Program

Sunday, 17.7.2022

Time	Sun, 17. Jul *TU Graz – Rechbauerstraße*	
13:30	**Registration** *Hotel Weitzer*	
18:00	Laureate Chair: S. Enders	**Opening** **Michelsen Award - S. Kjelstrup, Norwegian University of Science and Technology** "Thermodynamics at small scales" sponsored by Elsevier
19:30 - 22:00	**Welcome Reception**	

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Program

Monday, 18.7.2022 08:30 - 13:30

Time	Monday, 18.07.2022 *Hotel Weitzer*			
08:30	**Keynote** **Chair: J. N. Jaubert**	**K1 Keynote Speaker - A. Singh, Jansen Pharmaceuticals** "Development of Amorphous Solid Dispersions: Significance and factors impacting phase-behavior"		
		K2 Keynote Speaker - M. Fischlschweiger, TU Clausthal "Thermodynamic principles for tailoring polymer properties"		
10:00	**Coffee Break**			
10:25	**Polymer 1** **Chair: K. Langenbach**	**S1 Kruppa:** "Ultrasound-Induced Polymer Degradation", KIT	**Electrolytes 1** **Chair: N. Voutsas**	**S2 Roa Pinto:** "Temperature dependence and short-range electrolytic interactions within the e-PPC-SAFT framework", IFPEN
		S3 Valsecchi: "The influence of tie-molecules and microstructure on the fluid solubility in semi-crystalline polymers", Imperial College		**S4 Silva:** "The limits of the Debye-Hückel models concerning the Poisson-Boltzmann equation", Technical University of Denmark
		S5 Atiq: "Prediction of hydrogen sorption in semi-crystalline polymers through a multi-scale modeling approach.", University of Bologna		**S6 De-Hemptinne:** "Best Practices for the parameterization of reactive electrolyte mixed-solvent systems: an EleTher JIP contribution", IFPEN
11:30	**Polymer 2** **Chair: G. Sadowski**	**S7 Fan:** "Solid-liquid equilibria of polydisperse polyethylene-solvent systems based on continuous thermodynamics and lattice cluster theory", TU Clausthal	**Electrolytes 2** **Chair: Y. Wei**	**S8 Velho:** "Insights on the thermodynamic modelling of ionic liquids using the Pitzer-Debye-Hückel Equation", University of Porto
		S9 Wolf: "Polymer Solutions: Equilibrium Clusters versus Shear clusters", University of Mainz		**S10 Yang:** "A benchmark database for mixed-solvent electrolyte solutions: Consistency analysis using e-NRTL", IFPEN
		S11 Nikiforova: "Linear polyelectrolyte chains with differing counterions in solution: a field theoretic modeling vs MD", St. Petersburg State University		**S12 Moine:** "Electrolyte models: good practices to parameterize them?", ProSim
12:30	**Lunch Break**			

