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# Event Agenda

22nd Symposium on Thermophysical Properties & 18th International Conference on Properties of Water and Steam

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## Sun, Jun 23, 2024

4:00 PM - 8:00 PM

### Registration & Social Event

Location: Glenn Miller Ballroom of the University Memorial Center (UMC)

8:00 PM - 11:00 PM

### Evening Social

Location: TBD

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## Mon, Jun 24, 2024

8:30 AM - 10:00 AM

### Plenary 1

Location: Math100

Session Chair: Kenneth Kroenlein

#### Opening Ceremony

8:30 AM - 9:00 AM

Speaker: Kenneth Kroenlein

#### Keynote Lecture: Thermophysical Properties for Chemical Industry

9:00 AM - 10:00 AM

Speaker: Sumnesh Gupta

10:00 AM - 10:20 AM

### Coffee Break

Location: Math Plaza

10:20 AM - 12:30 PM

### Plenary 2

Location: Math100

Session Chair: Kenneth Kroenlein

#### IAPWS Gibbs Award Lecture: Thermodynamics of Water in the "Steam Engine" Climate

10:25 AM - 11:25 AM

Speaker: Rainer Feistel

#### Plenary Lecture: Understanding and Mitigating Bias in Autonomous Materials Characterization and Discovery

11:30 AM - 12:30 PM

Speaker: Jason Hattrick-Simpers

1:45 PM - 3:30 PM

### Wetting, Interfaces, Hydrates and Membranes 1: Wetting, Interfaces, and Membranes

Location: MATH100

#### The role of interaction range and buoyancy on the adhesion of vesicles

1:50 PM - 2:10 PM

Speaker: Marcus Müller

#### Comparison of Surface Tension Predictions from Butler's Method and Classical Density Functional Theory Based on Statistical Associating Fluid Theory

2:10 PM - 2:30 PM

Speaker: Le Wang

#### Effect of confinement and wetting on liquid-vapor equilibrium

2:30 PM - 2:50 PM

Speaker: Frédéric Caupin

#### Vapor-liquid Interfacial Properties of Mixtures: Experiment, Theory, and Molecular Simulation

2:50 PM - 3:10 PM

Speaker: Florian Fleckenstein

#### Scale-up of perfluoro(butenyl vinyl ether) (PBVE) and perfluoro(2,2-dimethyl-1,3-dioxole) (PDD) copolymers for the separation of R-410A

3:10 PM - 3:30 PM

Speaker: Abby Harders

1:45 PM - 2:50 PM

## Modeling and Calculations for the Power Industry 1

Location: ECCR1B40

### Proposal for the Development of a New Industrial Formulation for the Properties of Water and Steam

1:50 PM - 2:10 PM

Speaker: Matthias Kunick

### Influence of Equations of State and Mixture Models on the Design of Heat Exchangers for Supercritical Power Cycles using CO<sub>2</sub> based mixtures

2:10 PM - 2:30 PM

Speaker: Sebastian Rath

### Sulfuric Acid Dew Point for Gas Turbine Combined Cycle Power Plants

2:30 PM - 2:50 PM

Speaker: Nobuo Okita

1:45 PM - 3:30 PM

## Properties of Working Fluids Including Refrigerants 1: Measurements I

Location: ECCR265

### Dew-point/bubble-point measurements for HFC/HFO refrigerant mixtures

1:50 PM - 2:10 PM

Speaker: Yohei Kayukawa

### Bubble-Point Measurements of Three Mixtures of cis-1,1,1,4,4,4-hexafluorobutene (R-1336mzz(Z)) + trans-1,2-dichloroethylene (R-1130(E))

2:10 PM - 2:30 PM

Speaker: Stephanie L. Outcalt

### Vapor-Liquid Equilibrium Measurements of Binary Refrigerant Blends R1234yf + R1123, R1132(E), R32, and R1243zf

2:30 PM - 2:50 PM

Speaker: Naoya Sakoda

### Experimental Compressed Liquid Density Measurements and Correlation of the Binary Mixture {3,3,3-trifluoropropene (R1243zf) + isobutane (R600a)}

2:50 PM - 3:10 PM

Speaker: Davide Menegazzo

### Liquid (p-rho-T) Measurements of R1130(E)

3:10 PM - 3:30 PM

Speaker: Tara Fortin

1:45 PM - 3:30 PM

## Physical Chemistry of Aqueous Systems 1: Thermodynamics and Transport Properties

Location: ECCR200

### A Revised Formulation for the Ionization Constant of Water over a Wide Range of Temperatures and Densities, Including Near-Critical Conditions

1:50 PM - 2:10 PM

Speaker: Hugues Arcis

### Improvements in Internal Consistency of Inorganic Thermodynamic Data at 298.15 K

2:10 PM - 2:30 PM

Speaker: D. Kirk Nordstrom

### The Observation of Molecular Symmetry Evolutions in Extremely Supersaturated Aqueous Solution

2:30 PM - 2:50 PM

Speaker: Yong Chan Cho

### Equilibria of Aqueous Solutions of Disodium Terephthalate, Terephthalic Acid, and Compressed Carbon Dioxide for Separations

2:50 PM - 3:10 PM

Speaker: Diego Trevisan Melfi

### Protein Diffusion in Aqueous Solution for Revealing Spectrally Silent Conformation Change

3:10 PM - 3:30 PM

Speaker: Masahide Terazima

1:45 PM - 3:30 PM

## Properties of Metastable, Nucleating, and Glassy Systems 1: Supercooled Liquids

Location: ECCR245

### Refractive Index of Supercooled Water between 535 nm and 670 nm

1:50 PM - 2:30 PM

Speaker: Claudia Goy

### New First Principles Based Water Model Predicts Liquid Water Anomalies in the Supercooled Regime in Good Agreement with Experiments

2:30 PM - 2:50 PM

Speaker: Feng Wang

### Density of Supercooled Waters - Overview of Measurements using Dual-capillary Dilatometer

2:50 PM - 3:10 PM

Speaker: Aleš Blahut

### No Structural Transitions in Solid Fe

3:10 PM - 3:30 PM

Speaker: Geun Woo Lee

1:45 PM - 3:10 PM

## Theory of Thermophysical Properties 1

Location: ECCR 105

### Virial Equation of State Using Volume-Dependent Coefficients

1:50 PM - 2:10 PM

Speaker: David Kofke

### Accounting for Intra-molecular Hydrogen-bond Formation in Modeling Aqueous Solutions of Glycine Homopeptide Using the SAFT- $\gamma$ Mie Equation of State

2:10 PM - 2:30 PM

Speaker: Shubhani Paliwal

### Molecular association in the chemical and the physical picture: pure fluids, binary mixtures and ionic solutions

2:30 PM - 2:50 PM

Speaker: Wolfram Schröder

### Prediction of Transport Coefficients in Dense, Cryogenic Gases using Revised Enskog Theory

2:50 PM - 3:10 PM

Speaker: Vegard Gjeldvik Jervell

1:45 PM - 3:30 PM

## Fluid Property Measurements 1

Location: BESC180

### Measuring and modelling of water dew points in with hydrogen enriched natural gas

1:50 PM - 2:30 PM

Speaker: Christoph Sulberg

### Freeze-out Measurements of Impurities in Hydrogen with a Microwave Resonant Cavity

2:30 PM - 2:50 PM

Speaker: Emma Bond

### First Results of Density and Dielectric Virial Coefficients of Hydrogen

2:50 PM - 3:10 PM

Speaker: Mathis Manzel

### Density and Speed of Sound Measurements in (H<sub>2</sub> + n-Butane) for Decarbonizing the Gas Grid

3:10 PM - 3:30 PM

Speaker: David Vega-Maza

3:30 PM - 3:50 PM

## Coffee Break

Location: Math Plaza

3:50 PM - 5:35 PM

## Non-Equilibrium Thermodynamics 1: Computational and Theoretical Methods for Non-Equilibrium Systems

Location: ECCR1B40

### Nonequilibrium Steady States: Theory and Simulation

3:55 PM - 4:35 PM

Speaker: Debra J. Bernhardt

### Effective Emerging Interactions and Ordered Phases in Active Suspensions

4:35 PM - 4:55 PM

Speaker: Ignacio Pagonabarraga

### Non-equilibrium Grand-canonical Molecular Dynamics Simulations in the Adaptive Resolution Method

4:55 PM - 5:15 PM

Speaker: Robin Cortes-Huerto

### Stochastic Thermodynamics of Silicon Nanostructures

5:15 PM - 5:35 PM

Speaker: Albert Beardo

3:50 PM - 5:35 PM

## Wetting, Interfaces, Hydrates and Membranes 2: Hydrate Kinetics

Location: MATH100

### Dependence of gas hydrate formation kinetics on system-size and kinetic inhibitor concentration from stirred lag time experiments

3:55 PM - 4:15 PM

Speaker: Chenglong Li

### Experimental Indication of Regimes of Heterogeneous and Homogeneous Nucleation of Carbon Dioxide Gas-Hydrates

4:15 PM - 4:35 PM

Speaker: Bernd Rathke

### Growth rate of CO<sub>2</sub> and CH<sub>4</sub> hydrates by means of molecular dynamics simulations

4:35 PM - 4:55 PM

Speaker: Samuel Blázquez

### Novel Pipeline Materials for Managing Hydrate Formation

4:55 PM - 5:15 PM

Speaker: Bruce Norris

### Hydrate Agglomeration in Oil-Dominated Systems at Different Driving Forces

5:15 PM - 5:35 PM

Speaker: Jose Delgado

3:50 PM - 5:35 PM

## Properties of Working Fluids Including Refrigerants 2: Measurements II

Location: ECCR265

### Viscosity Measurements of Binary Mixtures of Difluoromethane (R-32) and 2,3,3,3-Tetrafluoropropene (R-12324yf) Refrigerants and Their Empirical Models

3:55 PM - 4:15 PM

Speaker: Monjur Morshed

### Speed of sound measurements on select ternary refrigerant mixtures

4:15 PM - 4:35 PM

Speaker: Karim Al-Barghouti

### Measurement and Correlation of Dielectric Permittivity for Difluoromethane (R32) with a Microwave Cavity Resonator

4:35 PM - 4:55 PM

Speaker: Taka-aki Hoshina

### Freezing Point Temperature Measurements of Lower GWP Alternative Mixtures for Ultra-low Temperature Refrigeration

4:55 PM - 5:15 PM

Speaker: Sebastiano Tomassetti

### Measurements and Modeling of Binary Adsorption for Separating Refrigerant R-410A

5:15 PM - 5:35 PM

Speaker: Andrew Yancey-Jardon

3:50 PM - 5:35 PM

## Physical Chemistry of Aqueous Systems 2: High Temperatures-High Pressures, Electrochemistry, and Corrosion

Location: ECCR200

### High Pressure, High Temperature Rotating Cylinder Electrode for Electrochemical Corrosion Studies in Flowing Systems.

3:55 PM - 4:15 PM

Speaker: Andrei Yermalayeu

### Electrochemical and Fluid Properties of Electrolyte Solutions in All-Vanadium Redox Flow Batteries

4:15 PM - 4:35 PM

Speaker: Jana HeiB

### Microscopic Investigations towards the Practical Implementation of Film Forming Amines as Corrosion Inhibitors in High-Temperature Aqueous Systems

4:35 PM - 4:55 PM

Speaker: Ken Yoshida

### Hydrolysis of Trivalent Lanthanides at High Temperatures and Pressures

4:55 PM - 5:15 PM

Speaker: Essmaïl Djamali

### Gibbs Energy Local Basis Function Representations for Aqueous NaCl and Ammonia-Water Solutions to 10 GPa and 2000 K

5:15 PM - 5:35 PM

Speaker: J. Michael Brown

3:50 PM - 5:35 PM

## Photothermal and Photoacoustic Thermophysics 1: Novel Phenomena and Applications

Location: ECCR135

### Phonon-Polariton Thermal Waves

3:55 PM - 4:35 PM

Speaker: Jose Ordonez-Miranda

### Thermophysical Properties Characterization based on ET-Raman and FET-Raman: Down to nm size

4:35 PM - 4:55 PM

Speaker: Xinwei Wang

### Thermal Transport in Biopolymers with Borax as Crosslinking Agent

4:55 PM - 5:15 PM

Speaker: Juan José Alvarado-Gil

### Joule Effect in Electrically Aligned CNFs: Towards Ultrafast Heating of Liquids

5:15 PM - 5:35 PM

Speaker: Juan José Alvarado-Gil

3:50 PM - 4:55 PM

## Fluid Property Measurements 2

Location: BESC180

### Cryogenic Speeds of Sound of Gaseous Mixtures of Hydrogen for the Hydrogen Liquefaction Process

3:55 PM - 4:15 PM

Speaker: Subash Dhakal

### Density measurements of hydrogen-isobutane and hydrogen-pentane mixtures

4:15 PM - 4:35 PM

Speaker: Raffaella Romeo

### Wide-ranging Speed of Sound Measurements in Supercritical Helium at High Pressures

4:35 PM - 4:55 PM

Speaker: Tobias Dietl

3:50 PM - 5:55 PM

## Theory of Thermophysical Properties 2

Location: ECCR 105

### Combining Theoretical Tools to Characterize the Thermophysical Profile of Deep Eutectic Solvents for CO<sub>2</sub> and F-Gas Capture Applications

3:55 PM - 4:35 PM

Speaker: Fèlix Llovel

### Time-dependent Surface Properties of a Quaternary Mixture for an Esterification Reaction in Reactive Distillation

4:35 PM - 4:55 PM

Speaker: Sabine Enders

### On the Continuity of the Equation of State of Fluid and Solid Phases

4:55 PM - 5:15 PM

Speaker: Gustavo Chaparro

### Predicting Phase Behavior and Obtaining Molecular-level Insight Using the Solubility Parameter Method MOSCED: Entrainer Selection, Solubility Enhancement, and Beyond!

