Agenda

Computational Approaches for Modeling Molten Salts

Molten Salt Thermal Properties Working Group

Virtual Meeting: November 10-11, 2020
Organizer: Matthew Christian (mchristi@cec.sc.edu)
University of South Carolina

November 10, 2020, Times in EST

9:30 AM	**Introduction and Goals**	Matthew Christian, U. of SC
9:40 AM	**DFT**	
9:40 AM	Prediction of the Properties of Fluorinated Compounds for Molten Salt Reactors	David Dixon, U. of AL
9:50 AM	Challenging Applications for DFT in Solid-State Chemistry	Erin Johnson, Dalhousie U.
10:00 AM	Multi-Scale Modelling of Molten Salts for Molten Salt Reactors	Matthew Christian, U. of SC
10:10 AM	Thermophysical and Transport Properties of Chloride Salts	Ben Beeler, NCSU
11:20 AM	Ab-Initio Molecular Dynamics Simulations of Actinide-Containing Molten Chloride Properties	David Andersson, LANL
10:30 AM	**Discussion : How DFT Issues Affect Salt Modeling**	Matthew Christian, U. of SC
11:00 AM	**Break**	
11:15 AM	**AIMD/MD I**	
11:15 AM	Ab Initio Molecular Dynamics Studies of MOlten Salt Mixtures (K,Li)Cl and (K,Na)Cl	Manh-Thuong Nguyen, PNNL
11:25 AM	Local Coordination Strucutrein Molten Chloride Salts from Ab Initio MD and Computational Spectroscopy	Slava Bryantsev, ORNL
11:35 AM	Key Recent Studies/Contributions for MSEE Modeling	Claudio Margulis, U. of IA
11:45 AM	Computing Melting Points of Molten Salts from Molecular Simulation	Ed Maginn, U. of Notre Dame
11:55 PM	**Discussion: AIMD or MD ? Where and Why**	David Andersson, LANL
12:25 PM	**Adjourn Day 1**	

November 11, 2020

9:30 AM	**AIMD/MD II**	
9:30 AM	AIMD Modeling of Ternary Chloride Molten ($MgCl_2$-KCl-NaCl) Salts for Concentrated Solar Power (CSP) Purposes	Kemal Ramic, Rensselaer Polytechnic
9:40 AM	First Principles Free Energies of Molten Salts by Hybrid Thermodynamic Integration	Ravishankar Sundararaman, Rensselaer Polytechnic
9:50 AM	FPMD Simulations for Accurate Description of Composition and Temperature Dependency Properties of Molten Salts	Aimen Gheribi, Polytechnique Montréal
10:00 AM	High-Throughput First-Principles Calculations and CALPHAD Modeling	Zi-Kui Liu, Penn. State U.
10:10 AM	**Discussion : MD and AIMD**	Slava Bryantsev, ORNL
10:40 AM	**Break**	
10:55 AM	**MD/Machine Learning**	
11:10 AM	Development of Spatial Density Neural Netowork Force Fields with First-Principles Level Accuracy and Potential Application to Thermodynamics and Transport	Ming Hu, U. of SC
11:20 AM	Using Chemically and Structurally Diverse Datasets to Train Robust Neural Network Interatomic Potentials	Stephen Lam, U. Mass, Lowell
11:30 AM	Comparative Studies of the Structural, Dynamic and Thermodynamic Properties of molten FLiNaK Using Machine-Learned Neural Network and Analytical Forcefields	Y Z, U. of IL
11:40 AM	Modeling Molten Salts in MSR Design and Safety Evalulation	Pavel Tsvetkov, Texas A&M
11:50 AM	Discussion : Promise and Pitfalls of Machine Learned Potentials	Matthew Christian, U. of SC
12:20 PM	**Break**	
12:30 PM	**Discussion : Experimental Feedback**	Theodore Besmann, U. of SC
1:00 PM	**Adjourn**	Theodore Besmann, U. of SC