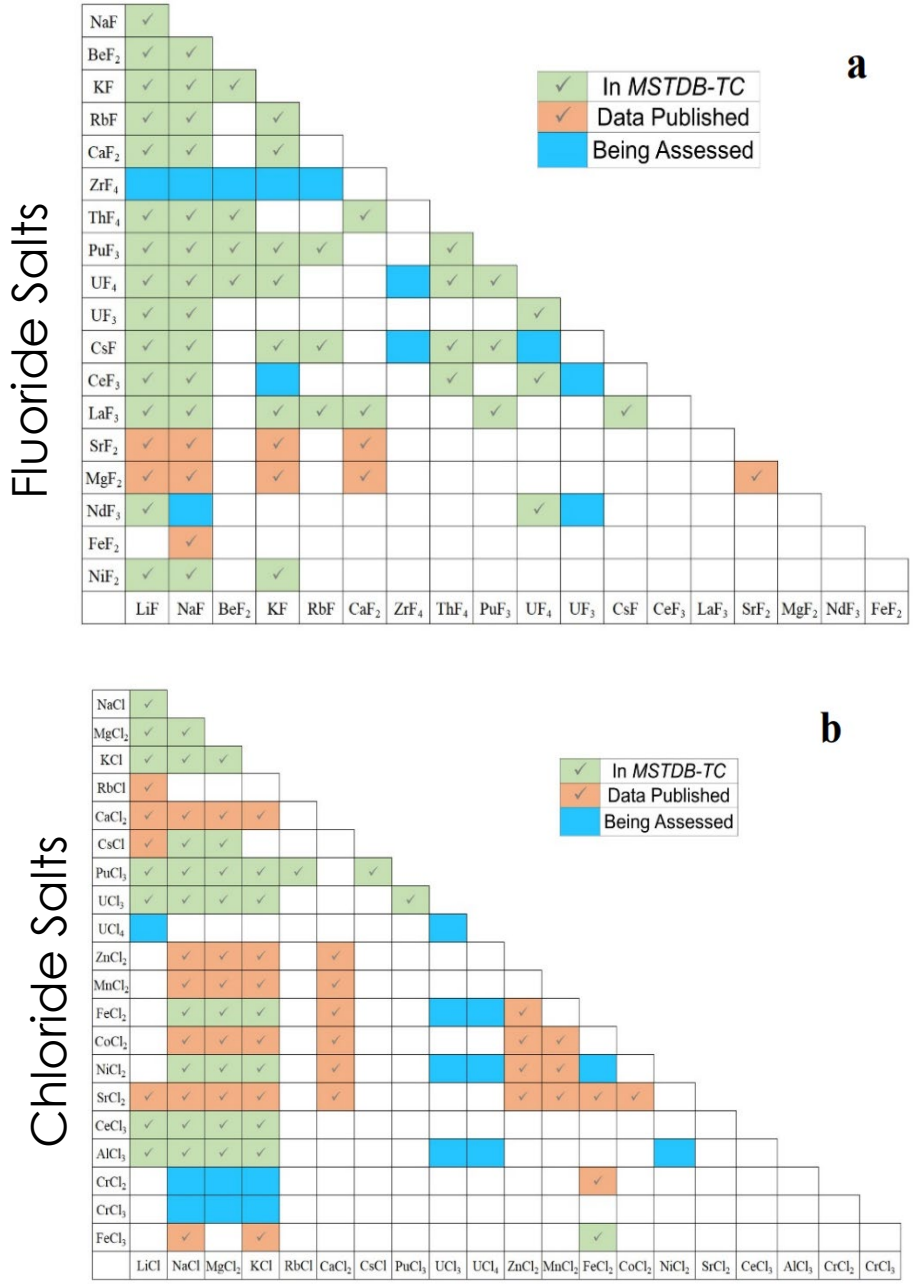
[14] https://doi.org/10.2172/1778081

MSTDB-TC Overview

- Contains Gibbs energy models and values for molten salt components and related systems of interest
- Requires Gibbs energy minimizer to process "Chemsage".dat format
  - FactSage (Licensed)
  - Thermochimica (open source)
- Allows for phase diagrams and associated values:
  - Heat capacity
  - Enthalpy of mixing
  - Vapor pressures
- More information can be found on the MSTDB-TC website