5:15 PM - 5:35 PM

Speaker: Andrew Paluch

### The State of the Art in Entropy Scaling Applied To Transport Property Modeling

5:35 PM - 5:55 PM

Speaker: Ian Bell

3:50 PM - 5:35 PM

## Properties of Metastable, Nucleating, and Glassy Systems 2: Nucleation

Location: ECCR245

### Non-Classical Vapor and Ice Nucleation from Metastable Water

3:55 PM - 4:15 PM

Speaker: Rakesh S. Singh

### Homogeneous Nucleation of Water Droplets: Role of the Real Gas Behavior of the Vapor-carrier Gas Mixture

4:15 PM - 4:35 PM

Speaker: Jan Hrubý

### Homogeneous Nucleation Rate of Methane and Carbon Dioxide Hydrates Formation under Experimental Conditions from Seeding Simulations

4:35 PM - 4:55 PM

Speaker: Felipe Blas

### Extreme Value Statistics of Heterogeneous Ice Nucleation and Applications in Supercooled Biopreservation

4:55 PM - 5:15 PM

Speaker: Tony Consiglio

### The Phenomenon of Superheat: to the 100th Anniversary of Wismer's Pioneering Experiments

5:15 PM - 5:35 PM

Speaker: Pavel Skripov

7:30 PM - 9:15 PM

### Physical Chemistry of Aqueous Systems 3: Thermodynamic Modeling

Location: ECCR200

#### **A Novel Standard Gibbs Energy of Formation Model for High-Enthalpy Water Systems**

7:35 PM - 7:55 PM

Speaker: Derek Hall

#### **Modeling Speciation and Phase Equilibria of Aqueous Boric Acid and Metal Borates from Ambient to Hydrothermal Conditions**

7:55 PM - 8:15 PM

Speaker: Andre Anderko

#### **A Thermodynamically Sound and Numerically Robust Modelling Framework for Mixed Aqueous Electrolyte Solutions and for Redefining pH**

8:15 PM - 8:35 PM

Speaker: Eric May

#### **Quantifying Ion-Ion Association in Mixed Electrolyte Systems using Bulk Thermodynamic Experimental Data**

8:35 PM - 8:55 PM

Speaker: Elizabeth Ploetz

#### **PVTx Thermodynamic Modeling of Aqueous Solutions and Applications for Isochoric Cryopreservation**

8:55 PM - 9:15 PM

Speaker: Tony Consiglio

7:30 PM - 9:15 PM

### Theory of Thermophysical Properties 3

Location: ECCR 105

#### **Something New in Thermodynamics: Excess Properties and Density Fluctuations from Free Energy Perturbation Theories for Polar, Polarizable, and Associating Molecules**

7:35 PM - 7:55 PM

Speaker: Walter G. Chapman

#### **Spectroscopic Quantification of Cooperative Bonding of Alcohols**

7:55 PM - 8:15 PM

Speaker: Carl Lira

#### **Modeling Thermodynamic and Transport Properties of Hydrogen-Containing Mixtures**

8:15 PM - 8:35 PM

Speaker: Fufang Yang

#### **Towards Transferable User-Friendly Machine Learning for thermophysical Property Prediction**

8:35 PM - 8:55 PM

Speaker: Frank Mtetwa

#### **Entropy Scaling Framework for Modeling Transport Properties using Molecular-based Equations of State**

8:55 PM - 9:15 PM

Speaker: Dennis Alt

7:30 PM - 8:55 PM

### Non-Equilibrium Thermodynamics 2: Foundations and Interdisciplinary Applications

Location: ECCR1B40

#### **The Coming of Age of Nonlinear Response Theory: Rheology and Tribology at Experimentally Accessible Rates of Strain**

7:35 PM - 7:55 PM

Speaker: Billy Todd

#### **Non-equilibrium Thermodynamics of Active Particles Self-assembly**

7:55 PM - 8:15 PM

Speaker: Miguel Rubi

#### **Size-effects in Polymer Stretching**

8:15 PM - 8:35 PM

Speaker: Sondre K. Schnell

#### **Kinetic Description of Viral Self-assembly using Mesoscopic Nonequilibrium Thermodynamics**

8:35 PM - 8:55 PM

Speaker: David Reguera

7:30 PM - 8:55 PM

### Properties of Metastable, Nucleating, and Glassy Systems 3: Anomalies of Metastable Liquids

Location: ECCR245

#### Deciphering the Breakdown of the Stokes-Einstein Relation in Supercooled Water and Aqueous Solution using Translational Jump-diffusion Approach

7:35 PM - 7:55 PM

Speaker: Snehasis Daschakraborty

#### Anomalies of Heavy Water at Negative Pressure

7:55 PM - 8:15 PM

Speaker: Frédéric Caupin

#### Peculiar Thermodynamics of Interconverting Species

8:15 PM - 8:35 PM

Speaker: Mikhail A. Anisimov

#### Extrapolation into the Meta and Unstable Regions of the Phase Diagram of Fluids

8:35 PM - 8:55 PM

Speaker: Morten Hammer

7:30 PM - 9:15 PM

### Photothermal and Photoacoustic Thermophysics 2: Non-Destructive Methodologies

Location: ECCR135

#### Advances in Photothermal Science and Techniques: A Route for NDT from Macro to Nanoscale

7:35 PM - 7:55 PM

Speaker: Roberto Li Voti

#### Simultaneous Density and Thermal Conductivity Depth Profile Reconstructions from Noised Thermal-wave Amplitude and Phase Data using a Combined Integral-equation and Imperialist Competitive Algorithm Method

7:55 PM - 8:15 PM

Speaker: Andreas Mandelis

#### Three-dimensional Super-resolution Crack Imaging in Industrial Manufactured Components: A Truncated Correlation Photothermal Coherence Tomography Approach

8:15 PM - 8:35 PM

Speaker: Andreas Mandelis

#### First QEPAS Measurements on Solid Samples

8:35 PM - 8:55 PM

Speaker: Judith Falkhofen

#### Thermal Characterization by Front Flash Laser of Composites Loaded with Graphite Rod Inclusions and the Influence of their Distribution on the Thermal Properties

8:55 PM - 9:15 PM

Speaker: Juan José Alvarado-Gil

7:30 PM - 9:15 PM

### Fluid Property Measurements 3

Location: BESC180

#### Early Solid Detection Sensor for Production Line Monitoring

7:35 PM - 8:15 PM

Speaker: Frederik Hahn

#### Adiabatic Calorimetry of Hydrocarbons Presented as a Combination of the Simplest Mixtures of the Gas-Condensate Hydrocarbon System

8:15 PM - 8:35 PM

Speaker: Valery Buleiko

#### Isochoric Heat Capacity Measurements of Multicomponent Mixtures for Natural Gas at Temperatures from (77 to 340) K

8:35 PM - 8:55 PM

Speaker: Jintao Xie

#### Solid-Fluid Equilibrium Measurements of Benzene in Mixed Solvents & Hydrogen Sulfide in Methane

8:55 PM - 9:15 PM

Speaker: Wanying Wu

9:00 PM - 11:00 PM

### Evening Social

Location: TBD

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Tue, Jun 25, 2024

8:30 AM - 10:15 AM

### Non-Equilibrium Thermodynamics 3: Thermodiffusion

Location: ECCR1B40

#### **Soret Vector for Description of Multicomponent Mixtures**

8:35 AM - 8:55 AM

Speaker: Valentina Shevtsova

#### **Diffusion and Thermodiffusion of CO<sub>2</sub> Mixtures at the Extended Critical Region**

8:55 AM - 9:15 AM

Speaker: Gabriela Guevara Carrion

#### **DCMIX4 Microgravity Experiment Evaluation of C<sub>60</sub>-THN-Tol Ternary Mixtures**

9:15 AM - 9:35 AM

Speaker: Ane Errarte

#### **A Double-pass Optical Beam Deflection Instrument for the Measurement of Diffusion, Thermodiffusion and Soret Coefficients in Liquid Mixtures and its Application to Polymer Analysis**

9:35 AM - 9:55 AM

Speaker: Roman Reh

#### **The Working Limit Conditions for the FJO Theory**

9:55 AM - 10:15 AM

Speaker: Antton Sanjuan Esnaola

8:30 AM - 9:55 AM

### Power Cycle Chemistry 1

Location: ECCR135

#### **How IAPWS Technical Guidance Documents Address the Major Cycle Chemistry Influenced Problems in Fossil and Combined Cycle Plants**

8:35 AM - 9:15 AM

Speaker: Barry Dooley

#### **IAPWS PCC Special Task Group - Update on the IAPWS Technical Guidance Document for Geothermal Steam Purity**

9:15 AM - 9:35 AM

Speaker: David Addison

#### **Grain Unit Preservation and Return to Service**

9:35 AM - 9:55 AM

Speaker: Paul McCann

8:30 AM - 10:15 AM

### Wetting, Interfaces, Hydrates and Membranes 3: Hydrates - Storage and Capture

Location: MATH100

#### **Facile storage of methane in sH hydrates under broader thermodynamic conditions by utilizing pre-constructed sII hydrate seeds**

8:35 AM - 8:55 AM

Speaker: Jae W Lee

#### **Natural gas capture and storage by hydrates in the presence of promoters**

8:55 AM - 9:15 AM

Speaker: Yu Wei

#### **Hydraulic Yield Strength Measurements of CO<sub>2</sub> Gas Hydrate**

9:15 AM - 9:35 AM

Speaker: Christopher Brock

#### **Thermodynamic Properties of Hydrogen-Natural Gas Blends in the Presence of Salt**

9:35 AM - 9:55 AM

Speaker: Zoe Taylor Adkins

#### **Omni Tester for Rapid Hydrate Equilibrium Prediction**

9:55 AM - 10:15 AM

Speaker: Litao Chen

8:30 AM - 10:15 AM

#### Fluid Property Measurements 4

Location: BESC180

##### **Viscosity of Methane, Nitrogen, and their mixtures at temperatures between (95 and 225) K at pressures up to 10 MPa**

8:35 AM - 8:55 AM

Speaker: Xinzi Zhou

##### **Speed of Sound Measurements in Isopentane at Temperatures from (230 to 350) K and Pressures up to 20 MPa**

8:55 AM - 9:15 AM

Speaker: Lukas Soba

##### **Evaluation of the Crystallization Risk in LNG Production. The Solubility of neo-Pentane in Methane-Rich Mixtures Down to Cryogenic Temperatures**

9:15 AM - 9:35 AM

Speaker: Marco Campestrini

##### **Measurements of p-p-T data for He-CH<sub>4</sub> binary mixtures at temperatures from 110 K-190 K and pressures up to 15 MPa**

9:35 AM - 9:55 AM

Speaker: Jiadong Sun

##### **Solubility of Dimethyl Sulfide in Water**

9:55 AM - 10:15 AM

Speaker: Kurt A.G. Schmidt

8:30 AM - 10:15 AM

#### Physical Chemistry of Aqueous Systems 4: Aqueous Solution Chemistry

Location: ECCR200

##### **MB-pol Data-Driven Many-Body Potential: Realistic Simulations of Water Across All Phases**

8:35 AM - 8:55 AM

Speaker: Francesco Paesani

##### **Structure and Dynamics of Water-in-Salt LiTFSI Electrolytes from First-Principles Molecular Dynamics Simulations**

