29th European Symposium on Applied Thermodynamics – ESAT 2017

May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Thursday, May 18th, 2017		
10.00-18.00	***Registration (Registration desk – Radisson Blu Hotel, Atlas Foyer)***	
14.45-15.05	**Opening Ceremony – Romanian Athenaeum (across Radisson Blu Hotel)** *Catinca Secuianu, Mihnea Costoiu, Eugenia Macedo*	
15.05-15.15	**BASF** – *Diana Neacșu, Communications and Government Relations*	
15.15-16.45	**Invited lectures (Romanian Athenaeum)** *Chairs: Catinca Secuianu and Georgios Kontogeorgis*	
15.15-16.00	**IL1**	***Phase Behaviour, Interfacial and Single-Phase Properties of CO_2-Brine Mixtures for Applications in Carbon Storage*** *J.P. Martin Trusler* – Imperial College London, UK
16.00-16.45	**IL2**	***Fast and robust volume-based phase equilibrium calculations*** *Dan Nichita* – University of Pau and Pays de l'Adour, France
17.00-19.30	***Coffee Break (Radisson Blu Hotel, Prefunction area)*** ***Poster Session – Radisson Blu Hotel (Prefunction Area, Atlas Foyer)***	
19.30-22.00	**Welcome Cocktail**	

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Friday, May, 19th 2017						
8.00-10.00	***Registration (Registration desk – Radisson Blu Hotel, Atlas Foyer)***					
8.30-10.45	**Invited lectures (Atlas 1)** *Chairs: Ioannis Economou, Alexey Victorov, and Urszula Domańska-Żelazna*					
8.30-9.15	**IL3**	***Electrolyte solutions: Simulation challenges and the quest for better models*** *Athanassios Z. Panagiotopoulos* – Princeton University, USA				
9.15-10.00	**IL4**	***Solubility of precombustion gasses and sulfur components in ionic liquids and physical solvents by Monte Carlo simulations*** *Thijs Vlugt* – Delft University of Technology, The Netherlands				
10.00-10.45	**IL5**	***Polymer – based nanocomposites. New methods and concepts*** *Horia Iovu* – University Politehnica of Bucharest, Romania				
10.45-10.50	***BASF presentation***					
10.50-11.15	***Coffee Break (Radisson Blu Hotel, Prefunction area)*** ***Poster Session – Radisson Blu Hotel (Prefunction Area, Atlas Foyer)***					
11.15-13.00	**Parallel sessions**					
	Atlas 1		**Merope 1+2**		**Electra 1+2**	
	Session: Phase equilibria & transport properties (experimental & modelling) *Chairs: Dan Nichita and Martin Trusler*		**Session: Molecular & statistical thermodynamics** *Chairs: Athanassios Z. Panagiotopoulos and Thijs Vlugt*		**Session: Phase equilibria & transport properties (experimental & modelling)** *Chairs: Xuqiang Guo and Horia Iovu*	
11.15-11.30	O1	Electrolyte Thermodynamics: Current Status, Future Challenges and some applications of an electrolyte CPA equation of state *Georgios M. Kontogeorgis* – Technical University of Denmark	O8	Beyond "simple" COSMO-RS theory: Current developments and future perspectives for the improvement and extension of a successful model *Andreas Klamt* – COSMOlogic GmbH&CoKG/University of Regensburg	O15	Extraction of 2–phenylethanol (PEA) from aqueous phase using ionic liquids *Urszula Domańska-Żelazna* – Warsaw University of Technology
11.30-11.45	O2	***Sponsored by BASF*** Phase equilibria for CO_2 + 1,2-dimethoxy-ethane at high-pressures *Sergiu Sima* – University Politehnica of Bucharest	O9	Round Robin Study of Molecular Simulation Programs *Michael Schappals* – University of Kaiserslautern	O16	High pressure vapor-liquid equilibria for Diethyl + methane and + carbon dioxide *Silvana Mattedi* – University Federal of Bahia

11.45-12.00	O3	Accurate modelling of high-pressure phase-equilibria of mixtures containing non-condensable components *Silvia Lasala* – University of Lorraine	O10	Perturbation based activity coefficient model for hard-sphere chain mixtures *Gerard J.P. Krooshof* – DSM Ahead B.V/ Eindhoven University of Technology	O17	Thermodynamic stability of ethane clathrate hydrate under an external field *Matthew Lasich* – University of KwaZulu-Natal
