Thermodynamics 2015
Tivoli Congres Hotel
15-18. September 2015

Final program

Tuesday 15 September		
12:00 – 14:00	**Registration** (Harlekin/Columbine)	
14:00 – 14:15	**Welcome Session** (Harlekin/Columbine) Georgios Kontogeorgis & Erling H. Stenby (Conference chairs)	
14:15 – 15:00	Venue: Harlekin/Columbine Chair: George Jackson	
	Taylor & Francis Molecular Physics Lecture: Thermodynamics and Kinetics of Deeply Supercooled Water: a Computational Perspective Pablo G. Debenedetti – Princeton University	
15.00 – 15:45	Venue: Harlekin/Columbine Chair: Andrew Masters	
	Session: Invited Talk	
	Towards a coarse grained molecular representation valid both for static and transport properties Guillaume Galliero - Université de Pau et des Pays de l'Adour	
15:45 – 16:15	*Coffee/Tea Break*	
16:15 – 18:00	**Parallel Sessions**	
	Venue: Harlekin/Columbine	Venue: Pjerrot

	Chair: Erich A. Müller		Chair: Kim Knudsen	
	Session: Simulation – 1		**Session: Engineering applications**	
16:15 – 16:35	OP1	**Comparison of absolute free energy calculation methods for fluids and solids** Martin B. Sweatman - University of Edinburgh	OP6	**CO_2 Capture and Transport: Thermodynamic Investigation of Relevant Fluid Mixtures** Dimitra Aslanidou - Aristotle University of Thessaloniki
16:35 – 16:55	OP2	**Surface Tension Calculations of Liquid Metals** Olivier Durand - CEA	OP7	**Thermophysical Properties of Aqueous Amine Solutions for CO_2 Capture** Jiafei Zhang - Imperial College London
16:55 – 17:15	OP3	**Calculating free energies of atmospherically relevant clusters using non-equilibrium molecular dynamics** Gabriel Lau - Imperial College London	OP8	**MD Simulations of Low-Salinity Enhanced Oil Recovery. A molecular-level description of interactions between charged colloid particles, organic oil molecules and simple salt ions.** Thomas Underwood - Durham University
17:15 – 17:35	OP4	**The thermodynamics of low dimensional materials: Finding solvents for graphene, carbon nanotubes and their relatives** Henry Bock - Heriot Watt University	OP9	**Liquid-Liquid Equilibrium of Aqueous Two-phase Systems for Protein Partitioning from goat milk whey in-nature** Camila G. Pereira - Federal University of Rio Grande do Norte
17:35 – 17:55	OP5	**Mixtures of Hydrogenated and Fluorinated Alcohols: Thermodynamics, Spectroscopy and Simulation** Eduardo J. M. Filipe - Universidade de Lisboa	OP10	**Modeling of the phase equilibrium and the thermodynamic properties of aqueous systems from an industrial point of view** Eirini K. Karakatsani - Haldor Topsoe A/S
19:00 –	*Welcome Reception – Copenhagen Town Hall*			

Wednesday 16 September				
09:00 – 10:30	Venue: Harlekin/Columbine Chair: Georgios Kontogeorgis			
	Session: Invited Talks			
09:00 – 09:45	**Understanding the Self-Assembly and Phase Behavior of Skin Lipids** Clare McCabe – Vanderbilt University			
09:45 – 10:30	**Modelling at the appropriate lengthscale for industrial applications** Massimo Noro – Unilever			
10:30 – 11:00	*Coffee/Tea Break*			
11:00 – 12:30	**Parallel Sessions**			
	Venue: Harlekin/Columbine Chair: Ioannis Economou		Venue: Pjerrot Chair: Stefano Brandani	
	Simulation – 2		**Equations of State – 1**	
11:00 – 11:20	OP11	**Molecular simulation of ionic liquid solvents: bulk properties and the effect of confinement** Niki Vergadou - Demokritos	OP15	**Phase behaviour of the system (carbon dioxide + n-heptane + methylbenzene) and (carbon dioxide + methane + methylbenzene): a comparison between experimental data and SAFT-γ-Mie predictions** Saif. Z Al Ghafri - Qatar Carbonates and Carbon Storage Research Centre

