Introduction Contents

Introduction

It is with great pleasure that the International Steering Comittee, the local Organising committee and the University of Edinburgh welcome you to **ESAT 2024**, marking the **50th anniversary** of the European Symposium on Applied Thermodynamics series. When it started, in 1974, Europe was still divided in blocks and the conference took place in west Berlin. Since then, ESAT has been hosted by Northern, Southern, Eastern and Western European Countries to represent the diversity and richness of our culture. We will celebrate this with a special anniversary ceremony during our social dinner. We will also present the EFCE Michael L. Michelsen Award 2024 to Prof. Jean Noel Jaubert, who will give a speech entitled „*Some insights on the development of equations of state over the past 30 years*“ and award three Helmut Knapp prizes to the best poster presenters.

ESAT is a truly European conference with a global flavour that proudly hosts contributions from all continents. As British scientists, we are particularly excited to celebrate our Association to European scientific schemes such as Horizon and continue a tradition of succesful collaborations. As a Scottish Institution, we are proud to celebrate the numerous Scottish scientists who have contributed to the field of Applied Thermodynamics, who built their strenght through mutual **collaborations**, such as those between Joseph Black and James Watt, Peter Tait and Lord Kelvin, James C. Maxwell and James Dewar. As the challenges we are facing, such as sustainability, energy transition and climate change, become ever more pressing, we need to collaborate and interact and we hope that ESAT 2024 will strengthen existing connections and foster new ones.

On behalf of the organizing and IS committee, welcome to Edinburgh!

The ESAT conference series

EDITION	Year	ORGANISER	LOCATION	COUNTRY
33rd	**2024**	**University of Edinburgh**	**Edinburgh**	**Scotland (UK)**
32nd	2022	TU Graz	Graz	Austria
31st	2021	IFP Energies nouvelles	Paris / online	France
30th	2018	The Czech Academy of Sciences	Prague	Czech Republic
29th	2017	Polytechnic Univ. Bocarest	Bucarest	Romania
28th	2015	Nat. Tech. Univ. Athens	Athens	Greece
27th	2014	Eindhoven University of Technology	Eindhoven	The Netherlands
26th	2012	TU Berlin and DECHEMA	Potsdam	Germany
25th	2011	St. Petersburg State Univ, Russian Acad.Sci, The Mendeleev Russian chem. Soc.	St. Petersburg	Russia
24th	2009	ETSE.Univ, Santiagp de Compostela	Santiago de Compostela	Spain
23rd	2008	ENSIC-INPL, Nancy	Cannes	France
22nd	2006	Tech. Univ. Denmark	Elsinore	Denmark
21st	2005	Warsaw Univ. of Tech.	Jurata	Poland
20th	2003	VDI-GVC, Dusseldorf + Bayer AG, Leverkusen + Univ. Kaiserslautem	Lahnstein	Germany
19th	2002	Nat. Tech. Univ. Athens	Santorini	Greece
18th	2000	ICT, Prague + ICPF, Prague	Kutna Hora	Czech Republic
17th	1999	Univ. Porto + Univ. Aveiro	Vilamoura	Portugal
16th	1997	Univ. Metz + ENSIC-INPL, Nancy	Pont-a-Mousson	France
15th	1996	ICI, Runcom	Runcom	United Kingdom
14th	1994	Nat. Tech. Univ. Athens	Marathon	Greece
13th	1993	Univ. Marseille	Marseille	France
12th	1991	Tech. Univ. Berlin	Berlin	Germany
11th	1990	Tech. Univ. Denmark	Rungsted	Denmark
10th	1988	Univ. Porto	Ofir	Portugal
9th	1987	Norsk Hydro, Posgrunn	Bergen	Norway
8th	1985	Univ. Trieste	Trieste	Italy
7th	1983	Univ. Dortmund	Dortmund	Germany
6th	1982	Institut Français du pétrol	Rueil Malmaison	France
5th	1980	Linde AG, Munchen	Sachrang	Germany
4th	1979	Shell, Amsterdam	Amsterdam	The Netherlands
3nd	1978	Tech. Univ. Denmark	Lyngby	Denmark
2nd	1976	Tech. Univ. Berlin	Berlin (West)	Germany
1st	1974	Tech. Univ. Berlin	Berlin (West)	Germany