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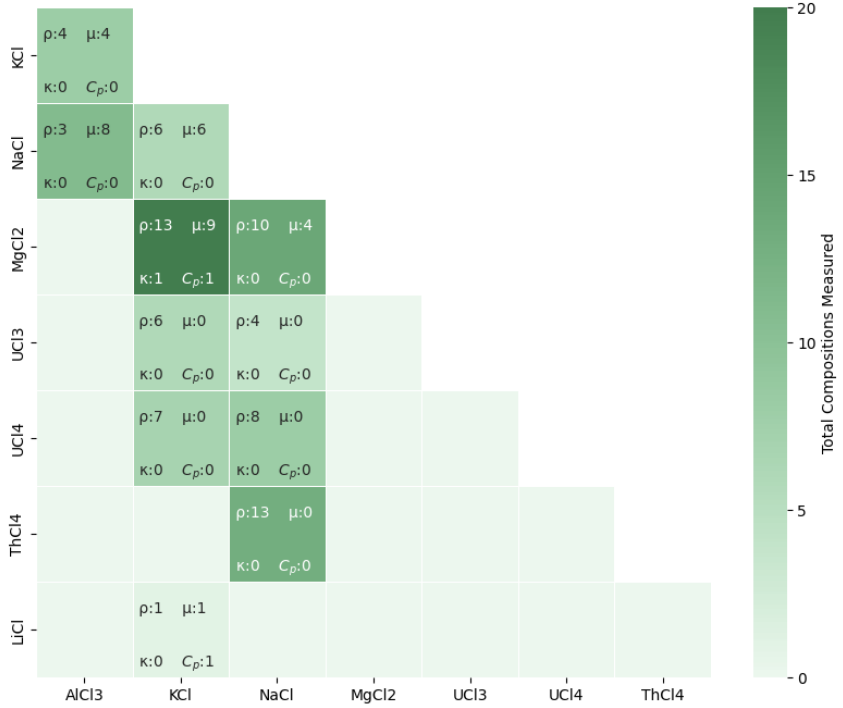
MSTDB-TP Overview

- The MSTDB-TP contains empirical relations for the following properties:
  - Melting and boiling points
  - Density
  - Viscosity
  - Heat Capacity
  - Thermal Conductivity
- As per the current version release (v2.0) There are 273 entries, including:
  - 33 pure compounds
  - 214 pseudo-binaries
  - 20 pseudo-ternaries
  - 6 pseudo-quaternaries
- Each property entry in the database includes a margin of experimental error dictated by the report or by our review process
- The data is based on the outputs of 140+ independent experimental studies.

