Sunday 9 June

Start	End	Programme
15:00	18:00	**Registration**
18:00	18:15	Pentland Theatre **Conference Opening** Prof. Maria Eugénia MACEDO, ESAT International Steering Committee Chair
18:15	19:15	Pentland Theatre **Michael M. Michelsen Award Lecture** Sponsored by **Fluid Phase Equilibria** - an Elsevier Journal - Introduced by Prof. Jean-Charles de Hemptinne and Prof. Georgios Kontogeorgis Prof. Jean- Noel **JAUBERT** - Michelsen Awardee 2024
19:15	21:00	**Centro-JM Conference Centre** **Welcome Reception**

Monday 10 June

Pentland Theatre

Chairs: Ralf Dohrn, Sabine Enders

Start	End			
08:30	09:15	**Plenary talk** - **255** - *Atomistic and Mesoscopic Modeling of Structure-Property Relations in Polymers* - Prof. Doros N. **THEODOROU**, National Technical Univ. of Athens, Greece		
09:15	10:00	**Plenary talk** - **264** - *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 Denibigh's session)** **Chair: Tina Düren** *Prestonfield*	**Molecular design: membranes & interfaces** **Chair: Doros Theodorou** *Pentland West*
10:30	10:50	**278** - *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	**250** - **Keynote** - *On Adsorption Azeotropy and a Classification Based on the Dual Site Langmuir Isotherm* - Prof. Stefano **BRANDANI**, Univ. of Edinburgh, UK (10:30–11:10)	**207**-*Dynamically Switchable Monolayer Coatings: Improved Understanding of Group Contribution to Surface Tension* - Nicholas **CRAVEN**, Vanderbilt Univ. USA
10:50	11:10	**289** - *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		**55** - *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	**272** - *Understanding the CO_2 Capture Performance of amine-functionalized Silica and Carbon-based materials Using Molecular Simulations*, Prof. Lourdes **VEGA**, Khalifa Univ., UAE	**128**-*Predicting Adsorption with 3D classical Density Functional Theory based on PC-SAFT* - Nadine **THIELE**, Univ. of Stuttgart, Germany	**299** - *Wetting, adsorption, and desorption behaviour of polymers on surfaces* - Prof. Vasileios **KOUTSOS**, Univ. of Edinburgh, UK
11:30	11:50	**268** - *Integrating Theoretical Approaches for Profiling the Thermophysical Behavior of DESs in Greenhouse Gas Treatments* - Dr. Fèlix **LLOVELL**, Univ. Rovira i Virgili, Spain	**204**-*Impact of Force Field Choice on Adsorption Predictions in MOFs* -Connaire **McCREADY**, University of Strathclyde, UK	**5** - *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	**31** - *Improvement of diffusion coefficient prediction by active learning* - Zeno **ROMERO,** RPTU Kaiserslautern, Germany	**43** - *Predicting Gas Solubilities in Semi-crystalline Branched Polyolefin Systems with the Lattice-Cluster-Theory-EoS* - Simon **LEUBE**, KIT, Germany	**242** - *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	**70** - *Predicting solvation free energy in binary solvents using graph neural networks* - Roel **LEENHOUTS**, KU Leuven, Belgium	**46** - *High throughput screening of polymers: properties prediction and structures discovery* - Dr. Vittoria **FANTAUZZO**, Univ. of Liverpool, UK	**271** - *Decorrelating equation of state parameters with mixture data* - Dr. Philippe **REHNER**, ETH Zurich, Switzerland
12:40	13:00	**37** - *Thermodynamic Modeling of Poorly Specified Mixtures using NMR Spectroscopy and Machine Learning* - Dr. Thomas **SPECHT**, RPTU Kaiserslautern, Germany	**64** - *Thermodynamics characterization of CO_2 sorption in polymers for CO_2 transport applications* - Virginia **SIGNORINI**, Univ. of Bologna, Italy	**35** - *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**		
