Monday 10 June Morning

Plenary talks - Pentland Theatre

Chairs: Ralf Dohrn, Sabine Enders

08:30	09:15	*Atomistic and Mesoscopic Modeling of Structure-Property Relations in Polymers* Prof. Doros N. **THEODOROU**, National Technical Univ. of Athens, Greece
09:15	10:00	*Exploiting active learning for porous material screening* Prof. Tina **DÜREN**, University of Bath, UK
10:00	**10:30**	**Coffee Break**

SESSIONS		**Carbon capture & Storage (CCS) I** **Chair: Sandra Kentish** *Pentland East*	**Adsorption (the Kenneth Denbigh's session)** **Chair: Tina Düren** *Prestonfield*	**Molecular design: membranes & interfaces** **Chair: Doros Theodorou** *Pentland West*
10:30	10:50	*Modelling the phase behaviour of fluid systems relevant for carbon-capture processes: the importance of SOx and NOx* Dr. Andrew **HASLAM**, Imperial College London, UK	**Keynote** - *On Adsorption Azeotropy and a Classification Based on the Dual Site Langmuir Isotherm* Prof. Stefano **BRANDANI**, Univ. of Edinburgh, UK	*Dynamically Switchable Monolayer Coatings: Improved Understanding of Group Contribution to Surface Tension* Nicholas **CRAVEN**, Vanderbilt Univ. USA
10:50	11:10	*A robust and efficient augmented free-water flash method for CO_2 -water-hydrocarbon mixtures* Dr. Dan **NICHITA**, Univ. de Pau et des Pays de l'Adour, France		*Computational Design and Assessment of Mixed Matrix Membranes using Coarse-Grained Molecular Modeling* Dr. Amro **MOHAMED**, Texas A&M University at Qatar, Qatar
11:10	11:30	*Understanding the CO_2 Capture Performance of amine-functionalized Silica and Carbon-based materials Using Molecular Simulations* Prof. Lourdes **VEGA**, Khalifa Univ., UAE	*Predicting Adsorption with 3D classical Density Functional Theory based on PC-SAFT* Nadine **THIELE**, Univ. of Stuttgart, Germany	*Wetting, adsorption, and desorption behaviour of polymers on surfaces* Prof. Vasileios **KOUTSOS**, Univ. of Edinburgh, UK
11:30	11:50	*Integrating Theoretical Approaches for Profiling the Thermophysical Behavior of DESs in Greenhouse Gas Treatments* Dr. Félix **LLOVELL**, Univ. Rovira i Virgili, Spain	*Impact of Force Field Choice on Adsorption Predictions in MOF* Connaire **McCREADY**, University of Strathclyde, UK	*Decoding the Interplay Between Topology and Surface Charge in Graphene Oxide Membranes During Humidity Induced Swelling* Prof. Paola **CARBONE**, Univ. of Manchester, UK
11:50	12:00	Break		

SESSIONS		**Machine Learning I** **Chair: Erich Müller** *Pentland*	**Polymers I** **Chair: Michael Fischlschweiger** *Prestonfield*	**Equations of State (the Peter G. Tait Session)** **Chair: Ioannis Economou** *Pentland West*
12:00	12:20	*Improvement of diffusion coefficient prediction by active learning* Zeno **ROMERO**, RPTU Kaiserslautern, Germany	*Predicting Gas Solubilities in Semi-crystalline Branched Polyolefin Systems with the Lattice-Cluster-Theory-EoS* Simon **LEUBE**, KIT, Germany	*Can we hope for a revival of the equations of state by coupling the Peng-Robinson model and an uncharted activity-coefficient model?* Prof. Romain **PRIVAT**, Univ. de Lorraine, France
12:20	12:40	Predicting solvation free energy in binary solvents using graph neural networks Roel **LEENHOUTS**, KU Leuven, Belgium	High throughput screening of polymers: properties prediction and structures discovery Dr. Vittoria **FANTAUZZO**, Univ. of Liverpool, UK	Decorrelating equation of state parameters with mixture data Dr. Philipp **REHNER**, ETH Zurich, Switzerland
12:40	13:00	*Thermodynamic Modeling of Poorly Specified Mixtures using NMR Spectroscopy and Machine Learning* Dr. Thomas **SPECHT** , RPTU Kaiserslautern, Germany	*Thermodynamics characterization of CO_2 sorption in polymers for CO_2 transport applications* Virginia **SIGNORINI**, Univ. of Bologna, Italy	*Comparison of CP-PC-SAFT and CS-SAFT-VR-Mie in predicting fluid phase behavior in systems of phenolic compounds, aromatic amines, acetophenone and benzaldehyde* Prof. Ilya **POLISHUK**, Ariel Univ., Israel
13:00	**14:00**	**Lunch**		