12.00-12.15	O4	Investigation of Mass Transfer in Liquid-Liquid Systems based on Density Gradient Theory *Tim Zeiner* – TU Dortmund	O11	CO_2 solubility in carboxylic acids: PC-SAFT modeling and Monte Carlo simulations *Mahinder Ramdin* – Delft University of Technology	O18	Viscosity of long-chain molecules *Velisa Vesovic* – Imperial College London
12.15-12.30	O5	Influence of temperature on liquid-liquid equilibria of water+alcohol+entrainer systems *Cara E. Schwarz* – Stellenbosch University	O12	Combining the reaction ensemble with the Continuous Fractional Component Monte Carlo technique *Ali Poursaeidesfahani* – Delft University of Technology	O19	Gas hydrates in, on and around water droplets *Daniel Broseta* – University of Pau and Pays de l'Adour
12.30-12.45	O6	A methodology for the development of an extensive databank containing Gibbs-energy-of-solvation data of pure and mixed solutes *Edouard Moine* – University of Lorraine	O13	Technology Predicting Liquid-Liquid Equilibria with Associating Lattice Cluster Theory *Kai Langenbach* – University of Kaiserslautern/Rice University	O20	Modeling of aggregates in ionic surfactant solutions and concentration effect *Nikolai A. Volkov* – Saint Petersburg State University
12.45-13.00	O7	Calculation of water content of natural gases using the PC-SAFT equation of state *Khashayar Nasrifar* – Shiraz University of Technology	O14	Renewable platform-chemicals and materials: Thermochemical study of levulinic acid esters *Sergey Verevkin* – University of Rostock *Christoph Held* – TU Dortmund University	O21	Study on the thermodynamics and kinetics of CH_4 hydrate in the presence of bio-additives *Qiang Sun* – China University of Petroleum
13.00-14.30	***Lunch*** ***Poster Session- Radisson Blu Hotel (Prefunction Area, Atlas Foyer)***					
14.30-16.30	**Parallel sessions**					
	Atlas 1		**Merope 1+2**		**Electra 1+2**	
	Session: Phase equilibria & transport properties (experimental & modelling) *Chairs: Romain Privat and Michael Kleiber*		**Session: Molecular & statistical thermodynamics** *Chairs: Joachim Gross and Jean-Charles de Hemptinne*		**Session: Phase equilibria & transport properties (experimental & modelling)** *Chairs: Sergey Verevkin and Antonio Marcilla*	
14.30-14.45	O22	How accurate can be the predictions of critical and subcritical phase behavior in	O30	Pitfalls in vapor-liquid equilibrium simulations: Reliability of published data	O38	A thermodynamic approach for the prediction of mixed gas transport and solubility in glassy polymers

		aqueous systems without fitting binary parameters? *Ilya Polishuk* – Ariel University		*Ivo Nezbeda* – Czech Academy of Sciences/J.E. Purkinje University		*Giulio C. Sarti* – University of Bologna
14.45-15.00	O23	Statistical significance of modelling factors in high-pressure phase equilibria *Johannes H. Knoetze* – Stellenbosch University	O31	Finite-Size Effects of Kirkwood-Buff Integrals from Molecular Simulations *Noura Dawass* – Delft University of Technology	O39	Uncertainties in the determination of reaction equilibria *Karsten Müller* – Friedrich-Alexander-Universität Erlangen-Nürnberg
15.00-15.15	O24	Volume-translation in cubic EoS: which parameterization for pure-components and which mixing rule for multicomponent systems *Yohann Le Guennec* – University of Lorraine	O32	Computing Chemical Potentials of Water, Methanol, Carbon Dioxide, and Hydrogen Sulfide at Low Temperatures Using Continuous Fractional Component Gibbs Ensemble Monte Carlo *Ahmadreza Rahbari* – Delft University of Technology	O40	Experimental and Modelling study of the HPHT Phase Equilibria of crude oil *Emmanuel Chidi Efika* – Imperial College London
