Poster Presentations – Session 1

Monday, 18.07. 16:00 – 18:00

Hotel Weitzer, Room: Nikolai

ID	Presenting Author	Affiliation	Title
P1-1	A. Alhadid	Technical University of Munich, Germany	Modeling of Solid Complexes Formation in Deep Eutectic Solvents Using COSMO-RS
P1-2	O. Atiq	Università di Bologna, Italy	Solubility in semi-crystalline polymers: A comparative review of the available modeling strategies.
P1-3	B. Bursik	University of Stuttgart, Germany	Predicting Solvation Free Energies from the MNSol database using Classical Density Functional Theory based on PC-SAFT
P1-4	I. Cachadiña Gutiérrez	Universidad de Extremadura, Spain	A pressure-surface tension-temperature equation of state for n-alkanes
P1-5	R. Canales	Pontificia Universidad Católica de Chile, Chile	Thermodynamic selection of solvents for in situ recovery of b-ionone from a fermentation broth
P1-6	E. Cea-Klapp	Universidad de Concepción, Chile	Interfacial properties of deep eutectic solvents by density gradient theory
P1-7	S. Enders	Karlsruhe Institute of Technology (KIT), Germany	Modeling the salt influence on swelling of crosslinked Poly(N-isopropyacrylamide) in aqueous solution
P1-8	T. Esper	University of Stuttgart, Germany	(group contribution-) equation of state parametrization using large experimental databases
P1-9	M. Fermeglia	University of Trieste, Italy	A Molecular Dynamics approach to investigate the tribological behaviour of Al-Si and α-Al2O3-Si interfaces at the nanoscale
P1-10	A. Gonçalves	University of Campinas, Brazil	Investigation of cross-association between CO2 and H2S using the SAFT-VR-Mie EoS
P1-11	R. Haghbakhsh	University of Isfahan, Iran	More than 100 deep eutectic solvents of different natures investigated by the PC-SAFT EoS for their CO2 solubility
P1-12	N. Hayer	TU Kaiserslautern, Germany	Prediction of Temperature-Dependent Henry's Law Constants by Matrix Completion
P1-13	M. De Angelis	University of Edinburgh, UK	The Determination of Equation of State (EoS) Parameters Using Machine Learning Methods: A Case Study of The Sanchez-Lacombe EoS.
P1-14	S. Khennache	University of PAU, France	Thermophysical properties prediction: towards a generic coarse grained force field
P1-15	A. Kłosińska	Warsaw University of Technology, Poland	Ionic liquids in Separation of butadiene from C4- fraction
P1-16	A. Kroyan	Norwegian University of Science and Technology, Norway	Molecular Dynamics simulations for RNA : benchmark and folding-stretching experiments
P1-17	S. Wagner	Graz University of Technology, Austria	Modeling liquid absorption of highly cross-linked epoxy resins
P1-18	S. Leube	Karlsruhe Institute of Technology (KIT), Germany	Gas Solubility in Semi-crystalline Branched Polyolefins
P1-19	P. Ndiaye	Federal University of Rio de Janeiro, Brazil	Barotropic inversion in carbon dioxide rich systems
P1-20	D. Nichita	CNRS-University of Pau, France	Rapid three-phase equilibrium calculations in water-hydrocarbon mixtures
P1-21	K. Papchenko	University of Edinburgh, United Kingdom	Molecular Screening Of Sustainable Alternatives To Polymeric Membranes: The Case Of Poly(Hydroxy Alkanoates)