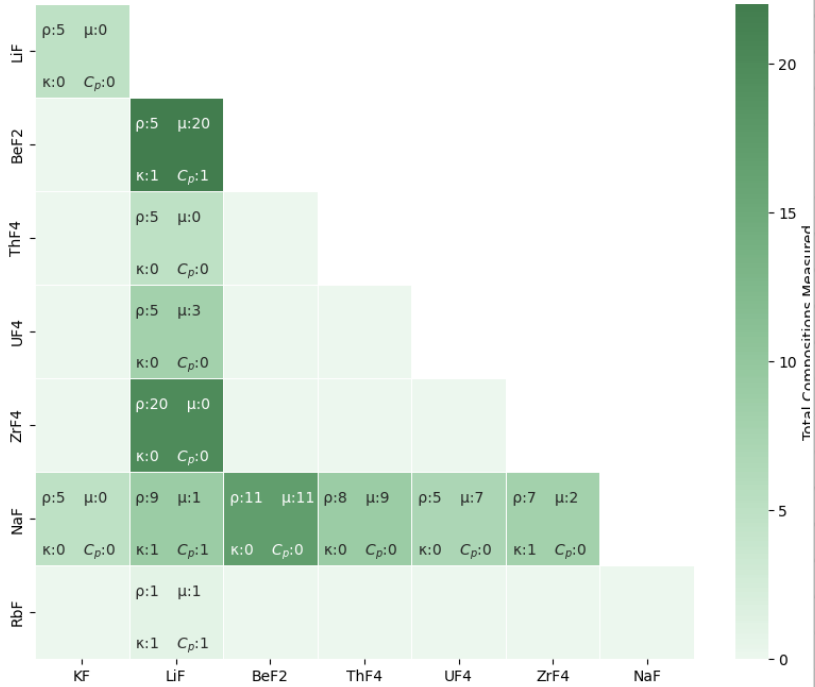
MSTDB-TP Experimental Efforts

Binaries:

Chlorides



Fluorides



Pure:

Salt	Measurements			
	ρ	μ	κ	c_p
AlCl3	1	1	0	1
BeCl2	1	0	0	1
BeF2	1	1	1	1
CaCl2	1	1	1	1
CaF2	1	1	1	1
GdCl3	1	1	0	1
GdF3	0	0	0	1
KCl	1	1	1	1
KF	1	1	1	1
LaCl3	1	1	0	1
LaF3	1	0	0	1
LiCl	1	1	1	1
LiF	1	1	1	1
MgCl2	1	1	1	1
MgF2	1	1	1	1
NaCl	1	1	1	1
NaF	1	1	1	1
NdCl3	1	1	0	1
NdF3	0	0	0	1
NpCl3	0	0	0	1
NpF3	0	0	0	1
PuCl3	0	0	0	1
PuF3	0	0	0	1
SrCl2	1	1	1	1
SrF2	1	1	1	1
ThCl4	1	0	0	1
ThF4	1	0	0	1
UCl3	1	0	0	1
UCl4	1	0	0	0
UF3	0	0	0	1
UF4	1	1	0	1
ZrCl4	1	1	0	0
ZrF4	1	0	0	0

Ternary:

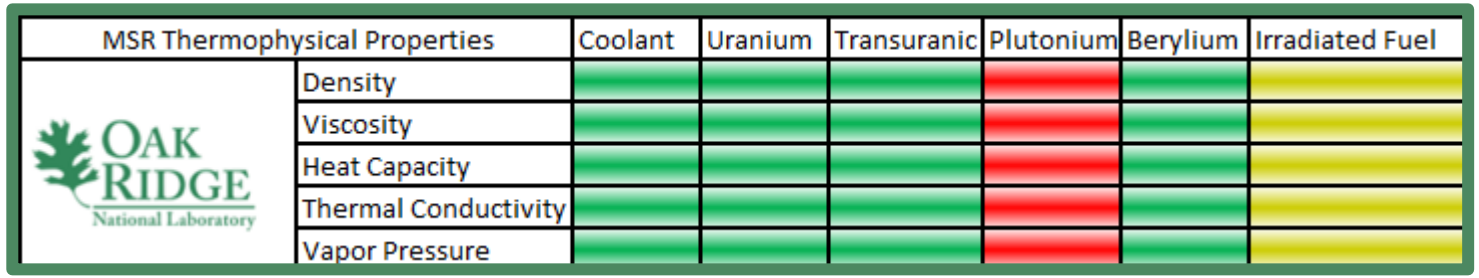
Salt	Measurements			
	ρ	μ	κ	c_p
BeF2-LiF-ThF4	3	2	0	0
BeF2-LiF-ZrF4	1	0	0	0
BeF2-LiF-NaF	5	5	1	1
KF-LiF-NaF	1	1	1	1
BeF2-KF-NaF	1	1	0	0
KF-NaF-UF4	1	1	1	1
KF-NaF-ZrF4	1	1	0	0
LiF-NaF-ZrF4	1	1	0	1
NaF-UF4-ZrF4	3	3	2	3
RbF-UF4-ZrF4	2	2	1	1