11:20 – 11:40	OP12	**Determining the Factors that Govern the Permeation of Ions into Graphene Oxide Membranes using Molecular Simulation** Christopher D. Williams - University of Manchester	OP16	**A Comprehensive Investigation on CO_2 Solubility and Kinetics in Tricyanomethanide-based Ionic Liquids: Experiments and ePC-SAFT Modeling** Lawien F. Zubeir - Eindhoven University of Technology
11:40 – 12:00	OP13	**Non-equilibrium molecular dynamics simulations of water permeation through graphene-based membranes** Frederike Jaeger - Imperial College London	OP17	**Multi-scale modelling of polyamide thin films** Jordan Muscatello - Imperial College London
12:00 – 12:20	OP14	**Wetting on Grafted Thermo-responsive Polymer Brushes: A Molecular Dynamics Study** Debdip Bhandary - Indian Institute of Technology Kanpur	OP18	**Modeling thermodynamic derivative properties of ionic liquids with ePC-SAFT** Xiaoyan Ji - Lulea University of Technology
12:30 – 13:30	*Lunch*			
13:30 – 14:00	Venue: Harlekin/Columbine Chair: Georgios Kontogeorgis			
	Christopher Wormald Award: Entropic Control over Nanoscale Colloidal Crystals Nathan A. Mahynski – Princeton University			
14:00 – 14:30	Venue: Harlekin/Columbine Chair: Ioannis Economou			
	Guggenheim Medal Award: The Legacy of Edward Guggenheim to Statistical Thermodynamics George Jackson – Imperial College London			
14:30 – 15:10	Venue: Harlekin/Columbine Chair: Martin Trusler			
	Contributed Plenary Lectures			

14.30 – 14:50	OP19	**Modeling coarse grained linear alkanes and polymers using SAFT-γ Mie using molecular dynamics simulations** Erich A. Müller - Imperial College London		
14:50 – 15:10	OP20	**Combining quantum chemistry and statistical mechanics for thermodynamic property prediction involving natural complex materials: ligno-cellulosic biomass, kerogen, asphaltenes, clay minerals, and micro emulsions.** Philippe Ungerer - Materials Design S.A.R.L.		
15:10 – 15:30	**Group Photo**			
15:30 – 16:00	*Coffee/tea break*			
16:00 – 18:00	**Parallel Session**			
	Venue: Harlekin/Columbine Chair: Philippe Ungerer		Venue: Pjerrot Chair: Andrew Haslam	
	Simulation – 3		**Equations of state – 2, Electrolytes**	
16:00 – 16:20	OP21	**Phase equilibria of methane and carbon dioxide hydrates using molecular dynamics simulations** Vasileios K. Michalis - Texas A&M University at Qatar	OP27	**Thermodynamic Modelling with SAFT of the properties of Aqueous Electrolyte solutions for Nuclear Waste Processing** Mark Bankhead - National Nuclear Laboratory
16:20 – 16:40	OP22	**Multi-scale simulation of the early stages of zeolite nucleation** Carlos Nieto-Draghi - IFP Energies nouvelles	OP28	**Evaluation of the quadrupolar CPA EoS for modeling multicomponent CO_2-mixtures** Martin G. Bjørner - Technical University of Denmark
16:40 – 17:00	OP23	**Spatial resolution of thermal transport properties in simulated nanomaterials** Niall Jackson - Imperial College London	OP29	**Predicting the formation of liquid-liquid phase splits from mixing rules** **thermodynamically correct in the limit of zero pressure** Stefano Brandani - University of Edinburgh

17:00 – 17:20	OP24	**Taming Thermophoretic transport across nanopores: novel approaches for nanofluidic analytical devices** Silvia Di Lecce - Imperial College London	OP30	**Modelling electrolytes using a single-parameter molecular-based equation of state: improving solvation energies** Daniel Kunisch Eriksen - Imperial College London
17:20 – 17:40	OP25	**Hydrogen bonding in hybrid scale models** Richard J. Gowers - University of Manchester	OP31	**Pressure-Driven Molecular Dynamics Simulations of an Electrolytes Solution through a polyamide membrane** Aziz Ghoufi - Université de Rennes
17:40 – 18:00	OP26	**Self-Assembly of High-Symmetry Planar Rings** Carlos Avendano - University of Manchester	OP32	**The complementing rôles of Coulombic forces and association in the thermodynamics of selected room-temperature ionic liquids** Fernando del Río - Universidad Autónoma Metropolitana
19:00 –	*Conference Dinner (Grøften – Tivoli)*			