8:55 AM - 9:15 AM

Speaker: J. Ilja Siepmann

##### **Ion Dehydration under Operating Conditions for Brine Treatment**

9:15 AM - 9:35 AM

Speaker: Nathanael Schwindt

##### **Solubility Effects at the Critical Point of Solution**

9:35 AM - 9:55 AM

Speaker: Jim Baird

##### **Optimization of the route to produce magnetic nanofluids**

9:55 AM - 10:15 AM

Speaker: Anja Meyer

8:30 AM - 10:15 AM

#### Properties of Working Fluids Including Refrigerants 3: Engineering Applications

Location: ECCR265

##### **Properties of Engineering Liquids Based on Hydrofluoroethers – Modeling and Experiments at 0.1 MPa**

8:35 AM - 8:55 AM

Speaker: Václav Vinš

##### **Molecular dynamics studies on phase transition behavior of liquid film of R450A on solid copper surface**

8:55 AM - 9:15 AM

Speaker: Muhammad Asif Shakoori

##### **Mapping the Flammability Space of Complex Refrigerant Mixtures Through Artificial Neural Networks based on Molecular Descriptors**

9:15 AM - 9:35 AM

Speaker: Carlos G. Albà

##### **New parametrization approach for molecular models, and predictive simulation studies on refrigerant blends and refrigerant-lubricant mixtures**

9:35 AM - 9:55 AM

Speaker: Gabriele Raabe

##### **Simulation studies on thermophysical properties during condensation of R450A+PEC4 on different surfaces**

9:55 AM - 10:15 AM

Speaker: Misbah Khan

8:30 AM - 10:15 AM

**Properties for Fuels and Energy Systems 1: Phase Behavior and Transport Properties I**

Location: ECCR245

**Diffusivities in Electrolyte Systems from Dynamic Light Scattering (DLS)**

8:35 AM - 9:15 AM

Speaker: Tobias Klein

**Self-diffusion Coefficients of Methane in Gaseous Binary Mixtures**

9:15 AM - 9:35 AM

Speaker: Sam Kobeissi

**Study on Thermal Conductivity of Semiclathrate Hydrate by the Transient Hot-wire Method**

9:35 AM - 9:55 AM

Speaker: Kento Doi

**High Pressure Vapor Liquid Equilibrium Measurements of binary hydrocarbon and water mixtures using Nuclear Magnetic Resonance (NMR) Spectroscopy**

9:55 AM - 10:15 AM

Speaker: Samantha L. Miller

10:15 AM - 10:35 AM

**Coffee Break**

Location: Math Plaza

10:35 AM - 12:20 PM

**Wetting, Interfaces, Hydrates and Membranes 4: Thermodynamics-Invited session**

Location: MATH100

**The Cage Specific Hydrate Equilibrium Electrolyte (CaSH-e) Model**

10:40 AM - 11:20 AM

Speaker: Eric May

**Study of the univariant two-phase dissociation line of the tetrahydrofuran hydrate from molecular dynamics**

11:20 AM - 11:40 AM

Speaker: Felipe Blas

**Simulation of the carbon dioxide hydrate-water interfacial free energy along its aqueous-hydrate two-phase equilibrium line**

11:40 AM - 12:00 PM

Speaker: Felipe Blas

**Dissociation line and driving force for nucleation of the nitrogen hydrate from computer simulation**

12:00 PM - 12:20 PM

Speaker: Jesús Algaba

10:35 AM - 12:00 PM

**Properties for Fuels and Energy Systems 2: Phase Behavior and Transport Properties II**

Location: ECCR245

**Exploring Lattice Thermal Transport in Methane Hydrates: Insights from Deep Neural Network-Enhanced Interatomic Potentials**

10:40 AM - 11:00 AM

Speaker: Yan Wang

**Thermophysical Properties of Liquid Organic Hydrogen Carriers**

11:00 AM - 11:20 AM

Speaker: Michael H. Rausch

**Measurement and Modelling of Density, Viscosity, and Speed of Sound of Methyl Dodecanoate, Ethyl Tetradecanoate and Two Oxymethylethers as Alternative Fuels**

11:20 AM - 11:40 AM

Speaker: Sebastian Klink

**Characterization and Commingling of Oils based on semi-continuous thermodynamics**

11:40 AM - 12:00 PM

Speaker: Sergio E. Quiñones-Cisneros

10:35 AM - 12:00 PM

**Power Cycle Chemistry 2**

Location: ECCR135

**Commissioning of a 49 MW Electrical Boiler in Denmark**

10:40 AM - 11:00 AM

Speaker: Monika Nielsen

**Water Quality Aspects for PEM Electrolysis**

11:00 AM - 11:20 AM

Speaker: David De Vos

**Electrochemical Investigation of Boiler Steel Corrosion Under Chloride and Sulphate Contamination**

11:20 AM - 11:40 AM

Speaker: Benjamin Loder

**IAPWS PCC Special Task Group - Update on the IAPWS Technical Guidance Document for Electrode Boilers**

11:40 AM - 12:00 PM

Speaker: David Addison

10:35 AM - 12:20 PM

## Fluid Property Measurements 5

Location: BESC180

### Measuring Intermolecular Interactions in Solution

10:40 AM - 11:20 AM  
Speaker: Angela Stelson

### Thermophysical Properties of Lubricants at Extreme Conditions: Experiments, Molecular Simulation and Modelling

11:20 AM - 11:40 AM  
Speaker: Dennis Alt

### Metrological Use of Thermophysical Properties of Gases from Ab Initio Calculations and Precision Experiments

11:40 AM - 12:00 PM  
Speaker: Christof Gaiser

### Liquid-Liquid Equilibria from a more General Point of View: Mixtures of Alkanes with Ethanol or Acetonitrile

12:00 PM - 12:20 PM  
Speaker: Bernd Rathke

10:35 AM - 12:20 PM

## Non-Equilibrium Thermodynamics 4: Thermodiffusion/ Mass Transport

Location: ECCR1B40

### Mass Diffusion and Thermodiffusion in Multicomponent Fluid Mixtures

10:40 AM - 11:20 AM  
Speaker: Jan Sengers

### Diffusion and Thermodiffusion of the Ternary System Polystyrene+Toluene+Cyclohexane

11:20 AM - 11:40 AM  
Speaker: Werner Köhler

### Thermal Marangoni Effects, Thermodiffusion, and Thermo-osmosis in Membranes

11:40 AM - 12:00 PM  
Speaker: Bjørn Hafskjold

### Using Non-equilibrium Thermodynamics to Develop a Consistent Model of Non-isothermal, Multi-phase Flow through Porous Media

12:00 PM - 12:20 PM  
Speaker: Øivind Wilhelmsen

10:35 AM - 12:20 PM

## Properties of Working Fluids Including Refrigerants 4: Modeling

Location: ECCR265

### Automatic Fitting of Refrigerant Thermodynamic Models

10:40 AM - 11:00 AM  
Speaker: Ian Bell

### Modelling the thermodynamic properties of reactive working fluids for thermodynamic cycles

11:00 AM - 11:20 AM  
Speaker: Silvia Lasala

### Application of Extended Corresponding States (ECS) for Modelling Viscosity of Several Refrigerants

11:20 AM - 11:40 AM  
Speaker: Junwei Cui

### A New Fundamental Equation of State for cis-1-Chloro-2,3,3,3-tetrafluoropropene (R-1243zf)

11:40 AM - 12:00 PM  
Speaker: Ryo Akasaka

### Development of equation of state and vapour-liquid equilibrium models for refrigerant mixtures containing R-1132a

12:00 PM - 12:20 PM  
Speaker: Robert Low

10:35 AM - 12:00 PM

## Thermophysical Properties of Aqueous Systems 1: Aqueous Mixtures and Electrolyte Solutions I

Location: ECCR 105

### "Cenotectic": On the Equilibrium Limit of Liquid Stability in Aqueous Systems

10:40 AM - 11:00 AM

Speaker: Matthew Powell-Palm

### Examining the Equilibrium Thermodynamics of High-pressure Ice Polymorphs and Aqueous NaCl

11:00 AM - 11:20 AM

Speaker: Ula Jones

### Comparison of the Surface Tension of Aqueous Binaries with Methanol, Ethanol, and Ethylene Glycol in the Low Temperature Region Including Supercooled State

11:20 AM - 11:40 AM

Speaker: Václav Vinš

### Hygroscopic Properties of Assam Silk Fibers under Thermal Condition

11:40 AM - 12:00 PM

Speaker: Dip Saikia

1:45 PM - 3:30 PM

## Non-Equilibrium Thermodynamics 5: Mass and Heat Transport/ Interfaces

Location: ECCR1B40

### Innovative Space Cooling Solutions: Evaporative Technologies with Radiative Enhancements

1:50 PM - 2:10 PM

Speaker: Pietro Asinari

### Insights into the Mass Transfer through Vapor-Liquid Interfaces from Molecular Dynamics Simulations

2:10 PM - 2:30 PM

Speaker: Simon Stephan

### Comprehensive Description of Transport Phenomena in Soap-film Functional Membranes

2:30 PM - 2:50 PM

Speaker: Eliodoro Chiavazzo

### Thermal Transport across Heterogeneous Surfaces

2:50 PM - 3:10 PM

Speaker: Fernando Bresme

### Self-propulsion at the Nano-scale by Exponential Kicks

3:10 PM - 3:30 PM

Speaker: Arnau Jurado Romero

1:45 PM - 3:10 PM

## Properties for Fuels and Energy Systems 3: Properties of Fuels and Biofuels

Location: ECCR245

### Speed of sound measurements in pure n-octane and ethylcyclohexane and their mixtures at saturation

1:50 PM - 2:10 PM

Speaker: Ilmutdin Abdulgatov

### Phase-Equilibria of Renewable Fuel Blends, Water, and Additives

2:10 PM - 2:30 PM

Speaker: Justus Arweiler

### Consistent Prediction of Thermodynamic Properties for Sustainable Aviation Fuel Components

2:30 PM - 2:50 PM

Speaker: Eugene Paulechka

### Modeling Mass Transport Properties of Oxyfuel-relevant Species in the Porous Structure of Solid Biomass Fuel Particles

2:50 PM - 3:10 PM

Speaker: Tim Eisenbach

1:45 PM - 3:30 PM

## Thermophysical Properties of Aqueous Systems 2: Pure Water

Location: ECCR 105

### Shear and Bulk Viscosity of Water up to 1.5 GPa

1:50 PM - 2:30 PM

Speaker: Frédéric Caupin

### Gas-phase Refractivity Measurement of Ordinary and Heavy Water

2:30 PM - 2:50 PM

Speaker: Patrick Egan

### Toward a Replacement for the Standard Equation of State for Water

2:50 PM - 3:10 PM

Speaker: Allan Harvey

### Current Status of Correlations for the Surface Tension of Ordinary Water

3:10 PM - 3:30 PM

Speaker: Václav Vinš

1:45 PM - 3:30 PM

## Carbon Capture, Transportation, and Storage 1: Thermophysical Properties for CO<sub>2</sub> Transport

Location: ECCR135

### Modelling the phase behaviour of fluid systems relevant for carbon-capture processes: the importance of SO<sub>x</sub> and NO<sub>x</sub>

1:50 PM - 2:30 PM

Speaker: Andrew Haslam

### New density data and Equations of State assessment for CO<sub>2</sub>-based mixtures at conditions relevant to CO<sub>2</sub> transport for the CO<sub>2</sub> Capture and Storage chain

2:30 PM - 2:50 PM

Speaker: Manuele Gatti

### Investigation of property methods for CO<sub>2</sub> conditioning, transport and sequestration

2:50 PM - 3:10 PM

Speaker: Shu Wang

### Microfluidic Measurements of CO<sub>2</sub> Hydrates: Equilibrium Water Content, Film Thickening, and Raman Spectroscopy

3:10 PM - 3:30 PM

Speaker: Lindsey Wadsworth

1:45 PM - 3:30 PM

## Wetting, Interfaces, Hydrates and Membranes 5: Hydrate Confinement and Transport/Interfaces

Location: MATH100

### Determination of local crystal orientation of Methane hydrates in tailored confined media using polarized Raman spectroscopy

1:50 PM - 2:10 PM

Speaker: Mrityunjay Sharma

### Gas Hydrate Plugging Conceptual Mechanistic Model during Transient Shut-in/Restart Operation in Fully-Dispersed Systems

2:10 PM - 2:30 PM

Speaker: Anqi Qu

### Rheological Perspective on Hydrate Agglomeration Tendency in Crude Oils at Different Thermodynamic Conditions

2:30 PM - 2:50 PM

Speaker: Oliver Greener

### Microscale Evaluation of Hydrate Interparticle Interactions

2:50 PM - 3:10 PM

Speaker: Ramon Castrejon Miranda

### Impact of Subcooling on Gas Condensate Systems: Insights into Hydrate Plugging with Methanol and Kinetic Hydrate Inhibitor (KHI)