Quaternary:

Salt	Measurements			
	ρ	μ	κ	c_p
BeF2-LiF-ThF4-UF4	1	1	0	0
BeF2-LiF-UF4-ZrF4	1	0	0	0
BeF2-LiF-NaF-UF4	1	1	0	0
KF-LiF-NaF-UF4	2	2	1	1
LiF-NaF-UF4-ZrF4	1	1	0	1

National Lab Experimental Capabilities:

- Density
  - Archimedean Method*
  - Dilatometry*
  - Method of maximum bubble pressure
- Viscosity
  - Rolling Ball Method*
  - Rotational viscometry
  - Oscillation damping method
  - Capillary viscometry
- Thermal Conductivity
  - Variable gap technique*
  - Coaxial cylinder technique
  - Transient hot wire method
  - Laser flash
- Heat Capacity
  - DSC Ratio method*
  - Drop calorimetry



Institution	Property measurement capabilities	Systems of focus
Oak Ridge (ORNL)	ρ, ν, κ, Cp, p*, m.p, and compositional analysis	• U and Be bearing fluorides • U bearing Be chlorides
Argonne (ANL)	ρ, ν, κ, Cp, m.p, and compositional analysis	• Actinide and Be bearing fluorides • Actinide and Be bearing chlorides
Idaho (INL)	ρ, ν, κ, Cp, m.p, compositional analysis	• Actinide bearing chlorides • Irradiated salts
Pacific Northwest (PNNL)	ρ, ν, κ, Cp, p*, m.p, $\Delta H^{f.}$ ΔH^{mix} and compositional analysis	• U and Be bearing fluorides • U bearing chlorides
Los Alamos (LANL)	ρ, ν, κ, Cp, m.p, compositional analysis	• Actinide and Be bearing fluorides • Actinide and Be bearing chlorides