P1-22	H. Polat	TotalEnergies S.E., France	A Major Update to the Open Source Monte Carlo Software Brick-CFCMC: Thermodynamic Integration and Hybrid MD/MC Trial Moves
P1-23	T. Poppe	Karlsruhe Institute of Technology (KIT), Germany	Calculation of Caloric Properties using EoS
P1-24	S. Raeissi	University of Isfahan, Iran	Global models for estimating electrical and thermal conductivities of deep eutectic solvents
P1-25	M. Sekulla	Chemnitz University of Technology, Germany	Linking molecular adsorption simulations and density measurements: The key to more accurate dew-point densities?
P1-26	A. Serban	Romanian Academy, Romania	A thermodynamic study of the protein interaction with magnetic dextran iron oxide nanoparticles
P1-27	F. Shaahmadi	Stellenbosch University, South Africa	Monomer Fraction Measurement of Ethanol+ Ketones Binary Mixtures Using FTIR Spectroscopy
P1-28	G. Silva	Technical University of Denmark, Denmark	The specificities of the different derivations of the Debye-Hückel equations
P1-29	M. Singer	Graz University of Technology, Austria	Interfacial Behavior and Droplet Interaction in Liquid-Liquid Systems
P1-30	A. Somoza	Universidade de Santiago de Compostela, Spain	Mixtures of sodium dodecylbenzenesultonate and surface active ionic liquids for Enhaced Oil Recovery processes
P1-31	A. Soto	Universidade de Santiago de Compostela, Spain	Amino Acid solubility in acetate ionic liquids
P1-32	M. Tariq	Universidade NOVA de Lisboa, Portugal	CO2 Hydrates Phase Behaviour and Dissociation Enthalpies in Presence of Novel Ionic Liquids
P1-33	E. Tsochantaris	Technical University of Denmark, Denmark	Evaluation of associated reference thermodynamic models for water's anomalies
P1-34	S. Tzima	National Technical University of Athens, Greece	Evaluation of conventional and novel technologies for H2S and CO2 recovery from natural gas
P1-35	T. van Westen	University of Stuttgart, Germany	uv-Theory for Lennard-Jones chain fluids
P1-36	R. Villablanca Ahues	Technische Universität Clausthal, Germany	Phase Equilibria and Interfacial Properties at Elevated Pressure
P1-37	E. Voutsas	National Technical University of Athens, Greece	Extraction of Chlorella vulgaris using a deep eutectic solvent
P1-38	Ø. Wilhelmsen	SINTEF Energy Research, Norway	Using thermodynamics and equations of state to describe the thermal effects of sorption in porous media
P1-39	M. Willger	TU Freiberg, Germany	Activity Coefficients from Excess Raman Spectra
P1-40	B. Wilthan	NIST, United States of America	API accessible free NIST thermophysical property database for metal systems
P1-41	W. Yan	DTU Chemistry, Denmark	RAND-based Chemical and Phase Equilibrium Computation: From Standalone Calculation to Dynamic Simulation
P1-42	J. Yip	University of Innsbruck, Austria	Transient diffusion investigated with irreversible thermodynamics and molecular simulation

