EUROPEAN SYMPOSIUM ON APPLIED THERMODYNAMICS

LISBON
10-13 MAY 2026

34th ESAT
PROGRAMME

E-MAIL: esat2026@fct.unl.pt
WEBSITE: esat-2026.sci-meet.net/

NOVA SCHOOL OF SCIENCE & TECHNOLOGY
requimte LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE
U.PORTO FEUP FACULDADE DE ENGENHARIA UNIVERSIDADE DO PORTO
ALiCE ASSOCIATE LABORATORY IN CHEMICAL ENGINEERING
SREC M LABORATORY OF SEPARATION AND REACTION ENGINEERING LABORATORY OF CATALYSIS AND MATERIALS

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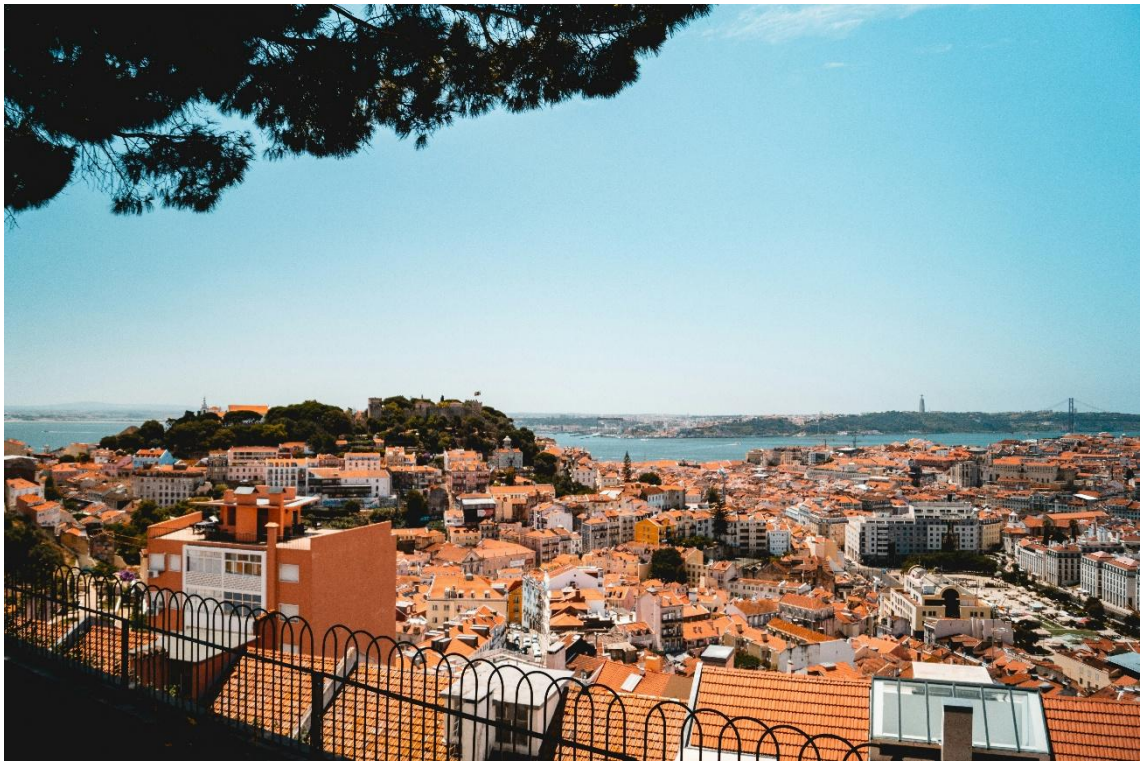
General information: Lisbon



Lisbon, awarded Europe's Leading City Destination 2024 by the World Travel Awards, stands out as a vibrant and welcoming capital. Renowned for its safety, visitors can explore its streets comfortably at any hour, discovering a city where tradition and modernity coexist seamlessly. Its rich culinary heritage is exemplified by the countless ways to prepare its iconic "bacalhau", while a diverse range of hotels and restaurants ensures options for every preference and budget. With its unique blend of authenticity, historic charm, cultural vitality, and forward-looking innovation, Lisbon offers an inspiring setting for both visitors and events alike.