15.15-15.30	O25	Experimental and Modeling Study of the Phase Behavior of (Butanoic Acid + Carbon Dioxide) and (Propanoic Acid Methyl Ester + Carbon Dioxide) at Temperatures Between (323.15 and 423.15) K and Pressures up to 20 MPa *Sultan S. A. Al Habsi* – Imperial College London	O33	Molecular dynamics simulation of homogeneous bubble nucleation *Martin Horsch* - University of Kaiserslautern	O41	Modeling of Multicomponent Phase Equilibria in Ionic Liquid Systems Using Leading Thermodynamic Approaches: PC-SAFT vs COSMO-RS *Kamil Paduszyński* – Warsaw University of Technology
15.30-15.45	O26	Thiophene Removal from {Aliphatic + Thiophene} Mixtures Using Tetrahexylammonium-based Deep Eutectic Solvents *Samah E.E Warrag* – Eindhoven University of Technology/The Petroleum Institute	O34	Adsorption of CO_2/N_2 mixtures on MFI: a molecular simulation study *Lucienne L. Romanielo* – Federal University of Uberlândia	O42	Liquid-Liquid Equilibrium for Extraction of Dilute Aqueous Furfural Mixtures *Mikael Männistö* – Aalto University
15.45-16.00	O27	Predicting the viscosity of *n*-alkane liquid mixtures *Thanh-Binh Nguyen* – Imperial College London	O35	Interfacial Properties of the Lennard Jones Truncated and Shifted Fluid by Molecular Simulations and a New	O43	Calculation of Multiphase Chemical Equilibrium by Non-Stoichiometric Methods

				Equation of State Combined with Density Gradient Theory *Simon Stephan* - University of Kaiserslautern		*Christos Tsanas* – Technical University of Denmark
16.00-16.15	O28	A new association scheme and CPA parameterization for monoethylene glycol *Francois Kruger* – Technical University of Denmark	O36	Association equilibrium, kinetics, and gelation in a solution of cross-associating chains with inactive fragments *Igor Gotlib* – Saint Petersburg State University	O44	Necessity of assessment of the LLE correlation parameters prior to publication *Antonio Marcilla* – University of Alicante
16.15-16.30	O29	Phase Behaviour of the Ternary System (CO_2 + Methylcyclohexane + N_2) *Geraldine A. Torín-Ollarves* – Imperial College London	O37	A Novel Force Field Development Algorithm to Improve the Quantitative Predictability of Thermophysical Properties with Molecular Simulation *Richard A. Messerly* – National Institute of Standards and Technology	O45	Predictive Models Evaluation for Physical Properties of Pure Ionic Liquids *Kamil Oster* – The University of Manchester/ Queen's University Belfast
16.30-17.30	**WP-TTP meeting (by invitation only) – Merope 1+2**					
17.30-19.30	***Guided visit***					
19.30-22.00	***Dinner at Manuc's Inn (La Hanu' lui Manuc)***					

Saturday, May, 20th 2017						
8.30-10.45	**Invited lectures (Atlas 1)** *Chairs: Sabine Enders, Ralf Dohrn, and Cor Peters*					
8.30-9.15	**IL6**	***ATPS for the Recovery of Biomolecules: Characterisation and Application*** *Eugenia Macedo* – University of Porto, Portugal				
9.15-10.00	**IL7**	***Thermodynamics of fluids in confinement: Molecular models and property predictions*** *Ioannis Economou* – Texas A&M University at Qatar, Qatar				
10.00-10.45	**IL8**	***How to parameterize SAFT and cubic equations of state to boost their performance*** *Romain Privat* – University of Lorraine, France				
10.45-11.15	***Coffee Break (Radisson Blu Hotel, Prefunction area)*** ***Poster Session – Radisson Blu Hotel (Prefunction Area, Atlas Foyer)***					
	Parallel Sessions					
	Atlas 1		**Merope 1+2**		**Electra 1+2**	