3:10 PM - 3:30 PM

Speaker: Seetharaman Navaneetha Kannan

1:45 PM - 3:30 PM

## Optical and Thermal Radiative Properties 1: Particles and Particulate Media

Location: ECCR200

### Modeling and Measurements of Spectral Radiative Properties of Solid Particles, Particle Beds, and Inhomogeneous Layers

1:50 PM - 2:30 PM

Speaker: Zhuomin Zhang

### Design of near-perfect absorption with random particulate materials

2:30 PM - 2:50 PM

Speaker: Cédric Blanchard

### Infrared micro-reflectance measurements and modeling of silicate nanopowders

2:50 PM - 3:10 PM

Speaker: Mireia Sainz-Menchón

### Thermal emission by dielectric particles

3:10 PM - 3:30 PM

Speaker: Joseph McKay

1:45 PM - 3:30 PM

### Fluid Property Measurements 6

Location: BESC180

#### **Solubility of N<sub>2</sub>, O<sub>2</sub> and CH<sub>4</sub> in Ionic Liquids for CH<sub>4</sub> Purification from Low-concentration Coal-bed Gas**

1:50 PM - 2:10 PM

Speaker: Shaoxuan Huang

#### **Effect of temperature and organic solvent structure on ternary liquid-liquid equilibria of (water + short-chain normal alcohol + organic solvent) systems**

2:10 PM - 2:30 PM

Speaker: Cara Schwarz

#### **Phase behavior and physical properties (density and viscosity) of supercritical carbon dioxide + (1 octanol and/or n alkanes)**

2:30 PM - 2:50 PM

Speaker: Cara Schwarz

#### **Phase Behaviour of Methanol + CO<sub>2</sub> at Temperatures between 230 and 423.15 K**

2:50 PM - 3:10 PM

Speaker: Riley Latcham

#### **Modeling on multiple scales establishes the atomistic details of ion-solvent and ion-ion interactions in experimental, PT-dependent NMR chemical shifts of aqueous alkali fluorides**

3:10 PM - 3:30 PM

Speaker: Demian Riccardi

3:30 PM - 3:50 PM

### Coffee Break

Location: Math Plaza

3:35 PM - 5:35 PM

### Posters, Exhibits, and Software Demonstrations

Location: Glenn Miller Ballroom of the University Memorial Center (UMC)

Session Chair: Jason Widegren, Joseph Magee, Ian Bell, Kirk Buecher

7:00 PM - 8:15 PM

### IAPWS Award Lecture and General Meeting

Location: Math100

Session Chair: Daniel Friend

#### **IAPWS Helmholtz Lecture: From Accurate Viscosity Measurements to Wide-ranging Viscosity Formulations including the Near-critical Region Applying a Structural-optimization Method**

7:05 PM - 7:45 PM

Location: Math100

Speaker: Sebastian Herrmann

#### **IAPWS General Meeting**

7:45 PM - 8:15 PM

Location: Math100

Speaker: Daniel Friend

8:00 PM - 11:00 PM

### Evening Social

Location: TBD

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## Wed, Jun 26, 2024

8:30 AM - 10:15 AM

### Wetting, Interfaces, Hydrates and Membranes 6: Hydrates - Modeling at Interfaces

Location: MATH100

#### **Thermophysical Properties Relevant for Gas Hydrate Management Obtained from Atomistic Molecular Simulations**

8:35 AM - 8:55 AM

Speaker: Alberto Striolo

#### **Analysis of methane hydrate crystallization under oceanic conditions using Molecular Dynamics**

8:55 AM - 9:15 AM

Speaker: Manuel M. Piñeiro

#### **Factors Governing the Performance of Chemical Promoters for Gas Hydrate Growth**

9:15 AM - 9:35 AM

Speaker: Anh Phan

#### **Extension of the van der Waals and Platteeuw Gas Hydrate Model for Hydrogen Hydrates**

9:35 AM - 9:55 AM

Speaker: Felix Fiedler

#### **Porous Materials for Hydrogen Storage at Low Temperatures: A Review**

9:55 AM - 10:15 AM

Speaker: Maria-Sophie Günther

8:30 AM - 9:55 AM

## Properties for Fuels and Energy Systems 4: Utilization of Fuels and Energy Systems

Location: ECCR245

**Challenges on the determination of the thermophysical properties of molten eutectic Li, Na and K carbonate mixtures for thermal storage applications**

8:35 AM - 8:55 AM

Speaker: Maria José V. Lourenço

**Combustion Calorimetry: Yesterday, Today and Tomorrow.**

8:55 AM - 9:15 AM

Speaker: Andrei Yermalayeu

**A practical Stirling cycle heat engine utilizing a non-ideal working fluid subjected to the Van der Waals attractive intermolecular forces to boost the thermodynamic efficiency theoretically in excess of the Carnot efficiency**

9:15 AM - 9:35 AM

Speaker: Matthew Marko

**Utilization of clayey freshwater sediments through geopolymerization**

9:35 AM - 9:55 AM

Speaker: Jan Fořt

8:30 AM - 9:55 AM

## Thermophysical Properties of Aqueous Systems 3: Hydrates and Electrolyte Solutions

Location: ECCR 105

**Interactions of Hydrate Promoters Sodium Dodecyl Sulfate and Tetrahydrofuran near Hydrate Forming Conditions**

8:35 AM - 8:55 AM

Speaker: Zoe Taylor Adkins

**Experimental Measurements and Modeling of CO<sub>2</sub>-rich Gas Hydrates**

8:55 AM - 9:15 AM

Speaker: Amadeu Sum

**Screening of Electrolyte Solutions as Phase Change Materials using COSMO-SAC and Numerical Optimization**

9:15 AM - 9:35 AM

Speaker: Erik Mickoleit

**Choline Chloride Thermophysical and Phase Change Studies: Relevance for the Representation of Eutectic Systems**

9:35 AM - 9:55 AM

Speaker: Simão P. Pinho

8:30 AM - 10:15 AM

## Correlations, Databases, and Engineering Equations of State 1: Transport Properties I

Location: ECCR265

**Combining Molecular Simulation with Residual Entropy Scaling to Correlate Self-Diffusivity**

8:35 AM - 8:55 AM

Speaker: J. Richard Elliott

**Reference Correlation of the Viscosity of Ethene from the Triple Point to 580 K and up to 200 MPa**

8:55 AM - 9:15 AM

Speaker: Sofia Sotiriadou

**Entropy Scaling of Viscosity IV: Application to 124 Industrially Important Fluids**

9:15 AM - 9:35 AM

Speaker: Viktor Martinek

**A new estimation scheme for liquid metal thermal conductivity**

9:35 AM - 9:55 AM

Speaker: Ian Bell

**Prediction Model for Fick Diffusion Coefficients in Liquids with Dissolved Gases Close to Infinite Dilution**

9:55 AM - 10:15 AM

Speaker: Frances D. Lenahan

8:30 AM - 10:15 AM

## Non-Equilibrium Thermodynamics 6: Fluctuations and Transport Phenomena in Fluids

Location: ECCR1B40

**Fluctuating Hydrodynamics for Fun and Profit**

8:35 AM - 9:15 AM

Speaker: Alejandro Garcia

**Can a Mesoscopic Model Describe Stick-slip Flow?**

9:15 AM - 9:35 AM

Speaker: Peter Daivis

**Green-Kubo and Einstein-Helfand Expressions for Transport Properties from Dissipative Particle Dynamics Simulations**

9:35 AM - 9:55 AM

Speaker: Josep Bonet Avalos

**The Role of Thermal Fluctuations in the Motion of Free Bodies: Viscoelasticity vs. Orientational Diffusion**

9:55 AM - 10:15 AM

Speaker: Jaime Arturo de la Torre

8:30 AM - 9:55 AM

## Carbon Capture, Transportation, and Storage 2: Thermophysical Properties of Amine Systems for CO<sub>2</sub> Capture

Location: ECCR135

### High-Pressure Speed of Sound Measurements in Monoethanolamine Aqueous Solutions with Carbon Dioxide (CO<sub>2</sub>)

8:35 AM - 8:55 AM

Speaker: Simona Lago

### Density and Isobaric Heat Capacity Of CO<sub>2</sub>-Loaded Aqueous Amines For Carbon Capture

8:55 AM - 9:15 AM

Speaker: David Vega-Maza

### A New Approach to the Calculation of the Interfacial Tension for the (Carbon Dioxide + Water) System

9:15 AM - 9:35 AM

Speaker: Sergio E. Quiñones-Cisneros

### Amine Functionalized Supported Ionic Liquid Membranes (SILMs) for CO<sub>2</sub>/N<sub>2</sub> Separation

9:35 AM - 9:55 AM

Speaker: Antoine Chamoun-Farah

8:30 AM - 10:15 AM

## Fluid Property Measurements 7

Location: BESC180

### Density Measurements of Squalane using Single-sinker and Vibrating-tube Densimeters

8:35 AM - 8:55 AM

Speaker: Aleš Blahut

### Density Measurements on Helium, Neon, and Three Mixtures at Temperatures from (100 to 283.15) K Utilizing a Single-Sinker Densimeter

8:55 AM - 9:15 AM

Speaker: Nils von Preetzmann

### The Effect of Molecular Structure on Liquid Viscosity and Density

9:15 AM - 9:35 AM

Speaker: Brayton Young

### Density Measurements of (Argon + Carbon Dioxide) over the Temperature Range from (253.15 to 453.15) K at Pressures up to 20 MPa

9:35 AM - 9:55 AM

Speaker: Robin Wegge

### High-Pressure Vibrating-Tube Densimeters – Performance Limit and Uncertainty at Low Densities

9:55 AM - 10:15 AM

Speaker: Dennis Panke

8:30 AM - 10:15 AM

## Properties for Materials Science at High Temperatures 1: Levitation I

Location: ECCR200

### High-temperature studies of the structure and molar volume of metallic alloys by using electromagnetic levitation and synchrotron X-ray diffraction

8:35 AM - 9:15 AM

Speaker: Ivan Kaban

### Melting and Solidification Behavior of Type 316L Austenitic Stainless Steel Containing 30mass% B<sub>4</sub>C

9:15 AM - 9:35 AM

Speaker: Hiroyuki Fukuyama

### Thermal Conductivity Measurements by Non-Contact Modulation Calorimetry through Magnetohydrodynamic Modeling

9:35 AM - 9:55 AM

Speaker: Lydia Ellen Tonani

### Inductive Measurement of Electrical Resistivity and Density of Fe<sub>90</sub>Ni<sub>10</sub>, Fe<sub>72</sub>Cr<sub>13</sub>Ni<sub>15</sub> and Fe<sub>72</sub>Cr<sub>17</sub>Ni<sub>11</sub> using the Sample Coupling Electronics on board the ISS Space Station

9:55 AM - 10:15 AM

Speaker: Peace Muusha

10:15 AM - 10:35 AM

## Coffee Break

Location: Math Plaza

10:35 AM - 12:40 PM

## Properties of Polymers 1: Interfaces and Films

Location: ECCR245

### Can Cyclic Block Copolymers Meet the Needs for Next-Generation Nanolithography?

10:40 AM - 11:20 AM

Speaker: Julie Albert

### Microscopic Insights into Compatibilized Semicrystalline Blends

11:20 AM - 11:40 AM

Speaker: Robert Ivancic

### Modelling of Shear-induced Mixing Behaviour of Polymer Blends

11:40 AM - 12:00 PM

Speaker: Jonas Jaske

### Low Thermal Resistance Insulating Thin Film Primer using Oriented Mesogenic Epoxy Resin

12:00 PM - 12:20 PM

Speaker: Yoshitaka Takezawa

### Expanding the TUFF and TUTTUT Methods: Stretching Ultrathin Rubbery Polymers Films and Microbial Biopolymer Films

12:20 PM - 12:40 PM

Speaker: Konane Bay

10:35 AM - 12:20 PM

## Correlations, Databases, and Engineering Equations of State 2: Transport Properties II

Location: ECCR265

### Reference Correlations of the Viscosity and Thermal Conductivity of Tetrahydrofuran from the Triple Point to High Temperatures and Pressures

10:40 AM - 11:00 AM

Speaker: Eleftheria Ntonti

### State of the Art and Challenges in the Development of Models for the Calculation of Transport Properties of Asymmetric Mixtures

