Day 1

	time	Room A
	10.00	**Registration (entrance Pathe)**
	13.00	**Welcome** from chair **Othon Moultos**
Invited talks (chair: **Carmelo Herdes**)	13.15	**I1.1a Lourdes Vega:** Design of catalysts for CO2 conversion and hydrogen production by computational modeling tools
	14.00	**I1.2a Andre Bardow:** Do Androids Dream of Equations of State?
	14.45	**Coffee break (foyer)**
Invited talks (chair: **Catinca Secuianu**)	15.15	**I1.3a Erika Eiser:** Thermodynamics of Multivalent Nanoparticles in Bacterial Genome Detection
	16.00	**I1.4a Antoon ten Kate:** Thermochemical perspective on a Transient World (a personal view from an industrial practitioner)
	16.45	**Poster session 1 / snacks (foyer)** **List of posters (P1.1 - P1.32) are available in the List of Talks section**

Day 2

	time	Room A		Room B	
(chair: **George Jackson**)	9.00	**S2.1a Molecular Physics Lecture, Tyler Josephson:** Writing Bug-Free Software Using Lean			
	9.45	**S2.2a Christopher Wormald Prize lecture, Stefanie Walter:** Application of thermodynamic modeling in the design and manufacturing of pharmaceutical formulations			
	10.30	**Coffee break (foyer)**			
		theme	**presentation**	**theme**	**presentation**
Oral presentations	11.00	**CO_2 and H_2** (chair: Tim Nijssen)	**O2.1a Thijs van Westen:** Corresponding-states principle for classical and quantum fluids	**Batteries** (chair: Sondre Schnell)	**O2.1b S. Kjelstrup:** The Effect of Ion, Solvent, and Thermal Onsager Coefficients on the Lithium Battery Voltage
	11.15		**O2.2a Daniel T. Banuti:** Pseudo boiling and molecular network structure in near-critical hydrogen		**O2.2b Olav Galteland:** Multi-scale modelling of redox-mediated hybrid zinc-air flow batteries
	11.30		**O2.3a Catinca Secuianu:** Are the clathrate hydrates a solution for CCS?		**O2.3b Florian Baakes:** Assessing Li-ion battery safety: The role of solvents, gas solubility, and salts in pressure evolution
	11.45		**O2.4a Felix Llovell:** A Consistent Multiscale Simulation for the Characterization of Phosphonium-Based Ionic Liquids in CO2 Capture Applications		**O2.4b Henk Huinink:** Hydration transitions: water is both reactant and catalyst
	12.00		**O2.5a Riccardo Cremona:** CO2 capture via solvent-based chemical absorption in an hollow fiber membrane contactor: experimental tests and modelling activities	**Electrolytes** (chair: Nefeli Novak)	**O2.5b Xiaodong Liang:** Molecular thermodynamics for water and electrolytes
	12.15	**Machine learning** (chair: Frederick de Meyer)	**O2.6a Yongchul G. Chung:** PACMAN: A Robust Partial Atomic Charge Predicter for Nanoporous Materials Based on Crystal Graph Convolution Networks		**O2.6b S. Blázquez:** Computation of Electrical Conductivities of Aqueous Electrolyte Solutions: Two Surfaces, One Property
	12.30		**O2.7a Gustavo Chaparro:** A continuous machine-learned molecular Equation of State to describe the vapor, liquid, and solid states		**O2.7b C. Nieto-Draghi:** Critical Micelle Concentration of Perfluoroalkyl Substances in Ionic Aqueous Phase: a combined experimental, Machine Learning and Coarse-Grained molecular simulation study
	12.45		**O2.8a Thomas Bernet:** A machine-learning approach to predict the surface tension of amine-based solvents		**O2.8b Rasmus Fromsejer:** Reliable and fast predictions of the thermochemical properties of solids
	13.00		**O2.9a Kyrylo Klimenko:** ML modeling of acid gases VLE in aqueous MDEA solvents		**O2.9b Felipe M. Coelho:** Thermodiffusion of CO2 in Brine Solutions via Molecular Dynamics Simulations
	13.00	**Lunch break (foyer)**			
Invited talks (chair: **Gennady Gor**)	14.00	**I2.1a Randall Snurr:** Insights into Capillary Condensation and Hysteresis in Nanoporous Materials from New Simulation Methods			
	14.45	**I2.2a Hans Hasse:** Machine Learning and Physical Modeling of Thermodynamic Properties of Mixtures			
	15.30	**Poster session 2 / coffee break (foyer)** **P2.1 - P2.32**			
	16.30	Free time			
	18.00	**Prinsenhof Museum Tour**			
	19.30	**Conference Dinner at Prinsenhof**			