	Session: Phase equilibria & transport properties (experimental & modelling) ***Sponsored by IFP Energies Nouvelles*** *Chairs: Ilya Polishuk and Ana Soto*		**Session: Molecular & statistical thermodynamics** *Chairs: Patrice Paricaud and Andreas Klamt*		**Session: Gas & oil (downstream and upstream), petrochemicals, hydrofracking** *Chairs: Ivo Nezbeda and Nicolas von Solms*	
11.15-11.30	O46	Measurement of Phase Equilibria at High Pressure: Trends and Systems Investigated *Ralf Dohrn* – Bayer AG	O53	Extension of the BMCSL equation of state for hard spheres to the metastable disordered region: Application to the PC-SAFT model *Patrice Paricaud* – Université Paris-Saclay	O60	General Multiphase PH Flash and Its Application in Thermal Recovery *Wei Yan* – Technical University of Denmark
11.30-11.45	O47	On the condition of electroneutrality in liquid-liquid equilibria *Saifuddin Ahmed* – IFP Energies Nouvelles	O54	Modification of the Wolf Summation and Application to Molecular Simulation of Phase Equilibria for Molecules with Partial Charges and Induced Dipoles *Christian Waibel* – University of Stuttgart	O61	Transport of gases confined in kerogen: Diffusion paths, diffusion coefficients and permeability *Manolis Vasileiadis* – National Center for Scientific Research "Demokritos"
11.45-12.00	O48	New Model for Liquid Adsorption Isotherms of Isomeric Mixtures *Thomas Goetsch* – TU Dortmund	O55	Computer simulations and theory of decorated soft disks in two dimensions *Stefan Sokołowski* – Maria Curie-Skłodowska University	O62	An extension of SAFT-VR Mie to predict confined fluid properties: application to adsorption isotherms *Luís F. M. Franco* – Texas A&M University at Qatar

12.00-12.15	O49	Saturated phase densities of (CO_2 + methylcyclohexane) at temperatures from (293 to 450) K and pressures up to 64 MPa *Yolanda Sanchez-Vicente* – Imperial College London	O56	Molecular Dynamics Prediction of the Phase Equilibria of the Ternary Methane-Carbon Dioxide-Water Hydrate System *Vasileios K. Michalis* – National Center for Scientific Research "Demokritos"	O63	Thermodynamic properties of fluids in the upstream petroleum engineering: from rigorous thermodynamics to soft computing *Vassilis Gaganis* – Technical University of Crete
12.15-12.30	O50	RAND-based Formulations for Isothermal Multiphase Flash *Wei Yan* – Technical University of Denmark	O57	Molecular Simulation of Activities in Electrolyte Solutions *Maximilian Kohns* – University of Kaiserslautern	O64	A simplified thermodynamic approach for reservoir fluid phase behavior mapping with depth *Nikos Varotsis* – Technical University of Crete
12.30-12.45	O51	In-situ Measurement of Physico-Chemical Properties of Liquids by Benchtop Nuclear Magnetic Resonance Spectroscopy *Anne Friebel* – TU Kaiserslautern	O58	Simple and accurate prediction of high-pressure densities of RTILs using fluctuation-based isothermal EoS *Mirosław Chorążewski* – University of Silesia	O65	Modelling mercury distribution in the oil and gas value chain *Eleni Panteli* – Statoil ASA
12.45-13.00	O52	An engineering perspective of a crossover equation of state *Andre P. C. M. Vinhal* – Technical University of Denmark	O59	Molecular thermodynamic modeling of bilayer perforations in solutions of ionic surfactants *Ksenia A. Emelyanova* – St. Petersburg State University	O66	Experimental Study on Asphaltene Aggregation Phenomena in a Microcapillary *Xingxun Li* – China University of Petroleum
13.00-14.15	***Lunch*** ***Poster Session- Radisson Blu Hotel (Prefunction Area, Atlas Foyer)***					
13.00-14.15	**Steering Committee Meeting (by invitation only)**					
14.15-16.00	**Parallel Sessions**					
	Atlas 1		**Merope 1+2**		**Electra 1+2**	