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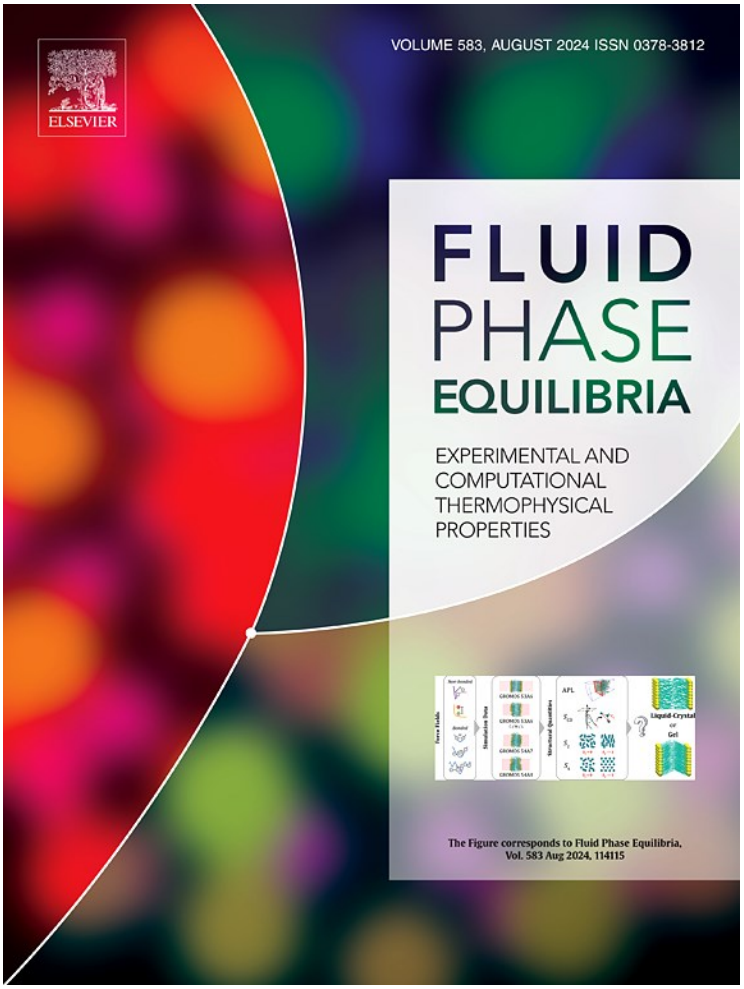

Fluid Phase Equilibria publishes high-quality papers dealing with experimental, theoretical, and applied research related to equilibrium and transport properties of fluids, solids, and interfaces. Subjects of interest include physical/phase and chemical equilibria; equilibrium and nonequilibrium thermophysical properties; fundamental thermodynamic relations; and stability. The systems central to the journal include pure substances and mixtures of organic and inorganic materials, including polymers, biochemicals, and surfactants, with sufficient characterization of composition and purity for the results to be reproduced. Naturally occurring systems that cannot be completely characterized will be considered only if they are of high practical interest and the work leads to significant new findings. In all cases, enough detail must be given to permit independent verification, and authors are also expected to provide physical or chemical interpretations of the results.

See more at: https://www.sciencedirect.com/journal/fluid-phase-equilibria


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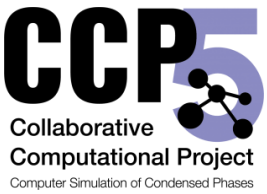
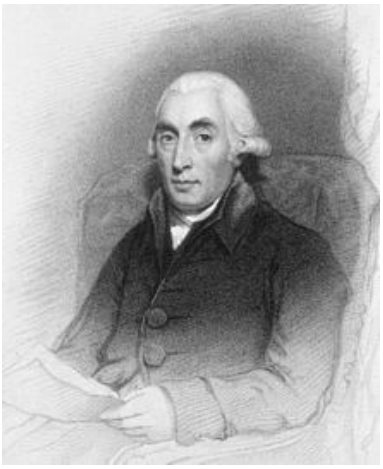

CCP5
Collaborative
Computational Project
Computer Simulation of Condensed Phases

Applied Thermodynamics in Scotland

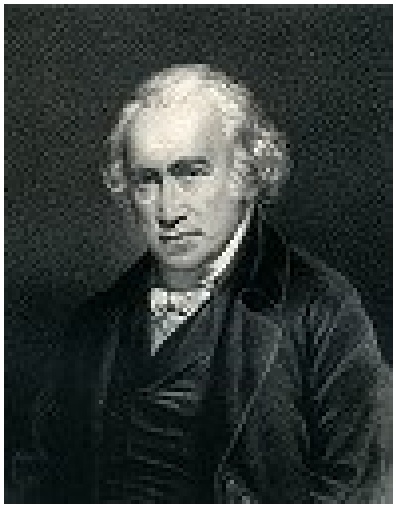
Scotland was the birthplace or workplace of many scientists who have contributed enormously to the field of applied thermodynamics. The section below, taken from open access sources such as Wikipedia and the Scottish Engineering hall of fame website, aims to pay a small tribute to their contribution to the advancement of this discipline and emphasise their mutual collaborations.