OAK RIDGE National Laboratory *indicates ORNL Capability

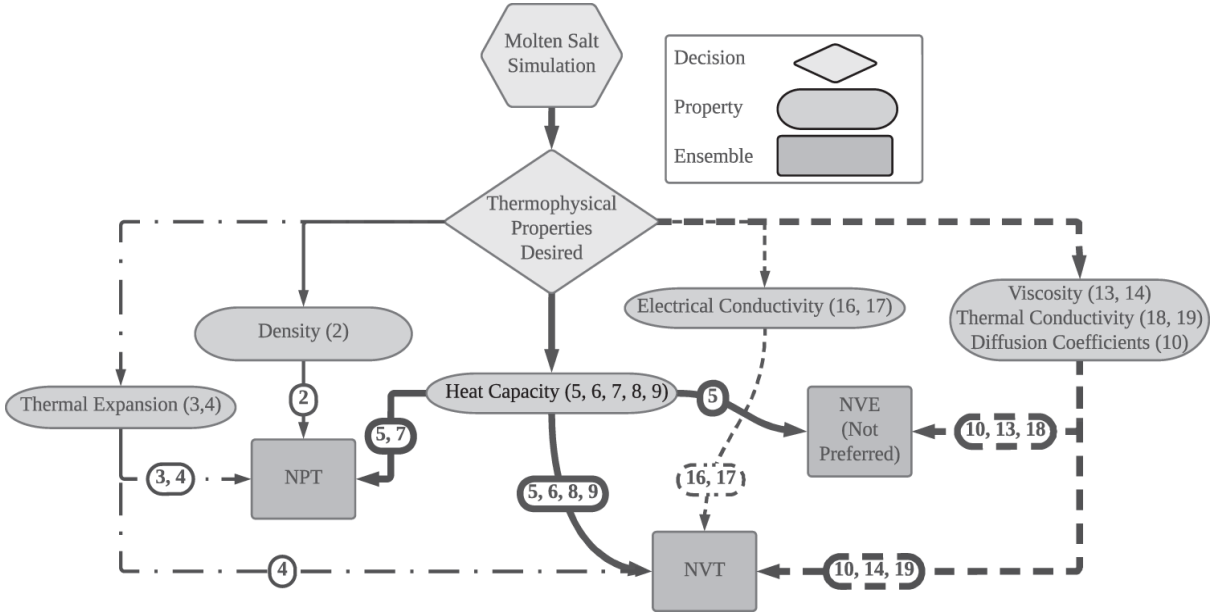
https://doi.org/10.2172/1778081

Computational Efforts:

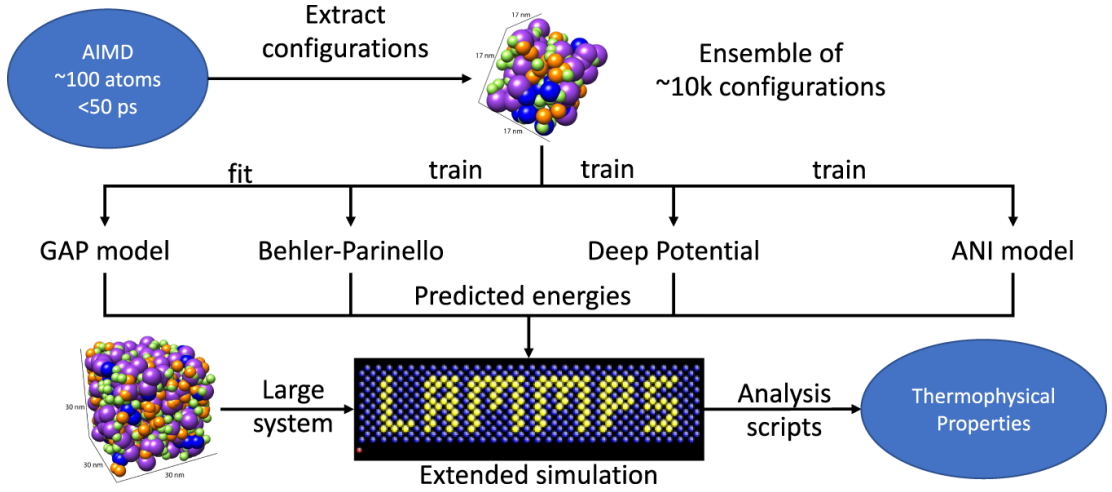
- Radiological and hazardous salts require major investment of time and money for just a single salt experimental measurement.
- Development of robust and accurate characterization of molten salts through computation methods can:
  - Flesh out compositional ranges of more experimentally characterized salts
  - Provide guidance to experiments on high interest salts for reactor development safely
- Computational techniques have two categories:
  - First principles modeling:
    - DFT-based Molecular dynamics
    - Machine Learning
  - Estimation:
    - Redlich-Kister expansion/Muggianu interpolation
    - Mixing models
- The database will clearly distinguish between experimental and synthetic data.

Computational Efforts: First Principles Modeling

- Current first principles modeling is mainly based on ab-initio molecular dynamics (AIMD)
- Size and length of simulation depends on property:
  - Short/small: density and heat capacity
  - Long/Larger: Viscosity, diffusion or thermal conductivity
- Quantifying the accuracy of models is incredibly difficult without experimental data will be difficult
  - Conservative estimates of uncertainty will be used in database for these calculations
- Advent of Machine learning may provide drastic improvements to design and use molten salts



Simulation Strategies to obtain thermophysical properties [12]



Machine learning methods for predicting molten salt properties [12]

