Virtual Workshop for the
Molten Salt Thermal Properties Working Group
Host: University of South Carolina
November 15-17, 2021

Monday, November 15 **ALL TIMES ARE *EASTERN STANDARD TIME***

12:00 pm	Meeting Site Opens	
1:00 pm	**Introductions and Goals**	Ted Besmann, UofSC
	DOE MS Programs	
1:15 pm	Molten Salt Reactor Campaign	Patricia Paviet, PNNL
1:35 pm	Joint Modeling and Simulation Program	Chris Stanek, LANL
1:55 pm	Severe Accident Modeling and Analysis	David Luxat, SNL
2:15 pm	Molten Salt in Extreme Environments EFRC	Jim Wishart, BNL
2:35 pm	Molten Salt Qualification Methodology	David Holcomb, ORNL
2:45 pm	***Break***	
3:00 pm	*Molten Salt Thermal Properties Database-Thermochemical* (*MSTDB-TC*)	Ted Besmann, UofSC
3:20 pm	*Molten Salt Thermal Properties Database-Thermophysical* (*MSTDB-TP*)	Dianne Ezell, ORNL
3:40 pm	**Poster Session**	***Gather Town***
5:30 pm	***Adjourn***	

Tuesday, November 16

	Thermal property measurements	***Chair: Jake McMurray***
1:00 pm	Mixing enthalpy of $LnCl_3$ in molten chloride salts	Xiaofeng Guo Washington State U.
1:20 pm	New approaches to thermal conductivity and viscosity measurements in molten salts	Alex Bataller North Carolina State U.
1:40 pm	Thermal Conductivity Probes for Molten Salts	Troy Munro Brigham Young Univ.
2:00 pm	Density Measurements in Molten Chloride Salts by Neutron Attenuation and Comparison with Redlich-Kister Model	Joanna McFarlane ORNL
2:20 pm	Molten Salt Density and Surface Tension Measurement with Archimedes' principle	Evan Wu ANL
2:40 pm	Remote density measurements of molten salts using neutron radiography	Alexander M. Long LANL
3:00 pm	***Break***	
	Thermodynamics and macro-analysis techniques	***Chair: Markus Piro***
3:20 pm	Measurements of kinetic and thermodynamic properties of molten salt”	Jinsuo Zhang Virginia Tech.
3:40 pm	Property databases and desired data accuracy through sensitivity/uncertainty evaluations	Pavel Tsvetkov Texas A&M U.
4:00 pm	Acceptance Criteria for Heat Capacity Measurements of Molten Salts by DSC	Timothy Lichtenstein, ANL
4:30 pm	**Molten Salt Collaboration Event**	***Gather Town***
6:00 pm	***Adjourn***	

Wednesday, November 17

	Chemistry and transport phenomena	***Chair: Wilson Chiu***
1:00 pm	Progress in multi-physics simulations of salt behavior and CALPHAD modelling	Markus Piro Ontario Tech
1:20 pm	Speciation and Local Structure of NaCl-$SrCl_2$ and LiF-ZrF_4 Molten Salts by X-ray Absorption Spectroscopy and Raman Spectroscopy	Wilson K. S. Chiu U. Conn.
1:40 pm	Analyzing Nitrate Salt Aerosol using Atomic Absorption Spectroscopy and Inductively Coupled Plasma Mass Spectrometry	Alli Mae Berry Abilene Christian U.
	Ab-initio and machine learning	***Chair: Ted Besmann***
2:00 pm	Active Learning Driven Automated Parametrization of Machine Learning Forcefields for Molten Salt Melts	Jicheng Guo ANL
2:20 pm	Ab Initio Molecular Dynamics Simulations of Molten Uranium Chloride Salts	David Andersson LANL
2:40 pm	***Break***	
3:00 pm	Computational Studies of Molten Salt Components	David Dixon U. Alabama
3:20 pm	Towards Multi-Element and High Accuracy Deep Learning Potential Development and its Application to Molten Salts	Ming Hu UofSC
3:40 pm	Comparative studies of the structural and transport properties of molten salt FLiNaK using 5 machine-learned neutral network and reparametrized classical forcefields	Yang Zhang U. Illinois – Champaign-Urbana
4:00 pm	Prediction of structure and transport properties in multivalent (Be^{2+}, Zr^{4+}) cation salt mixtures using neural network interatomic potentials	Stephen Lam U. Mass. - Lowell
4:20 pm	A theoretical framework for reliable predictions of thermal conductivity of multicomponent molten salts mixtures: KCl-NaCl-MgCl2 as a case study	Aimen Gheribi Polytechnique Montreal
4:40 pm	**Results & Next Phase of Round-Robin & Wrap-up**	Raluca Scarlat UC Berkeley
5:30 pm	***Adjourn***	

The list of posters and collaboration tables/topics can be found on the following two pages.

P-1	Microrheology of molten salts using Brownian motion	Hayden Bland	North Carolina State University
P-2	Optical Spectroscopy of Molten Fluorides	Will Derdeyn	University of Wisconsin-Madison
P-3	Purification of Thorium Tetrafluoride Using the Ammonium Bifluoride Method	Bernard Fitzpatrick	Ontario Tech University
P-4	Yellowjacket: Coupling Gibbs Energy Minimisation with Phase Field Method for Corrosion Modelling in Molten Salt Reactors	Parikshit Bajpai	Ontario Tech University
P-5	Ab initio simulation of the LiCl-KCl system	Kai Duemmler	North Carolina State University
P-6	Design and implementation of an experimental setup based on the three-omega method for thermal conductivity measurements of molten salts.	Maria del Rocio Rodriguez Laguna	Idaho National Laboratory
P-7	Measuring thermal conductivity of molten salts using time domain thermo-reflectance.	Syed Rizvi	North Carolina State University
P-8	Transport Properties of LiF and FLiBe Molten Salts with DeePot Potentials	Alejandro Rodriguez	University of South Carolina
P-9	Applications of Thermochimica for Molten Salt Systems	Max Poschmann	Ontario Tech University
P-10	Purification of Uranium Tetrafluoride via Solid-state Reaction with Ammonium Bifluoride	Kyle Foster	University of South Carolina
P-11	Viscosity measurements using rotating cylinder method	Levi Gardner	Argonne National Laboratory
P-12	Predicting enthalpy of mixing for trichloride salts	Juliano Schorne-Pinto	University of South Carolina
P-13	DSC measurements for molten salts: zero rate method coupled with error propagation & examples of misinterpretation of phase transitions	Jacob Yingling	University of South Carolina
P-14	Progress in Coupling Thermochimica and OpenFOAM for MSR Applications	Nikolas Scuro	Ontario Tech University

Collaboration Event Topic Areas

T-1: *DSC/phase equilibria measurements and optimizations* – Moderator: Tim Lichtenstein

T-2: *Conductivity and viscosity measurement* – Moderator: Dianne Ezell

T-3: *Density and other physical property measurements* – Moderator: Joanna McFarlane

T-4: *First principles and ab-initio molecular dynamics* – Moderator: David Andersson

T-5: *Determining uncertainty and applying machine learning* – Moderator: Zi-Kui Liu

T-6: *Structure, bonding, and speciation* – Moderator: Jim Wishart