Joseph Black (1728-1799)



Joseph Black was a physicist and chemist, known for his discoveries of magnesium, latent heat, specific heat, and carbon dioxide. He was Professor of Anatomy and Chemistry at the University of Glasgow for 10 years from 1756, and Professor of Medicine and Chemistry at the University of Edinburgh from 1766. The chemistry buildings at the University of Edinburgh are named after him. Around 1750, while still a student, Black developed the *analytical balance*, which far exceeded the accuracy of any other balance of the time and became an important scientific instrument. In 1761, he deduced that the application of heat to boiling water does not result in a rise in temperature of a water/steam mixture, but rather in an increase in the amount of steam. From these observations, he concluded that the heat applied must have combined with boiling water and become latent. *The theory of latent heat marks the beginning of thermodynamics*. Black also found that calcium carbonate could be heated or treated with acids to yield a gas (CO_2) he called "fixed air". In the last part of his career, he devoted himself exclusively to teaching. His lectures had a powerful effect in popularising chemistry and attendance at them even became a fashionable amusement. Black's grave is in Greyfriars Kirkyard in Edinburgh. In 2011, scientific equipment believed to belong to him was discovered during an archaeological dig at the University of Edinburgh. The session on ***Carbon Capture and Storage*** in **ESAT 2024** is dedicated to him.

James Watt (1736-1819)



James Watt was born in Greenock, near Glasgow. He was an inventor, mechanical engineer, and chemist who developed the *Watt steam engine* in 1776, which was fundamental to the Industrial Revolution.

After leaving school, he started working as a mathematical instrument maker and set up a workshop within the University of Glasgow in 1757. There, he became friends with chemist Joseph Black and economist Adam Smith.

There is a popular story that Watt was inspired to invent the *steam engine* by seeing a kettle boiling, the steam forcing the lid to rise and thus showing the power of steam. In reality, Watt did not invent the steam engine, but significantly improved the efficiency of the existing one by adding a separate condenser, consistent with the new principles of *thermal efficiency*. He came to realise the importance of *latent heat*, which his friend Joseph Black had previously discovered. The science of thermodynamics would not be formalised for nearly another 100 years.

Watt was a proficuous inventor, and, together with Matthew Boulton, who owned the Soho Manufactory works with some of the best iron workers in the world, formed a hugely successful partnership. Watt combined theoretical knowledge of science with the ability to apply it practically. The *watt*, the unit of power incorporated in the International System of Units is named after him. In 2009, the Bank of England released a £50 note depicting Boulton and Watt. Watt is commemorated by statuary in Princes Street, Edinburgh, while a painting „*James Watt contemplating the steam engine*“ is visible at the National Gallery of Scotland. **ESAT 2024** has dedicated the ***Electrochemical Process*** session to him, hoping that his work can inspire a new Industrial Revolution, based on a new energy transition.

John Leslie (1766-1832)

Leslie was born in Largo (Fife). At 13 years of age he entered the University of St Andrews. On completion of his course in 1784, he studied divinity at the University of Edinburgh but gained no further degrees. He then worked as a private tutor, employing his spare time in experimental research and continued his physical studies, which resulted in numerous papers and in the publication (1804) of the *Experimental Inquiry into the Nature and Properties of Heat*, a work which gained him the Rumford Medal of the Royal Society of London.

In 1805, after having been rejected in several attempts to obtain a Chair at a Scottish university, Leslie was elected to succeed John Playfair in the chair of mathematics at Edinburgh, despite violent opposition from a party who accused him of heresy (he was an atheist). With reference to his invention (in 1810) of a process of *artificial ice-making*, he published in 1813 *A Short Account of Experiments and Instruments depending on the relations of Air to Heat and Moisture.* When John Playfair died in 1819, Leslie was promoted to the more congenial chair of natural philosophy, which he held until his death. Leslie's main contributions to physics were made by the help of the differential thermometer, which he was able to employ to study photometry, hygroscopy and the temperature of space. The **ESAT 2024** will honour him through the ***Water and Aqueous*** solutions session.

Robert Stirling (1790-1878)

Robert Stirling was born in Perthshire. Though he had a natural inclination for engineering, he began attending Edinburgh University in 1805 at the age of 15 to study divinity in hopes of becoming a minister. He finished his studies there and continued at Glasgow University where he studied the classics, philosophy, theology and mathematics. Robert was licensed to preach in the Church of Scotland in 1816. Stirling is considered as one of the fathers of *hot air engines*. None of Stirling's experimental work or papers survived except for two model engines built by him when he was a Minister at Kilmarnock. At Edinburgh university Stirling's engine was

used in student classes and it is now on display in the Royal Scottish Museum. At Glasgow university the engine lay forgotten until discovered in 1847 by William Thomson, who later became Lord Kelvin. Thomson used the model in lectures to show that Stirling's machine worked on *a reversible cycle*. In 1816, at the age of 26 Stirling patented an engine which produced motive power from heated air. He continued to refine his ideas and, with his brother James, registered patents for improvements in 1827 and 1840. The principles of his revolutionary engine are increasingly being adopted and adapted as conventional fuels for internal combustion engines become scarcer. Today's applications include heat pumps; the NASA MOD I and II automotive engines; various hybrid electric vehicles; Stirling powered submarines - and many more. As conventional fuels become ever scarcer, the Scottish clergyman's ideas from almost 200 years ago are of more relevance today than ever. For his contributions, **ESAT 2024** has dedicated the ***New models*** session to him.