Poster Presentations – Session 2

Tuesday, 19.07. 16:00 – 18:00

Hotel Weitzer, Room: Nikolai

ID	Presenting Author	Affiliation	Title
P2-1	R. Amaral Coutinho Bartolomeu	State University of Campinas, Brazil	A molecular dynamics study on the role of Cholesterol in DPPC bilayers
P2-2	V. Bråten	Norwegian University of Science and Technology, Norway	Equation of State for Confined Nanosystems
P2-3	O. Cabeza	Universidade da Coruña, Spain	Monitoring of water contamination with a toxic ionic liquid through its physical properties
P2-4	Q. Chen	Imperial College London, London, UK	Solubility of Carbon Monoxide in Water and NaCl Aqueous Solutions at High Pressures
P2-5	J. Cripwell	Stellenbosch University, South Africa	Application of renormalization corrections to SAFT-VR Mie
P2-6	S. Dhakal	The University of Western Australia, Australia	Speeds of Sound in Gaseous, Liquid, and Supercritical Difluoromethane at Temperatures from 293 K to 373 K and at Pressures up to 40 MPa
P2-7	M. Fleck	University of Stuttgart, Germany	Transferable anisotropic Mie-potential (TAMie) force field for amines and alcohols
P2-8	O. Frotscher	Chemnitz University of Technology, Chemnitz, Germany	Optimal Experimental Design and Molecular Dynamics Simulations for Efficient Data Acquisition
P2-9	J. Gomez-Estevez	Universitat de Barcelona, Spain	The osmotic coefficient in implicit solvent simulations and the McMillan-Mayer theory of solutions
P2-10	A. Gonçalves	University of Campinas, Brazil	Capillary condensation: limitations of the multicomponent potential theory of adsorption (MPTA)
P2-11	R. Haghbakhsh	University of Isfahan, Iran	Thermodynamic Investigation on using Deep Eutectic Solvents as cosolvents for enhancing drug solubilities
P2-12	V. Jervell	PoreLab, Norway	Using Equations of State and Non-equilibrium Thermodynamics to Model Thermal Diffusion
P2-13	M. Kasterke	RWTH Aachen University, Germany	Single-droplet tracking in microfluidic plug-flow for automated Raman-based determination of liquid-liquid equilibria
P2-14	A. Keba	Universidade NOVA de Lisboa, Portugal	Effect of imidazolium-based ionic liquids on the formation and growth of tetrahydrofuran hydrates
P2-15	S. Khennache	University of PAU, France	Towards the development of a semi-rigid Lennard-Jones chain SAFT EoS
P2-16	Y. Leusmann	Chemnitz University of Technology, Germany	Improved Microwave Re-entrant Cavity Geometries for Dew-Point Measurements and Complete Phase Determination
P2-17	A. Marciniak	Warsaw University of Technology, Poland	Hansen Solubility Parameters for Ionic Liquids
P2-18	A. Moreau	University of Valladolid, Spain	Speed of sound measurements of propane with hydrogen
P2-19	S. Naseri Boroujeni	Technical University of Denmark (DTU), Denmark	A predictive analysis of electrical conductivity models for electrolyte solutions
P2-20	P. Ndiaye	Federal University of Rio de Janeiro, Brazil	Water content determination in natural gas streams
P2-21	S. Ormazábal-Latorre	Pontificia Universidad Católica de Chile, Chile	Liquid-liquid separation of guaiacol from n-hexane using glycols and their choline chloride-based eutectic mixtures

P2-22	F. Paes	Université de Lorraine, France	Prediction of solvation energies for biofuel oxidation stability: benchmarking of models and development of a method for radicals
P2-23	A. Reimer	University of Stuttgart, Germany	Highly accurate uv-theory for Lennard-Jones and Mie fluids
P2-24	M. Richter	The University of Western Australia, Australia	Is Raman spectroscopy appropriate for reliable sorption analysis?
P2-25	E. Safonova	Saint Petersburg State University, Russian Federation	Employing the Born term in modeling aqueous solutions of high valence electrolytes and water-miscible ionic liquids
P2-26	G. Segner	Graz University of Technology, Austria	A model to describe associating mixtures of structural isomers
P2-27	J. Skvara	The Czech Academy of Sciences, Czech Republic	Effect of Solvent on Ibuprofen Chiral Recognition: A Molecular Dynamic Study
P2-28	A. Somoza	Universidade de Santiago de Compostela, Spain	Activity maps as tools for surfactant enhanced oil recovery
P2-29	A. Soto	Universidade de Santiago de Compostela, Spain	Eutectic solvents for valorisation of fish processing industry waste: fundamental studies
P2-30	P. Stanwix	The University of Western Australia, Australia	Microwave Resonator Sensors for Detecting Solid Formation and Deposition
P2-31	R. Stierle	University of Stuttgart, Germany	Hydrodynamic Density Functional Theory for Coalescence of Mixtures
P2-32	M. Tariq	Universidade NOVA de Lisboa, Portugal	Effect of Host Framework on The Phase Behaviour and Nucleation of CO2 Hydrates: Isotopic Effects
P2-33	A. Tiwikrama	National Taipei University of Technology, Taiwan	EPPS-buffer effect on liquid-liquid equilibria of carboxylic acids (acetic acid/propionic acid/lactic acid)-water-methyl isobutyl ketone at elevated temperatures
P2-34	J. Trancoso Fernandes dos Santos	Danmarks Tekniske Universitet, Denmark	Vapor-Liquid Equilibrium Measurements and Cubic Plus Association (CPA) Modeling of Triethylene Glycol (1) + Methane/Ethane (2) + Water (3) Systems
P2-35	D. Vega-Maza	University of Valladolid, Spain	New technique for measuring humidity in gases
P2-36	P. Velho	University of Porto, Portugal	Partition Of Vitamins With Antioxidant Properties In Green Aqueous Two-Phase Systems
P2-37	F. Vermeire	Massachusetts Institute of Technology, USA	The Merit of Thermodynamics in Machine Learning
P2-38	M. Więckowski	Warsaw University of Technology, Poland	Eutectics of Diols and Ionic Liquids as Phase Change Materials
P2-39	B. Winter	ETH Zürich, Switzerland	Predicting limiting activity coefficients using natural language processing
P2-40	M. Wlazło	Warsaw University of Technology, Poland	Activity coefficients at infinite dilution of [C3(OH)2MIM][NTf2] ionic liquid for the separation processes
P2-41	S. Wünsche	Max-Planck-Institut für Dynamik komplexer technischer Systeme, Germany	Solubility measurement and modeling of artemisinin in toluene/n-heptane mixtures
P2-42	D. Grigorash	DTU Chemistry, Denmark	Diffusion Coefficients in Systems Related to Reservoir Fluids: Available Data and Evaluation of Correlations
P2-43	J. Zimmermann	Clausthal University of Technology, Germany	Simultaneous experimental determination of gas sorption and accompanied changes of caloric properties in glassy polymers