Find further information about Lisbon's top attractions, events, restaurants and more on this official website: https://www.visitlisboa.com/.

Time zone: The time zone in Lisbon is WEST (summer) and GMT (winter).

Water: Tap water in Portugal is considered safe.

Electricity: Standard voltage is 220V AC. Plugs are European style with two round pins.

Currency, banks and post offices: The national currency in Portugal is the Euro. Banks are open from Monday to Friday between 8h30 and 15h. Post offices are usually open between 8h30 and 18h. Exchange houses operate every day between 9h and 13h and from 14h to 19h.

Programme summary

Sunday, May 10th			Room
15h30	20h30	Registration	South foyer
17h30	18h30	Opening session	Arrábida I-II
18h30	19h30	Plenary session - Michael L. Michelsen Award	Arrábida I-II
19h30	20h30	Plenary session - Agílio Pádua	Arrábida I-II
20h30	22h30	Welcome reception	Near outdoor swimming pool

Monday, May 11th			Room
8h15	19h30	Registration	South foyer
8h30	9h30	Plenary session - Ellen Steimers	Arrábida I-II
9h30	10h30	Parallel sessions I	*(see programme)*
10h30	10h50	Coffee break	South foyer
10h50	12h30	Parallel sessions II	*(see programme)*
12h30	13h30	Lunch break	-
13h30	14h30	Parallel sessions III	*(see programme)*
14h30	15h20	Special session - John Prausnitz	Arrábida I-II
15h20	16h10	Parallel sessions John Prausnitz I	*(see programme)*
16h10	16h20	Group photo	-
16h20	16h40	Coffee break	South foyer
16h40	19h10	Parallel sessions John Prausnitz II & Round Table Discussion IUT	*(see programme)*
19h10	19h55	Poster session I	-
19h55	20h30	-	-
20h30	21h30	Dinner	-

Tuesday, May 12th			Room
8h15	19h30	Registration	South foyer
8h30	9h30	Plenary session - Hans Hasse	Arrábida I-II
9h30	10h30	Parallel sessions IV	*(see programme)*
10h30	10h50	Coffee break	South foyer
10h50	12h30	Parallel sessions V	*(see programme)*
12h30	13h30	Lunch break	-
13h30	14h30	Parallel sessions VI	*(see programme)*
14h30	16h10	Parallel sessions VII	*(see programme)*
16h10	16h30	Coffee break	South foyer
16h30	18h45	Special session - Maurizio Fermeglia	Arrábida I-II
18h45	19h30	Poster session II	-
19h30	20h30	-	-
20h00	23h00	Gala dinner	-

Wednesday, May 13th			Room
8h30	13h30	Registration	South foyer
8h30	10h45	Special session - Karel Aim	Arrábida I-II
10h45	11h05	Coffee break	South foyer
11h05	12h45	Parallel sessions VIII	*(see programme)*
12h45	13h15	Closing session	Arrábida I-II
13h15	14h15	Lunch break	-

Preface

Dear Participants,

We welcome you to the **34th European Symposium on Applied Thermodynamics** (ESAT 2026), in Lisbon, Portugal.

Established in 1974 in Berlin (West Germany) through the initiative of Professor Helmut Knapp, ESAT is the oldest and most respected conference of its kind in Europe. Since its inception, it has been hosted all over Europe, highlighting both the scientific excellence and cultural richness of the continent.

From the beginning, one of the core objectives of ESAT has been to strengthen university-industry collaboration, fostering joint research from fundamental studies to industrial applications, especially in separation processes and phase equilibria. Over the years, the scope has been broadened to include eco-friendly processes and components and other topics aligned with today's societal and environmental challenges.

ESAT has grown into a truly global conference, attracting, in 2026, more than 200 participants from 38 different countries, from Europe, North and South America, Asia, and Africa. Many of the most innovative works presented at ESAT are the basis of groundbreaking publications in high-impact international journals.