Thomas Graham (1805-1869)

Thomas Graham was born in Glasgow, the son of a textile manufacturer, who wanted him to join the Church of Scotland. Instead, he became a student at the University of Glasgow and developed a strong interest in chemistry. He later studied medicine at the University of Edinburgh. After taking a professorship at the University of London, he founded the Chemical Society of London in 1841.

Thomas Graham is known for his studies on the behavior of gases, which resulted in the formulation of two relationships, now known as "*Graham's Laws*," regarding gas *diffusion* and effusion. In applied areas, Graham also made fundamental discoveries related to *dialysis*, a process used in research and industrial settings, as well as in modern health care. Graham's study of colloids resulted in his ability to separate colloids and crystalloids using a so-called "dialyzer", using technology that is a rudimentary forerunner of technology in modern kidney dialysis machines. These studies were foundational in the field known as *colloid chemistry*, and Graham is credited as one of its founders. He also proposed the association theory which claimed that the substances such as cellulose that we now know are *polymers* are composed from smaller molecules hold together by unknown forces. A statue of Graham

in Glasgow was erected by the city in 1872. The **ESAT 2024** has decided to dedicate its session on ***Transport Properties*** to him.

William Rankine (1820-1872)

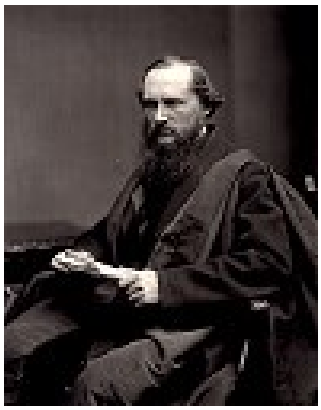
William John Macquorn Rankine, born in Edinburgh, was a mathematician and physicist. In 1836, he began to study a number of scientific topics at the University of Edinburgh, leaving it in 1838 without a degree and starting to work, as his father, in the Railways. There he developed a technique, the *Rankine's method*, for laying out railway curves. For Queen Victoria's visit to Scotland, he organised a large bonfire on Arthur's Seat, which served to initiate a chain of other bonfires across Scotland. From 1855 he was Professor of Civil Engineering and Mechanics at Glasgow University.

By 1849, he had discovered the relationship between saturated vapour pressure and temperature and between the temperature, pressure and density of gases, as well as for the latent heat of evaporation of a liquid. In 1851 he set out to calculate the *efficiency* of heat engines and used his theory to deduce the principle that the maximum efficiency possible is a function only of the two temperatures between which it operates. In 1853, he coined the term *potential energy*. From 1854, he made wide use of his thermodynamic function which he later realised was identical to the *entropy* of Clausius. He published a definition of energy in terms of capacity of performing work, which quickly became the standard general definition. In 1859 he proposed the *Rankine scale of temperature*, an absolute scale whose degree is equal to a Fahrenheit degree.

The *Rankine cycle* is an analysis of an ideal heat-engine with a condensor. One of King's Buidings campus buildings at the University of Edinburgh is named after him. The ESAT 2024 has decided to dedicate ***Fluid Phase Equilibria* IV** session to William Rankine for his studies on the relationship between thermodynamic quantities.

Lord Kelvin (1824-1907)

William Thomson, 1st Baron Kelvin, was a mathematician, mathematical physicist and engineer born in Belfast. He was the professor of Natural Philosophy at the University of Glasgow for 53 years, where he undertook significant research and mathematical analysis of electricity, the formulation of the *first and second laws of thermodynamics*, and contributed significantly to unifying physics, which was then in its infancy of development as an emerging academic discipline.



Absolute temperatures are stated in units of kelvin in his honour. While the existence of a coldest possible temperature, absolute zero, was known before his work, Kelvin determined its correct value as approximately −273.15 degrees Celsius. In 1892, he became the first British scientist to be elevated to the House of Lords. Thomson had a fruitful, though largely epistolary, collaboration with James P. Joule: Joule conducting experiments, Thomson analysing the results and suggesting further experiments. The collaboration produced discoveries including the Joule–Thomson effect.

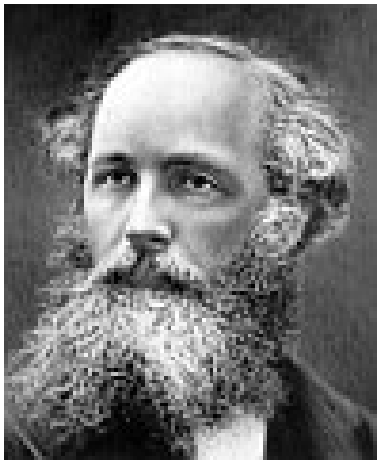
He also had a career as an electrical telegraph engineer and inventor which earned him wealth, fame, and honours. For his work on the transatlantic telegraph project, he was knighted in 1866 by Queen Victoria, becoming Sir William Thomson. He had extensive maritime interests and worked on the mariner's compass.

