# ICCT<sub>25</sub>

27<sup>th</sup> IUPAC International Conference on Chemical Thermodynamics

**July 20 to 24<sup>th</sup>, 2025** Faculty of Sciences University of Porto

# **PROGRAMME**



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## PARTNERS AND SPONSORS









































## **WELCOME**

Welcome to the ICCT2025 | 27<sup>th</sup> IUPAC International Conference on Chemical Thermodynamics, taking place in Porto, Portugal, from July 20 to 24th, 2025.

ICCT2025 is organized by the Faculty of Science of the University of Porto in partnership with the Portuguese Society of Chemistry (SPQ).

Contact email: icct2025@chemistry.pt

Website: https://icct2025.events.chemistry.pt/

## **ICCT Conference series**

The IUPAC International Conferences on Chemical Thermodynamics (ICCT) are a well-established international conference series that focuses on the topics of chemical thermodynamics, fundamentals, modulation, and applications.

ICCT comprehensively covers various topics, including the physicochemical and biological properties of organic and inorganic compounds and their potential applications. In recent years, the remarkable potential applications of Chemical Thermodynamics have captured the interest of researchers from various multidisciplinary fields such as chemistry, physics, biology, and materials engineering. As a result, Chemical Thermodynamics is a line topic for advancing science and technology in a diverse range of applications. The extensive research and utilization of Chemical Thermodynamics in various domains have significantly contributed to advancing knowledge.

ICCT2025 presents an unparalleled opportunity for researchers worldwide who specialize in Chemical Thermodynamics to showcase their latest achievements and exchange valuable experiences. By bringing together academic scientists from diverse regions of the world, this conference aims to provide a forum for discussing a wide range of related topics and their properties and applications. The overarching goal is to foster scientific discussions and collaborations in a socially dynamic and intellectually stimulating atmosphere that will inspire new applications in the field of sustainable development.

Thank you for joining us in Porto!





#### TOPICS

- So1 | Energy and Sustainability
- So2 | Bio and Pharmaceutical Materials
- So3 | Phase Equilibria and Fluid Properties So8 | Surfaces, Interfaces, and Confinement
- So4 | Organic Materials and Polymers
- So5 | Inorganic Materials and Metals
- So6 | Ionic Fluids and Eutectic Solvents
- So7 | Soft Matter, Colloids, and Complex Fluids
- Sog | Modelling and Simulation S10 | Instrumentation and Methods

#### **CONFIRMED SPEAKERS**

#### Rossini Lecture



#### IACT Junior Award



#### Plenary Lectures













#### **Keynote Lectures**























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# **PROGRAMME**

Sunday, 20 <sup>th</sup> July	
14:30 - 16:00	Registration
16:00 - 16:20	Opening Ceremony - Ferreira da Silva Auditorium/FC6
16:20 - 16:50	Keynote 1 - Ferreira da Silva Auditorium/FC6
16:50 - 17:50	Plenary 1 - Ferreira da Silva Auditorium/FC6
18:00	Welcome Reception
Monday, 21st July	
08:50 - 09:20	Keynote 2 - Ferreira da Silva Auditorium/FC6
09:20 - 10:20	Plenary 2 - Ferreira da Silva Auditorium/FC6
10:20 - 10:45	Coffee Break
10:45 - 12:35	<b>Oral Communications</b> Parallel Sessions - Rooms 1,2,3 - FC2/FC3
12:35 - 14:00	Lunch
14:00 - 14:30	Keynote 3 - Ferreira da Silva Auditorium/FC6
14:30 - 15:30	Plenary 3 - Ferreira da Silva Auditorium/FC6
15:30 - 15:45	Coffee Break
15:45 - 17:50	<b>Oral Communications</b> Parallel Sessions - Rooms 1,2,3 - FC2/FC3
Tuesday, 22 <sup>nd</sup> Jul	у
08:50 - 09:20	Keynote 4 - Ferreira da Silva Auditorium/FC6
09:20 - 10:20	Plenary 4 - Ferreira da Silva Auditorium/FC6
10:20 - 10:45	Coffee Break
10:45 - 12:35	Oral Communications Parallel Sessions - Rooms 1,2,3 - FC2/FC3
12:35 - 14:00	Lunch
14:00 - 14:30	Sponsor Lecture 1 - Ferreira da Silva Auditorium/FC6
14.00 - 14.30	Sporisor Lecture 1 - Ferreira da Sitva Auditorium/ FCo
14:30 - 15:30	Rossini Award/Lecture - Ferreira da Silva Auditorium/FC6

Wednesday, 23 <sup>rd</sup> July		
08:50 - 09:20	Keynote 5 - Ferreira da Silva Auditorium/FC6	
09:20 - 10:20	Plenary 5 - Ferreira da Silva Auditorium/FC6	
10:20 - 10:45	Coffee Break	
10:45 - 12:35	Oral Communications Parallel Sessions - Rooms 1,2,3 - FC2/FC3	
12:35 - 14:00	Lunch	
14:00 - 16:10	Oral Communications Parallel Sessions - Rooms 1,2,3 - FC2/FC3	
16:00	Free Time & Social Events	
19:15	Conference Dinner	
Thursday, 24 <sup>th</sup> Ju	ıly	
08:50 - 09:20	Keynote 6 - Ferreira da Silva Auditorium/FC6	
09:20 - 10:20	Plenary 6 - Ferreira da Silva Auditorium/FC6	
10:20 - 10:45	Coffee Break	
10:45 - 11:15	Sponsor Lecture 2 - Ferreira da Silva Auditorium/FC6	
11:15 - 11:45	Keynote 7 - Ferreira da Silva Auditorium/FC6	
11:45 - 12:15	IACT Junior Award/Lecture - Ferreira da Silva Auditorium/FC6	
12:15	Closing Ceremony & Farewell Party	

## **Day 1** - Sunday, 20<sup>th</sup> July

14:30 - 16:00	Registration
16:00 - 16:20	Opening Ceremony (Ferreira da Silva (FS) Auditorium/FC6)
	Pedro Fernandes (DQB/FCUP); Pedro Rodrigues (UP); Luís Santos (Chair ICCT2025); João Coutinho (Co-Chair ICCT2025); Kazuya Saito (IACT)
16:20 - 17:50	Lectures Session (FS Auditorium)
	Chairs: João Coutinho; Magdalena Bendová
16:20 - 16:50	Keynote 1 - Kenneth Kroenlein
	Maximizing the value of your data
16:50 - 17:50	Plenary 1 - Lourdes Vega
	Redefining energy: Thermodynamics at the heart of the hydrogen and carbon capture and utilization revolution
	Lecture sponsored by NETZSCH   Paralab
18:00	Welcome Reception