Monday 10 June Afternoon

SESSIONS		**Carbon capture & Storage (CCS) II - (The Joseph Black's session)** **Chair: Lourdes Vega** *Pentland East*	**Molecular Design: Materials** - sponsored by the Henry Royce Institute **Chair: Eleonora Ricci** *Prestonfield*	**Phase equilibria I** **Chair: Catinca Secuianu** *Pentland West*
14:00	14:20	*Exploring Thermophysical Properties of Phosphonium-Based Ionic Liquids in CO_2 Capture Applications through a Multiscale Approach* Dr. Sabrina **RODRIGUEZ REARTES**, Univ. Rovira i Virgili, Spain	*From Chemical Drawing to Electronic Properties of Semiconducting Polymers in Bulk: A Tool for Chemical Discovery* Dr. Hesam **MAKKI**, University of Liverpool, UK	*Liquid-Liquid Equilibria of the Binary Systems Biodiesel/Glycerol and Biodiesel/Water* Dr. Giulio **SANTORI**, Univ. of Edinburgh, UK
14:20	14:40	*Enhanced Acid Gas Removal from Natural Gas Using Phase Change Amine Solvents* Soultana **TZIMA**, National Technical Univ. of Athens, Greece	*Thermodynamic of Phase Change Material Based on Stearic Acid with Graphene Nanoplatelets* Dr. Yolanda **SANCHEZ VICENTE**, Northumbria University, UK	*A Robust Setup for Efficient Characterization of Multicomponent Vapor-Liquid Equilibria Using Raman Spectroscopy -* Marvin **KASTERKE**, RWTH Aachen Univ., Germany
14:40	15:00	*Predictive Post-Combustion CO_2 Reactive Absorption Framework Combining Electrolyte Thermodynamics with Electronic Structure and Atomistic Simulation Methodologies* Prof. William **SMITH**, Univ. of Guelph, Canada	*Rational Design of Nanoparticle Surface Patterning for Directed Self-Assembly* Dr. Thi **VO**, Johns Hopkins University, USA	*Investigating the solute + solute interactions observed in ternary mixtures of CO_2 + (n-alkanes and/or methyl esters and/or 1-alcohols and/or carboxylic acids)* Prof. Cara **SCHWARZ**, Stellenbosch Univ., South Africa
15:00	15:20	*Enrichment at fluid interfaces and its impact on mass transfer at elevated pressures* Prof. Tim **ZEINER**, Graz Univ. of Technology, Austria	*Sticky–MARTINI – A Reactive Coarse-Grained Model for Self-Assembly in Materials Synthesis* Dr. Miguel **JORGE**, Univ. of Strathclyde, UK	*Analysis of the quality of published experimental and correlated binary and ternary VLE data. Proposal for an adequate planning of their experimental determination and correlation* Prof. Antonio **MARCILLA**, Univ. of Alicante, Spain
15:20	**15:50**	**Coffee Break**		

SESSIONS		**Transport properties (the Thomas Graham's Session)** **Chair: Amparo Galindo** *Pentland East*	**Polymers II** **Chair: Tim Zeiner** *Prestonfield*	**New refrigerants (the David Boyle's session)** **Chair: Romain Privat** *Pentland West*
15:50	16:10	*Generalised dissipative particle dynamics with coupled energy and mass transfers: A coarse-grain framework for simulations of thermodiffusion* Prof. Martin **LISAL**, Czech Academy of Sciences, Czech Republic	*A multi-scale modeling approach for the prediction of hydrogen transport properties in semi-crystalline polymers* Dr. Omar **ATIQ**, Univ. of Bologna, Italy	*The Role of 4E Analysis and Thermodynamic Modeling in the Rational Design of Low-GWP Refrigerants as Drop-in Replacements* Carlos **ALBÁ**, Univ. Rovira i Virgili, Spain
16:10	16:30	*Entropy Scaling for Thermal conductivity with critical Enhancement -* Julia **BURKHARDT**, Univ. of Stuttgart, Germany	*Thermomechanical Modeling of Microstructural Influences on Gas Solubility in Semi-crystalline Polyethylenes* Jana **ZIMMERMANN**, TU Clausthal, Germany	*A comprehensive approach to incorporating intermolecular dispersion into COSMO-RS model* Daria **GRIGORASH**, TU Denmark
16:30	16:50	*Application of the Significant Structure Theory for the Viscosity Modeling of Ionic Fluids* Dr. Ricardo **MACIAS-SALINAS**, ESIQIE - Instituto Politecnico Nacional, Mexico	*Molecular insight on Energetic Interactions and their Contribution to Diffusion of Small Molecules in Polyesters* Dr. Kseniya **PAPCHENKO**, Univ. of Edinburgh, UK	*Biomass-derived working fluids as sustainable alternatives to classical absorption refrigeration systems* Dr. Gabriel **ZARCA**, Univ. de Cantabria, Spain
16:50	17:00	Break		
17:00	18:30	**Poster session I** - Afternoon Tea		
18:30	20:00	Break		
20:00	23:30	**Scottish Ceilidh dances and musical entertainment, South Hall (onsite), with food platters and drinks. Music by the Reel Time Band, Drinks and Food Platters**		