He was ennobled in 1892 in recognition of his achievements in thermodynamics. Despite offers of elevated posts from several world-renowned universities, Kelvin refused to leave Glasgow, remaining until his retirement in 1899. Active in industrial research and development, he was recruited around 1899 by George Eastman to serve as vice-chairman of the board of the British company Kodak Limited.

The Hunterian Museum at the University of Glasgow has a permanent exhibition on the work of Kelvin, which includes many of his original papers, instruments, and other artefacts, including his smoking pipe.

ESAT 2024 honours his contributions to applied thermodynamics, and the bicentennial of his birth, through the session ***Phase Equilibria* III**.

James Clerk Maxwell (1831-1879)



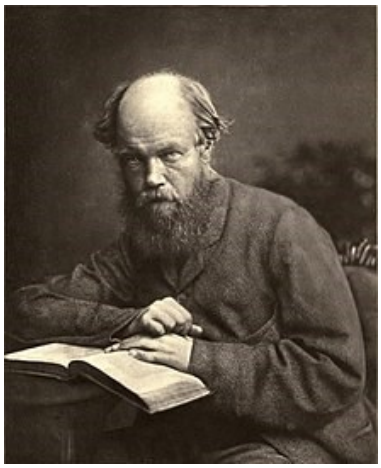
James Clerk Maxwell was born in 1831 at 14 India Street, Edinburgh, now hosting a museum operated by the omonomious Foundation. Maxwell was sent to the Edinburgh Academy where he became friend with Peter Tait. In 1850, he left Scotland for Cambridge, where in 1854, graduated from Trinity in mathematics. Maxwell was Chair of Natural Philosophy at Marischal College, Aberdeen and at King's College, London; and in 1871 became the first Cavendish Professor of Physics in Cambridge.

He was responsible for the classical theory of electromagnetic radiation, which was the first theory to describe electricity, magnetism and light as different manifestations of the same phenomenon and it is considered the "*second great unification in physics*" after the one of Newton. The unification of light and electrical phenomena led to his prediction of the existence of *radio waves*. Maxwell was the first to derive the *Maxwell–Boltzmann distribution*, a statistical mean of describing aspects of the kinetic theory of gases given the fraction of gas molecules moving at a specified velocity at any given temperature. His work on thermodynamics led him to devise the thought experiment that came to be known as *Maxwell's demon*, where the 2nd law of thermodynamics is violated by an imaginary being capable of sorting particles by energy. In 1871, he established *Maxwell's thermodynamic relations*, between the second derivatives of the thermodynamic potentials with respect to different thermodynamic variables. Maxwell proved that the rings of Saturn were made of small particles, winning the 1857 Adams prize, and providing an explanation that was confirmed by direct observations by the Voyager probe in the 1980s.

He is also known for presenting the first durable *colour photograph* in 1861 and he is responsible for modern *dimensional analysis*. Maxwell is also recognized for laying the groundwork for *chaos theory*. His discoveries helped usher in the era of modern physics, laying the foundation for such fields as *special relativity* and *quantum mechanics*. Many physicists regard Maxwell as the 19th-century scientist having the greatest influence on 20th-century physics.

ESAT 2024 decided to dedicate the session of ***Machine Learning*** to Maxwell, for his ability to utilise mathematical methods to describe physics laws.

Peter Guthrie Tait (1831-1901)



Tait was born in Dalkeith (Scotland) on 28 April 1831. He was educated at the Edinburgh Academy. He studied Mathematics and Physics at the University of Edinburgh, and then went to Peterhouse, Cambridge. Two years later he took up the professorship of mathematics at Queen's College, Belfast. His work on knot theory contributed to the eventual formation of *topology* as a mathematical discipline. His name is known in graph theory mainly for *Tait's conjecture* on cubic graphs. In 1860, Tait became professor of natural philosophy at the University of Edinburgh. In 1871, he emphasised the significance and future importance of the principle of the dissipation of energy (2nd law of thermodynamics). Researches on "Charcoal Vacua" with James Dewar led him to see the true dynamical explanation of the Crookes radiometer in the large mean free path of the molecules of highly rarefied air. From 1879 to 1888, he engaged in difficult experimental investigations on the corrections required for thermometers operating at high pressure, for the benefit of the Challenger expedition for observing deep-sea temperatures, which led to the *Tait equation* (of state). Between 1886 and 1892 he published a series of papers on the foundations of the kinetic theory of gases. With Lord Kelvin, he collaborated in writing the well-known *Treatise on Natural Philosophy* an all-comprehensive treatise on physical science. He is buried in the second terrace down from Princes Street in the burial ground of St John's Episcopal Church, Edinburgh. Tait's house was at 17 Drummond Place, Edinburgh. He was a lifelong friend of James Clerk Maxwell. One of the chairs in the Department of Physics at the University of Edinburgh is the Tait professorship. Tait Road at the University of Edinburgh King's Buildings complex is named in his honour. The **ESAT 2024** session ***Equations of state*** is dedicated to him.