In this edition, the EFCE Michael L. Michelsen Award 2026 will be presented to Professor Ioannis G. Economou, who will deliver a lecture on "Multi-scale simulation of complex chemical systems: Structure and physical properties for novel material and process design". As usual, the Helmut Knapp award will be given to the best PhD Student poster.

Besides this, ESAT 2026 will include three special moments.

Monday afternoon will be reserved to honour Professor John Prausnitz, who has been the dominant figure of Applied Thermodynamics for many years. His prolific publications and prominent texts pioneering the breadth and depth of the area have been cited innumerable times, and his inspiring lectures are models of communication effectiveness. He attended many ESAT meetings and his friendship with Helmut Knapp, founder of the ESAT series, is legendary. The organizers of ESAT 2026 have chosen to show gratitude of the European Applied Thermodynamics Community for Professor Prausnitz's contributions to our vibrant community by dedicating sessions of invited lectures celebrating his significance in our work and his leadership in guiding our advancements. The first session has presentations by two of his closest colleagues, Edmundo Gomes de Azevedo of Instituto Superior Técnico (PT) and John P. O'Connell of University of Viginia (US) recounting Professor Prausnitz' accomplishments and impacts, as well as insights into his scholarly and personal values. Following these, are talks by prominent researchers connecting their work to the foundations and applications of Professor Prausnitz and the positive impacts he has had on their lives.

The Industrial Use of Thermodynamics round table also joins in acknowledging Professor John Prausnitz's accomplishments. We are happy to host this recognition in Portugal, since Professor Prausnitz is a very dear friend. We are deeply grateful to Professor John O'Connell for his valued advice and support during the preparation of these sessions.

The other two special moments constitute our most sincere tributes to Professor Karel Aim and Professor Maurizio Fermeglia, who sadly are missing. Professor Karel Aim, an outstanding colleague of the thermodynamic community, who was an esteemed member of the International Steering Committee of ESAT since 2000, a role in which he served with distinction for over two decades. Professor Maurizio Fermeglia was a distinguished researcher, former Rector of the University of Trieste, and a cherished participant of the ESAT conferences. It is a mark of our respect and appreciation to dedicate two plenary sessions to their memories.

We are happy to offer our grateful thanks to the invited speakers, to the members of the International Steering Committee for their valuable input, all communication contributors and all participants who bring and share their knowledge and expertise.

We would like to express our gratitude to our sponsors, whose valued support has been essential to the preparation of this conference.

We look forward to an outstanding programme filled with engaging scientific discussions, as well as the opportunity for you to experience the unique history, vibrant culture, and natural beauty of our country.

And now, it is our hope that when you return to your own homes with the happiest of memories and you remember the great Portuguese discoveries of another age, you will have made, in this age, some meaningful discoveries of your own in the field of Applied Thermodynamics.

On behalf of the Local Organising Committee,

Maria Eugénia Rebello de A. Macedo (Chair)

Ana B. Pereiro (Co-Chair)

João M. Mendes de Araújo (Co-Chair)

Committees

ORGANISING COMMITEE

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Sabine **Enders**, Germany (Vice-Chair)

Jean-Noël **Jaubert**, France (Vice-Chair)

Karel **Aim**, Czech Republic *(In memoriam)*

Maria Grazia de **Angelis**, Italy

Jean-Charles **de Hemptinne**, France

Ralf **Dohrn**, Germany

Georgios M. **Kontogeorgis**, Denmark

Catinca **Secuianu**, Romania

Ana **Soto**, Spain

Alexey **Victorov**, Russia

Epaminondas **Voutsas**, Greece

Tim **Zeiner**, Austria

Venue and maps

The event will take place at the **Design Tróia Hotel**, a five-star contemporary resort located in Tróia, a unique peninsula south of Lisbon and integrated within a protected Natural Reserve.

The Design Tróia Hotel offers excellent views of the Atlantic Ocean, extensive beaches, the Sado river, and the distinctive Arrábida mountain range, providing a calm and inspiring environment. The hotel combines a sophisticated and comfortable atmosphere, with thoughtful design in every detail, and offers high-quality facilities.

We are confident that this venue will provide an excellent setting for the conference and contribute positively to the overall experience of all participants.