SESSIONS		**Carbon capture & Storage (CCS) II - (The Joseph Black's session)** **Chair: Lourdes Vega** *Pentland East*	**Molecular Design: Materials** **Chair: Eleonora Ricci** *Prestonfield*	**Phase equilibria I** **Chair: Catinca Secuianu** *Pentland West*
14:00	14:20	**239** - *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	**72** - *From Chemical Drawing to Electronic Properties of Semiconducting Polymers in Bulk: A Tool for Chemical Discovery* -Dr. Hesam **MAKKI**, University of Liverpool, UK	**12** - *Liquid-Liquid Equilibria of the Binary Systems Biodiesel/Glycerol and Biodiesel/Water* - Dr. Giulio **SANTORI**, Univ. of Edinburgh, UK
14:20	14:40	**174** - *Enhanced Acid Gas Removal from Natural Gas Using Phase Change Amine Solvents*, Soultana **TZIMA**, National Technical Univ. of Athens, Greece	**202** - *Thermodynamic of Phase Change Material Based on Stearic Acid with Graphene Nanoplatelets*, Dr. Yolanda **SANCHEZ VICENTE**, Northumbria University, UK	**216** - *A Robust Setup for Efficient Characterization of Multicomponent Vapor-Liquid Equilibria Using Raman Spectroscopy*- Marvin **KASTERKE**, RWTH Aachen Univ., Germany
14:40	15:00	**71** - *Predictive Post-Combustion CO2 Reactive Absorption Framework Combining Electrolyte Thermodynamics with Electronic Structure and Atomistic Simulation Methodologies*, Prof. William **SMITH**, Univ. of Guelph, Canada	**135** - *Rational Design of Nanoparticle Surface Patterning for Directed Self-Assembly* - Dr. Thi **VO**, Johns Hopkins University, USA	**153** - *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	**110** - *Enrichment at fluid interfaces and its impact on mass transfer at elevated pressures* - Prof. Tim **ZEINER**, Graz Univ. of Technology, Austria	**132** - *Sticky-MARTINI – A Reactive Coarse-Grained Model for Self-Assembly in Materials Synthesis* - Dr. Miguel **JORGE**, Univ. of Strathclyde, UK	**42** - *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	**209** - *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	**215** - *A multi-scale modeling approach for the prediction of hydrogen transport properties in semi-crystalline polymers* - Dr. Omar **ATIQ**, Univ. of Bologna, Italy	**191** - *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	**58** - *Entropy Scaling for Thermal conductivity with critical Enhancement*, Julia **BURKHARDT**, Univ. of Stuttgart, Germany	**164** - *Thermomechanical Modeling of Microstructural Influences on Gas Solubility in Semi-crystalline Polyethylenes* - Jana **ZIMMERMANN**, TU Clausthal, Germany	**185** - *A comprehensive approach to incorporating intermolecular dispersion into COSMO-RS model* - Daria **GRIGORASH**, TU Denmark
16:30	16:50	**152** - *Application of the Significant Structure Theory for the Viscosity Modeling of Ionic Fluids* - Dr. Ricardo **MACIAS-SALINAS**, ESIQIE - Instituto Politecnico Nacional, Mexico	**167** - *Molecular insight on Energetic Interactions and their Contribution to Diffusion of Small Molecules in Polyesters* - Dr. Kseniya **PAPCHENKO**, Univ. of Edinburgh, UK	**295** - *Experimental method for VLE measurement of low GWP HFOs working fluid* - Dr. Zhiqiang **YANG**, Xi'an modern chemistry research institute, China
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**		