David Boyle (1837-1891)

Born in Johnstone (Scotland), he emigrated to the USA at 21 and studied refrigeration texts at the San Francisco Mechanics' Institute. Boyle developed an improved form of ice making machine in a time when most ice was harvested in winter from lakes and rivers, transported long distances and stored for months. He is credited with being the first person to make use of *ammonia* as the working fluid in *a vapour-compression refrigeration system* reliable and commercially successful and he established an *ice machine manufacturing* company in the very early days of mechanical refrigeration. He developed an improved form of compressor valve which became the standard way of achieving inlet and outlet control in many makes of compressors. Boyle's success with his ammonia compression system led to the rapid adoption of ammonia as the preferred refrigerant for industrial systems. This created a huge industry in America and Europe. Boyle's machines continued to be sold by his or successor companies after his death until about 1905. The **ESAT 2024** has named the session on ***New Refrigerants*** after him.

James Dewar (1842-1923)

James Dewar was born in Kincardine, Fife, in 1842. He studied Chemistry at the University of Edinburgh under Lyon Playfair, becoming his personal assistant. His investigations regarded the physiological action of light, the spectroscopic analysis of gases separated from atmospheric air at low temperatures, the electrical behaviour of substances at very low temperatures. His name is most widely associated to the liquefaction of the permanent gases at temperatures close to absolute zero. In 1874 he discussed the "*Latent Heat of Liquid Gases*" before the British Association. He built a machine from which the liquefied gas could be used as a cooling agent, and obtained solid oxygen.
Around 1892, he had the idea of using vacuum-jacketed vessels for the storage of liquid gases – the *Dewar flask* – the invention for which he became famous, although he did not patent it, and lost a court case against Thermos who exploited the design commercially.
In 1898, using a high-pressure machine based on the Joule–Thomson effect, he was able to collect liquid hydrogen for the first time, solid hydrogen following in 1899. He tried to liquefy the last remaining gas, helium, but owing to a number of factors, including a short

supply of helium, Dewar was preceded by Onnes as the first person to produce liquid helium, who would later be awarded the Nobel Prize in Physics – Dewar was nominated several times, but never succeeded in winning. In 1905, he began to investigate the gas-absorbing powers of charcoal when cooled to low temperatures and applied his research to the creation of high vacuum, which was used for further experiments in atomic physics. Dewar continued his research work into the properties of elements at low temperatures, specifically low-temperature calorimetry, until the outbreak of World War I. The Royal Institution laboratories lost a number of staff to the war, and his research during and after the war mainly involved investigating surface tension in soap bubbles, reason for which the **ESAT 2024** has dedicated the ***Surfactants*** session to him.

Kenneth Denbigh (1911-2004)

Kenneth George Denbigh was a chemical engineer and scientific philosopher. He wrote much on the issue of time in relation to thermodynamics.

He was born in Luton and attended the University of Leeds graduating with a BSc in 1932. He then undertook his doctorate under Robert Whytlaw-Gray gaining a PhD in 1934. He worked for Imperial Chemical Industries (ICI) until 1938 when obtained a post of Lecturer in Chemistry at the University of Southampton. In the Second World War he was taken back into industry, as head of the laboratories for the Royal Ordnance Factory at Bridgwater. This led him into his first hands-on experience with practical issues concerning thermodynamics. In 1948 he received a post lecturing at the Chemical Engineering Department at the University of Cambridge and this provided a stepping-stone to be Professor of Chemical Technology at the University of Edinburgh in 1955. This in turn took him to Imperial College, London in 1960. In 1966 his final move was to be principal of Queen Elizabeth College in London. The University of Edinburgh named the Kenneth Denbigh Building at King's Buildings in his honour. The School of Engineering of The University of Edinburgh awards the Kenneth Denbigh Medal in support of his scientific legacy. The Medal has been first established in 2023. Among his publications *The Thermodynamics of the Steady State* (1951), *Thermodynamics and the Sense of Time* (1953), *The Principles of Chemical Equilibrium* (1955), *Entropy in Relation to Incomplete Knowledge* (1985).

For his contributions to Chemical Engineering the **ESAT 2024** honors his memory with the Session on ***Adsorption***.

Venue

Located at the foot of Edinburgh's iconic extinct volcano, Arthur's Seat, the **John McIntyre Conference Centre** (JMCC) offers flexible state-of-the-art facilities.

Address: Pollock Halls, **18 Holyrood Park Rd**, Edinburgh EH16 5AY.