11:00 AM - 11:20 AM

Speaker: Monika Thol

### Reference Correlation for the Viscosity of Nitrogen

11:20 AM - 11:40 AM

Speaker: Marcia Huber

### Re-evaluation of Viscosity Measurements on Natural Gas

11:40 AM - 12:00 PM

Speaker: Sebastian Herrmann

### Squalane – a HTHP viscosity standard re-examined

12:00 PM - 12:20 PM

Speaker: Kurt A.G. Schmidt

10:35 AM - 11:40 AM

## Thermophysical Properties of Aqueous Systems 4: Aqueous Mixtures and Electrolyte Solutions II

Location: ECCR 105

### Characterization of the Hydrogen Carrier System Based on Aqueous Solutions of Isopropanol and Acetone by Optical and Conventional Techniques

10:40 AM - 11:00 AM

Speaker: Lena M. Braun

### Nuclear Magnetic Resonance Spectroscopy Experiments and Multiscale Modeling Give Insights into Ion-Solvent Interactions and Ion Pairing in Simple Aqueous Salt Solutions

11:00 AM - 11:20 AM

Speaker: Małgorzata Musiał

### Nuclear Magnetic Resonance Spectroscopy for Measurements of Ion Solvent and Ion Pairing Interactions in Aqueous Solutions

11:20 AM - 11:40 AM

Speaker: Christopher L. Suiter

10:35 AM - 12:20 PM

### Carbon Capture, Transportation, and Storage 3: Thermophysical Properties for Next-Generation CO<sub>2</sub> Capture

Location: ECCR135

#### Thermodynamic Modeling of CO<sub>2</sub> Absorption in Aqueous Potassium Carbonate Solution with Association eNRTL Model

10:40 AM - 11:00 AM

Speaker: Cheng-Ju Hsieh

#### A Novel Generation of Sorbents Capable of Capturing Carbon Dioxide Using Ionic Liquids and Deep Eutectic Solvents

11:00 AM - 11:20 AM

Speaker: Ardila Hayu Tiwiktama

#### Molecular Modeling of Amine-based Deep Eutectic Solvents for CO<sub>2</sub> Capture Employing COSMO-RS and Soft-SAFT Equation of State

11:20 AM - 11:40 AM

Speaker: Safique Anwer

#### Thermophysical Properties of Amino Acid Salt Solutions for Carbon Capture Applications

11:40 AM - 12:00 PM

Speaker: Hossam Qusty

#### Are clathrate hydrates a solution for CCS?

12:00 PM - 12:20 PM

Speaker: Catinca Secuianu

10:35 AM - 12:20 PM

### Wetting, Interfaces, Hydrates and Membranes 7: Inorganic Clathrates & New Hydrates - Synthesis

Location: MATH100

#### Structural diversity and stabilization of substituted silicon and carbon clathrates

10:40 AM - 11:00 AM

Speaker: Timothy Strobel

#### Inorganic Clathrates: Structure-property Relations and Potential Applications

11:00 AM - 11:20 AM

Speaker: George Nolas

#### Formation of Type II Silicon Clathrate with Lithium Guests

11:20 AM - 11:40 AM

Speaker: Yinan Liu

#### Spin dynamics of Na guest in type II Si clathrate

11:40 AM - 12:00 PM

Speaker: Joseph P. Briggs

#### New class of stable NaCl hydrates: On the role of pressure in hydration and ionic dissociation in hydrogen bounded solids.

12:00 PM - 12:20 PM

Speaker: Baptiste Journaux

10:35 AM - 12:00 PM

### Fluid Property Measurements 8

Location: BESC180

#### Surface Light Scattering Close to the Critical Damping of Surface Fluctuations and in the Presence of Molecular Orientation Effects

10:40 AM - 11:00 AM

Speaker: Thomas M. Koller

#### Determination of Sound Speed for 1-Alcohols between 303 and 473 K and up to 10 MPa by Dynamic Light Scattering

11:00 AM - 11:20 AM

Speaker: Junwei Cui

#### Automated Measurement, Modeling, and Interpretation of Diffusion Coefficients in Multicomponent Liquids

11:20 AM - 11:40 AM

Speaker: Carsten Flake

#### Final Experimental Results for the Virial Coefficients of Argon and Neon and their Utilization in Gas Metrology

11:40 AM - 12:00 PM

Speaker: Christian Günz

10:35 AM - 12:20 PM

## Properties for Materials Science at High Temperatures 2: Levitation II

Location: ECCR200

### **Thermophysical Property Measurement of Molten Materials by the Electrostatic Levitation Furnace (ELF) on the International Space Station (ISS)**

10:40 AM - 11:00 AM

Speaker: Rina Shimonishi

### **Thermophysical properties of molten metal oxides**

11:00 AM - 11:20 AM

Speaker: Richard Weber

### **Comparison of thermophysical properties of Ni-based superalloys using electrostatic levitation**

11:20 AM - 11:40 AM

Speaker: Brandon Phillips

### **Precise Density Measurements of Refractory Liquid Metals over 3000 K by Using Electrostatic Levitation**

11:40 AM - 12:00 PM

Speaker: Geun Woo Lee

### **Effect of hypercooling limit for supercooling behavior and glass formation**

12:00 PM - 12:20 PM

Speaker: Lei Wang

1:45 PM - 3:10 PM

## Non-Equilibrium Thermodynamics 7: Electrified Interfaces and Interdisciplinary Topics

Location: ECCR1B40

### **The Effect of Ion, Solvent and Thermal Interaction Coefficients on Battery Voltage. The Case of the Lithium-ion Battery Electrolyte**

1:50 PM - 2:10 PM

Speaker: Øystein Gullbrekken

### **Reactive Molecular Dynamics Frameworks for Describing Transport of Lithium in Solid Electrolyte Interphases**

2:10 PM - 2:30 PM

Speaker: Paolo De Angelis

### **The Impact of Potential on Thermal Conductance**

2:30 PM - 2:50 PM

Speaker: Aidan Chapman

### **Liquid CO<sub>2</sub> Jets at Atmospheric Pressure for Cutting Applications**

2:50 PM - 3:10 PM

Speaker: Laura Göhlich

1:45 PM - 3:30 PM

## Optical and Thermal Radiative Properties 2: Measurement and Metrology

Location: ECCR 105

### **Development of a new test bench for measuring emissivity at low temperature for the space sector**

1:50 PM - 2:10 PM

Speaker: Jean-Pierre Monchau

### **Emissivity measurements of vitreous silica from 4 K to 2500 K in static and dynamic conditions**

2:10 PM - 2:30 PM

Speaker: Iñigo González de Arrieta

### **Apparatus for measuring the emissivity of polished and rough NiTi samples at different temperatures**

2:30 PM - 2:50 PM

Speaker: Muhammad Ali Javed

### **Micro BRDF measurements with infrared quantum cascade laser sources**

2:50 PM - 3:10 PM

Speaker: Patrick McArdle

### **Towards an open database of optical and thermal radiative data**

3:10 PM - 3:30 PM

Speaker: Jon Gabirondo-López

1:45 PM - 3:30 PM

### Properties for Materials Science at High Temperatures 3: Levitation III

Location: ECCR200

#### **Density and surface tension of binary and ternary Al-Ti-V liquid alloys and the influence of oxygen on the surface tension**

1:50 PM - 2:10 PM

Speaker: Jürgen Brillo

#### **Thermophysical properties of selected Nickel based superalloys by voestalpine BÖHLER Edelstahl GmbH & Co KG measured with an Electromagnetic Levitation Apparatus and a Furnace Rheometer System**

2:10 PM - 2:30 PM

Speaker: Thomas Leitner

#### **Thermal Expansion Mechanism of Elemental Liquids**

2:30 PM - 2:50 PM

Speaker: Geun Woo Lee

#### **Thermophysical properties of 10, 20 mol% Ga-Fe melts measured by electromagnetic levitation**

2:50 PM - 3:10 PM

Speaker: Masayoshi Adachi

#### **The Use of Multiphysics Modeling Assists in Determining the Thermophysical Properties of Liquid Metals Obtained Through Aerodynamic Levitation**

3:10 PM - 3:30 PM

Speaker: Mickael Courtois

1:45 PM - 3:30 PM

### Carbon Capture, Transportation, and Storage 4: Thermophysical Properties for CO<sub>2</sub> Storage

Location: ECCR135

#### **Interfacial Properties of Live Fluids at Reservoir Conditions**

1:50 PM - 2:10 PM

Speaker: David Uko

#### **Solid-State and Gas-Phase NMR Spectroscopy for Characterizing CO<sub>2</sub> Uptake in Solids**

2:10 PM - 2:30 PM

Speaker: Christopher L. Suiter

#### **Convective Plume Spreading in Model Transparent Porous Media**

2:30 PM - 2:50 PM

Speaker: Happiness Imuetinyan

#### **Investigation of the chalk dissolution kinetics in brines loaded with carbon dioxide**

2:50 PM - 3:10 PM

Speaker: Marc Cassiède

#### **Viscosity and density of decane and hexylbenzene with dissolved carbon dioxide and/or methane**

3:10 PM - 3:30 PM

Speaker: Iusiph Eiubovi

1:45 PM - 3:30 PM

### Nuclear Reactor and Fuel Cycle Chemistry 1

Location: ECCR245

#### **Impact of KOH Primary Coolant Chemistry on Pressurized Water Reactor's Operating with Fuel Crud**

1:50 PM - 2:10 PM

Speaker: Hugues Arcis

#### **Phase Behavior and Thermodynamic Solubility Constants for Novel Nickel Sulfate Phases Formed Under Secondary Coolant Hideout Conditions**

2:10 PM - 2:30 PM

Speaker: Maryanne Stones

#### **A Re-evaluation of the Boric Acid Thermodynamics for PWR Systems**

2:30 PM - 2:50 PM

Speaker: Hugues Arcis

#### **Modernization of a Radioactivity Transport Code to Support the CANDU Industry**

2:50 PM - 3:10 PM

Speaker: Cassidy Perry

#### **Experiments for a "What If" Scenario –Deep Geological Repository Groundwater Leak Tests with SMR Fuel Cladding**

3:10 PM - 3:30 PM

Speaker: Olga Palazhchenko

1:45 PM - 3:10 PM

**Correlations, Databases, and Engineering Equations of State 3: Helmholtz-Energy Equations of State: Pure Fluids**

Location: ECCR265

**Mutating Thermodynamic Properties for Use in Fitting Equations of State**

1:50 PM - 2:30 PM

Speaker: Eric W. Lemmon

**New Methods for Fitting Equations of State with Application to cis-Decalin**

2:30 PM - 2:50 PM

Speaker: Hiroyuki Miyamoto

**Current Status on Thermodynamic Properties of Ortho-, Para- and Normal Hydrogen**

2:50 PM - 3:10 PM

Speaker: Tan-Trieu-Giang Nguyen

1:45 PM - 3:10 PM

**Fluid Property Measurements 9**

Location: BESC180

**Supporting Scientific Reviewing of Publications on Experimental Thermophysical and Thermochemical Research**

1:50 PM - 2:10 PM

Speaker: Ala Bazyleva

**Temperature dependence on flow property of blood based on modified Herschel-Bulkley equation**

2:10 PM - 2:30 PM

Speaker: Hideki Yamamoto

**Vapor pressure measurements on cannabinoids and cannabis-associated terpenes to support cannabis breathalyzer development**

2:30 PM - 2:50 PM

Speaker: Jason Widegren

**Experimental and Modeling of Electrical Permittivity, Density, Solubility and Viscosity of Carbon Dioxide/Dodecane Liquid Mixtures**

2:50 PM - 3:10 PM

Speaker: Moisés Alves Marcelino Neto

3:30 PM - 3:50 PM

**Coffee Break**

Location: Math Plaza

3:50 PM - 5:20 PM

**Plenary 3: Touloukian Award Ceremony**

Location: Math100

Session Chair: Kenneth Kroenlein, J. Ilja Siepmann

**Touloukian Lecture: Clathrate Hydrates in Energy and Carbon Capture Applications**

3:55 PM - 4:55 PM

Location: Math100

Speaker: Carolyn Koh

**Presentation of the Yeram S. Touloukian Awards**

4:55 PM - 5:20 PM

Speaker: J. Ilja Siepmann

5:30 PM - 6:30 PM

**Awards Reception**

Location: Stadium Club

7:00 PM - 10:00 PM

**IAPWS Banquet**

Location: Chatauqua Dining Hall

8:00 PM - 11:00 PM

**Evening Social**

Location: TBD

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**Thu, Jun 27, 2024**

8:30 AM - 10:15 AM

## Molecular Simulation 1: Applications

Location: ECCR245

### Designing Selective Nanoporous Materials for VOC Capture Applied to Breath Diagnostics: Insights from Simulation and Experiments