## Day 2 - Monday, 21st July

09.20 - 10.20	Ion trios: Cause of ion specific interactions in aqueous solutions and path to a better pH definition
09:20 - 10:20	Plenary 2 - Eric May
	Turning a curse into an opportunity: How thermodynamics can help selecting the right organic crystal phase for a specific application
08:50 - 09:20	Keynote 2 - Manuel E. Minas da Piedade
	Chairs: Brian Woodfield; Margarida Bastos
08:50 - 10:20	Lectures Session (FS Auditorium)

	Oral Communications	<b>S</b> (Rooms 1,2,3 - FC2/FC3)	
10:45 - 12:35	Phase Equilibria & Fluid Properties (Room 1) Chairs: Jean Jaubert; Inês Vaz	lonic Fluids and Deep Eutectic Solvents (Room 2) Chairs: João Coutinho; Olga Ferreira	Bio and Pharmaceutical Materials (Room 3) Chairs: Margarida Bastos; Eduardo Filipe
10:45 - 11:05	HO3.1 - Margarida Costa Gomes Thermodynamics of water- driven separation of ionic liquid mixtures	HO6.1 - <u>Aaron Scurto</u> Phase equilibria and thermophysical properties of ionic liquids or deep eutectic solvents with hydrofluorocarbon gases	HO2.1 - <u>Marko Popović</u> Insulin - the detailed story: Biothermodynamic analysis of insulin
11:05 - 11:20	O3.2 - Alexandre Jorge Assessing the polarity of polymer/polymer aqueous two-phase systems via the Owens-Wendt method	O6.2 - <u>Dinis</u> <u>Abranches</u> Al-enabled discovery of deep eutectic solvents based lubricants	<b>O2.2</b> - Evgenyi Shalaev Chemical stability of amorphous pharmaceuticals: Water clusters and acid/base relationships
11:20 - 11:35	<b>O3.3</b> - <u>Jorge Pereira</u> Hydrodynamics of aqueous two-phase systems separation	O6.3 - Murilo Alcantara Screening of high- temperature solvents for methanol separation	<b>02.3</b> - <u>Ricardo Castro</u> Relative thermodynamic stability of famciclovir polymorphs
11:35 - 11:50	<b>O3.4</b> - Bruno Pinheiro Thermophysical properties and environmental relevance of three dichlorobenzaldehyde isomers	O6.4 - Luan Corso Enhancing the bioavailability of antimalarial drugs with natural excipients	O2.4 - Sahar Nasrallah Solubility enhancement of active pharmaceutical ingredients through hydrotropy: Experimental investigation and thermodynamic modeling
11:50 - 12:05	O3.5 - Moisés Neto Thermophysical properties of high CO <sub>2</sub> mixtures: Experiments and theory	O6.5 - <u>Letícia Souza</u> Stepwise conformational disorder in an ionic plastic crystal	O2.5 - <u>Dmitriy Moreira</u> Structural and thermodynamic insights into photoresponsive liposomes
12:05 - 12:20	O3.6 - Guillaume Depraetère Assessing solid-liquid equilibrium by isothermal titration calorimetry	O6.6 - <u>Lucas Zini</u> Phase equilibria of binary and ternary deep eutectic solvents	
12:20 - 12:35	O3.7 - Fufang Yang PC-SAFT and residual entropy scaling for thermodynamic and transport properties of hydrogen-containing mixtures	O6.7 - Rodrigo Silva Anion chain length effect on the thermodynamic properties of bis(fluoroalkylsulfonyl)imi de-based ionic liquids	

12:35 - 14:00	Lunch		
14:00 - 15:30	Lectures Session (FS Auditorium)		
	Chairs: Margarida Costa Go	mes; Simão Pinho	
14:00 - 14:30	Keynote 3 - Adriaan van den Bruinhorst		
	Assessing concealed therm constituents	odynamic properties of deep	eutectic solvents & their
14:30 - 15:30	<b>Plenary 3</b> - Mirjana M	linceva	
	Thermodynamic insights int mixture, and cocrystal form	o the solubility enhancement. ation	hydrotropy, eutectic
	Lecture sponsored by ANT	ON PAAR   MTBrandão	
15:30 - 15:45	Coffee Break		
	Oral Communication	<b>S</b> (Rooms 1,2,3 - FC2/FC3)	
15:45 - 17:35	Phase Equilibria and Fluid Properties (Room 1)	Surfaces, Interfaces, and Confinement (Room 2)	Modelling and Simulation (Room 3)
	Chairs: Simão Pinho; Bernd Rathke	Chairs: José Costa; Natália Cordeiro	Chairs: Costas Patrickios; Julien Joliat
15:45 - 16:05	HO3.8 - Jean Jaubert Al-driven fluid modeling: predicting input parameters of pure-component equations of state with ensemble learning	HO8.1 - Gennady Gor Derivative thermodynamic properties of confined fluids based on density functional theory	HO9.1 - Fuyu Jiao Detailed simulation of a liquid H₂ plant including ortho-para hydrogen conversion
16:05 - 16:20	O3.9 - Anastasiia Maslechko Evaluation of the surface properties for fluids through the isomorphism with lattice models	O8.2 - Miguel Jorge Quantifying the uncertainty of force field selection on adsorption predictions in metal-organic framework materials	Og.2 - Ashish Verma Investigating air- nanobubbles stability in water using a classical thermodynamic model for dispersed nanophase
16:20 - 16:35	<b>O3.10</b> - <u>Aline Zambom</u> Polyglycols as mass separating agents for fuel and terpene processing	<b>08.3</b> - <u>Shaoheng Wang</u> Water vapor sorption of salt nanoparticles in porous silica: experimental insights and thermodynamic modelling	<b>Og.3</b> - <u>José Fonseca</u> The challenge of reliable property data in process modelling
16:35 - 16:50	<b>O3.11</b> - <u>Vito Cimmelli</u> Nonlocal internal variable and superfluid state in liquid helium	<b>O8.4</b> - <u>Soraia Silva</u> Tailoring morphology and wetting behavior of films of ionic liquid mixtures with varied alkyl chain lengths	Og.4 - Carlos Bernardes Advancing molecular force fields of organic molecules for molecular dynamics simulations from ab initio calculations, single crystal data, and sublimation enthalpies

16:50 - 17:05	<b>03.12</b> - <u>Catinca</u>	<b>08.5</b> - <u>Eva Mühlegger</u>	<b>09.5</b> - <u>Dinis Abranches</u>
	Secuianu  High-pressures phase behavior of CO₂ with n- alkane isomers	Surface cleaning procedure using gas for contact angle measurement	Fast and furious: Accelerating OpenCOSMO- RS with graph convolutional networks
17:05 - 17:20	O3.13 - Marc Tshibangu	<b>08.6</b> - Artur Farinha	
	Investigation of perfluorohexane as a potential physical solvent for flue gas cleaning: Experimental vapor-liquid equilibrium data and modelling	Giant crystalline film growth of organic semiconductors on engineered ionic liquid surfaces in vacuum	
17:20 - 17:35	<b>03.14</b> - <u>Leslie</u> <u>Woodcock</u>	<b>08.7</b> - <u>Sonia Losada-</u> <u>Barreiro</u>	
	Universality of scaled pure fluid equations of state	Antioxidant efficiency in tween and cyclodextrin- stabilized emulsions	