Thursday 17 September			
09:00 – 09:45	Venue: Harlekin/Columbine Chair: Amparo Galindo		
	Lennard-Jones Prize and Lecture: Liquid crystal structure and dynamics: what can computer simulations tell us? Michael P. Allen – University of Warwick		
9:45 – 10:45	Venue: Harlekin/Columbine Chair: Andrew Masters		
	Session: Plenary Lectures		
09:45 – 10:05	OP33	**Simulations of mean ionic activity coefficients and solubilities in aqueous electrolyte solutions** Athanassios Panagiotopoulos - Princeton University	
10:05 – 10:25	OP34	**Atomistic Molecular Dynamics Simulations of Transport Properties for the H_2O+CO_2+NaCl mixture at conditions relevant to CCS processes** Ioannis G. Economou - Texas A&M University at Qatar	
10:25 – 10:45	OP35	**Molecular simulation of polarizable models of electrolytes: Concentration dependence of the chemical potentials, density and solubility** Ivo Nezbeda - J .E. Purkinje University	
10:45 – 11:00	*Coffee/Tea Break*		
11:00 – 12:30	**Parallel Sessions**		
	Venue: Harlekin/Columbine Chair: Athanassios Panagiotopoulos		Venue: Pjerrot Chair: Kai Langenbach
	Simulation – 4		**Equations of state – 3**

11:00 – 11:20	OP36	**Nanoparticle thermophoresis under thermal gradients: thermophobic or thermophilic, … and why?** Irene Iriarte-Carretero - Imperial College London	OP40	**Coarse graining of polymer systems employing SAFT** Jos Tasche - Durham University
11:20 – 11:40	OP37	**The molecular segregation of tri-butyl phosphate in an organic diluent and its relevance to nuclear extraction processes.** Junju Mu - University of Manchester	OP41	**Computer-Based Discovery of Surfactants** Mariah Ritz - North Carolina State University
11:40 – 12:00	OP38	**Developing Peptoid Simulation Models** Laura J. Weiser - North Carolina State University	OP42	**Mixing rules for modelling asymmetric systems with water** Duncan Paterson - Technical University of Denmark
12:00 – 12:20	OP39	**Computer Simulation of chromonic materials: the influence of molecular structure on self-assembly** Mark R. Wilson - Durham University	OP43	**Prediction of the phase behaviour of hydrocarbon and water mixtures with the SAFT-γ Mie group-contribution equation of state: properties at infinite dilution** Panatpong Hutacharoen - Imperial College London
12:30 – 13:30	*Lunch*			
13:30 – 15:30	**Parallel Sessions**			
	Venue: Harlekin/Columbine Chair: Jadran Vrabec		Venue: Pjerrot Chair: Peter Ahlström	
	Interfaces		**Materials – 1**	
13:30 – 13:50	OP44	**Molecular modelling of interfacial properties by multi-criteria optimization** Martin Horsch - University of Kaiserslautern	OP50	**Solubility and diffusion of small molecules in polymers** Peter Ahlström - University of Borås

13:50 – 14:10	OP45	**First Principles Prediction of Liquid/Liquid Interfacial Tension** Martin P. Andersson - University of Copenhagen	OP51	**Impact of Ions on the Vitamin C Uptake and Release Using Hydrogels** Daniel Althans - TU Berlin
14:10 – 14:30	OP46	**Phase behaviour and interfacial properties of ternary system CO_2 + n-butane + n-decane: Coarse-Grained theoretical modelling and Molecular Simulations** Andrés Mejía - Universidad de Concepción	OP52	**Thermodynamic properties of inverse patchy colloids** Gerhard Kahl - Technische Universität Wien
14:30 – 14:50	OP47	**Molecular Modelling and Simulation of Wetting on Solid Surfaces** Maximilian Kohns - University of Kaiserslautern	OP53	**Surface photografting of acrylic acid on poly(dimethylsiloxane). Experimental and dissipative particle dynamics studies** Carlos Nieto-Draghi - IFP Energies nouvelles
14:50 – 15:10	OP48	**Thermodynamics and statistical mechanics of wetting transitions: fluid phase behavior in prototypical nanostructured substrates** P. Yatsyshin - Imperial College London	OP54	**Application of Lattice Cluster Theory to Solid-Liquid-Liquid Equilibria of Semi-crystalline Polymer Solutions** Kai Langenbach - Technical University of Berlin
15:10 – 15:30	OP49	**Prediction of Interfacial Properties of Industrially Relevant Fluid Mixtures by Molecular Simulation and Density Gradient Theory + PC-SAFT** Stephan Werth - University of Kaiserslautern	OP55	**Solubility predictions for active pharmaceutical ingredients using the SAFT-γ Mie approach** Simon Dufal - Imperial College London
15:30 – 16:00	*Coffee/Tea Break*			
16:00 – 17:00	**Short oral presentation of selected Posters**			
	Venue: Harlekin/Columbine		Venue: Pjerrot	