Program

Monday, 18.7.2022 13:30 - 21:00

Time	Monday, 18.07.2022 *Hotel Weitzer*			
13:30	**Phase Equilibria 1** **Chair: W. Chapman**	**S13 Rehner:** "Helmholtz energy model for fused-sphere chains", University of Stuttgart	**Pharma** **Chair: M. Fischlschweiger**	**S14 Danzer:** "Release Behaviour of Amorphous Solid Dispersion: Thermodynamics and kinetics" TU Dortmund
		S15 Wehbe: "Thermodynamic modeling of the nature of speciation and phase behavior of binary and ternary mixtures of formaldehyde, water and methanol", Imperial College		**S16 Serban:** "Thermodynamic characterization of plasma proteins interactions with sphingomyelin based nanoemulsions", Romanian Academy
		S17 Arroyo-Avirama: "2-Phenylethanol Extraction from an Aqueous Phase: Solvent Selection Using PC-SAFT and Experimental Data", Pontificia Universidad Católica de Chile		**S18 Borrmann:** "Measuring and modeling simultaneous water sorption and crystallization kinetics in ASDs", TU Dortmund
14:35	**Phase Equilibria 2** **Chair: J. Trusler**	**S19 Tenberg:** "Phase Equilibria and Separation of Solid Solutions Using Solvent Mixtures in Counter-Current Crystallizers", MPI Magdeburg	**Supercritical Fluids** **Chair: P. Jaeger**	**S20 Dhakal:** "Speeds of Sound in Binary Mixtures of Water and CO2 at Temperatures from 273.15 K to 313.15 K and at Pressures up to 50 MPa", University of Western Australia
		S21 Aasen: "Perturbation theories for fluids with short-ranged attractive forces", Norwegian University of Science and Technology		**S22 Secuianu:** "High-pressure phase equilibrium for carbon dioxide + branched alkanes", University Politehnica of Bucharest
		S23 Nezbeda: "Thermodynamic properties of water from SAFT and CPA equations of state: Critical assessment", Czech Academy of Sciences		**S24 Georgiopoulou:** "Optimization and comparison of supercritical CO2 and microwave assisted extraction of bioactive compounds from Chlorella vulgaris", National Technical University Athens
15:35	**Coffee Break**			
16:00	**Chair: F. Jirasek**			
	Online Poster Session 1		**Poster Session 1**	
18:00	**Break**			
19:00 - 21:00	**Dinner** *Hotel Weitzer*			

Program

Tuesday, 19.7.2022 08:30 - 13:30

Time	Tuesday, 19.07.2022 *Hotel Weitzer*			
08:30	**Keynote** **Chair: S. Enders**	**K3 Keynote Speaker - C. Miqueu, Univ. Pau & Pays Adour** "Thermodynamics of inhomogeneous fluids with molecular Density Functional Theory (DFT)"		
		K4 Keynote Speaker - C. Brandenbusch, TU Dortmund "Transformation to a sustainable (bio-) chemical production - what thermodynamics has to offer"		
10:00	**Coffee Break**			
10:25	**Interface 1** **Chair: Ø. Wilhelmsen**	**S25 Nagl:** "Interfacial Properties of Reactive Liquid-Liquid Systems", TU Graz	**Data Driven Modeling** **Chair: J.-C. de Hemptinne**	**S26 Jirasek:** "Hybrid Models for Predicting Fluid Properties of Mixtures", TU Kaiserslautern
		S27 Hajjar: "Time-dependent Interfacial Properties", KIT		**S28 Jaubert:** "Performance evaluation of cubic and SAFT-type equations of state over 300,000 experimental data points from 1800 pure components", Université de Lorraine
		S29 Trusler: "Experimental and Modelling Study of the Interfacial Tension of (n-Decane + Carbon Dioxide + Water) in the Three Phase Region", Imperial College		**S30 Gond:** "Molecular Descriptors from Mixture Data", TU Kaiserslautern
11:30	**Interface 2** **Chair: C. Miqueu**	**S31 Hammer:** "Classical DFT for Hydrogen: Vapour-liquid interfaces and confined systems", Norwegian University of Science and Technology	**Electrolytes 3** **Chair: C. Held**	**S32 Naseri Boroujeni:** “Electrical conductivity of associative electrolyte solutions", Technical University of Denmark
		S33 Brettschneider-Lazaro: "Surface Properties of Water containing Mixtures using ARPC-SAFT Equation of State", KIT		**S34 Polishuk:**"Wide-ranging prediction of phase behaviour in the systems of [Cxmim][BF4] and [Cxmim][PF6] (2≤x≤12) ionic liquids by CP-PC-SAFT with universal kij value.", Ariel University
		S35 Wachsmann: "Investigation of droplet and bubble coalescence using the Navier-Stokes-Korteweg approach with the PeTS equation of state", University of Innsbruck		**S36 Velho:** "Determining the dissociation degree of ionic liquids in aqueous binary mixtures", University of Porto
12:30	**Lunch Break**			