Conference contact: esat2024@ed.ac.uk

Registration: ESATregistration@ed.ac.uk

Pollock Halls E-mail: estates.helpdesk@ed.ac.uk

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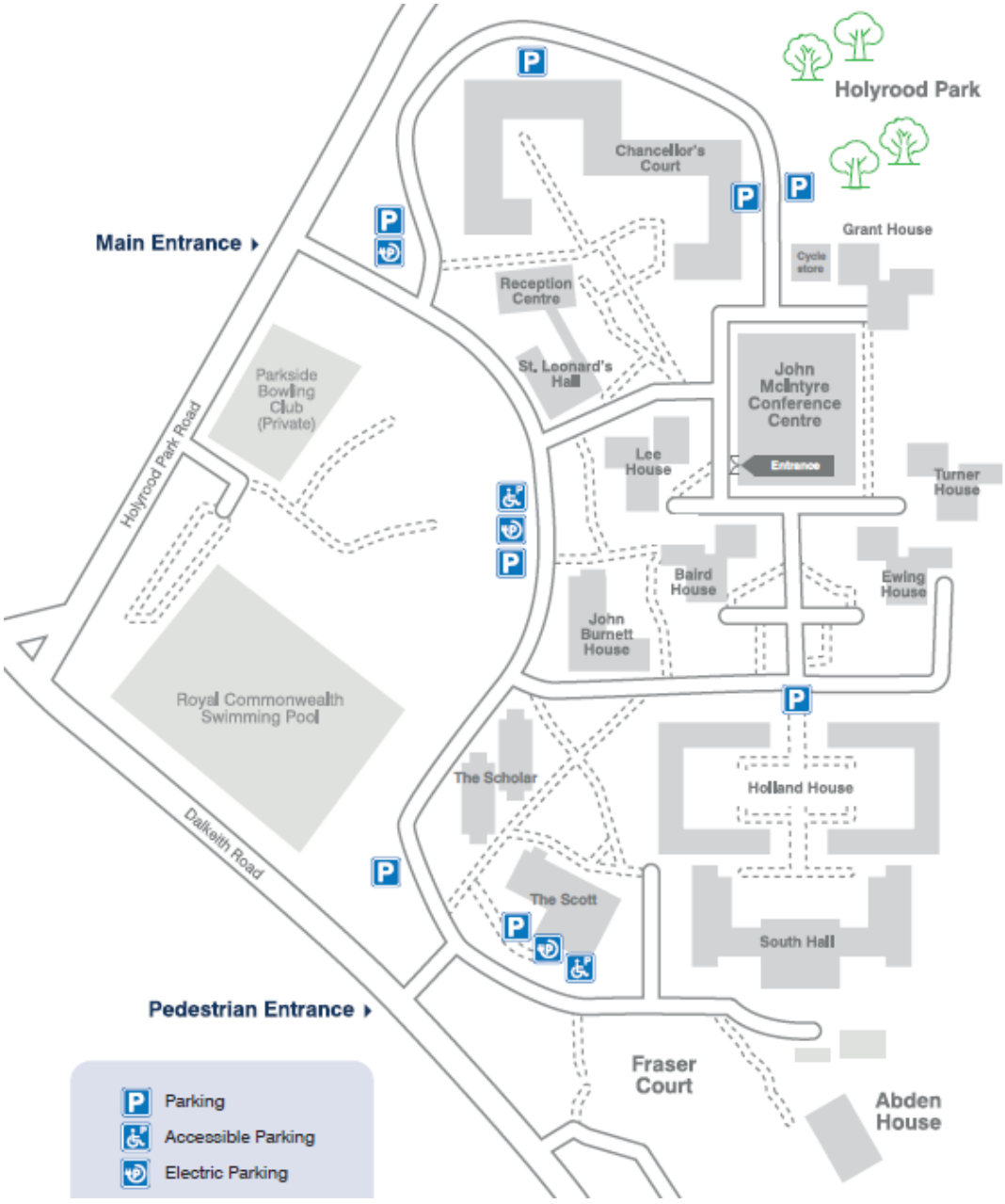
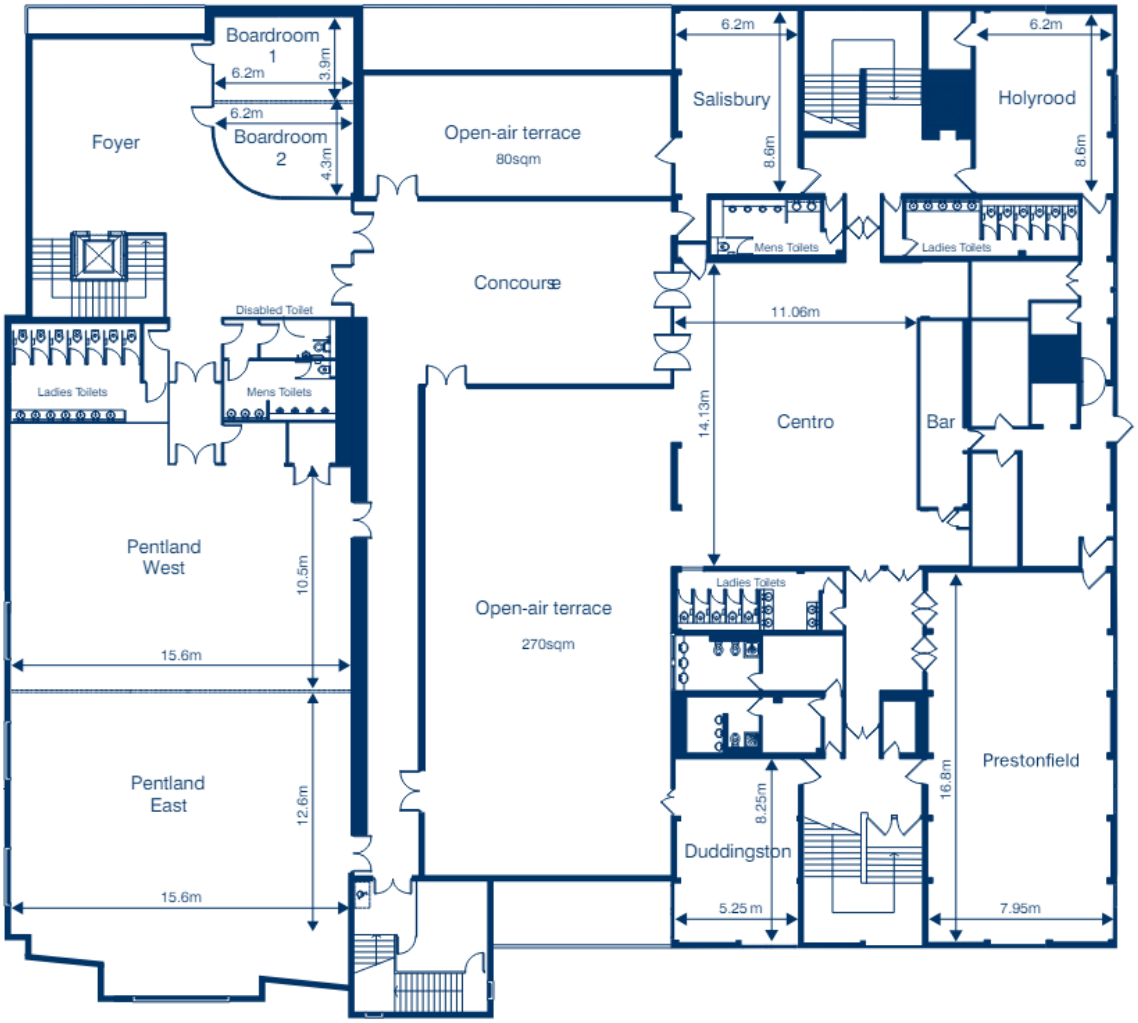