	Chair: Ivo Nezbeda		Chair: Carlos Nieto-Draghi	
16:00 – 16:05	PP1	**Comparison of GERG-2008 and Soave-BWR for modeling of natural gas mixtures** Farhad Varzandeh – Technical University of Denmark	PP10	**A predictive square-gradient route to the interfacial tension of fluids** Daniel Kunisch Eriksen – Imperial College London
16:05 – 16:10	PP2	**High pressure phase equilibrium measurement of methane + n-decane** Teresa Regueira – Technical University of Denmark	PP11	**Coarse-Grained SAFT-γ Mie for Understanding Wax Deposition in Crude Oil** Sara Shahruddin – Imperial College London
16:10 – 16:15	PP3	**Water structure effects of anions and their volumes** Yizhak Marcus – Hebrew University of Jerusalem	PP12	**Extension of SAFT-VRE to reacting systems by application to aqueous solutions of weak electrolytes** Georgia Lazarou – Imperial College London
16:15 – 16:20	PP4	**Prediction of Self Diffusion Coefficients from Chapman-Enskog-Theory in Combination with PC-SAFT or LCT-EOS** Hendryk Rudolph – TU Berlin	PP13	**Experimental study of phase equilibria of systems involved in CH_4 hydrate production coupled with CO_2 sequestration** Ludovic Legoix – IFREMER
16:20 – 16:25	PP5	**Thermodynamic Equilibrium** Richard M. Gibbons	PP14	**Development of Predictive Association Models for the Description of Multifunctional Molecules with the CPA EoS** André M. Palma – University of Aveiro
16:25 – 16:30	PP6	**Thermodynamic investigation of ternary electrolyte system $NiCl_2$ + Triton X-100 + H_2O) at T = 298.15 K** Mohammad.A. Bagherinia – Islamic Azad University	PP15	**Applications of The Virial Expansion** Tom Bourne – University of Manchester

16:30 – 16:35	PP7	**Parameterization and Evaluation of the Electrolyte CPA Equation of State** Anders Schlaikjer – Technical University of Denmark	PP16	**Universal scaling behavior of short flexible Mie n-6 chains: A simple and accurate correlation for the influence parameters** José Matías Garrido – Universidad de Concepción
16:35 – 16:40	PP8	**Interfacial Supermittivity of Confined Water at the Nanoscale** Aziz Ghoufi – Université de Rennes	PP17	**Asphaltene aggregation process analyzed by scattering experiments and molecular simulation** Carlos Nieto-Draghi – IFP Energies Nouvelles
16:40 – 16:45	PP9	**The effect of accounting for the contribution of the heat capacity in solubility predictions** Sara Febra – Imperial College London	PP18	**Volumetric and ultrasonic study of mixtures of Benzyl alcohol with 1-propanol, 2-propanol, and 1, 2-propandiol, 1, 3-propandiol and t-butanol at T= (298.15–323.15) K and atmospheric pressure: Measurement and prediction** Mohammad M. Alavianmehr – Shiraz University of Technology
17:00-19:00	**Poster session with refreshments**			

Friday 18 September				
09:00 – 10:30	**Parallel Sessions**			
	Venue: Harlekin Chair: Sabine Enders		Venue: Columbine Chair: Guillaume Galliero	
	Materials – 2		**Materials – 3**	
09:00 – 09:20	OP56	**Temperature-dependent sublimation enthalpy for molecular crystals obtained from high-level quantum chemistry calculations** Ctirad Červinka - Institute of Chemical Technology Prague	OP60	**Transport of Gases in Polymers for Offshore Applications** Susana Almeida - Technical University of Denmark
09:20 – 09:40	OP57	**Structure of water confined in nanopores** Malgorzata Sliwinska-Bartkowiak - North Carolina State University	OP61	**Clay suspensions in and out of equilibrium** Jeroen S. van Duijneveldt - University of Bristol
09:40 – 10:00	OP58	**Confinement Effect on Chemical Reaction Yield: The Nitric Oxide Dimer Reaction** Deepti Srivastava - North Carolina State University	OP62	**Optimisation of Interactions and Pathways for Self Assembly** Mark A. Miller - Durham University
10:00 – 10:20	OP59	**Modelling the self-assembly of polyphilic molecules via coarse-grained simulations** Maziar Fayaz-Torshizi - Imperial College London		
10:30 – 11:00	*Coffee/Tea Break*			
11:00 – 11:45	Venue: Harlekin/Columbine Chair: Erling H. Stenby			
	Plenary Invited Talk			

	The Role of Interfacial Water on Water Desalination, Hydrates Management, and Oil & Gas Production Alberto Striolo – University College London
11:45 – 12:00	Venue: Harlekin/Columbine Presentation of Thermodynamics 2017 – Martin Sweatman
12:00 – 12:30	Venue: Harlekin/Columbine Closing Thermodynamics 2015
12:30 – 13:30	*Lunch*