Tuesday 11 June Morning

Plenary talks - Pentland Theatre

Chairs: Maria Eugenia Macedo, Alex Victorov

08:30	09:15	*Towards linking engineering workflows: Phase behavior, self-assembly, and fluctuations from thermodynamic perturbation* Prof. Walter **CHAPMAN**, Rice University, USA
09:15	10:00	*Applied Thermodynamics – Examples from Industrial Applications* Dr. Stephanie **PEPER**, Bayer AG, Germany
10:00	**10:30**	**Coffee Break**

SESSIONS		**Phase equilibria II** **Chair: Felix Llovell** *Pentland East*	**Electrochemical processes (the James Watt's session)** **Chair: Georgios Kontogeorgis** *Prestonfield*	**Surfactants (the James Dewar's session)** **Chair: Helena Passos** *Pentland West*
10:30	10:50	*A Comparison of the UNIFAC Model vs. Graph Neural Network-based Models for the Prediction of Binary Vapor-Liquid Equilibria* Egdar **SANCHEZ MEDINA**, Otto-von-Guericke Univ., Germany	**Keynote**-*Molecular Simulation of Supercapacitors*	*Investigation of coalescence and Ostwald ripening of bubbles of varying sizes and distance using the Navier-Stokes-Korteweg approach* Christian **WACHSMANN**, Univ. of Innsbruck, Austria
10:50	11:10	*Thermodynamic modelling of the systems involved in TEG dehydration of Natural Gas* George **TASIOS**, National Technical Univ. of Athens, Greece		*Polarizable water models for dissipative particle dynamics simulations of micellar solutions* Dr. Rachel **HENDRIKSE**, Durham Univ. UK
11:10	11:30	*Vapor-Liquid Equilibria for Tri-ethylene glycol in high pressure methane: Experiments and Modelling* Prof. Sandra **KENTISH**, Univ. of Melbourne, Australia	*Alkali metal ion intercalation of molybdenite for enhanced CO_2 reduction* Eszter **MADAI**, Delft Univ. of Technology, NL	*Computer-Aided Molecular Design of Surfactants Using Classical Density Functional Theory* Pierre **WALKER**, California Institute of Technolgy, USA
11:30	11:50	*Phase Equilibria and Fluid Properties Modelling for a Hydrogen-based Economy* Dr. Antonio **QUEIMADA**, KBC, UK	*Exergy Based Conceptual Design of Hybrid Electrolyser Systems for PtX* Faisal **SEDEQI**, German Aerospace Centre (DLR), Germany	*Describing Hydrophobic Interactions Using Heterosegmented PC-SAFT – Application to Surfactants* Marius **ROTHER**, TU Dortmund, Germany
11:50	12:00	Break		

SESSIONS		**Polymers III** **Chair: Walter Chapman** *Pentland East*	**Machine Learning II (the James Clark Maxwell's session)** **Chair: Gabriele Sadowski** *Prestonfield*	**Electrolytes I - sponsored by IFPEN** **Chair: Christoph Held** *Pentland West*
12:00	12:20	*Direct shock simulations of several polymer melts* Claire **LEMARCHAND**, Université Paris-Saclay, France	*Coarse Grained Molecular Simulations of Polymers using Machine Learned Potentials* Dr. Eleonora **RICCI**, Univ. of Edinburgh, UK	*ElecTher.IIP: A quaternary system for investigating the effect of acid-base equilibria on volatilities* Dr.Jean-Charles **DE HEMPTINNE,** IFPEN, France
12:20	12:40	*Modeling Swelling and Drying in Electronic Encapsulation* Stefan **WAGNER**, Graz Univ. of Technology, Austria	*Differentiable Equations of State for Machine Learning Thermodynamic-Property Prediction* Michael **GADALOFF**, Imperial College London, UK	*Thermodynamics-assisted kinetic model for esterfication reactions based on ePC-SAFT: Application to levulinic acid* Marcel **KLINKSIEK**, TU Dortmund, Germany
12:40	13:00	*Solubility of Organic Fluid Mixtures in Glassy Polymers* Lorenzo **MERLONGHI**, Univ. of Bologna, Italy	*Modeling Transport Properties of Aqueous Potassium Hydroxide with Machine Learning Molecular Force Fields* Dr. Jelle **LAGERWEIJ**, Delft Univ. of Technology, NL	*Ion-pairing in BMSA ePPC-SAFT for aqueous and mixed-solvent alkali halide solution* Abtin **RAEISPOUR SHIRAZI**, IFPEN, France
13:00	**14:00**	**Lunch**		