For more information, please visit: https://www.troiadesignhotel.com/pt/

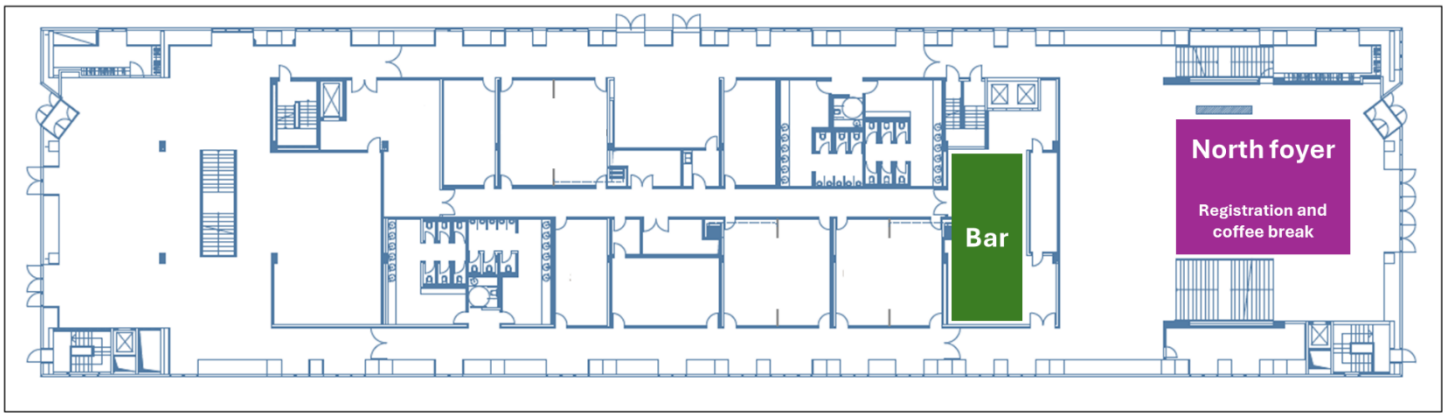
Address:

Tróia Design Hotel, Marina de Tróia - Península de Tróia

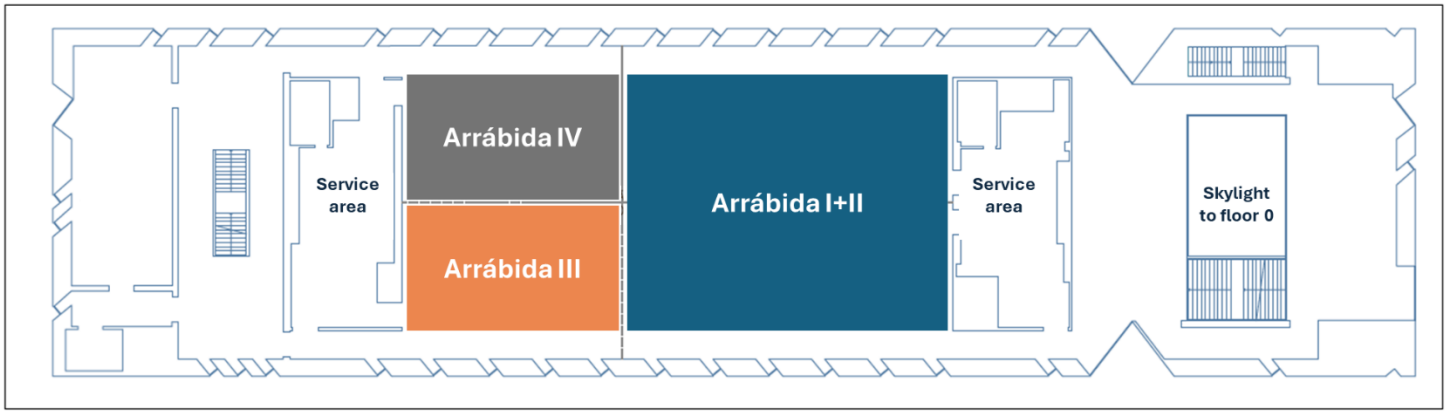
7570-789 Carvalhal, Grândola

Portugal

GROUND FLOOR | Conference centre



FIRST FLOOR | Conference centre



OPEN WIFI

Conference Centre: Troia Eventos

Troia Design Hotel: Troia Design Hotel

Technical information

LECTURES

Plenary Lectures | **PL**

50 (talk) + 10 (Q&A) min

Invited Lectures – John M. Prausnitz | **IL**

20 (talk) + 5 (Q&A) min

Oral Lectures | **OL**

15 (talk) + 5 (Q&A) min

Flash Lectures | **FL**

5 (talk) + 5 (Q&A) min

Please help keep our conference programme on schedule by adhering to these time limits.

Please prepare your PowerPoint presentations in 16:9 format and send them to esat2026@fct.unl.pt before the start of the conference. Alternatively, you may deliver them in person in the designated presentation room, no later than the session preceding your own.

POSTER SESSION

Monday, May 11th | 19h10 – 19h55

Tuesday, May 12th | 18h45 – 19h30

Room: Conference centre

Posters can be mounted from the morning of May 10th. **The posters will be exhibited from May 10th to 13th.**

Each poster has been assigned a number, which will also be displayed on the movable wall. Our staff will be on hand to assist you in finding your designated poster spot and will provide mounting material as well as assistance. Please remember to remove your posters at the end of the conference.

SOCIAL PROGRAMME

Welcome reception | Sunday, May 10th | 20h30 – 22h30

After gathering in the Arrábida I–II room for the opening session and for the first two plenary sessions, we will proceed to the welcome reception, which will take place near the outdoor swimming pools at the Troia Design Hote

Gala dinner | Tuesday, May 12th | 20h00 – 23:00

The Conference dinner will be held at the Restaurant of the Show Centre in the Troia Design Hotel and will include a surprise cultural moment during the evening.

Group photo

Monday, May 11th | 16h10 – 16h20

The official group photo will be taken on the staircase between the ground and first floors of the Conference Centre.

Scientific programme: Talks

Sunday, May 10th

OPENING SESSION

Room: Arrábida I-II

17h30 – 18h30	**OPENING SESSION**

PLENARY SESSION - Michael L. Michelsen Award

Room: Arrábida I-II
Chairs: A. Gonçalves da Silva and Grazia de Angelis

18h30 – 19h30	**MULTI-SCALE SIMULATION OF FISCHER-TROPSCH SYNTHESIS FOR THE GAS-TO-LIQUID PROCESS: FROM DENSITY FUNCTIONAL THEORY CALCULATIONS TO PHYSICAL PROPERTY PREDICTIONS**
PS	**Ioannis G. Economou**, Texas A&M University, Qatar

PLENARY SESSION – Agílio Pádua

Room: Arrábida I-II
Chairs: A. Gonçalves da Silva and Grazia de Angelis

19h30 – 20h30	**POROUS IONIC LIQUIDS FOR SEPARATIONS, CONVERSIONS AND DELIVERY**
PS	**Agílio Pádua**, ENS de Lyon, France

WELCOME RECEPTION

Room: near the outdoor swimming pools (Troia Design Hotel)

20h30 – 22h30	**WELCOME RECEPTION**

Scientific programme: Talks

Monday, May 11th

PLENARY SESSION - Ellen Steimers

Room: Arrábida I-II
Chair: Georgios M. Kontogeorgis

8h30 – 9h30	**FROM PREDICTION TO PRACTICE: PHYSICAL PROPERTY DATA FOR INDUSTRIAL PROCESS SOLUTIONS**
PS	**Ellen Steimers**, BASF, Germany