Tuesday 11 June

Pentland Theatre

Chairs: Maria Eugenia Macedo, Alex Victorov

Start	End			
08:30	09:15	**Plenary Talk** - **294** - *Towards linking engineering workflows: Phase behavior, self-assembly, and fluctuations from thermodynamic perturbation theory and molecular simulation* - Prof. Walter **CHAPMAN**, Rice University, USA		
09:15	10:00	**Plenary Talk** - *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: Epaminondas Voutsas** *Prestonfield*	**Surfactants (James Dewar's session)** **Chair: Helena Passos** *Pentland West*
10:30	10:50	**273** - *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	189 - **Keynote**-*Molecular Simulation of Supercapacitors* - Prof. Peter **CUMMINGS**, Heriot-Watt Univ, UK (10:30–11:10)	**127**-*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	**170** - *Thermodynamic modelling of the systems involved in TEG dehydration of Natural Gas* - George **TASIOS**, National Technical Univ. of Athens, Greece		**276** - *Polarizable water models for dissipative particle dynamics simulations of micellar solutions* - Dr. Rachel **HENDRIKSE**, Durham Univ. UK
11:10	11:30	**52** - *Vapor-Liquid Equilibria for Tri-ethylene glycol in high pressure methane: Experiments and Modelling*. Prof. Sandra **KENTISH**, Univ. of Melbourne, Australia	**254** - *Alkali metal ion intercalation of molybdenite for enhanced CO_2 reduction* -Eszter **MADAI**, Delft Univ. of Technology, NL	**74** - *Computer-Aided Molecular Design of Surfactants Using Classical Density Functional Theory* - Pierre **WALKER**, California Institute of Technolgy, USA
11:30	11:50	**223** - *Phase Equilibria and Fluid Properties Modelling for a Hydrogen-based Economy* - Dr. Antonio **QUEIMADA**, KBC, UK	**114** - *Exergy Based Conceptual Design of Hybrid Electrolyser Systems for PtX* - Faisal **SEDEQI**, German Aerospace Centre (DLR), Germany	**54** - *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** **Chair: Christoph Held** *Pentland West*
12:00	12:20	**129** - *Direct shock simulations of several polymer melts* - Claire **LEMARCHAND**, Université Paris-Saclay, France	**235** - *Coarse Grained Molecular Simulations of Polymers using Machine Learned Potentials* - Dr. Eleonora **RICCI**, Univ. of Edinburgh, UK	**212** - EleTher JIP: A quaternary system for investigating the effect of acid-base equilibria on volatilities **-** Dr.Jean-Charles **DE HEMPTINNE,** IFPEN, France
12:20	12:40	**158** - *Modeling Swelling and Drying in Electronic Encapsulations* - Stefan **WAGNER**, Graz Univ. of Technology, Austria	**292** - *Differentiable Equations of State for Machine Learning Thermodynamic-Property Prediction* - Luc **PAOLI**, Imperial College London, UK	**79 -** Thermodynamics-assisted kinetic model for esterification reactions based on ePC-SAFT: Application to levulinic acid- Marcel **KLINKSIEK,** TU Dortmund, Germany
12:40	13:00	**130** - *Solubility of Organic Fluid Mixtures in Glassy Polymers* - Lorenzo **MERLONGHI**, Univ. of Bologna, Italy	**17** - *Modeling Transport Properties of Aqueous Potassium Hydroxide with Machine Learning Molecular Force Fields* -Dr. Jelle **LAGERWEIJ**, Delft Univ. of Technoloy, NL	**65 -** Ion-pairing in BiMSA ePPC-SAFT for aqueous and mixed-solvent alkali halide solutions- Abtin **RAEISPOUR SHIRAZI**, IFPEN, France
13:00	**14:00**	**Lunch**		
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** **Chair: Eirini Karakatsani** *Pentland West*
14:00	14:20	**266 -** *Phase equilibria of clathrate hydrates of carbon dioxide and different substrates* - Prof. Catinca **SECUIANU,** National Univ. of Science and Technology Politehnica Bucharest, Romania	**251 -** *Acidic aqueous biphasic systems: a novel approach for recovering critical metals from e-waste* - Prof. Helena **PASSOS**, Univ. of Porto, Portugal	**8 -** *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	**49 -** *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	**221 -** *Choline-Amino Acid Ionic Liquids: from synthesis to application in ATPS* - Pedro **VELHO**, University of Porto, Portugal	**260 -** *First-order perturbation theory using a short-range Lennard-Jones fluid reference* - Dr.Andrij **TROKHYMCHUK,** Univ. of Ljubljana, Slovenia
14:40	15:00	**57 -** *Solid-Liquid Equilibria of Selected Ternary Systems Containing Diphenyl Carbonate, Alcohol, Dialkyl Carbonate, and Phenol* - Prof. Hiroyuki **MATSUDA**, Nihon University, Japan	**113 -** *Eutectic solvents for fish skin valorization. From fundamentals to application* - Cristina **GALLEGO,** Univ. de Santiago de Compostela, Spain	**90 -** *A general method for calculating metastable fluid properties* - Dr. Ailo **AASEN**, SINTEF Energy Research, Norway
15:00	15:20	**248** - *Hydrogen and air storage in salt caverns: a thermodynamic model for phase equilibrium calculations* - Dr. Nicolas **FERRANDO**, IFPEN, France	**233** - *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	**249 -** *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 (the Robert Stirling's session)** **Chair: Jean-Charles de Hemptinne** Pentland West
15:50	16:10	**138 -** *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	**126 -** *In-silico approach to screen new nanoporous materials for urea capture from spent dialysate* - Thomas **FABIANI**, Univ. of Edinburgh, UK	**243** - *Overview of the ERC project: "New Paradigm in Electrolyte Thermodynamics"* - Prof. Georgios **KONTOGEORGIS**, TU Denmark
16:10	16:30	**228** - *Machine learning paradigm for parametrizing soft-SAFT molecular models for pure refrigerants* - Dr. Ismail **ALKHATIB,** Khalifa Univ. of Science and Technology**,** UAE	**104 -** *Designing selective nanoporous materials for VOC capture applied to breath diagnostics: insights from simulation and experiments* - Dr.Scott **BOBBITT**, Sandia National Lab., USA	**66 -** *Analysing Helmholtz energy contributions of model electrolyte systems using molecular simulations* - Anja **REIMER**, Univ. of Stuttgart, Germany
16:30	16:50	**143 -** *Neural Network-Based Tensor Completion: Advancing Predictions of Activity Coefficients and Beyond* - Tobias **AVERBECK**, TU Dortmund, Germany	**13 -** *On the formation of colloidal clathrates and diamond crystals* - Dr.Łukasz **BARAN**, Univ. Lublin, Poland	**41 -** *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 CCP++**		