8:35 AM - 8:55 AM

Speaker: Scott Bobbitt

### New Interpretation of NMR Relaxation Response from MD Simulations: Material Properties and MRI Contrast Agents

8:55 AM - 9:15 AM

Speaker: Walter G. Chapman

### Molecular Insights into NMR Relaxation of Gd(III)-based Contrast Agents for MRI Applications

9:15 AM - 9:35 AM

Speaker: Thiago J. Pinheiro dos Santos

### An Molecular Dynamics Investigation of the Shear Rate Dependency of the Thermophysical Properties for Molten Fe-C

9:35 AM - 9:55 AM

Speaker: John Shelton

### Molecular Dynamics meets Gravimetry: Progress in Highly Accurate Dew-Point Density Measurements

9:55 AM - 10:15 AM

Speaker: Markus Sekulla

8:30 AM - 9:55 AM

## Properties of Polymers 2: Nanocomposites

Location: ECCR135

### Thermal, Optical and Electrical Characterization of Silver Tetraiodomercurate Polymeric Composite

8:35 AM - 8:55 AM

Speaker: Fernando Cervantes-Alvarez

### Flexible Nanocomposite Polymer Materials for Energy Harvesting and Heat Management

8:55 AM - 9:15 AM

Speaker: Zdravko Kutnjak

### Soft Caloric Materials for New Heat-management Technologies

9:15 AM - 9:35 AM

Speaker: Brigita Rozic

### Polymer Crosslinking Regulates Local, Multimodal Drug Release to Skin

9:35 AM - 9:55 AM

Speaker: Nicole Day

8:30 AM - 9:55 AM

## Correlations, Databases, and Engineering Equations of State 4: Helmholtz-Energy Equations of State: Mixtures

Location: ECCR265

### Towards Modeling Mixtures with Increased Asymmetry

8:35 AM - 9:15 AM

Speaker: Andreas Jäger

### New Approaches for the Development of Helmholtz-Energy Based Multi-Parameter Property Models for Fluid Mixtures with Limited Data

9:15 AM - 9:35 AM

Speaker: Jessica Buchenfeld

### New approach to modeling mixtures based on Helmholtz energy equations for the components

9:35 AM - 9:55 AM

Speaker: Jan Hrubý

8:30 AM - 10:15 AM

### Optical and Thermal Radiative Properties 3: Tunable Radiative Properties

Location: ECCR 105

#### Self-adaptive radiative cooling and solar thermal for smart thermal management

8:35 AM - 8:55 AM

Speaker: Kegui Lu

#### Modulation of Nonreciprocal Thermal Radiative Properties Through Temperature

8:55 AM - 9:15 AM

Speaker: Bo Zhao

#### From the perspective of transmission line theory to view the fitting constants of the circuit models

9:15 AM - 9:35 AM

Speaker: Yiquan Gong

#### Optical and Thermal Characterizations of Metal-Insulating Phase Transition Titanium(III) Oxide

9:35 AM - 9:55 AM

Speaker: Richard Zhang

#### Improved Thermal Radiative Properties of Tungsten Doped VO<sub>2</sub> Thin Films Grown by High-Temperature Oxidation and Reduction Processes in Low-Oxygen Environment

9:55 AM - 10:15 AM

Speaker: Liping Wang

8:30 AM - 9:55 AM

### Instrumentation and Measurement Techniques 1: Diffusion

Location: ECCR1B40

Session Chair: Markus Richter

#### Diffusion Coefficients in Fluid Mixtures and Particulate Systems by Using Dynamic Light Scattering

8:35 AM - 9:15 AM

Speaker: Andreas P. Fröba

#### Determination of Mutual Diffusivities by the Shadowgraph Method

9:15 AM - 9:35 AM

Speaker: Patrick S. Schmidt

#### A New Pulse Method for the Measurement of the Thermal Diffusivity of Solids over a Wide Temperature Range

9:35 AM - 9:55 AM

Speaker: William Wakeham

8:30 AM - 9:55 AM

### Fluid Property Measurements 10

Location: BESC180

#### Experimental observations of the effects of intermolecular Van der Waals force on entropy

8:35 AM - 8:55 AM

Speaker: Matthew Marko

#### Accelerated Test Method to Quantify Changes in the Composition of CO<sub>2</sub>/air Reference Gases in Cylinders

8:55 AM - 9:15 AM

Speaker: Tamae Wong

#### Experimental Thermal Conductivity Measurements for the Hydrofluoroolefin R1225ye(Z)

9:15 AM - 9:35 AM

Speaker: Giulia Lombardo

#### Thermophysical Properties of n-alkane systems for low temperature thermal energy storage

9:35 AM - 9:55 AM

Speaker: Maria C.M. Sequeira

8:30 AM - 9:55 AM

### Ocean and Atmospheric Applications 1: Ocean Salinity and pH

Location: ECCR200

#### How to End Confusion Over pH and Influence National Standards

8:35 AM - 9:15 AM

Speaker: Eric May

#### Traceability and Uncertainty of pHT Values of Artificial Seawater Standards over Wide Temperature and Salinity Ranges

9:15 AM - 9:35 AM

Speaker: Rieke Schäfer

#### Estimation of Sensitivity Coefficients for Indirect Determination of Seawater Salinity

9:35 AM - 9:55 AM

Speaker: Evgeniy Sychov

10:15 AM - 10:35 AM

### Coffee Break

Location: Math Plaza

10:35 AM - 12:20 PM

## Instrumentation and Measurement Techniques 2: VLE and Phase Behavior

Location: ECCR1B40

Session Chair: Markus Richter

### Development of a Custom High-Temperature, High-Pressure Phase Behavior Apparatus

10:40 AM - 11:00 AM

Speaker: Aaron Rowane

### The Four Sinker Densimeter: A Journey Towards Accurate Dew-point Densities

11:00 AM - 11:20 AM

Speaker: Luca Bernardini

### Characterization of Ignitable Liquids in Simulated Fire Debris using Dynamic Vapor Microextraction, NMR Spectroscopy, and Sensitivity Analysis

11:20 AM - 11:40 AM

Speaker: Christopher L. Suiter

### Isochoric freezing: A high-throughput, high-accuracy tool for thermodynamic characterization of multiphase coexistence in high-pressure low-temperature aqueous solutions

11:40 AM - 12:00 PM

Speaker: Matthew Powell-Palm

### A new fully instrumental optical method for determining critical parameters of liquid mixtures

12:00 PM - 12:20 PM

Speaker: Vitaly Podnek

10:35 AM - 12:20 PM

## Correlations, Databases, and Engineering Equations of State 5: Prediction of Thermophysical Properties

Location: ECCR265

### Advancing Group-Contribution Methods for Thermophysical Properties of Mixtures

10:40 AM - 11:00 AM

Speaker: Nicolas Hayer

### Predicting Pure-Component Vapor Pressures with Graph Neural Networks

11:00 AM - 11:20 AM

Speaker: Marco Hoffmann

### Autoignition Temperature Family Trends and an Improved Prediction Method

11:20 AM - 11:40 AM

Speaker: Cassandra Guffey

### Thermodynamics-informed Symbolic Regression

11:40 AM - 12:00 PM

Speaker: Viktor Martinek

### Symbolic regression used to develop a new cubic equation of state for improved liquid density calculations

12:00 PM - 12:20 PM

Speaker: Xiaoxian Yang

10:35 AM - 12:00 PM

## Ocean and Atmospheric Applications 2: Thermophysical Properties of Seawater and Humid Air

Location: ECCR200

### Absolute Measurements on Density of Sea-Water Under Controlled Pressure

10:40 AM - 11:00 AM

Speaker: Yohei Kayukawa

### Measurements of Constant Pressure Specific Heat Capacity of IAPSO Standard Seawater

11:00 AM - 11:20 AM

Speaker: P. Alberto Giuliano Albo

### A New Approach to a Comprehensive Formulation of Thermodynamic Properties of Seawater

11:20 AM - 11:40 AM

Speaker: Jan Hrubý

### Comparison Between Experimental Determinations and Theoretical Modelling of Speed of Sound in Humid Air

11:40 AM - 12:00 PM

Speaker: Roberto M. Gavioso

10:35 AM - 12:20 PM

### Molecular Simulation 2: Methods

Location: ECCR245

#### **Appraising the Surface Thermodynamics of Nanoscopic Liquid Drops: From a Mechanical to a Quantum Description**

10:40 AM - 11:20 AM

Speaker: George Jackson

#### **Determination of Surface Tension of Simple Fluids using Temperature-dependent Intermolecular Potential Parameters (TDIP)**

11:20 AM - 11:40 AM

Speaker: Ali Al-Matar

#### **Reproducibility of Computational Methods for Modeling Thermophysical Properties**

11:40 AM - 12:00 PM

Speaker: Florian Fleckenstein

#### **Diffusivities in Electrolyte Systems from Equilibrium Molecular Dynamics Simulations**

12:00 PM - 12:20 PM

Speaker: Chathura J. Kankanamge

10:35 AM - 12:20 PM

### Properties of Polymers 3: Innovations and Applications

Location: ECCR135

#### **Higher-order Structural Analysis of Transparent and Flexible High Thermal Conductive Liquid Crystalline Elastomer Sheet and its Composite**

10:40 AM - 11:00 AM

Speaker: Yoshitaka Takezawa

#### **Utilization of Recycled Brick Waste in Geopolymers: Investigating Shrinkage Behavior and Heat Evolution**

11:00 AM - 11:20 AM

Speaker: Martin Mildner

#### **High-Pressure Torsional Braid Analysis for Rational Selection of Polymer Foaming Conditions with Physical Blowing Agents**

11:20 AM - 11:40 AM

Speaker: Erdogan Kiran

#### **Thermophysical Properties of Polymer Melts with Dissolved Blowing Agents by Optical Techniques**

11:40 AM - 12:00 PM

Speaker: Julius H. Jander

#### **Experimental Study of the Influence of Molecular Architecture and Morphology on the Gas Solubility in Polyethylene Grades**

12:00 PM - 12:20 PM

Speaker: Jana Zimmermann

10:35 AM - 12:00 PM

### Ionic Liquids 1: Structure and Modeling

Location: BESC180

#### **A Multiscale Approach for the Thermophysical Characterization of Phosphonium-based Ionic Liquids in CO<sub>2</sub> capture Applications**

10:40 AM - 11:00 AM

Speaker: Félix Llovel

#### **Exploring the Impact of Cation Diversity on Properties of Bis(trifluoromethylsulfonyl)imide Ionic Liquids**

11:00 AM - 11:20 AM

Speaker: Pranav Thacker

#### **Water harvesting by thermoresponsive ionic liquids: A molecular dynamics study of the water absorption kinetics and of the role of nanostructuring**

11:20 AM - 11:40 AM

Speaker: Robin Cortes-Huerto

#### **Data Driven Development of Binary IL-IL Systems**

11:40 AM - 12:00 PM

Speaker: Kimia Fereydooni

10:35 AM - 12:40 PM

## Optical and Thermal Radiative Properties 4: Applications

Location: ECCR 105

### Emissivity and Reflectivity Measurements for Passive Radiative Cooling Technologies

10:40 AM - 11:20 AM

Speaker: Albert Adibekyan

### Thermal control characteristics of dielectric multilayer films for space use

11:20 AM - 11:40 AM

Speaker: Hiroto Fukuhara

### Enhanced Radiative Heat Transfer for High Performance Thermophotovoltaics

11:40 AM - 12:00 PM

Speaker: Mohammad Habibi

### A thermoelectric converter with four-layer selective emitters for efficient thermophotovoltaic applications

12:00 PM - 12:20 PM

Speaker: Shuni Chen

### Enhancement of the Non-Radiative Conversion Efficiency and Thermal Property Analysis for Natural Pigments Employed as Sensitizers in DSSC Solar Cells