Hotels:

- Scholar Hotel https://www.uoecollection.com/hotels/the-scholar/
- Scott Hotel https://www.uoecollection.com/hotels/the-scott/
- Chancellors Court https://www.uoecollection.com/summer-stays-at-the-university-of-edinburgh/chancellors-court/

  Catering options (meals during the Conference will be provided)
- Scholar Restaurant: Offers an informal evening à la carte service. https://www.uoecollection.com/hotels/the-scholar/the-brasserie-lounge-bar/
- JMCC Restaurant**:** Buffet. Breakfast: 07:30 - 10:00. Dinner: 18:00 – 20:00
- Arthur's Food & Drink: barista coffee, cookies, classic pub food and Crafty pizza alongside craft tap beers and a range of spirits, wines and seltzers. Monday – Sunday: 12:00-23:00. Serving food: 12:00-21:30

JMCC Floorplan



Programme

Sunday Afternoon

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
18:15	19:15	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**

Monday Morning

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. Fèlix **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 Afternoon

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 Morning

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 theory and molecular simulation* 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* Prof. Peter **CUMMINGS**, Heriot-Watt Univ, UK	*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	*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	*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 esterification 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 BiMSA ePPC-SAFT for aqueous and mixed-solvent alkali halide solution* Abtin **RAEISPOUR SHIRAZI**, IFPEN, France
13:00	**14:00**	**Lunch**		

Tuesday Afternoon

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.Łukasz **BARAN**, Univ. Lublin, Poland	*Applying open COSMO-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	19:20	Break		
19:20	23:00	**Social Dinner, Playfair Library** **Knapp Poster Awards, sponsored by CCP5++**		

Wednesday Morning

Plenary Talks - Pentland Theatre			
Chairs: Ana Soto, Jean-Noel Jaubert			
08:30	09:15	*Measurement of Vapour Liquid Equilibrium Thermodynamic Properties Until the Critical Point and modelling* - Prof. Cristophe **COQUELET**, IMT Mines Albi, France	
09:15	10:00	*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 - 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-g 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**	

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