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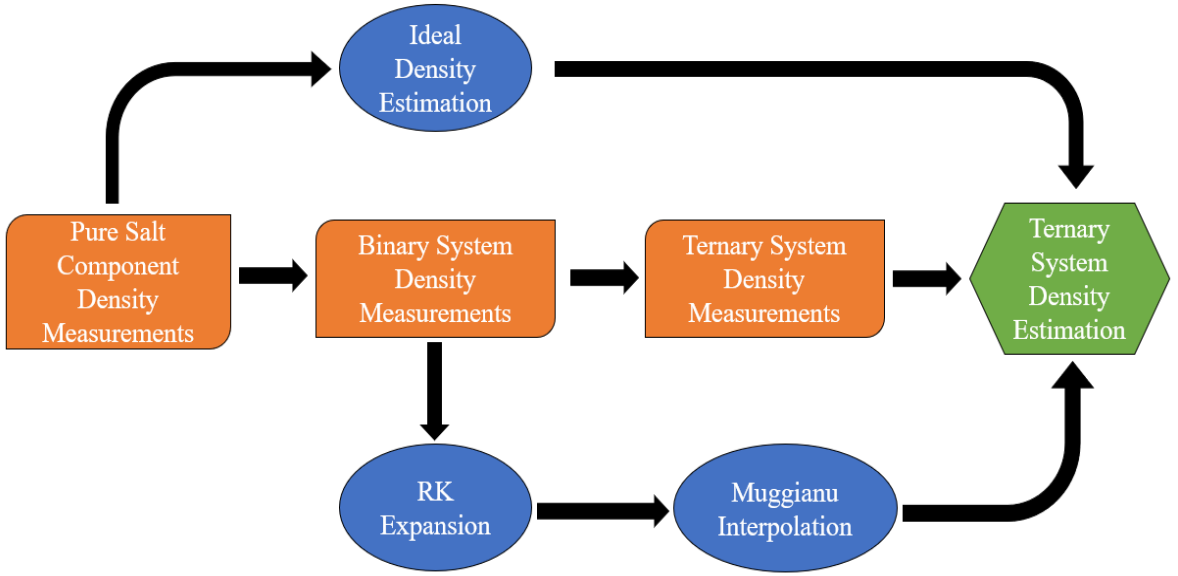
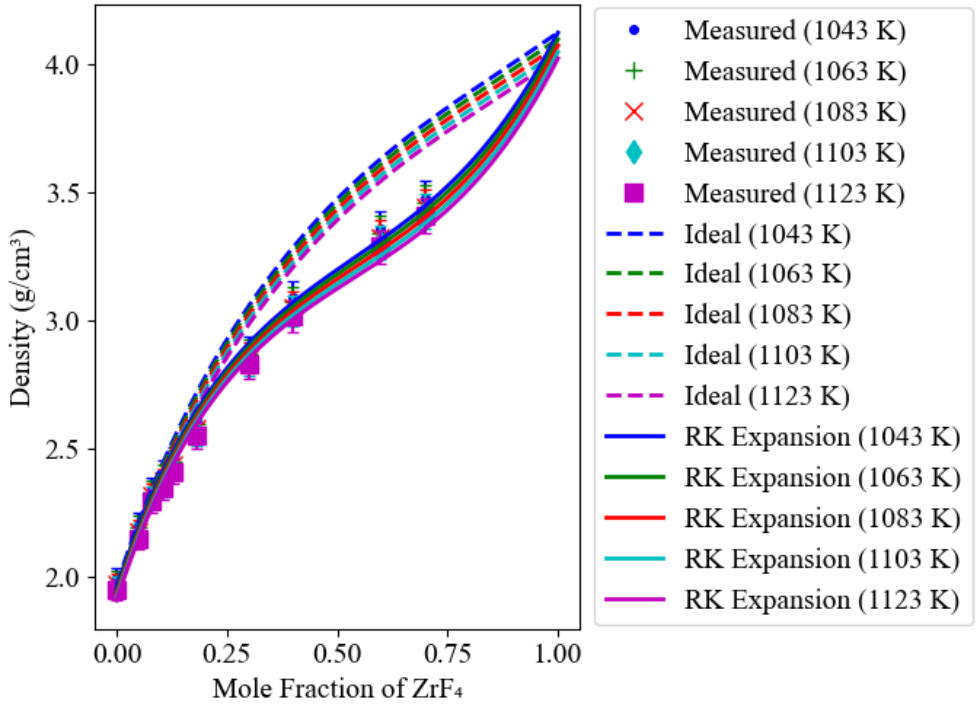
[12] https://doi.org/10.1038/s42004-022-00684-6