12:20 PM - 12:40 PM

Speaker: Cindy Lorena Gomez-Heredia

1:45 PM - 3:10 PM

## Correlations, Databases, and Engineering Equations of State 6: Data Assessment and Correlation

Location: ECCR265

### Estimation of Paraffin Pour Points

1:50 PM - 2:10 PM

Speaker: Paul Mathias

### ASSURE X23 project: Revision of the benchmark for sublimation enthalpy calculations

2:10 PM - 2:30 PM

Speaker: Vojtěch Štejfá

### Integration of Data and Models in the ThermoData Engine Software

2:30 PM - 2:50 PM

Speaker: Vladimír Diky

### High-pressure fluid-phase equilibria: New trends, experimental methods, and systems investigated (2017–2020)

2:50 PM - 3:10 PM

Speaker: Jose M.S. Fonseca

1:45 PM - 3:30 PM

## Molecular Simulation 3: Hydrates, Clathrates, and Interfaces

Location: ECCR245

### Analyzing Cage Occupancy Rates in Structure II Clathrate Hydrates Using Gibbs Ensemble Monte Carlo Simulations

1:50 PM - 2:10 PM

Speaker: Hirotaka Kishimoto

### Graph Neural Network Based Parameter Design Method for Liquid, Ice, and Clathrate Hydrate Phase Analysis

2:10 PM - 2:30 PM

Speaker: Kenji Yasuoka

### Molecular Simulation of the Hydrate - Water Interfacial Free Energies of Carbon Dioxide and Methane Hydrates

2:30 PM - 2:50 PM

Speaker: Felipe Blas

### Heterogeneous Molecular Dynamics in Quasi-liquid Layers of Ice Surface using Molecular Dynamics Simulation

2:50 PM - 3:10 PM

Speaker: Ikki Yasuda

### Interaction of Glycine with Ice

3:10 PM - 3:30 PM

Speaker: Yevgeniy Kviring

1:45 PM - 3:30 PM

### Instrumentation and Measurement Techniques 3: VLE and Microwave Cavities

Location: ECCR1B40

Session Chair: Aaron Rowane

#### VLE Measurements of Polar Binary Mixtures with Microwave Resonators

1:50 PM - 2:10 PM

Speaker: Liam D. Tenardi

#### Improved Microwave Re-entrant Cavity Design for binary VLE Measurements Including Complete Phase Description

2:10 PM - 2:30 PM

Speaker: Yvonne Leusmann

#### A microwave reentrant cavity resonator for the measurement of mixture dew points

2:30 PM - 2:50 PM

Speaker: Mark McLinden

#### New Frontiers in Mixture Vapor-Liquid Equilibria Measurement I: Can the Unconventional Become the Norm?

2:50 PM - 3:30 PM

Speakers: Mark McLinden, Markus Richter, Paul L. Stanwix

1:45 PM - 3:30 PM

### Ionic Liquids 2: Solutions and Solubility

Location: BESC180

#### Sustainable Extraction of Micropollutants and Heavy Metals: Harnessing the Potential of Ionic Liquids and Deep Eutectic Solvents

1:50 PM - 2:10 PM

Speaker: Ramesh Gardas

#### Prospects for Separation of Rare Earth Elements by Liquid Extraction with Protonated Betaine Bis(trifluoromethylsulfonyl)imide

2:10 PM - 2:30 PM

Speaker: Jaeseong Lee

#### Thermal Stability and CO<sub>2</sub> Uptake of Dicationic Ionic Liquids Containing 2-Cyanopyrrolide Anions

2:30 PM - 2:50 PM

Speaker: Junwon Park

#### Thermodynamic integration calculations for helium solubility in lead-lithium alloys.

2:50 PM - 3:10 PM

Speaker: Edgar Alvarez-Galera

#### Surface tension of glycol-based eutectic solvents in water

3:10 PM - 3:30 PM

Speaker: Esteban Cea-Klapp

1:45 PM - 3:30 PM

### Thermal Properties of Nanostructured Materials 1: Novel Thermal Characterization Techniques

Location: ECCR 105

#### Ultrafast, Nanometric Spatiotemporal Mapping for Measurement of Transport Properties of Thin Film Semiconductors

1:50 PM - 2:30 PM

Speaker: Xianfan Xu

#### Nanoscale Thermal Behaviors of Wide-bandgap Materials via Non-contact Deep-ultraviolet Transient Gratings

2:30 PM - 2:50 PM

Speaker: Brendan McBennett

#### Particle Diffusivity in Particulate Systems by Using Photon Correlation Spectroscopy

2:50 PM - 3:10 PM

Speaker: Wenchang Wu

#### Interface Thermal Resistance at Single-Walled Carbon Nanotube/Silicon Interface by Raman Thermometry

3:10 PM - 3:30 PM

Speaker: Ibrahim Al Keyyam

1:45 PM - 3:30 PM

## Properties for Materials Science at High Temperatures 4: Advanced Techniques

Location: ECCR200

### The NIST Alloy Database: Enhancing Accessibility and Reliability for Thermophysical Property Data

1:50 PM - 2:10 PM

Speaker: Boris Wilthan

### Monitoring of sintering with and without shrinkage via the impulse excitation technique (IET)

2:10 PM - 2:30 PM

Speaker: Willi Pabst

### Thermophysical Properties of Near-Eutectic Gallium-Indium-Tin Alloy

2:30 PM - 2:50 PM

Speaker: Matthias H. Buschmann

### $3\omega$ contact resistance measurement at pressure

2:50 PM - 3:10 PM

Speaker: Isaac Cutler

### Specific heat measurement of refractory metals and their binary alloys at temperatures above 1500°C

3:10 PM - 3:30 PM

Speaker: Veeraraahavan R S

1:45 PM - 3:10 PM

## Properties of Solids 1: Thermochemistry

Location: ECCR135

### Water ice polymorphs Gibbs energy Local Basis Functions up to 2,300 MPa: reconciling water thermodynamics with the water phase diagram

1:50 PM - 2:30 PM

Speaker: Baptiste Journaux

### Heat Capacity and Thermodynamic Functions of NaREF4

2:30 PM - 2:50 PM

Speaker: Brian Woodfield

### A CALPHAD-type database for Co-base Superalloys

2:50 PM - 3:10 PM

Speaker: Ursula R. Kattner

3:30 PM - 3:50 PM

## Coffee Break

Location: Math Plaza

3:50 PM - 5:35 PM

## Correlations, Databases, and Engineering Equations of State 7: Thermophysical Properties of Fluids

Location: ECCR265

### High-Accuracy Equations of State – Continued Progress Through Art + Science

3:55 PM - 4:35 PM

Speakers: Mark McLinden, Markus Richter

### Development of Helmholtz Equations of State with Symbolic Regression

4:35 PM - 4:55 PM

Speaker: Ophelia Frotscher

### Thermophysical Property Model of Lubricant Oils and Their Mixtures with Refrigerants

4:55 PM - 5:15 PM

Speaker: Xiaoxian Yang

### Thermodynamic characterization of (H<sub>2</sub> + iC<sub>4</sub>H<sub>10</sub>) for flow metering applications

5:15 PM - 5:35 PM

Speaker: P. Alberto Giuliano Albo

3:50 PM - 5:35 PM

## Instrumentation and Measurement Techniques 4: Thermal Techniques

Location: ECCR1B40

Session Chair: J.P. Martin Trusler

### The thermal needle-probe instrument revisited

3:55 PM - 4:35 PM

Speaker: William Wakeham

### The application of Differential Scanning Calorimetry (DSC) for determination of thermodynamic and kinetic properties of pure compounds and mixtures.

4:35 PM - 4:55 PM

Speaker: Dzmityr Zaitsau

### Development of Miniaturized Peltier Element Towards Temperature Control within Microfluidic Systems

4:55 PM - 5:15 PM

Speaker: Muhammad Taha

### Measuring Thermophysical Properties of Magnetic Nanofluid by Lock-in Thermography

5:15 PM - 5:35 PM

Speaker: Abdulkareem Alasli

3:50 PM - 5:35 PM

## Thermal Properties of Nanostructured Materials 2: Nanostructured Materials for Advanced Thermal Applications

Location: ECCR 105

### Powerless $\mu\text{m}$ -scale Photon Sensing Enabled by Functional Grading in Carbon Microstructures

3:55 PM - 4:15 PM

Speaker: Amin Karamati

### Axial Direction Structure Thermal Domain Size of Highly Aligned Single-Walled Carbon Nanotube Bundles

4:15 PM - 4:35 PM

Speaker: Mahya Rahbar

### Thermal Conductivity Mapping of Graphitized Polydimethylsiloxane Thin Film

4:35 PM - 4:55 PM

Speaker: Yuto Kibe

### Characterizing Highly-confined Heat Flow, Elastic Properties, and Porosity in a Semiconductor Metalattice

4:55 PM - 5:15 PM

Speaker: Emma Nelson

### Experimental Demonstration of Thermal Conductivity Reduction by Localized Phonon Resonances

5:15 PM - 5:35 PM

Speaker: Mahmoud Hussein

3:50 PM - 5:35 PM

## Properties for Materials Science at High Temperatures 5: Nuclear Materials

Location: ECCR200

### Spectro-pyrometric measurements on solid and liquid uranium-ameridium mixed oxides near their melting transition

3:55 PM - 4:15 PM

Speaker: Konstantinos Boboridis

### Surface Tension Measurements of Uranium Melts at High Temperatures

4:15 PM - 4:35 PM

Speaker: Jules Delacroix

### A novel and comprehensive approach to the thermophysical characterization of a SiC-based ATF cladding

4:35 PM - 4:55 PM

Speaker: Andrea Cavaliere

### Synthesis and thermodynamic behaviour of (U,Am,Pu)O<sub>2</sub> solid solutions

4:55 PM - 5:15 PM

Speaker: Sorin-Octavian Vălu

### New developments on Uranium Carbide systems for ISOL targets

5:15 PM - 5:35 PM

Speaker: Beatriz Aguiar Santos

3:50 PM - 5:35 PM

## Molecular Simulation 4: QM-Informed Thermodynamics

Location: ECCR245

### Ab Initio Prediction of the Thermophysical Properties and Vapor-Liquid Equilibria of Hydrogen

3:55 PM - 4:15 PM

Speaker: Richard Sadus

### Mie-FH: A Quantum-corrected Potential in LAMMPS Simulation Package

4:15 PM - 4:35 PM

Speaker: Thuat Trinh

### Cross Second Virial Coefficients for Mixtures of Hydrogen with Nitrogen, Oxygen, Carbon Dioxide, Methane, Ethane, and Propane from First-principles Calculations

4:35 PM - 4:55 PM

Speaker: Robert Hellmann

### Calculation of Thermodynamic Properties of Helium and Neon by Path Integral Monte Carlo Simulations using ab initio Potentials

4:55 PM - 5:15 PM

Speaker: Philipp Marienhagen

### Fully Quantum Calculation of Dielectric Virial Coefficients for Molecular Gases

5:15 PM - 5:35 PM

Speaker: Giovanni Garberoglio

3:50 PM - 5:35 PM

### Ionic Liquids 3: Equilibrium Properties

Location: BESC180

#### **Estimating Critical Solution Temperatures above the Decomposition Temperature: Ternary Mixtures of the Protic Ionic Liquid Ethyl-Ammonium Nitrate and Mixtures of n-Alkyl Alcohols**

3:55 PM - 4:15 PM

Speaker: Bernd Rathke

#### **Experimental Interfacial Tension of Refrigerants, HFC-32 and HFC-125 in a Mixture with Ionic Liquid, [C1C2im][Tf2N]**

4:15 PM - 4:35 PM

Speaker: Julia Espinoza Mejia

#### **Thermophysical Properties of Ionic Liquids and Compressed Gas Mixtures: Experiment and Modeling**

4:35 PM - 4:55 PM

Speaker: Karim Al-Barghouti

#### **Acoustic Method as a Precise Tool for Determining pVT Data of Liquids**

4:55 PM - 5:15 PM

Speaker: Marzena Dzida

#### **Acoustic method as a tool for searching new applications of ionic liquids**

5:15 PM - 5:35 PM

Speaker: Małgorzata Musiał

3:50 PM - 5:35 PM

### Properties of Solids 2: Measurement of Thermal Transport

Location: ECCR135

#### **Measurement of thermophysical properties for the development of a flexible thermal protection system (FTPS) for Mars entry**

3:55 PM - 4:35 PM

Speaker: Erhard Kaschnitz

#### **Measurement of thermal-contact-resistance distribution for semiconductor heat dissipation substrate by using lock-in thermography periodic heating method**

4:35 PM - 4:55 PM

Speaker: Harumi Niida

#### **Thermal diffusivity measurement for high thermal diffusivity materials by applying undersampling to the lock-in thermography**

4:55 PM - 5:15 PM

Speaker: Yudai Kaneko

#### **Measurement of the thermal conductivity and diffusivity at cryogenic temperature**

5:15 PM - 5:35 PM

Speaker: Jean-Pierre Monchau

6:00 PM - 10:00 PM

### Conference Banquet

Location: Stadium Club

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**Fri, Jun 28, 2024**

8:30 AM - 10:15 AM

### Thermal Properties of Nanostructured Materials 3: Propagation of Energy Carriers

Location: ECCR 105

#### **Harnessing Wave and Particle Properties of Phonons for Enhanced Control over Lattice Thermal Transport**

8:35 AM - 9:15 AM

Speaker: Yan Wang

#### **Energy and Charge Carrier Dynamics in Nanoscale Thermal Characterization**

9:15 AM - 9:35 AM

Speaker: Xinwei Wang

#### **Direct Atomistic Wave-packet Simulation of Coherent Phonon Transport in Superlattice Structures**

9:35 AM - 9:55 AM

Speaker: Theodore Maranets

#### **Extending Characterization of Non-diffusive Thermal Transport in Silicon to $\ll 1 \mu\text{m}$ Length Scales using Deep-ultraviolet Transient Gratings**