Tuesday 11 June Afternoon

SESSIONS		**Phase equilibria III (the Lord Kelvin's session)** **Chair: Cara Schwarz** *Pentland East*	**New trends in Ionic liquids** **Chair: Sabine Enders** *Prestonfield*	**New models (the Robert Stirling's session)** **Chair: Eirini Karakatsani** *Pentland West*
14:00	14:20	*Phase equilibria of clathrate hydrates of carbon dioxide and different substrates-* Prof. Catinca **SECUIANU,** National Univ. of Science and Technology Politehnica Bucharest, Romania	*Acidic aqueous biphasic systems: a novel approach for recovering critical metals from e-waste* Prof. Helena **PASSOS**, Univ. of Porto, Portugal	*Multilayer Quasichemical Model of a Nonuniform Fluid Mixture that Contains Chainlike and Associating Species* Prof. Alexey **VICTOROV**, St. Petersburg State Univ., Russian Federation
14:20	14:40	*A general Gibbs free energy minimization algorithm for modelling solid-fluid equilibria involving miscible solids, pure solids, hydrates, and cocrystals* Wen Hwa **SIAH**, ARMINES Mines Paris - PSL,France	*Choline-Amino Acid Ionic Liquids: from synthesis to application in ATPS* Pedro **VELHO**, University of Porto, Portugal	*First-order perturbation theory using a short-range Lennard-Jones fluid reference* Dr.Andrij **TROKHYMCHUK,** Univ. of Ljubljana, Slovenia
14:40	15:00	*Solid-Liquid Equilibria of Selected Ternary Systems Containing Diphenyl Carbonate, Alcohol, Dialkyl Carbonate, and Phenol* Prof. Hiroyuki **MATSUDA**, Nihon University, Japan	*Eutectic solvents for fish skin valorization. From fundamentals to application* Cristina **GALLEGO,** Univ. de Santiago de Compostela, Spain	*A general method for calculating metastable fluid properties* Dr. Ailo **AASEN**, SINTEF Energy Research, Norway
15:00	15:20	*Tunable alkali-aluminosilicates geopolymers and composites as solid adsorbents for CO_2 capture applications* Prof. Matteo **MINELLI**, Univ. of Bologna, Italy	*Development of a hybrid platform for molecular design and selection of Ionic Liquids for CO_2 capture and conversion* Dr. Felipe **PERDOMO**, Univ. of Edinburgh, UK	*Cluster-Based Discrete Modeling Approach for Activity Coefficients of Molecular Liquids* Prof. Thomas **WALLEK**, Graz Univ. of Technology, Austria
15:20	**15:50**	**Coffee Break**		

SESSIONS		**Machine Learning II** **Chair: Joao Coutinho** *Pentland East*	**Molecular Design: porous & crystalline materials** **Chair: Matteo Minelli** *Prestonfield*	**Electrolytes II** **Chair: Jean-Charles de Hemptinne** Pentland West
15:50	16:10	*Estimating Gas Sorption in Polymeric Membranes from The Molecular Structure: A Machine Learning Based Group Contribution Method For The Non-Equilibrium Lattice Fluid Model (ML-GC-NELF)* Hasan **ISMAEEL** , Univ. of Edinburgh, UK	*In-silico approach to screen new nanoporous materials for urea capture from spent dialysate* Thomas **FABIANI**, Univ. of Edinburgh, UK	Overview of the ERC project: "New Paradigm in Electrolyte Thermodynamics" Prof. Georgios **KONTOGEORGIS**, TU Denmark
16:10	16:30	*Machine learning paradigm for parametrizing soft-SAFT molecular models for pure refrigerants* Dr. Ismail **ALKHATIB,** Khalifa Univ. of Science and Technology**,** UAE	*Designing selective nanoporous materials for VOC capture applied to breath diagnostics: insights from simulation and experiments* Dr.Scott **BOBBITT** , Sandia National Lab., USA	*Analysing Helmholtz energy contributions of model electrolyte systems using molecular simulations* Anja **REIMER**, Univ. of Stuttgart, Germany
16:30	16:50	*Neural Network-Based Tensor Completion: Advancing Predictions of Activity Coefficients and Beyond* Tobias **AVERBECK**, TU Dortmund, Germany	*On the formation of colloidal clathrates and diamond crystals-* Dr.ukasz **BARAN**, Univ. Lublin, Poland	*Applying openCOSMO-RS to Electrolyte Systems from Infinite Dilution to the Ionic Liquid State* Dr. Simon **MÜLLER**, TU Hamburg, Germany
16:50	17:00	Break		
17:00	18:30	**Poster session II**		
18:30	20:00	Break		
20:00	23:00	**Social Dinner, Playfair Library** **Knapp Poster Awards, sponsored by CCPS++**		