	Session: Phase equilibria & transport properties, Nanoscience & nanotechnology *Chairs: Daniel Broseta and Olivier Baudouin*		**Carbon capture & storage** *Chairs: Velisa Vesovic and Alireza Shariati*		**Teaching Thermodynamics Workshop** *Chairs: Jean-Nöel Jaubert, Nontas Voutsas, and Peter Ahlström*	
14.15-14.30	O67	Calculation of bubble and dew points of mixtures with minimization of the tangent plain distance to a modified Gibbs free energy surface	O74	Catalytic CO_2 Capture directly from Air: a Molecular Modeling Study *Wim Buijs* – Delft University of Technology	W1	Teaching Chemical Engineering Thermodynamics at DTU: How, why, impressions and some personal thoughts

		Ilias K. Nikolaidis – National Center for Scientific Research "Demokritos"/Texas A&M at Qatar				*Georgios M. Kontogeorgis* – Technical University of Denmark
14.30-14.45	O68	Ion based Electrolyte CPA for Aqueous Single- and Multiple-Salt Solutions *Anders Schlaikjer* – Technical University of Denmark	O75	Liquid-liquid phase separation of {amine – H_2O – CO_2} systems: New methods for key data *Karine Ballerat-Busserolles* – Chemistry Institute of Clermont-Ferrand		
14.45-15.00	O69	Modelling of the equilibrium properties in {water- polyol} solutions *Oumar Toure* – ROQUETTE Freres	O76	Supported Ionic Liquid Membranes with Finest CO_2 Separation Performances: Insights into Structure-Property Relationships *Isabel M. Marrucho* – University Nova of Lisbon	W2	Thermath-XSEOS-YouThermo: from an alphabet soup to an educational project *Marcelo Castier* – Texas A&M University at Qatar
15.00-15.15	O70	Phase equilibrium of CO_2-CH_4-brine systems at elevated temperature: application to Enhanced Geothermal System (EGS) *Clémentine Pouget* – University of Pau and Pays de l'Adour	O77	Experimental study of CO_2 solubility in NaCl solutions under high pressure and temperature *Hamdi Messabeb* – Université de Pau et des Pays de l'Adour		
15.15-15.30	O71	Incorporating uncertainty in molar volume modelling of liquid metal chlorides *Lesley J. Beyers* – KU Leuven	O78	Screening new amines for energy efficient absorption of CO_2 from synthesis gas *Elmar Kessler* – TU Kaiserslautern	W3	Teaching Molecular Thermodynamics with COSMO-RS *Andreas Klamt* – COSMOlogic GmbH & CoKG / University of Regensburg
15.30-15.45	O72	Nanothermodynamics of water clusters *Signe Kjelstrup* – Norwegian University of Science and Technology	O79	Environomic optimization of the coal and natural gas fired power plants with carbon dioxide capture process *Cristian Dincă* – University Politehnica of Bucharest	W4	Innovative tools for teaching applied thermodynamics *Jean-Charles de Hemptinne* – IFP Energies Nouvelles
15.45-16.00	O73	Correlation between thermodynamic properties, synthesis conditions and different compositional variables in nanometer-sized materials	O80	A multiscale method to predict the mixed gas performance of polymeric membranes for CO_2 capture *Eleonora Ricci* – University of Bologna		

		Speranţa Tănăsescu – "Ilie Murgulescu" Institute of Physical Chemistry of the Romanian Academy				
16.00-16.25	***Coffee Break (Radisson Blu Hotel, Prefunction area)*** ***Poster Session – Radisson Blu Hotel (Prefunction Area, Atlas Foyer)***					
16.25-17.55	**Parallel Sessions**					
	Atlas 1		**Merope 1+2**		**Electra 1+2**	
	Session: Colloids, surfactants & interfacial phenomena *Chairs: Kamil Paduszyński and Giulio Sarti*		**Session: Novel reaction & separation technologies** *Chairs: Wim Buijs and Christoph Held*		**Teaching Thermodynamics Workshop** *Chairs: Jean-Nöel Jaubert, Nontas Voutsas, and Peter Ahlström*	