## Day 3 - Tuesday, 22<sup>nd</sup> July

08:50 - 10:20	<b>Lectures Session</b> (F Chairs: José Costa; Olga		
08:50 - 09:20	<b>Keynote 4</b> - Vojtěch Path from experiment to s sublimation properties	n Štejfa standard: development of refer	ence data for
09:20 - 10:20	Plenary 4 - Taichi A Thermodynamic quantitie	be es in the phase diagram databo	ase
10:20 - 10:45	Coffee Break		
	Oral Communication	ons (Rooms 1,2,3 - FC2/FC3)	
10:45 - 12:35	Phase Equilibria & Fluid Properties (Room 1) Chairs: Jean Jaubert; Mónia Martins	Energy and Sustainability (Room 2) Chairs: Helena Passos; Nicolas Schaeffer	Modelling and Simulation (Room 3) Chairs: Luís Varela; José Fonseca
10:45 - 11:05	HO3.15 - Mark Thies Phase behavior of both woody and grassy lignins with aqueous renewable solvents: Ternary phase diagrams & thermodynamic modeling	HO1.1 - Sergey Verevkin Does the oxygen functionality really improve the thermodynamics of reversible hydrogen storage with LOHC?	HO9.6 - Julien Joliat Characterization of reactive working fluids by Monte Carlo simulations
11:05 - 11:20	O3.16 - Maria Sequeira Towards thermal performance: Di-n- alkyl adipates for efficient low- temperature thermal energy storage	O1.2 - Leslie Woodcock Thermodynamics of C-net zero: Investigations of 'free' energy from 2nd law bypass processes for climate sustainability and mobility	O9.7 - Miguel Jorge Polarization- consistent force fields to predict solvation and dielectric properties of mixtures
11:20 - 11:35	O3.17 - Caleb Narasigadu Measurement and modelling of liquid- liquid equilibrium for the water + propan-2- ol + cyclopentanol system	O1.3 - Yongchai Kwon Aqueous redox flow batteries using iron complex materials as redox couple	O9.8 - <u>Takashi</u> <u>Tokumasu</u> Molecular analyses of mass transport phenomena in polymer electrolyte fuel cell

11:35 - 11:50	O3.18 - Fernanda Pelaquim Volumetric properties and bubble point pressures of synthetic oil under gas injected	O1.4 - Arthur Nascimento A qualitative methodology for antisolvent selection for partial acylglycerols removal from biodiesel + glycerol systems using the COSMO-SAC model	Og.g - Micha Polak Unraveling the role of mixing entropy in equilibrated nano- confined reactions by statistical- thermodynamics modelling
11:50 - 12:05	O3.19 - Markus Sekulla Molecular dynamics meets gravimetry: Paving the way to accurate dew-point densities	O1.5 - <u>Jorge Pereira</u> Extraction of microalgal chlorophyll for eco- friendly wool dyeing: From Chemistry to the process thermodynamics	Og.10 - André Gomes Optimizing QM workflows for drug solubility prediction: The impact of conformer generation methods
12:05 - 12:20	<b>03.20</b> - <u>Rui Zhang</u> Accurate predictions	<b>01.6</b> - <u>Margarida</u> Pinhão	
	of phase equilibria & thermophysical properties: A CALPHAD-based approach for metals and slag	Aqueous solubility enhancement with Al designed hydrotropes	
12:20 - 12:35		<b>01.7</b> - <u>Brian</u> Woodfield	
		Incorporating positional entropy into statistical thermodynamics: Phase changes, colligative properties, & concentration batteries	
12:35 - 14:00	Lunch		
14:00 - 15:30	Lectures Session (FS	Auditorium)	
	Chairs: Luís Santos; Kazuy	a Saito	
14:00 - 14:30	Sponsor Lecture 1		
	Ligia de Souza (PARAL	.AB & NETZSCH)	
	Applications of kinetic and	ılysis using kinetics Neo Softwa	re
14:30 - 15:30	Rossini Award/Lect	ure	
	Christoph Schick		
	,	nd its contribution to chemical the TTLER TOLEDO   Soquímica	ermodynamics
15:30 - 17:30	Poster Session	·	
	Sponsored by MALVERN	PANALYTICAL   Paralab	

Lectures Session (FS Auditorium)

## Day 4 - Wednesday, 23rd July

08:50 - 10:20

	Chairs: Eduardo Marques; Ricardo Torre		
08:50 - 09:20	<b>Keynote 5</b> - Markus F Mastering fluid properties: T	Richter The hidden science behind eve	eryday technologies
09:20 - 10:20	<b>Plenary 5</b> - Quan Shi Chemical thermodynamics s	study of energy materials	
10:20 - 10:45	Coffee Break		
	Oral Communications	(Rooms 1,2,3 - FC2/FC3)	
10:45 - 12:35	Phase Equilibria & Fluid Properties (Room 1) Chairs: Simão Pinho; Jorge Pereira	Instrumentation and Methods (Room 2) Chairs: Luís Santos; Christoph Schick	Soft Matter, Colloids, and Complex Fluids (Room 3) Chairs: Eduardo Marques; Sonia Losada-Barreiro
10:45 - 11:05	HO3.21 - Bernd Rathke The crucial factors of liquid-liquid equilibria: The proper choice of reference systems	HO10.1 - Hal Suzuki Development of a differential scanning calorimeter equipped with a shearing system	HO7.1 - Eduardo Filipe Towards compartmentalized micelles: How the phobicity between hydrogenated and fluorinated chains determines organization
11:05 - 11:20	<b>03.22</b> - <u>Olivia Fandino</u>	O10.2 - Kazuya Saito	<b>07.2</b> - <u>Isabel Oliveira</u>
	Geological and thermodynamic influences on gas hydrate stability: Insights from the black sea and sea of marmara	Chemical thermodynamics as data-driven science/technology	Thermoresponsive poloxamers with varying hydrophobic/hydrophilic balance: Self-assembly and rheological behavior
11:20 - 11:35	<b>O3.23</b> - <u>Mark Barwood</u> Measurements of the solubility of H₂S in CH₄ at cryogenic temperatures using optical microscopy	O10.3 - Martin Trusler Acoustic resonator for sound speed measurements in light gases at high pressures	O7.3 - Mariko Noguchi Identification of various crystalline phases of thermotropic liquid crystal OHMBBA by DSC-XRD and DSC-Raman spectroscopy
11:35 - 11:50	O3.24 - Wanying Wu Measurements and modelling of solubility of solid methanol in liquid methane	O10.4 - Inès Vaz Advancing two-phase isothermal calorimetry: ITC for metal extraction with eutectic solvents	O7.4 - Teresa Iglesias Approximation for determining effective nanolayer thickness in nanofluids of spherical NPs through permittivity