Wednesday 12 June

Pentland Theatre

Chairs: Ana Soto, Jean-Noel Jaubert

Start	End		
08:30	09:15	**Plenary Talk** - **23** -*Measurement of Vapour Liquid Equilibrium Thermodynamic Properties Until the Critical Point and modelling* - Prof. Cristophe **COQUELET**, IMT Mines Albi, France	
09:15	10:00	**Plenary Talk** - **261** - *Utilizing the Molecular Simulation Design Framework (MoSDeF) to Screen Soft Matter Systems* - **Prof. Clare McCABE,** Heriot-Watt University, UK	
10:00	10:30	**Coffee Break**	
SESSIONS		**Pharmaceutical applications** **Chair: Ilya Polishuk** *Prestonfield*	**Statistical Mechanics** **Chair: Peter Cummings** *Pentland*
10:30	10:50	**259** - *Water in glassy carbohydrates: thermodynamic analysis and molecular dynamics simulations* - Prof. Vitaly **KOCHERBITOV**, Malmö University, Sweden	**38**-**Keynote**- *Computational Design of Peptides as Sensors and Drugs* - Prof. Carol **HALL**, North Carolina State Univ., USA (10:30–11:10)
10:50	11:10	**14** - *Influence of pH and Salts on the Solubilities of Active Pharmaceutical Ingredients*, Espen **FRITSCHKA**, TU Dortmund, Germany	
11:10	11:30	**134** - *Prediction of API solubility: an overview of the recent developments of the SAFT-γ Mie approach*, Dr. Thomas **BERNET**, Imperial College London, UK	**133**-*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** *Pentland East*	**Phase Equilibria IV (the William Rankine's session)** **Chair: Clare McCabe** *Prestonfield*
11:40	12:00	**22**-*Prediction of water anomalous properties by introducing the two-state theory in SAFT* -Dr. Nefeli **NOVAK**, TU Denmark	**218**- *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	**18**-*Maximizing solubilities in aqueous solutions* -Prof. Joao **COUTINHO**, Univ. of Aveiro, Portugal	**302** - *MCA+PZ and MCA+AMP aqueous solutions: CO_2 solubility experiments and modelling* - Dr. Fragkiskos **TZIRAKIS**, CeRTH, Greece
12:20	12:40	**25** - *The shape of water – how cluster formation explains the hydrophobic effect* - Dr. Martin **ANDERSSON**, King Fahd Univ., Saudi Arabia	**162** - *Phase equilibrium behavior of the acetonitrile + methane system, application to planetary science and methane transportation* - Nicholas **GASSIES**, MinesParis PSL, France
12:40	**13:00**	**Conclusive remarks, PPEPPD 2025 and ESAT 2026**	
13:00	**14:00**	**Lunch**	