16.25-16.40	O81	Molecular thermodynamics for branched networks and bicontinuous phases in water+oil+surfactant microemulsions *Alexey Victorov* – St. Petersburg State University	O87	An environmentally attractive CO_2-capturing technology for natural and industrial gas streams using gas hydrates *Cornelis J. Peters* – The Petroleum Institute/ Colorado School of Mines	W5	Presentation of second law and derivation of its main consequences *Giulio Sarti* – University of Bologna
16.40-16.55	O82	Effects of alkyl-alcohols on the interface tension of asphaltene solutions *Ronaldo G. Santos* – Industrial Engineering Faculty	O88	Transport properties of Ionic Liquids with gold nanoparticles *Oscar Cabeza* – University of Coruña		
16.55-17.10	O83	Nonuniformity of Droplets with Solid Charged or Uncharged Cores *Alexander Shchekin* – St Petersburg State University	O89	Separation of Azeotropic Mixtures using Ionic Liquids *Eleni Boli* – National Technical University of Athens	W6	Beloved like aTax Increase – Thermodynamics in Industry *Michael Kleiber* – thyssenkrupp Industrial Solutions AG
17.10-17.25	O84	A new methodology for liquid-adsorption experiments on porous solids *Thomas Hähnel* – University of Applied Sciences Dresden	O90	Solubility of Carbon Dioxide and Hydrogen Sulfide in the Ionic Liquid 1-Butyl-3-methylimidazolium Trifluoromethanesulfonate *Amir H. Jalili* – Research Institute of Petroleum Industry	W7	Gibbs energy minimization: a path to introduce this tricky concept to undergraduate students *Romain Privat* – Université de Lorraine, ENSIC-LRGP
17.25-17.40	O85	Influence of additives in Triton X solutions on micellar properties and solute partitioning for the design of bioprocesses	O91	Modelling CO reactive absorption into ionic liquid/metal salt mixtures with soft-SAFT EoS *Gabriel Zarca* – University of Cantabria	W8	Teaching Thermodynamics with MOOC: Motivations and Results *Arnaud Delebarre* – MINES ParisTech

		Alina Koneva – St. Petersburg State University				
17.40-17.55	O86	Fast and accurate determination of protein equation of state using microfluidic device *Sébastien Teychené* – University of Toulouse	O92	Structure of the Electric Double Layer in Ionic Liquid Mixtures *Luis M. Varela* – University of Santiago de Compostela	W9	Thermodynamics from theory to praxis; Laboratory Project in Chemical Engineering *Juha-Pekka Pokki* – Aalto University
17.55-18.00	***Break***					
18.00-19.15	**Parallel Sessions**					
	Maia		**Merope 1+2**		**Electra 1+2**	
	Session: Biological systems & health, Pharmaceuticals & cosmetics **Chairs:** *Oscar Rodriguez and Masahide Terazima*		**Session: Alternative solvents, Novel reaction & separation technologies,** *Chairs: Isabel Marrucho and Cara E. Schwarz*		**Session: Product & process design** *Chairs: Thomas Wallek and Juha-Pekka Pokki*	
18.00-18.15	O93	Time-resolved thermodynamics reveals transient fluctuation of proteins *Masahide Terazima* – Kyoto University	O97	Solute-solute binary interaction parameters for the ternary system CO2+1-decanol+n-tetradecane *Cara E. Schwarz* – Stellenbosch University	O101	Optimization of the extraction process of TMTZ, a prospective future propellant *Anne-Julie Bougrine* – Claude Bernard Lyon 1 University
18.15-18.30	O94	***Sponsored by BASF*** New Oxidized Compounds and Polyketides from Wheat Cuticular Waxes *Radu C. Racoviţă* – University of British Columbia/National Institute of Research and Development for Food Bioresources	O98	Influence of additives on equilibrium limited enzymatic reactions *Matthias Voges* – TU Dortmund University	O102	Application of graph theory to process design and analysis *Florian Pöllabauer* – Graz University of Technology
18.30-18.45	O95	Co-solvent induced changes of bioreaction kinetics and equilibria *Anton Wangler* – TU Dortmund University	O99	Volumetric properties versus mass transfer in membranes processes *Johanne Teychené* – University of Toulouse	O103	Thermodynamic property modelling for Lipids Based Process and Product Design *Olivia A. Perederic* – Technical University of Denmark