#### 11:50 - 12:05

#### O3.25 - Xiona Xiao

Cryogenic speed of sound of gaseous mixtures of mixed refriaerants employed for hydrogen liauefaction

#### O10.5 - Alexandre Alves

AdsorptionCAL - design and construction of a gas-adsorption microcalorimetry svstem

#### 07.5 - Yasuhiro Nakazawa

Electron correlation mechanism to make glassy state of phonons in organic charge transfer complexes

#### 12:05 - 12:20 O3.26 - Fabian Luther

Solubilities of refrigerants in surrogates for refrigeration oils using Raman spectroscopy

#### 07.6 - Rui Machado

Inversely coupled thermogelation: designing a polymer/surfactant hydroael for smart topical delivery

#### 12:20 - 12:35

#### O3.27 - Guinevere Sellner

Revisiting the static dielectric constant of hydrogen: Improved

modeling at cryogenic conditions

#### Lunch 12:35 - 14:00

#### Oral Communications (Rooms 1.2.3 - FC2/FC3)

#### 14:00 - 16:10

#### Ionic Fluids and Deep **Eutectic Solvents** (Room 1)

Chairs: Dinis Abranches: Aaron Scurto

#### Organic Materials and Polymers & Inorganic Materials and Metals

Chairs: Carlos Lima: Sergey Verevkin

(Room 2)

#### Modelling and Simulation (Room 3)

Chairs: Miquel Jorge: Carlos Bernardes

#### 14:00 - 14:20

#### HO6.8 - Marzena Dzida

Thermodynamic speed of sound in ionic liquids

#### HO4.1 - Ivo Rietveld

A benchmark of physical properties of the organic solid state for crystal structure prediction by COST Action BEST-CSP

#### HO9.11 - Antonio Sellitto

Phonon-boundary scatterina and boundary conditions: Application to the heat transfer in thin nanowires

#### 14:20 - 14:35

#### O6.9 - Krzysztof Cwynar

Quest to find the holy grail of ionanofluids. Brief story on isobaric heat capacity of ionanofluids

#### O4.2 - Aaron Scurto

Phase equilibria and modeling involved in the CO₂-assisted recovery of terephthalic acid from PET upcycling

#### **09.12** - Rachid Hadjadj

Molecular design, thermochemical and kinetics characterization of reactive working fluids

#### 14:35 - 14:50

#### **06.10** - Bastián González-Barramuño

Absorption of hydrofluorocarbons in fluorine-based eutectic solvents: Insights from molecular modeling

#### O4.3 - Riko Siewert

Determination of the intramolecular hydrogen bonding strength in diols

#### **09.13** - Costas **Patrickios**

Strain-induced morphological transitions in amphiphilic polymer conetwork bulk melts: A computational thermodynamic study

#### 14:50 - 15:05 **06.11** - Gabriel O4.4 - Yoshitomo 09.14 - Martín Otero-Teixeira Furushima Lema Polyol-based deep Influence of pre-thermal Thermochemistry analysis eutectic solvents: A treatment on the of solid-electrolyte comparative study of isothermal interfaces using neural betaine and choline crystallization of network forcefields chloride as hydrogen bond isotactic polypropylene acceptors O6.12 - Alexandre O4.5 - Monica Corea 09.15 - Luís Varela 15:05 - 15:20 Jorae Isothermal titration Water dissociation and calorimetry applied to proton transport in ionic Eutectic solvents as rare earth recovery sustainable dve baths for liquids process with cotton dveina , functionalized polymeric particles O6.13 - Joana Dias HO5.1 - Brian 15:20 - 15:35 Woodfield Pressurized hot water and deep eutectic solvents as Low-temperature heat additives for extracting capacities and absolute cannabinoids from entropies of a variety of Cannabis sativa I inorganic salts, oxides, and metals 06.14 - Natália 05.2 - Flavia Braga 15:35 - 15:50 Cordeiro Expanding aluminum salt-based recovery of Predictina heat capacity in PGMs from mixed spent deep eutectic solvents automotive catalytic using machine learning for converters sustainable design 15:50 - 16:05 O5.3 - Nicolas Schaeffer Thermodynamics of solvent extraction in Type V DES, an evolution or a revolution

from conventional systems?

## Day 5 - Thursday, 24th July

08:50 -10:20	Lectures Session (FS Auditorium)
	Chairs: Luís Varela; Natália Cordeiro
08:50 - 09:20	Keynote 6 - Hadrián Montes-Campos
	Simulation of thermodynamic properties in complex liquids. The role and opportunities of machine learning techniques
09:20 - 10:20	Plenary 6 - Frederico Tavares
	Equilibrium and non-equilibrium thermodynamics using 1-D and 3-D density functional theory
10:20 - 10:45	Coffee Break
10:45 - 12:15	Lectures Session (FS Auditorium)
	Chairs: Martin Trusler; Marzena Dzida
10:45 - 11:15	Sponsor Lecture 2
	Laurent Zoppi (SOQUÍMICA & METTLER-TOLEDO)
	An advanced heat flux DSC operated in the power compensation mode
11:15 - 11:45	Keynote 7 - Cara Schwarz
	The value and limitations of phase boundary data in high-pressure phase behavior studies
11:45 - 12:15	IACT Junior Award/Lecture
	Liam Tenardi - Magnetic refrigeration for hydrogen liquefaction
12:15	Closing Ceremony & Farewell Party

## LIST OF COMMUNICATIONS

#### ICCT Awards/Lectures

RL	Christoph Schick	Fast scanning calorimetry and its contribution to chemical thermodynamics
IACT_L	Liam Tenardi	Magnetic refrigeration for hydrogen liquefaction

#### **Plenary Lectures**

PL1	Lourdes Vega	Redefining energy: Thermodynamics at the heart of the hydrogen and carbon capture and utilization revolution
PL2	Eric May	lon trios: Cause of ion specific interactions in aqueous solutions and path to a better pH definition
PL3	Mirjana Minceva	Thermodynamic insights into the solubility enhancement: hydrotropy, eutectic mixture, and cocrystal formation
PL4	Taichi Abe	Thermodynamic quantities in the phase diagram database
PL5	Quan Shi	Chemical thermodynamics study of energy materials
PL6	Frederico Tavares	Equilibrium and non-equilibrium thermodynamics using 1-D and 3-D density functional theory