9:55 AM - 10:15 AM

Speaker: Theodore Culman

8:30 AM - 10:15 AM

## Properties for Materials Science at High Temperatures 6: Laser Techniques I

Location: ECCR200

**Development of laser-based experimental platforms for the study of thermophysical properties of nuclear irradiated fuels at high temperature.**

8:35 AM - 9:15 AM

Speaker: Thomas Doualle

**Emissivity and melting temperature of dual-phase high-entropy boride-carbide ultra-high temperature ceramics**

9:15 AM - 9:35 AM

Speaker: Patrick Hopkins

**Unveiling Front Surface Dynamics in Laser Flash Analysis: Modeling and Fitting for Enhanced Thermophysical Insights**

9:35 AM - 9:55 AM

Speaker: Amir Narymany Shandy

**Melting temperature and high-temperature emissivity of rare-earth silicates**

9:55 AM - 10:15 AM

Speaker: Milena Milich

8:30 AM - 10:15 AM

## Molecular Simulation 5: Phase Equilibria

Location: ECCR245

**Hydrogen Fluoride: A Tale of Four Fluids**

8:35 AM - 9:15 AM

Speaker: J. Ilja Siepmann

**Extensive Molecular Simulation Computation of Thermophysical Properties for Pure Component Refrigerant Molecules and their Mixtures**

9:15 AM - 9:35 AM

Speaker: Barnabas Agbodekhe

**Investigation of the Structure, Stability, and Relative Solubility of Psilocybin in Water and Pure Organic Solvents**

9:35 AM - 9:55 AM

Speaker: Andrew Paluch

**High Pressure Closure of Melting and Freezing Behavior**

9:55 AM - 10:15 AM

Speaker: Karl Travis

8:30 AM - 9:55 AM

## Correlations, Databases, and Engineering Equations of State 8: Theoretically Based EOS Approaches I

Location: ECCR265

**Gibbs and Helmholtz Local Basis Function Representations for Fluids, Solids, and Binary Phases**

8:35 AM - 8:55 AM

Speaker: J. Michael Brown

**An Improved Approach to Cryogenic Solid Solubility Prediction via the Poynting Factor Approximation**

8:55 AM - 9:15 AM

Speaker: Xiong Xiao

**Modelling solid-liquid equilibrium properties of amino-acid and oligopeptide solutions using the SAFT- $\gamma$  Mie group-contribution framework**

9:15 AM - 9:35 AM

Speaker: Ahmed Alyazidi

**An accurate equation of state based on the virial theorem in the statistical mechanics of the square-well potential**

9:35 AM - 9:55 AM

Speaker: Lloyd Lee

8:30 AM - 10:15 AM

### Instrumentation and Measurement Techniques 5: Hydrogen and Raman

Location: ECCR1B40

Session Chair: Paul L. Stanwix

#### **Advanced Test Facility to Characterise Ortho-Para Hydrogen Conversion and Liquid Hydrogen Boil-off**

8:35 AM - 8:55 AM

Speaker: Kwanghee Jeong

#### **Experimental Comparison of Raman Spectroscopy and Microwave Resonant Cavities as ortho-para Hydrogen Composition Sensors**

8:55 AM - 9:15 AM

Speaker: Guinevere M. Sellner

#### **A Magnetic-Suspension Balance for Measurements of Hydrogen at temperatures down to 77 K with pressures up to 15 MPa**

9:15 AM - 9:35 AM

Speaker: Maria-Sophie Günther

#### **A Robust Setup for Efficient Characterization of Multicomponent Vapor-Liquid Equilibria Using Raman Spectroscopy**

9:35 AM - 9:55 AM

Speaker: Marvin Kasterke

#### **Raman Spectroscopy – A Swiss Army Knife for Thermophysical Property Research**

9:55 AM - 10:15 AM

Speaker: Fabian Luther

8:30 AM - 10:15 AM

### Properties of Solids 3: Building and Geological Materials

Location: ECCR135

#### **Geopolymer mortars based on reactive ultra-fine fly ash doped with carbon admixture: Thermoelectric potential**

8:35 AM - 8:55 AM

Speaker: Petr Hotěk

#### **Ultra-Fine Fly Ash Geopolymer Mortars: Influence of Carbonaceous Admixture on New Functional Properties**

8:55 AM - 9:15 AM

Speaker: Lukáš Fiala

#### **Materials structure changes due to irradiation: comparison of impact on radionuclide transport performance of selected porous materials**

9:15 AM - 9:35 AM

Speaker: Václav Kočí

#### **Investigation of convective heat transfer in the surface boundary layers of building envelopes by means of a computational analysis of wind tunnel experiments**

9:35 AM - 9:55 AM

Speaker: Jan Kočí

#### **On the temperature-pressure behavior of effective thermal conductivity of rocks**

9:55 AM - 10:15 AM

Speaker: Boris Grigoriev

8:30 AM - 9:55 AM

### Ionic Liquids 4: Transport Properties I

Location: BESE180

#### **Density, Refractive Index and Thermal Conductivity of [C2mim][C7H15COO] + H2O Mixtures**

8:35 AM - 8:55 AM

Speaker: Rafael M. Almeida

#### **Electrolytic Conductivity Measurements and Models for Ten Ionic Liquids**

8:55 AM - 9:15 AM

Speaker: Joseph Magee

#### **Influence of Different Gases and Molecular Catalysts on Interfacial Tension and Viscosity of Ionic Liquids**

9:15 AM - 9:35 AM

Speaker: Ziwen Zhai

#### **The Thermal Conductivity of Ionic Liquids. Experiment and Molecular Interpretation**

9:35 AM - 9:55 AM

Speaker: Carlos Nieto de Castro

10:15 AM - 10:35 AM

### Coffee Break

Location: Math Plaza

10:35 AM - 12:00 PM

## **Ionic Liquids 5: Transport Properties II**

Location: BESC180

### **Explaining Nonmonotonic Ionic Conductivity in Binary Ionic Liquid-Solvent Mixtures**

10:40 AM - 11:00 AM

Speaker: Amey Thorat

### **Using Machine Learning to Predict Ionic Conductivity of Ionic Liquid Mixtures**

11:00 AM - 11:20 AM

Speaker: Masrur Ahmed

### **A Viscosity Model for Deep Eutectic Solvents Using a Density Scaling Approach**

11:20 AM - 11:40 AM

Speaker: Ricardo Macias-Salinas

### **Thermoelectric properties of ionic liquid/dimethyl sulfoxide hybrid materials**

11:40 AM - 12:00 PM

Speaker: Xiangyang Liu

10:35 AM - 12:20 PM

## **Instrumentation and Measurement Techniques 6: Extreme Conditions**

Location: ECCR1B40

Session Chair: Aaron Rowane

### **Experimental Measurements of Cryogenic Vapor-Liquid and Solid-Fluid Equilibria for the Hydrogen Liquefaction Process**

10:40 AM - 11:00 AM

Speaker: Mark Barwood

### **Measurement of Sound Speeds in Fluids at High Pressure from Near Freezing to Super Critical Temperatures**

11:00 AM - 11:20 AM

Speaker: Olivier Bollengier

### **Progress Toward a Gas Flow Standard for Metering Semiconductor Gases from 10 $\mu\text{L}/\text{min}$ to 1 L/min**

11:20 AM - 11:40 AM

Speaker: Keith Gillis

### **Manufacturing and characterization of the low volume fixed-point of carbon dioxide (CO<sub>2</sub>)**

11:40 AM - 12:00 PM

Speaker: Peter Pavlasek

### **Construction and characterisation of eutectic fixed points of Cobalt carbon (Co-C) and Palladium carbon (Pd-C) for non-contact calibration.**

12:00 PM - 12:20 PM

Speaker: Peter Pavlasek

10:35 AM - 12:20 PM

## **Properties for Materials Science at High Temperatures 7: Laser Techniques II**

Location: ECCR200

### **Structure and thermodynamics of ceramics above 2000 °C**

10:40 AM - 11:00 AM

Speaker: Sergey V. Ushakov

### **Environmental conical nozzle levitator equipped with dual lasers**

11:00 AM - 11:20 AM

Speaker: Scott McCormack

### **Novel contactless measurement technique to determine the thermal conductivity and spectral emissivity of UHTCs at ultra-high temperatures (>2000 °C)**

11:20 AM - 11:40 AM

Speaker: Hunter Schonfeld

### **Validation of Thermal Conductivity Technique for Low Conductivity Oxides at Extreme Temperatures**

11:40 AM - 12:00 PM

Speaker: Scott Bender

### **A new approach for estimating the thermal diffusivity of molten metals at very high temperature**

12:00 PM - 12:20 PM

Speaker: Jad Houssein

10:35 AM - 12:20 PM

## Molecular Simulation 6: Polymers and Surfactants

Location: ECCR245

### Atomistic Modeling of Thermochemical Processes for Efficient Recycling of Polymer Composite Materials

10:40 AM - 11:00 AM

Speaker: Marina Provenzano

### Thermophysical Property Prediction of Aerospace Thermoplastic Polymers with Coarse-grained Models

11:00 AM - 11:20 AM

Speaker: Chris Jones

### The Frank Elastic Constants of Liquid Crystals from Orientational Perturbations

11:20 AM - 11:40 AM

Speaker: Paul Brumby

### SDS Surfactants in Cylindrical Alumina Nanopores

11:40 AM - 12:00 PM

Speaker: Felipe Perez

### Efficient and Accurate Simulation of Surfactant Properties in Aqueous Solutions

12:00 PM - 12:20 PM

Speaker: Martin Richter

10:35 AM - 12:00 PM

## Properties of Solids 4: Theory and Prediction

Location: ECCR135

### Getting Solid Predictions: Solid-state Thermodynamics from Quantum Chemistry

10:40 AM - 11:00 AM

Speaker: Rasmus Fromsejer

### Predicted Dehydration of Brucite ( $\text{Mg}(\text{OH})_2$ ) to Periclase ( $\text{MgO}$ ) at High Pressures and Temperatures Using Local Basis Function Energy Representations

11:00 AM - 11:20 AM

Speaker: J. Michael Brown

### The Quasi-Harmonic Approximation: Solid Equation of State for the Prediction of Thermodynamic Properties and Solid Formation in Fluid Mixtures

11:20 AM - 11:40 AM

Speaker: Tage W. Maltby

### Nanocomposite Solid Materials for Novel Biomechanical Energy Harvesting and Dielectric Cooling

11:40 AM - 12:00 PM

Speaker: Zdravko Kutnjak

10:35 AM - 12:20 PM

## Thermal Properties of Nanostructured Materials 4: Technologies for Tailoring Thermal Conductivity

Location: ECCR 105

### Effective Thermal Conductivity of Dispersions with a Continuous Liquid Phase

10:40 AM - 11:00 AM

Speaker: Francisco E. Berger Bioucas

### Thermal Transport in Nanoengineered Poly-azobenzene Fibers

11:00 AM - 11:20 AM

Speaker: Sai Yelishala

### Investigating the Possibilities for Enhancement of Thermal Conductivity in High Temperature Alloys Through Nanostructuring

11:20 AM - 11:40 AM

Speaker: Douglas Barlow

### Propagation Characteristics of Narrowband Thermal Phonons under Atomic-scale Local Resonance Conditions

11:40 AM - 12:00 PM

Speaker: Prajit Rawte

### Effects of Surface Roughness on Nanophononic Metamaterial Performance

12:00 PM - 12:20 PM

Speaker: Chia-Nien Tsai

10:35 AM - 12:00 PM

**Correlations, Databases, and Engineering Equations of State 9: Theoretically Based EOS Approaches II**

Location: ECCR265

**Maximizing cubic EoS potential by fusing a theoretically sound mixing rule with an uncharted activity coefficient model**

10:40 AM - 11:00 AM

Speaker: Jean-Noël Jaubert

**Comparison of CP-PC-SAFT and CS-SAFT-VR-Mie in predicting fluid phase behavior in systems of phenolic compounds, aromatic amines, acetophenone and benzaldehyde.**

11:00 AM - 11:20 AM

Speaker: Ilya Polishuk

**Fundamental Reverse van der Waals Equation of State**

11:20 AM - 11:40 AM

Speaker: Sergio E. Quiñones-Cisneros

**WHIA: A Novel Cubic Equation of State for Accurate Modeling of Water Properties**

11:40 AM - 12:00 PM

Speaker: Ehsan Heidaryan