PARALLEL SESSIONS I – Equations of state

Room: Arrábida I-II
Chair: Fèlix Llovell

09h30 – 09h50	**APPLICATION OF CP-PC-SAFT WITH UNIVERSAL K_{12} VALUE FOR SIMULTANEOUS PREDICTION OF VLE, LLE AND CRITICAL LOCI IN SYSTEMS OF GASES AND ALIPHATIC HYDROCARBONS WITH SUBSTITUTED AROMATIC AND HETEROCYCLIC COMPOUNDS**
Oral	**Ilya Polishuk**, Ariel University, Israel
09h50 – 10h10	**USING THE HELMHOLTZ FREE-ENERGY EQUATION OF STATE FOR MIXTURES**
Oral	**Jan Foeke Kikstra**, Cargill, Netherlands
10h10 – 10h30	**DEVELOPMENT AND COMMERCIAL IMPLEMENTATION OF A COMPUTATIONALLY EFFICIENT POLAR PC-SAFT EQUATION OF STATE FOR LARGE SCALE INDUSTRIAL APPLICATIONS**
Oral	**Bennett D. Marshall**, ExxonMobil Technology and Engineering Company, USA

PARALLEL SESSIONS I – Absorption & Adsorption

Room: Arrábida III
Chair: Nicolas von Solms

09h30 – 09h50	**FROM POULTRY WASTE TO CRITICAL RAW MATERIAL RECOVERY: THERMODYNAMIC INSIGHTS INTO PLATINUM GROUP METAL ADSORPTION**
Oral	**Helena Passos**, FEUP, Portugal
09h50 – 10h10	**THERMODYNAMIC VS KINETIC CONTROL OF BRUSH COMPOSITION IN GRAFTING TO REACTIONS: A COMBINED EXPERIMENTAL AND GRAND CANONICAL MONTE CARLO STUDY**
Oral	**Cosimo Brondi**, Universitas Mercatorum, Italy
10h10 – 10h30	**HYDROGEN ADSORPTION WITH 3D CLASSICAL DENSITY FUNCTIONAL THEORY**
Oral	**Nadine Thiele**, University of Stuttgart, Germany

PARALLEL SESSIONS I – General

Room: Arrábida IV
Chair: Hiroyuki Matsuda

09h30 – 09h50	**PREDICTIVE COSMO-SAC CARBON-BASED MAGNETIC KINETIC PROMOTERS FOR ACCELERATED AND EFFICIENT CO_2 HYDRATE FORMATION**
Oral	**Mawadda A. A. Adam**, King Fahd University of Petroleum and Minerals, Saudi Arabia
09h50 – 10h10	**MULTISCALE MODELING FROM PREDICTIVE THERMODYNAMICS TO PROCESS SUSTAINABILITY: THE SCIENTIFIC LEGACY OF MAURIZIO FERMEGLIA**
Oral	**Andrea Mio**, University of Trieste, Italy

PARALLEL SESSIONS II – General

Room: Arrábida I-II
Chair: António Queimada

10h50 – 11h10	**A CLASSIFICATION FOR ELECTROLYTES BASED ON INTERMOLECULAR INTERACTIONS**
Oral	**Gabriel M. Silva**, Technical University of Denmark, Denmark
11h10 – 11h30	**MEASUREMENTS OF CARBON DIOXIDE SOLUBILITY IN CYRENE FOR CO_2 REMOVAL APPLICATIONS**
Oral	**Valentina Schiattarella**, Politecnico di Milano, Italy
11h30 – 11h50	**PHASE BEHAVIOUR OF HARD CLOVER-SHAPED PARTICLES FROM MONTE CARLO SIMULATIONS**
Oral	**Nathan B. de Souza**, Universidade Estadual de Campinas, Brazil
11h50 – 12h10	**STATISTICAL THERMODYNAMICS OF SUPERCOOLED WATER**
Oral	**Claudio Cerdeiriña**, University of Vigo, Spain