#### **Keynote Lectures**

KL1	Kenneth Kroenlein	Maximizing the value of your data
KL2	Manuel E. Minas da Piedade	Turning a curse into an opportunity: How thermodynamics can help selecting the right organic crystal phase for a specific application
KL3	Adriaan van den Bruinhorst	Assessing concealed thermodynamic properties of deep eutectic solvents and their constituents
KL4	Vojtěch Štejfa	Path from experiment to standard: development of reference data for sublimation properties
KL5	Markus Richter	Mastering fluid properties: The hidden science behind everyday technologies
KL6	Hadrián Montes- Campos	Simulation of thermodynamic properties in complex liquids. The role and opportunities of machine learning techniques
KL7	Cara E. Schwarz	The value and limitations of phase boundary data in high- pressure phase behavior studies
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#### **Sponsor Lectures**

SP_L1	Ligia de Souza	PARALAB & NETZSCH - Applications of kinetic analysis using kinetics Neo Software
SP_L2	Laurent Zoppi	SOQUÍMICA & METTLER-TOLEDO - An advanced heat flux DSC operated in the power compensation mode

#### **Oral Communications**

#### ORAL\_O1 - Energy and Sustainability

J. U 11_U1	Enorgy and Sastamasiaty	
HO1.1	Sergey Verevkin	Does the oxygen functionality really improve the thermodynamics of reversible hydrogen storage with LOHC?
01.2	Leslie Woodcock	Thermodynamics of C-net zero: Investigations of 'free' energy from 2nd law bypass processes for climate sustainability and mobility
O1.3	Yongchai Kwon	Aqueous redox flow batteries using iron complex materials as redox couple
01.4	Arthur Nascimento	A qualitative methodology for antisolvent selection for partia acylglycerols removal from biodiesel • glycerol systems using the COSMO-SAC model
O1.5	Jorge F. B. Pereira	Extraction of microalgal chlorophyll for eco-friendly wool dyeing: From Chemistry to the process thermodynamics
O1.6	Margarida Pinhão	Aqueous solubility enhancement with AI designed hydrotropes
01.7	Brian Woodfield	Incorporating positional entropy into statistical thermodynamics: Phase changes, colligative properties, and concentration batteries

#### ORAL\_O2 - Bio and Pharmaceutical Materials

HO2.1	Marko E. Popović	Insulin - the detailed story: Biothermodynamic analysis of insulin
O2.2	Evgenyi Shalaev	Chemical stability of amorphous pharmaceuticals: Water clusters and acid/base relationships
02.3	Ricardo Castro	Relative thermodynamic stability of famciclovir polymorphs
02.4	Sahar Nasrallah	Solubility enhancement of active pharmaceutical ingredients through hydrotropy: Experimental investigation and thermodynamic modeling
02.5	Dmitriy Moreira	Structural and thermodynamic insights into photoresponsive liposomes

#### ORAL\_O3 - Phase Equilibria and Fluid Properties

HO3.1	Margarida Costa Gomes	Thermodynamics of water-driven separation of ionic liquid mixtures
03.2	Alexandre Jorge	Assessing the polarity of polymer/polymer aqueous two- phase systems via the Owens-Wendt method
03.3	Jorge Pereira	Hydrodynamics of aqueous two-phase systems separation
03.4	Bruno Pinheiro	Thermophysical properties and environmental relevance of three dichlorobenzaldehyde isomers
03.5	Moisés Neto	Thermophysical properties of high CO <sub>2</sub> mixtures: Experiments and theory

О3.6	Guillaume Depraetère	Assessing solid-liquid equilibrium by isothermal titration calorimetry
O3.7	Fufang Yang	PC-SAFT and residual entropy scaling for thermodynamic and transport properties of hydrogen-containing mixtures
HO3.8	Jean-Noël Jaubert	Al-driven fluid modeling: predicting input parameters of pure-component equations of state with ensemble learning
O3.9	Anastasiia Maslechko	Evaluation of the surface properties for fluids through the isomorphism with lattice models
O3.10	Aline Zambom	Polyglycols as mass separating agents for fuel and terpene processing
O3.11	Vito Cimmelli	Nonlocal internal variable and superfluid state in liquid helium
O3.12	Catinca Secuianu	High-pressures phase behavior of CO₂ with n-alkane isomers
03.13	Marc Tshibangu	Investigation of perfluorohexane as a potential physical solvent for flue gas cleaning: Experimental vapor-liquid equilibrium data and modelling
HO3.14	Mark C. Thies	Phase behavior of both woody and grassy lignins with aqueous renewable solvents: Ternary phase diagrams and thermodynamic modeling
O3.15	Maria Sequeira	Towards thermal performance: Di-n-alkyl adipates for efficient low-temperature thermal energy storage
O3.16	Caleb Narasigadu	Measurement and modelling of liquid-liquid equilibrium for the water + propan-2-ol + cyclopentanol ternary system
O3.17	Fernanda Pelaquim	Volumetric properties and bubble point pressures of synthetic oil under gas injected
O3.18	Markus Sekulla	Molecular dynamics meets gravimetry: Paving the way to accurate dew-point densities
O3.19	Rui Zhang	Accurate predictions of phase equilibria and thermophysical properties: A CALPHAD-based approach for metals and slag
O3.20	Leslie Woodcock	Universality of scaled pure fluid equations of state
HO3.21	Bernd Rathke	The crucial factors of liquid-liquid equilibria: The proper choice of reference systems
03.22	Olivia Fandino	Geological and thermodynamic influences on gas hydrate stability: Insights from the black sea and sea of marmara
03.23	Mark Barwood	Measurements of the solubility of H2S in CH4 at cryogenic temperatures using optical microscopy
03.24	Wanying Wu	Measurements and modelling of the solubility of solid methanol in liquid methane
O3.25	Xiong Xiao	Cryogenic speed of sound of gaseous mixtures of mixed refrigerants employed for hydrogen liquefaction
O3.26	Fabian Luther	Solubilities of refrigerants in surrogates for refrigeration oils using Raman spectroscopy
O3.27	Guinevere Sellner	Revisiting the static dielectric constant of hydrogen: Improved modeling at cryogenic conditions

#### ORAL\_O4 - Organic Materials and Polymers

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HO4.1	Ivo Rietveld	A benchmark of physical properties of the organic solid state for crystal structure prediction by COST Action BEST-CSP
04.2	Aaron Scurto	Phase equilibria and modeling involved in the CO <sub>2</sub> -assisted recovery of terephthalic acid from PET upcycling
04.3	Riko Siewert	Determination of the intramolecular hydrogen bonding strength in diols
04.4	Yoshitomo Furushima	Influence of pre-thermal treatment on the isothermal crystallization of isotactic polypropylene
04.5	Mónica Corea	Isothermal titration calorimetry applied to rare earth recovery process with functionalized polymeric particles

#### ORAL\_O5 - Inorganic Materials and Metals

HO5.1	Brian Woodfield	Low-temperature heat capacities and absolute entropies of a variety of inorganic salts, oxides, and metals
05.2	Flavia N. Braga	Expanding aluminum salt-based recovery of PGMs from mixed spent automotive catalytic converters
O <sub>5.3</sub>	Nicolas Schaeffer	Thermodynamics of solvent extraction in Type V DES, an evolution or a revolution from conventional systems?