Wednesday 12 June Morning

Plenary Talks - Pentland Theatre

Chairs: Ana Soto, Jean-Noel Jaubert

08:30	09:15	*Measurement of Vapour Liquid Equilibrium Thermodynamic Properties Until the* Prof. Cristophe **COQUELET**, IMT Mines Albi, France
09:15	10:00	*Utilizing the Molecular Simulation Design Framework (MoSDeF) to Screen Soft Matter* Prof. Clare **McCABE**, Heriot-Watt University, UK
10:00	**10:30**	**Coffee Break**

SESSIONS		**Pharmaceutical applications** **Chair: Ilya Polishuk** *Prestonfield*	**Statistical Mechanics - Sponsored by the RSC** **Chair: Peter Cummings** *Pentland*
10:30	10:50	*Water in glassy carbohydrates: thermodynamic analysis and molecular dynamics simulations* Prof. Vitaly **KOCHERBITOV**, Malmö University, Sweden	***Keynote*** *- Computational Design of Peptides as Sensors and Drugs* Prof. Carol **HALL**, North Carolina State Univ., USA
10:50	11:10	*Influence of pH and Salts on the Solubilities of Active Pharmaceutical Ingredients* Espen **FRITSCHKA**, TU Dortmund, Germany	
11:10	11:30	*Prediction of API solubility: an overview of the recent developments of the SAFT-γ Mie approach* Dr. Thomas **BERNET**, Imperial College London, UK	*Runaway Transition in Irreversible Polymer Condensation with Cyclisation* Dr. Maria **PANOUKIDOU**, Univ. of Edinburgh, UK
11:30	11:40	**Break**	

SESSIONS		**Water & aqueous solutions (the John Leslie's session)** **Chair: Giulio Santori** *Prestonfield*	**Phase Equilibria IV (the William Rankine's session)** **Chair: Clare McCabe** *Pentland*
11:40	12:00	*Prediction of water anomalous properties by introducing the two-state theory in SAFT* Dr. Nefeli **NOVAK**, TU Denmark	*Application of DFT calculations in the correlation of phase equilibria: estimating non-randomness factors* Prof. Eugénia A. **MACEDO,** Univ. de Porto, Portugal
12:00	12:20	*Maximizing solubilities in aqueous solutions* Prof. Joao **COUTINHO**, Univ. of Aveiro, Portugal	*MCA+PZ and MCA+AMP aqueous solutions: CO_2 solubility experiments and modelling* Dr. Fragkiskos **TZIRAKIS**, CERTH, Greece
12:20	12:40	*The shape of water – how cluster formation explains the hydrophobic effect* Dr. Martin **ANDERSSON**, King Fahd Univ., Saudi Arabia	*Crystallization risk of aromatic compounds in LNG production: Part III: the solubility of o-xylene in methane-rich mixtures down to cryogenic temperatures* Dr. Salem **HOCEINI**, ARMINES MinesParis PSL, France
12:40	13:00	**Conclusive remarks, PPEPPD 2025 and ESAT 2026**	
13:00	**14:00**	**Lunch**	

Sunday 9 June

15:00	18:00	**Registration**
18:00	18:15	Pentland Theatre **Conference Opening** Prof. Maria Eugénia **MACEDO**, ESAT International Steering Committee Chair, Prof. Maria Grazia **DE ANGELIS**, ESAT 2024 Chair
		Pentland Theatre **Michael M. Michelsen Award Lecture** Sponsored by **Fluid Phase Equilibria** - an Elsevier Journal - Introduced by Prof. Ioannis **Economou** *Some insights on the development of equations of state over the past 30 years* Prof. Jean- Noel **JAUBERT** - Université de Lorraine - Michelsen Awardee 2024
19:15	21:00	**Centro-JM Conference Centre** **Welcome Reception**