Computational Efforts: Estimation Techniques

- Redlich-Kister expansion allows the estimation of higher order systems based on the interactions of the lower order components
- Any composition can be estimated:
  - Can help in compositional gaps for salts
- Successfully been demonstrated for ternary systems for density [11],[12]
  - May be expanded to other properties
- Drawback:
  - Requires well characterized pseudo-binary and pure components of the ternary system.
  - Difficult to extrapolate without ternary anchor points



Obtaining ternary properties through Redlich-Kister process [11]



Measured and estimated density of NaF-LiF-ZrF4 [11].

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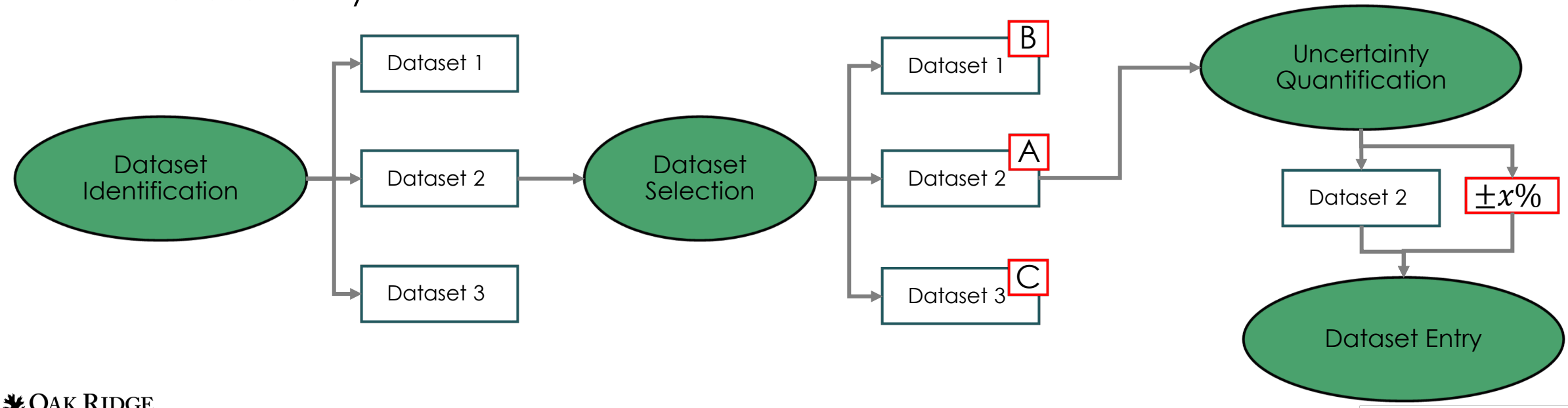
[11] https://doi.org/10.1016/j.ces.2022.117954

MSTDB-TP Review Process

- We utilize a 4-step process to populate the MSTDB-TP with thermophysical property data:
  1. Dataset Identification: Collection of multiple sources of literature which report a given thermophysical property measurement of a given system
  2. Dataset Selection: Down-selection to a particular data set which is of the highest quality
  3. Uncertainty Quantification: Assignment of experimental margin of error to the data
  4. Dataset entry



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MSTDB-TP Expansion Efforts

- New Salts:
  - New salts and relevant compositions are identified in literature and added
- New properties:
  - Surface Tension data is being processed and planned to be added to the database
- Filling in the gaps:
  - Datasets for existing systems are currently being processed to fill in the gaps in the database
  - Modeling and estimation will play a major role
- We need your input!