#### ORAL\_O6 - Ionic Fluids and Deep Eutectic Solvents

HO6.1	Aaron Scurto	Phase equilibria and thermophysical properties of ionic liquids or deep eutectic solvents with hydrofluorocarbon gases
O6.2	Dinis Abranches	Al-enabled discovery of deep eutectic solvents based lubricants
O6.3	Murilo Alcantara	Screening of high-temperature solvents for methanol separation
O6.4	Luan Corso	Enhancing the bioavailability of antimalarial drugs with natural excipients
O6.5	Letícia Souza	Stepwise conformational disorder in an ionic plastic crystal
O6.6	Lucas Zini	Phase equilibria of binary and ternary deep eutectic solvents
O6.7	Rodrigo Silva	Anion chain length effect on the thermodynamic properties of bis(fluoroalkylsulfonyl)imide-based ionic liquids
HO6.8	Marzena Dzida	Thermodynamic speed of sound in ionic liquids
O6.9	Krzysztof Cwynar	Quest to find the holy grail of ionanofluids. Brief story on isobaric heat capacity of ionanofluids
O6.10	Bastián González- Barramuño	Absorption of hydrofluorocarbons in fluorine-based eutectic solvents: Insights from molecular modeling
O6.11	Gabriel Teixeira	Polyol-based deep eutectic solvents: A comparative study of betaine and choline chloride as hydrogen bond acceptors
06.12	Alexandre Jorge	Eutectic solvents as sustainable dye baths for cotton dyeing

06.13	Joana Dias	Pressurized hot water and deep eutectic solvents as additives for extracting cannabinoids from Cannabis sativa L.
06.14	Natália Cordeiro	Predicting heat capacity in deep eutectic solvents using machine learning for sustainable design
ORAL_O7	- Soft Matter, Colloids, and	d Complex Fluids
H07.1	Eduardo Filipe	Towards compartmentalized micelles: How the phobicity between hydrogenated and fluorinated chains determines organization
07.2	Rui Machado	Inversely coupled thermogelation: designing a polymer/surfactant hydrogel for smart topical delivery
07.3	Mariko Noguchi	Identification of various crystalline phases of the thermotropic liquid crystal OHMBBA by DSC-XRD and DSC-Raman spectroscopy
07.4	Teresa Iglesias	Approximation for determining the effective nanolayer thickness in nanofluids of spherical nanoparticles through permittivity
07.5	Yasuhiro Nakazawa	Electron correlation mechanism to make glassy state of phonons in organic charge transfer complexes
ORAL_O8	- Surfaces, Interfaces, and	l Confinement
HO8.1	Gennady Gor	Derivative thermodynamic properties of confined fluids based on density functional theory
08.2	Miguel Jorge	Quantifying the uncertainty of force field selection on adsorption predictions in metal-organic framework materials
08.3	Shaoheng Wang	Water vapor sorption of salt nanoparticles in porous silica: experimental insights and thermodynamic modelling
08.4	Soraia Silva	Tailoring morphology and wetting behavior of films of ionic liquid mixtures with varied alkyl chain lengths
O8.5	Eva Mühlegger	Surface cleaning procedure using gas for contact angle measurement
O8.6	Artur Farinha	Giant crystalline film growth of organic semiconductors on engineered ionic liquid surfaces in vacuum
O8.7	Sonia Losada- Barreiro	Antioxidant efficiency in tween and cyclodextrin-stabilized emulsions
ORAL_O9	- Modelling and Simulatio	n
HO9.1	Fuyu Jiao	Detailed simulation of a liquid $\ensuremath{H}_{\!\scriptscriptstyle 2}$ plant including ortho-para hydrogen
Og.2	Ashish Verma	Investigating air-nanobubbles stability in water using a classical thermodynamic model for dispersed nanophase
O9.3	José Fonseca	The challenge of reliable property data in process modelling
O9.4	Carlos Bernardes	Advancing molecular force fields of organic molecules for molecular dynamics simulations from ab initio calculations, single crystal data, and sublimation enthalpies

O9.5	Dinis Abranches	Fast and furious: Accelerating OpenCOSMO-RS with graph convolutional networks
HO9.6	Julien Joliat	Characterization of reactive working fluids by Monte Carlo simulations
09.7	Miguel Jorge	Polarization-consistent force fields to predict solvation and dielectric properties of mixtures
09.8	Takashi Tokumasu	Molecular analyses of mass transport phenomena in polymer electrolyte fuel cell
09.9	Micha Polak	Unraveling the role of mixing entropy in equilibrated nano- confined reactions by statistical-thermodynamics modelling
09.10	André Gomes	Optimizing QM workflows for drug solubility prediction: The impact of conformer generation methods
HO9.11	Antonio Sellitto	Phonon-boundary scattering and boundary conditions: Application to the heat transfer in thin nanowires
09.12	Rachid Hadjadj	Molecular design, thermochemical and kinetics characterization of reactive working fluids
O9.13	Costas Patrickios	Strain-induced morphological transitions in amphiphilic polymer conetwork bulk melts: A computational thermodynamic study
O9.14	Martín Otero-Lema	Thermochemistry analysis of solid-electrolyte interfaces using neural network forcefields
O9.15	Luis M. Varela	Water dissociation and proton transport in ionic liquids

#### ORAL\_O10 - Instrumentation and Methods

HO10.1	Hal Suzuki	Development of a differential scanning calorimeter equipped with a shearing system
O10.2	Kazuya Saito	Chemical thermodynamics as data-driven science/technology
O10.3	Martin Trusler	Acoustic resonator for sound speed measurements in light gases at high pressures
O10.4	Inês Vaz	Advancing two-phase isothermal calorimetry: ITC for metal extraction with eutectic solvents
O10.5	Alexandre Alves	AdsorptionCAL – design and construction of a gas- adsorption microcalorimetry system