18.45-19.00	O96	Effect of operational variables of the synthesis in the solubility of ampicillin *Silvana Mattedi* – Federal University of Bahia	O100	Experimental and Theoretical Study on the Extraction of Aromatics from Aliphatic Hydrocarbons with Ionic Liquids *Amir Jalili* – Research Institute of Petroleum Industry	O104	Application of Thermodynamics in Industrial Slurry Catalytic Ethylene Polymerization Processes *Maryam Tamaddoni* – SABIC Technology Center
20.30-	***Helmut Knapp Poster Award sponsored by Heidi & Gala Dinner***					

Sunday, May, 21st 2017						
	Invited lectures (Atlas 1) *Chair: Eugenia Macedo and Karel Aim*					
9.00-9.45	**IL9**	***Thermodynamics in Qatar*** *Michael Kleiber* – thyssenkrupp Industrial Solutions AG, Germany				
9.45-10.00	***Simulis Thermodynamics: a bridge from research to industries*** *Olivier Baudouin* – ProSim					
10.00-10.30	**Ceremony EFCE Excellence Award** *Jean-Charles de Hemptinne, Ralf Dohrn, and Jean-Nöel Jaubert*					
10.30-10.45	***Presentation of ESAT 2018***					
10.45-11.15	***Coffee break – Radisson Blu Hotel (Prefunction Area)***					
11.15-12.30	**Parallel Sessions**					
	Atlas 1		**Merope 1+2**		**Electra 1+2**	
	Session: Carbon capture & storage, Renewable Energy *Chairs: Karine Ballerat-Busserolles and Cristian Dincă*		**Session: Food & functional food processing, Molecular & statistical thermodynamics** *Chairs: Marcelo Castier and Tim Zeiner*		**Session: Materials** *Chairs: Johannes Knoetze and Signe Kjelstrup*	
11.15-11.30	O105	On the use of exergy analysis for waste combustion *Peter Ahlström* – University of Borås	O110	Aqueous Two-Phase Extraction: Partition coefficients and phase diagrams *Oscar Rodríguez* – University of Santiago de Compostela	O115	Modeling and Measurement of Solubility and Swelling in Supercritical Carbon Dioxide – Polymer Systems *Nicolas von Solms*-Technical University of Denmark
11.30-11.45	O106	*E*-PPR78: a proper cubic EoS for modeling fluids of CCS processes *Xiaochun Xu* – University of Lorraine	O111	A new potential function to calculate second virial coefficients of polar gases *Alireza Shariati* – Shiraz University	O116	Impact of Polydispersity on Phase Equilibria of Branched Polyethylene Solutions *Christoph Walowski* – Karlsruhe Institute of Technology
11.45-12.00	O107	Temperature independent description of the adsorption equilibria of adsorption pairs with IUPAC type V adsorption behaviors *Kohler Tobias* – University of Erlangen-Nuremberg	O112	Deriving Equations of State based on a simple coupling parameter expansion *Spiros Kournopoulos* – Imperial College London	O117	A New Simulation Scenario for the Coil-to-globule Transition of Thermoresponsive Polymers *Edder J. García* – University of Kaiserslautern

12.00-12.15	O108	Use of reversible gas-solid-reactions to store thermal energy – screening and general thermodynamic assessment *Jonas Obermeier* – University of Erlangen-Nuremberg	O113	Modeling and Simulation of Wetting of Component Surfaces *Michaela Heier* – University of Kaiserslautern	O118	Solubility of gases in glassy and semicrystalline polymers *Michael Fischlschweiger* – OTTRONIC GmbH
12.15-12.30	O109	Uncertainties related to CO_2 Storage in deep brine aquifer *Mariana Laura Nistor* – Schlumberger	O114	Ionic Specificity of Alkali Cations Adsorption on Charged Silica *Sarah Hocine* – University of Montpellier	O119	Termodynamics of polyazulene based materials *Eleonora-Mihaela Ungureanu* – University Politehnica of Bucharest
12.30-12.45	**Atlas 1**					
	Closing Ceremony					
12.45-14.00	***Lunch***					