PARALLEL SESSIONS II – Novel solvents and supercritical fluids

Room: Arrábida III
Chair: Ilya Polishuk

10h50 – 11h10	**PHASE EQUILIBRIUM AND THERMOPHYSICAL PROPERTIES OF THE DEEP EUTECTIC SOLVENT CHOLINIUM CHLORIDE & ETHYLENE GLYCOL WITH HYDROFLUOROCARBON GASES**
Oral	**Aaron M. Scurto**, University of Kansas, USA
11h10 – 11h30	**ENHANCING LOW-CONCENTRATION CO_2 CAPTURE ABILITIES OF AMINIUM IONIC LIQUIDS THROUGH BLENDING WITH ACETATE IONIC LIQUIDS**
Oral	**Takashi Makino**, Nat. Inst. of Adv. Industrial Science and Technology, Japan
11h30 – 11h50	**THE STRUCTURE AND ORIGIN OF THE SUPERCRITICAL (WIDOM) ANOMALIES**
Oral	**Attila R. Imre**, Budapest University of Technology and Economics, Hungary
11h50 – 12h10	**SORPTION THERMODYNAMICS OF WATER AND METHANOL IN GLASSY POLYIMIDES: A MULTISCALE APPROACH COMBINING GRAVIMETRIC, FT-IR IN SITU EXPERIMENTS WITH A NON-EQUILIBRIUM STATISTICAL THERMODYNAMICS THEORY**
Oral	**Giuseppe Scherillo**, University of Naples Federico II, Italy

PARALLEL SESSIONS II – Molecular Modelling and Simulation

Room: Arrábida IV
Chair: Alberto Striolo

10h50 – 11h10	**ACCURATE THERMODYNAMIC MODELLING AND 3E CYCLE ANALYSIS FOR APPLICATIONS IN THE SEARCH FOR SUSTAINABLE ABSORPTION REFRIGERATION WORKING PAIRS**
Oral	**Fèlix Llovell**, Universitat Rovira i Virgili, Spain
11h10 – 11h30	**EXPLORING THE INTERACTION BETWEEN PLASMA PROTEINS AND POLYMERIC MATERIALS IN MEDICAL DEVICES: INSIGHTS FROM MOLECULAR SIMULATIONS**
Oral	**Amr Saleh**, Université Clermont Auvergne, France
11h30 – 11h50	**ELECTRO COALESCENCE OF IONIC LIQUID/ALKANOL LADEN WATER DROPLET: A MOLECULAR DYNAMICS STUDY**
Oral	**Sandip Khan**, Indian Institute of Technology Patna, India
11h50 – 12h10	**REVISION OF THE eSAFT-VR MIE EQUATION OF STATE FOR ELECTROLYTE SOLUTIONS**
Oral	**Ziyi Zhou**, Technical University of Denmark, Denmark
12h10 – 12h30	**FLASH LECTURES SESSION**
Flash	

PARALLEL SESSIONS III – Phase equilibria & Equations of state

Room: Arrábida I-II
Chair: William Smith

13h30 – 13h50	**COMMENTS ON THE CORRELATION OF AQUEOUS TWO-PHASE SYSTEMS (ATPS) INVOLVING POLYMERS**
Oral	**Antonio Marcilla**, University of Alicante, Spain
13h50 – 14h10	**IMPROVEMENT OF LIQUID PHASE SPLITTING OF WATER + ETHANOL + ISOBUTANOL MIXTURES IN THE PRESENCE OF ELECTROLYTE AT ATMOSPHERIC PRESSURE**
Oral	**Salal H. Khudaida**, Technische Universität Dortmund, Germany
14h10 – 14h30	**OPTIMAL STRATEGY FOR THE PARAMETRISATION OF THE ASSOCIATION TERM OF SAFT MODELS**
Oral	**Haziq Asmuni**, University of Lorraine, France

PARALLEL SESSIONS III – Multiscale models

Room: Arrábida III
Chair: Romain Privat

13h30 – 13h50	**MODELLING AMORPHOUS CHAIN TOPOLOGY IN SEMICRYSTALLINE POLYMERS AND ITS IMPACT ON POLYMER DEGRADATION**
Oral	**Michele Valsecchi**, Columbia University, USA
13h50 – 14h10	**AN INTEGRATED PHYSICS-BASED AND DATA-DRIVEN STRATEGY FOR MIXED-GAS SOLUBILITY IN POLYMER MEMBRANES**
Oral	**Eleonora Ricci**, University of Edinburgh, Scotland

14h10 – 14h30	**CONNECTING MICROSCOPIC WITH MESOSCOPIC TRANSPORT IN MODEL NANOPOROUS MATERIALS**
Oral	**Marcelle Spera**, University Grenoble Alpes, France