#### **Poster Communications**

#### POSTER\_P1 - Energy and Sustainability

P1.1	Sungjun Lee	The specific heat measurement of R1132a
P1.2	Yong Park	Enhanced thermodynamic performance of LiFePO <sub>4</sub> cathode with carbon coating layer formed by sulfur-modification
P1.3	Jinsoo Kim	Low-loading iridium and nickel alloys supported on titanium nitride applied for electrochemical hydrogen evolution reaction
P1.4	Emilie Bordes	Hydrogen storage in mixed hydrates: Effect of perchloric acid on thermodynamics
P1.5	Guinevere Sellner	Re-evaluating the role of purification adsorbents in ortho- para hydrogen conversion for liquefaction systems
P1.6	Rita Carvalho	Bio-based materials for selective and sustainable platinum group metal recovery
P1.7	Lillian Ladu	Thermophysical properties of sustainable liquid fuels
P1.8	Gabriel Camilo	Optimizing solubility of redox species to boost energy density in redox flow batteries
P1.9	Rita Carvalho	Membrane approaches for efficient separation of platinum group metals from leachate streams
P1.10	Bruno Ramos	Thermodynamic analysis of photocatalytic ammonia synthesis via quantum chemical calculations with process-level considerations
P1.11	Ana Pereira	Energetic study of α- and γ-pyrones
P1.12	Nuria Boluda-Botella	Development of a corn cob biochar anode with LDH (Ni-Fe) for the degradation of nicosulfuron
P1.13	Nuria Boluda-Botella	Structured design of a hydrochar-supported LDH/MOF composite for improved photocatalytic applications
P1.14	María Dolores Saquete	Photocatalytic-assisted hydrogenation over CuFe oxide derived from layered double hydroxides for nitro group reduction
P1.15	Aleksey Pimerzin	A thermochemical approach to catalytic hydrodeoxygenation of eugenol as a model for lignin valorization

#### POSTER\_P2 - Bio and Pharmaceutical Materials

P2.1	Luísa Amaral	3-Hydroxy-4-pyridine chelators: Exploring membrane interactions for enhanced metal ion management
P2.2	Roxana Pasca	Thermodynamic study on the stability of some oral anticoagulant drugs
		Danie autorita autoria familia anciale delli ami Calubilita and
P2.3	Vanessa Vieira	Deep eutectic systems for rifampicin delivery: Solubility and stability toward enhanced tuberculosis treatment

#### POSTER\_P3 - Phase Equilibria and Fluid Properties

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P3.1	Vojtěch Štejfa	PROFHET project: Thermodynamic characterization of hydrofluoroethers
P3.2	Maysa Nesti	Sensitivity analysis of epoxidation reaction effects on partition coefficients based on the UNIFAC model
P3.3	Murilo Alcantara	Strategies to increase the solubility of organic redox active materials using thermodynamic principles
P3.4	Jean-Luc Daridon	Measurement of density and speed of sound in biodiesel- nitrogen mixtures as surrogates for biodiesel-air systems in injection conditions
P3.5	Kuveneshan Moodley	Vapor-liquid equilibrium, density, and speed of sound measurements for butan-1-ol or butan-2-ol + oct-1-ene between 313.2-353.2 K
P3.6	Behnaz Asadzadeh	Solubility of CO <sub>2</sub> in the mixed DBN/ethylene glycol, along with physical properties of unloaded and CO <sub>2</sub> -loaded DBN with ethylene glycol
P3.7	Christopher Piske	Refining inconsistent data with stochastic machine learning: The salt effect on the solubility of amino acids
P3.8	Emilie Bordes	Phase behavior of polyethylenes in solvents
P3.9	Thomas Hughes	Improving calculations of vapor-liquid equilibria for hydrogen mixtures using the Peng-Robinson equation of state with quantum-corrections
P3.10	Mikołaj Więckowski	Supramolecular structures in systems containing halide organic salts: solid – liquid phase equilibria in systems with α.ω-alkanediols
P3.11	Mónia Martins	Green eutectic formulations for antimalarial drug delivery
P3.12	Juan Arroyave	Solubility of nitrous oxide and carbon dioxide in an aqueous mixture of 2-(Dimethylamino)ethanol + N-Methyl-1,3-propanediamine
P3.13	Alejandro Moreau	Density measurements of hydrogen + propane and hydrogen + butane mixtures for decarbonizing the gas grid
P3.14	María Dolores Saquete	Effect of lithium salts on the phase equilibrium of the water + 1-propanol binary system at 40°C
P3.15	Zuzana Součková	Molecular dynamics approach to solubility of amino acids in aqueous salt solutions
P3.16	Isabella Cordova	The influence of carbon chain length on hydrotropic effect using carbamazepine as a model compound
P3.17	Magdalena Bendová	Thermophysical properties, dissociation and partitioning of chiral imidazolium-based chloride salts in water-octanol systems
P3.18	Shaoheng Wang	Moisture-induced phase transitions in reciprocal quaternary salt mixtures
P3.19	Nivaar Brijmohan	Solvent selection methods in aromatic extraction processes towards optimal and sustainable design choices
P3.20	Ana Cunha	Influence of pressure and temperature on the physical properties of crude oil emulsions

P3.21	Olga Ferreira	Solubility of olive oil phenolic compounds in green solvents
P3.22	Osvaldo Chiavone- Filho	Vapor-liquid equilibrium behavior for ethanol and linoleic acid system
P3.23	Nouria Chiali	Modeling excess molar enthalpies of dimethyl carbonate with eight hydrocarbons (benzene, isopropylbenzene, nheptane, cyclohexane, hex-1-ene, hex-1-yne, hex-2-yne or hex-3-yne)
P3.24	Amal Ayad	Thermodynamic properties of N. N-dimethylacetamide with 1-butanol, 1-pentanol, furfural or furfuryl alcohol at temperatures from (293.15 to 323.15) K
P3.25	Aouicha Belabbaci	Thermodynamic, ultrasonic, and transport properties of binary mixtures containing 1-hexene and alcohols at (293.15 - 303.15) K
POSTER_F	P4 - Organic Materials and	Polymers
P4.1	Ibuki Tanizawa	Effects of solvent addition and crosslinking on the melting behavior of poly(dimethylsiloxane)
P4.2	Luísa Amaral	Thermochemical characterization of sulfur-containing furan derivatives: Experimental and theoretical Study
P4.3	Raluca Baron	Design of magnetic responsive cryogels based on hydroxypropyl cellulose derivatives for multi-functional sensors
P4.4	Gabriela Biliuta	Fabrication and characterization of a novel polysaccharide- based composite nanofiber with improved physical properties
P4.5	Artur Farinha	Thermodynamic properties of phenanthroline derivatives for thin film applications in organic optoelectronic devices
P4.6	Ana Luísa Silva	Alkyl substituent effects on the energetic properties of some 2-amino-5-R-1,3,4-thiadiazoles
P4.7	Filipe Ribeiro	Phase behavior of phenylnaphthalenes and phenylanthracenes: Influence of the central acene core and substituent position
P4.8	Marcin Smiglak	Influence of cation structure with allyl group and different anions on the glass transition and heat deflection temperatures of fiber reinforced epoxy composites
POSTER_F	<sup>9</sup> 5 - Inorganic Materials ar	nd Metals
P5.1	Min-Su Kim	Formation thermodynamics of TiN interlayer and its effect on the reliability of active metal brazed Cu/AlN substrate for power module packaging
P5.2	Cornelia Bandas	Aero-TiO₂ materials for evaluation of near-ultraviolet photodetector
P5.3	Riku Seiki	Relationship between heat storage properties and crystallite size of lambda-type trititanium pentoxide
P5.4	Nelson Nunes	Zeolites made from fly-ash wastes as Fenton catalysts for the degradation of methylene blue dye from aqueous media