Program

Tuesday, 19.7.2022 13:30 - 23:00

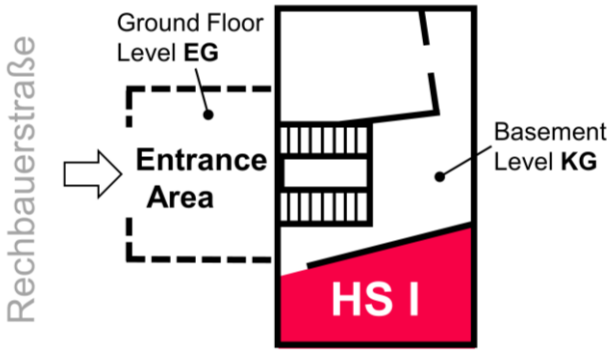
Time	Tuesday, 19.07.2022 *Hotel Weitzer*			
13:30	**Phase Equilibria 3** **Chair: C. Secuianu**	**S37 Held / Wangler**: "Predictive thermodynamic models: Gas solubility in acid-gas removal plants", TU Dortmund / BASF	**Molecular Modeling** **Chair: M. Fermeglia**	**S38 Habibi:** "Hydrogen Storage in 2D Boron-Based Materials", TU Delft
		S39 Castaneda: "Design and study of new tunable hydrophobicity solvents", Institut de Chimie de Clermont Ferrand		**S40 Pulido Lamas:** "Computing the phase diagram of the NaCl/water system via direct coexistence simulations", Universidad Complutense de Madrid
		S41 Novak: "Vapor-Liquid and Liquid-Liquid Equilibria in Electrolyte Solutions: Algorithms and Modeling", NCSR Demokritos		**S42 Bhendale:** "Insights into the thermodynamics and morphology of different phases of pluronic L64 from molecular simulations using derived coarse-grained model", Indian Institute of Technology Kanpur
14:35	**Phase Equilibria 4** **Chair: F. Llovell**	**S43 Bernet:** "Overview of thermodynamic properties of saturated lactones and extension of the SAFT-γ Mie approach", Imperial College London	**Associating Systems** **Chair: S. Kjelstrup**	**S44 Marx:** "Vapor-Liquid Equilibria of Mixtures of Fluids with Different Polarity", University of Innsbruck
		S45 Turner: "Molecular Simulation of Temperature Swing Solvent Extraction of High Salinity Brines", The University of Alabama		**S46 Chapman:** "Beyond Flory-Huggins: Activity coefficients from perturbation theory for polar, polarizable, and associating molecules from solvents to polymers", Rice University
		S47 Safonova: "Polymerized ionic liquids as new bioextraction agents", St. Petersburg State University		**S48 Cripwell:** "Structural (s)-SAFT-γ Mie Equation of State for Associating Compounds", Stellenbosch University
15:35	**Coffee Break**			
16:00	**Chair: N. Hansen**			
	Online Poster Session 2		**Poster Session 2**	
18:00	**Break**			
19:00 - 23:00	**Conference Dinner** *Schlossberg Restaurant* Knapp Award, sponsored by Digital Physics			