Day 3

	time	Room A		Room B	
		theme	**presentation**	**theme**	**presentation**
Oral presentations	9.00	Porous / confined media (chair: Greg Chung)	**O3.1a Nickolas Gantzler:** Self-diffusion of Volatile Organic Compounds in Zr-MOFs: A Joint Computational and Experimental Study	Aqueous systems (chair: Felix Llovell)	**O3.1b Callum Donaldson:** Green Solutions for Industrial Efficiency: Predicting Cyrene-Water Mixtures for Sustainable Processes
	9.15		**O3.2a Riya Sharma:** Optimizing adsorption refrigeration with MOF-propane integration: a sustainable approach		**O3.2b Lucía Fernández Sedano:** On the possible locus of the liquid–liquid critical point in real water from studies of supercooled water using the TIP4P/Ice model
	9.30		**O3.3a Gennady Gor:** Compressibility of Fluids in Nanopores: Molecular Modeling and Ultrasonic Experiments		**O3.3b Zoe Macpherson:** Exploring the Dipole Moment of Supercritical Water and the Hydrogen-Bonding Contributions Involved
	9.45		**O3.4a Tiong Wei Teh:** Effects of mobile framework cations on adsorption in zeolites: GPU-accelerated classical density functional theory		**O3.4b Willem Gispen:** Variational umbrella seeding for calculating nucleation barriers
	10.00		**O3.5a Thomas Fabiani:** Molecular screening of COFs for adsorption of uremic toxins from spent dialysate		**O3.5b James P.D. O'Connor:** Equation of State Informed Potentials: Towards a SAFT- γ-Mie based potential for Mesoscopic Simulation
	10.15		**O3.6a Samantha Corapi:** Understanding the Relationship between Pore Chemical Environment and Hysteresis using a Genetic Algorithm		**O3.6b Nefeli Novak:** Prediction of water anomalous properties by introducing the two-state theory in SAFT
	10.30	**Coffee break (foyer)**			
Oral presentations	11.00	Phase equilibria (chair: Ioannis Economou)	**O3.7a Cor Peters:** Brief Overview of Thermodynamic Achievements in the Period 1970 - 2000 at TU Delft	Thermodynamic modeling at differet scales (chair: Mahinder Ramdin)	**O3.7b Bjørn Hafskjold:** Local equilibrium in liquid-phase shock waves?
					O3.8b Asma Marzouk: Investigation of the Co-TiO2 Interaction in Fischer-Tropsch Synthesis through Multi-Scale Simulation Studies
	11.30		**O3.8a Happiness Imuetinyan:** Phase Behaviour and Density of CO2 + Toluene + Cyclohexanol Mixtures at T = 293.15 K to 353.15 K and P = 0.1 to 30 MPa		**O3.9b Jean-Marc Simon:** Application of the Kirkwood-Buff solution theory to solid solutions
	11.45		**O3.9a R. Bergmann:** Liquid-Liquid Phase Split of Associating Polymer Mixtures		**O3.10b Peter Krüger:** How to compute density fluctuations at the nanoscale
	12.00		**O3.10a Riley V. Latcham:** Automated Model-Assisted Phase Behaviour Measurements		**O3.11b Dick Bedeaux:** On How to Measure the Subdivision Potential in Nanothermodynamics
	12.15		**O3.11a Saman Naseri Boroujeni:** Benchmarking the Predictive Capabilities of the SAFT-γ Mie Eos for Properties of Interest in Pharmaceutical Systems		**O3.12b Jana Zimmermann:** Prediction of CO2 solubility in semicrystalline polyethylene and the influence of molecular architecture
	12.30		**O3.12a Gerard Alonso:** On the Compatibility of Butanol + Water + Dimethyl Carbonate blend at its Vapor-Liquid-Liquid Equilibrium		**O3.13b Sondre K. Schnell:** Stretching of nucleotide strains in the isometric- and isotensional ensemble
	12.45		**O3.13a Wilko Rohlfs:** ThermoQuiz: Game-based learning of basic thermodynamic principles		**O3.14b I.N. Tsimpanogiannis:** Simulation of a Fruit Juice Concentration Process Utilizing Hydrate Technology
	13.00	**Lunch break (foyer)**			
	14.00	**S3.1a Lennard-Jones Lecture, Mike Cates:** Surprises in the statistical mechanics of active matter (chair: Amparo Galindo)			
	14.45	**S3.2a Guggenheim Medal lecture, Amparo Galindo:** Following Guggenheim: from conformality to molecular modelling and property prediction (chair: Ioannis Economou)			
	15.30	**Poster award / Conference closure**			