Online Poster Presentations – Session 1

Monday, 18.07. 16:00 – 18:00

Hotel Weitzer, Room: Styria, Webex

ID	Presenting Author	Affiliation	Title
O1-1	K. Moodley	University of KwaZulu-Natal, South Africa	Application of the Truncated Perturbed Chain-Polar Statistical Associating Fluid Theory (tPC-PSAFT) to Alcohol/Alkane mixtures at high pressures
O1-2	A. Mansuri	INVITE GmbH, Cologne, Germany	Improved Free Volume Theory for the Self-Diffusion of Active Ingredients in Amorphous Polymers
O1-3	G. Tasios	National Technical University of Athens, Greece Equinor ASA, Norway	Development of a group contribution cubic equation of state with emphasis to natural gas mixtures
O1-4	N. Prinos	National Technical University of Athens, Greece	Development of a new solvation segment activity coefficient model based on COSMO-SAC
O1-5	A. González de Castilla	Hamburg University of Technology, Germany	Predicting the solubility of salts in non-aqueous solvents
O1-6	V. Gaganis	National Technical University of Athens, Greece	A generalized manifestation of the phase behavior problem for complex phase split calculations
O1-7	A. Nesterov	Lomonosov Moscow State University, Russian Federation	Thermodynamic Properties and Phase Equilibria in the Water–Aluminum Chloride–Aluminum Sulfate System
O1-8	G. Miyazaki	Mines Paristech, France	Vapor-Liquid Equilibria of alcohols in Deep Eutectic Solvent: Experimental data and modelling

Online Poster Presentations – Session 2

Tuesday, 19.07. 16:00 – 18:00

Hotel Weitzer, Room: Styria, Webex

ID	Presenting Author	Affiliation	Title
O2-1	K. Moodley	University of KwaZulu-Natal, South Africa	Design and Optimization of a Separation Process for Butanediol Dehydration for Use as a Biofuel
O2-2	Y. Chung	Massachusetts Institute of Technology, USA	Predicting solid solubility of organic solutes over a wide range of solvents and temperatures
O2-3	M. Campestrini	PSL University, France	On the crystallization of solid formers during liquefaction of gases
O2-4	K. SAITO	University of Tsukuba, Japan	Calorimetric Investigation of Crystalline p-Polyphenyls: Heat Capacity of p-Sexiphenyl
O2-5	G. DAS	OLI Systems Inc., USA	Thermodynamic modeling of rare earth fluorides in multi-component systems over a wide range of solution conditions
O2-6	M. S. Sadaghiani	The University of Western Australia, Australia	Vapour-Liquid Equilibria for 3,3,3-Trifluoropropene (HFO-1243zf) + Carbon Dioxide (CO2) Binary Mixtures
O2-7	Z. Zuo	Nanjing Tech University, China	A SAFT equation of state for the CH4–H2S–CO2–H2O–NaCl System: Phase equilibria at high temperatures and pressures
O2-8	G. Ivanis	University of Belgrade, Serbia	Thermodynamic properties of binary system eugenol + 4-propylguaiacol in wide ranges of temperature and pressure