P5.5	Bruno Ramos	On the distribution of ruthenium in nanostructured $WO_3$ synthesized by the Pechini method
POSTER_	P6 - Ionic Fluids and Deep	Eutectic Solvents
P6.1	Cleiton Beraldo	Predicting CO₂ solubility in hydrophobic deep eutectic solvents using SAFT-VR Mie - Impact of repulsive exponent
P6.2	Gabriel Teixeira	Melting properties of thermally unstable quaternary ammonium salts using fast-scanning calorimetry
P6.3	Antoni Maciejewski	Physicochemical properties of selected isoquinoline-, piperidine- and pyridine-based ionic liquids
P6.4	Ricardo B. Torres	Experimental and computational study on interactions in the ternary aqueous systems containing saccharides and 1-ethyl-3-methylimidazolium dicyanamide
P6.5	Isabella Souza	Ionic liquid incorporation in polymeric membranes for indoor air quality
P6.6	Rodrigo Silva	Bis(alkylsulfonyl)imide-based ionic liquids: Study of their thermodynamic properties
P6.7	Beatriz Esteves	Membranes functionalized with non-volatile solvents for gas separation
P6.8	Bruna Ferreira	Biopolymeric membrane using deep eutectic solvent for gas separation
P6.9	Bárbara Jesus	Understanding salicylic acid solubility in eutectic solvents: From predictions to experimental results and molecular simulations
POSTER_	P7 - Soft Matter, Colloids, a	and Complex Fluids
P7.1	Kosei Yoshida	Phase transition of cationic surfactant CTAB-water binary system: Effects of long-chain alcohol, carboxylic acid, and carboxylate additives
P7.2	Evgenyi Shalaev	Soft dynamics of water and solute in solutions of polyhydroxy compounds: inelastic and quasielastic neutron scattering and terahertz spectroscopy study
P7.3	Hiroki Fujimori	Heat capacity measurements of 2,5-dibromothiophene and 2,5-dichlorothiophene
P7.4	Teresa Iglesias	Volumetric study of zirconia (45 nm) + water nanofluid: thickness, molar volume and density of the nanolayer
P7.5	Isabel Oliveira	Tailoring thermotropic ionic liquid crystals: Chain mismatch and structural isomerism in lysine-based surfactants
P7.6	Nelson Nunes	Enhancing nimesulide solubility with sodium benzoate: A solvatochromic study to elucidate hydrotropic mechanisms
P7.7	Rui Machado	Phase behavior and rheological properties of thermoresponsive hydrogels

P7.9	Eduardo Filipe	Aneotropy: Unusual interfacial behaviour of mixtures of hydrogenated and fluorinated substances
POSTER_	P8 - Surfaces, Interfaces, a	and Confinement
P8.1	Ricardo Torres	Critical aggregation concentration of crude oil asphaltene
P8.2	Ricardo Torres	Properties of interfacial films containing crude oil asphaltenes
P8.3	Jiaqi Yan	Thin films of organic semiconductor materials: Structural, morphological, and thermodynamic study of polyphenylanthracenes
P8.4	João Pereira	Influence of alkyl chain length on the morphology of pyridinium-based ionic liquid films deposited by vacuum thermal evaporation
P8.5	Catarina Viegas	Crystalline film growth of pentacene and perylene via ionic liquid-assisted VLS mechanism followed by IL removal
P8.6	Soraia Silva	Ionic liquid-mediated vapor growth of thienoacenes for molecular electronics
P8.7	Sonia Losada- Barreiro	Inclusion complex of gallates with cyclodextrins: thermodynamic study and antioxidant activity
POSTER_	P9 - Modelling and Simula	ation
P9.1	Adrian Racki	Graph neural network framework for robust ionic liquid property prediction
P9.2	Sebastian Wohlrab	Shifting thermodynamic equilibria with membrane technology: Enhancing CO <sub>2</sub> conversion in catalytic processes
P9.3	Cleiton Beraldo	Predicting imidazolium-based ionic liquid phase equilibria via SAFT-VR Mie parameter correlations with molecular volume
P9.4	Kazuya Saito	Entropic order upon self-assembly: Antiferroic three-state potts model on reo net
P9.5	Frederico Tavares	The non-isothermal compositional grading problem specifying the overall composition of the mixed migrating streams
Pg.6	Ana Ferreira	Paving the way to a sustainable future: COSMO-RS as a tool to identify eutectic solvents for selective polymer dissolution
POSTER_	P10 - Instrumentation and	Methods
P10.1	Fabian Luther	Inherent single-point calibration for quantitative Raman analysis of hydrogen's isomeric composition
P10.2	Alexandre Alves	AdsorptionCAL – calibration and optimization of a Calvet microcalorimeter based gas-adsorption system
P10.3	Leonardo Oliveira	Experimental unit for absorption of gaseous mixtures in ionic liquids at high pressures
P10.4	Carlos Miranda	Novel small-volume electrical conductivity cell for ionic fluids

## **SOCIAL EVENTS**

Date: Wednesday, July 23rd

Venue: Port Wine Cellar / Caves Ferreira

Address: Av. de Ramos Pinto 70, 4400-082 Vila Nova de Gaia



Port Wine, a symbol of Portugal in the world, carries the history of a country and its people and has become a cultural landmark of work, experiences, knowledge, and art transmitted from generation to generation. Port Wine represents years of history and tradition of the Portuguese people.

The Conference Dinner will take place in Casa Ferreirinha, In the heart of the historic centre of Vila Nova de Gaia, with the River Douro as a backdrop, Casa Ferreira, part of Ferreira Cellars, is proud of its secular history and is today an excellent refurbished venue perfect to host memorable events.

# **CONFERENCE VENUE**

## Faculdade de Ciências da Universidade do Porto

Rua do Campo Alegre s/n, 4169-007 Porto, PORTUGAL

## FCUP CAMPUS - Campo Alegre





27th IUPAC International
Conference on Chemical
Thermodynamics

July 20 to 24th, 2025
Faculty of Sciences
University of Porto

U. PORTO