Program

Wednesday, 20.7.2022 08:30 - 14:00

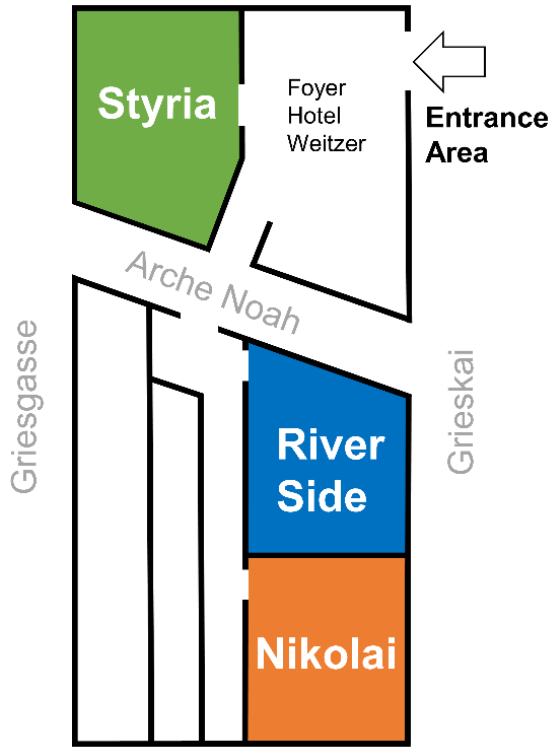
Time	Wednesday, 20.07.2022 *Hotel Weitzer*			
08:30	Keynote Chair: R. Dohrn	**K5 Keynote Speaker - Z. Knez, University of Maribor** "Fundamental Data for Design of Processes Using Sub- or Supercritical Fluids"		
09:20	COSMO Methods Chair: R. Dohrn	**S49 Klamt:** "Simulation of surfactants at interfaces with COSMOplex", DS Deutschland	Cycle Processes Chair: T. Zeiner	**S50 Albà:** "Thermodynamic design of low-GWP drop-in replacements for R134a and R410A by means of the polar soft-SAFT EoS", Universidad Rovira i Virgili
		S51 Dumouilla: "From numerical chemistry tools to the prediction of water activity in complex aqueous solutions containing carbohydrates and polyols", Roquette-Frères		**S52 Llovell:** "Thermodynamic characterization and energy analysis of hydrofluoroethers in Organic Rankine Cycles using soft-SAFT", Rovira i Virgili
		S53 Müller: "Efficient parameterization of openCOSMO-RS from the ground up", TU Hamburg		**S54 Tamson:** "New apparatus for the measurement of physical properties of cryogenic fluids", KIT
10:20	**Coffee Break**			
10:40	Novel Experimental Methods Chair: A. Soto	**S55 Ballerat-Busserolles:** "New Improvements for experimental thermodynamic characterization of brines loaded with Carbon Dioxide", Université Clermont Auvergne	Phase Equilibria 5 Chair: I. Nezbeda	**S56 Yan:** "Saturation Point and Phase Envelope Calculation for Systems with Simultaneous Chemical and Phase Equilibrium", Technical University of Denmark
		S57 Tenardi: "Characterization of a Novel Composite Microwave Resonator for Vapor-Liquid Equilibrium Measurements of Binary Mixtures", University of Western Australia		**S58 Thien:** "Microfluidics and Raman Spectroscopy for highly efficient and automated measurements of liquid-liquid equilibria", RWTH Aachen
		S59 Bernardini: "A new instrument for accurate dew-point density measurements of fluid mixtures", TU Chemnitz		**S60 Bauer:** "FeOs – an Open-Source Framework for Equations of State and Classical Density Functional Theory", University of Stuttgart
11:45	Cubic EOS Chair: E. Macedo	**S61 Fermeglia:** "50 years of Soave Equation of State (SRK): a source of inspiration for applied thermodynamics", University of Trieste	Phase Equilibria 6 Chair: M. Richter	**S62 Wang:** "Modeling CO2 absorption with chemical solvents via electrolyte thermodynamic models", AspenTech
		S63 Privat: "New insight on EoS/gE mixing rules for cubic equations of state: proposition of a unified approach", Université de Lorraine		**S64 Queimada:** "Modeling Hydrate Curves with a new Generalized Cubic-Plus-Association Equation of State (CPA EoS)", Aveiro University
12:45	**Closing Speech**			
13:15	**Lunch Break**			
14:00	**End of ESAT 2022**			

Floor Plan
Technical University Graz



- Lecture room HS I:
  - Opening of the 2022 ESAT conference
  - Michelsen Award
  - Welcome reception

Floor Plan
Hotel Weitzer



- Conference room **Styria** - Oral sessions:
  - Polymers 1 – 2
  - Phase Equilibria 1 – 4
  - Interface 1 – 2
  - Cosmo Methods
  - Novel Experimental Methods
- Conference room **River Side** - Oral sessions:
  - Electrolytes 1 – 3
  - Pharma
  - Supercritical Fluids
  - Data Driven Modeling
  - Molecular Modeling
  - Associating Systems
  - Cycle Processes
  - Phase Equilibria 5 – 6
- Conference room **Nikolai** - Poster sessions 1 & 2