Saline: An API for MSTDB-TP

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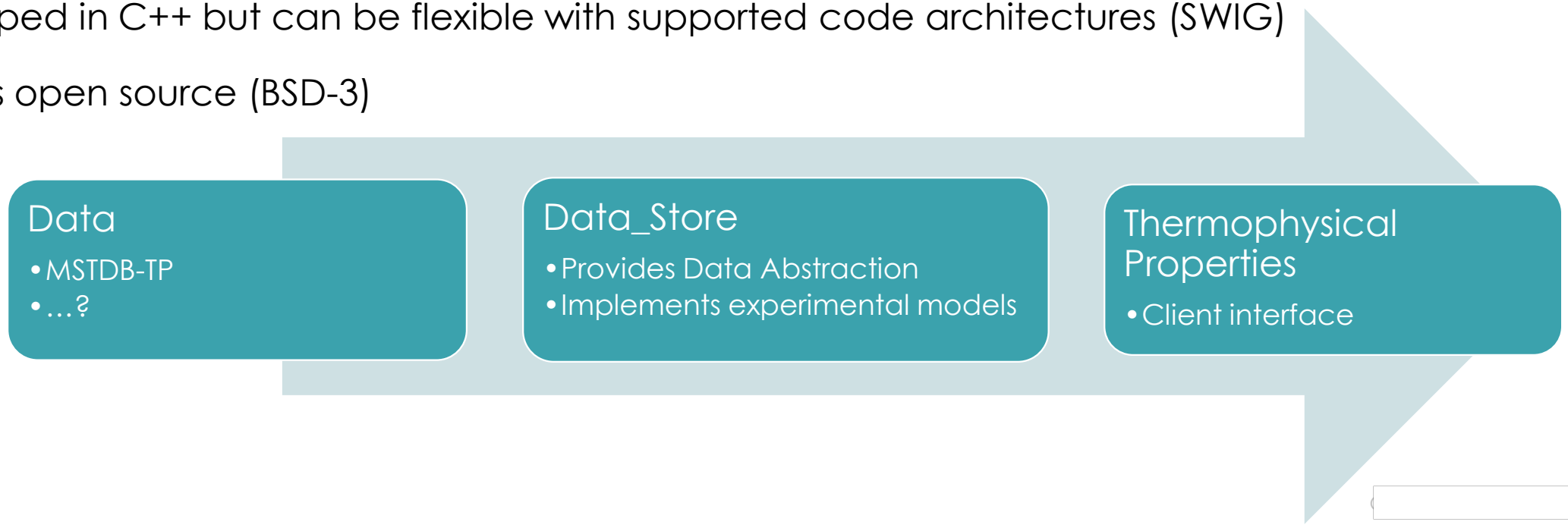
- The goal of Saline is to provide an independent interface between MSTDP-TP data and a user's code. (Safety calculations, simulations, machine learning.. etc.)
- Saline contains a list of functions to obtain supported properties in MSTDB-TP (density, viscosity, heat capacity, and thermal conductivity)
  - Can be extended to additional data models without affecting client codes
- Developed to provide estimations in the absence of experimental data through Riedlich-Kister approximations, and ideal mixing.
- Developed in C++ but can be flexible with supported code architectures (SWIG)
- Saline is open source (BSD-3)



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- We would like to acknowledge Ted Besmann for cooperation with MSTDB as Deputy Director of Structural Materials and Chemistry
- Abinitio – David Anderson (LANL)

GUI Demonstration

5.

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Questions?

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