PARALLEL SESSIONS III – Polymers and complex materials

Room: Arrábida IV
Chair: Aaron Scurto

13h30 – 13h50	**PREDICTION OF MASS TRANSPORT IN A GLASSY POLYETHERIMIDE IN PRESENCE OF SPECIFIC INTERACTIONS BASED UPON SELF-CONSISTENT NETGP-PC-SAFT DIFFUSION MODEL**
Oral	**Antonio Baldanza**, Scuola Superiore Meridionale, Italy
13h50 – 14h10	**MOLECULAR MODELLING OF GAS TRANSPORT AT A POLYMER/MOF INTERFACE**
Oral	**Tiziano Cavalieri**, University of Edinburgh, Scotland

SPECIAL SESSION – John M. Prausnitz

Room: Arrábida I-II
Chair: Doros Theodorou and Ralf Dohrn

14h30 – 14h55	**I FIRST MET JMP ON… AUGUST 1981**
Oral	**Edmundo G. de Azevedo**, Instituto Superior Técnico, Portugal
14h55 – 15h20	**HONORING JOHN M. PRAUSNITZ: GUIDING SPIRIT OF APPLIED THERMODYNAMICS**
Oral	**John O'Connell**, University of Virginia, USA

PARALLEL SESSIONS JOHN M. PRAUSNITZ I – Phase equilibria & Simulation

Room: Arrábida I-II
Chair: Ilja Siepmann and Mark Shiflett

15h20 – 15h45	**REVIEW SERIES ON HIGH-PRESSURE PHASE EQUILIBRIA: TRENDS, EXPERIMENTAL METHODS, AND SYSTEMS INVESTIGATED**
Oral	**Ralf Dohrn**, TU Hamburg, Bayer AG, Germany
15h45 – 16h10	**MORPHOLOGY DEVELOPMENT IN SEMICRYSTALLINE POLYETHYLENE: A MOLECULAR SIMULATION STUDY**
Oral	**Doros Theodorou**, Nat. Tech. University of Athens and Academy of Athens, Greece

PARALLEL SESSIONS JOHN M. PRAUSNITZ I – Sustainable processes

Room: Arrábida III
Chair: José Nuno C. Lopes and Phillip Choi

15h20 – 15h45	**EXTRACTION OF NATURAL COMPOUNDS USING SUSTAINABLE SOLVENTS – WHAT CAN THERMODYNAMICS BRING US?**
Oral	**Nicolas Papaiconomou**, Université Côte d'Azur, France

15h45 – 16h10	**DEVELOPMENT OF THERMO-CATALYTIC DECOMPOSITION PROCESS OF METHANE INTO HYDROGEN AND GRAPHITE AND OTHER MATTERS**
Oral	**Justin Salminen**, Hycamite TCD Technologies, Finland

PARALLEL SESSIONS JOHN M. PRAUSNITZ I – Phase equilibria & Interfaces

Room: Arrábida IV
Chair: David Kofke and Leo Lue

15h20 – 15h45	**ADSORPTION OF CHAINLIKE AMPHIPHILES ON SOLID NANOPARTICLES FROM AQUEOUS MIXTURES: PREDICTION FROM A MOLECULAR MODEL**
Oral	**Alexey Victorov**, St. Petersburg State University, Russia
15h45 – 16h10	**PEG/CITRATE AQUEOUS TWO-PHASE EXTRACTION OF FISH PROTEINS**
Oral	**Oscar Rodríguez**, Universidade de Santiago de Compostela, Spain

PARALLEL SESSIONS JOHN M. PRAUSNITZ II – Phase equilibria & Interfaces

Room: Arrábida I-II
Chair: Alexey Victorov and Nicolas Papaiconomou

16h40 – 17h05	**SEPARATION OF AZEOTROPIC REFRIGERANT MIXTURES USING IONIC LIQUIDS**
Oral	**Mark B. Shiflett**, University of Kansas, USA
17h05 – 17h30	**TRANSPORT PROPERTIES AND GLASS TRANSITION TEMPERATURES OF POLYMERS AS DETERMINED BY MACROMOLECULAR THEORY AND SIMULATIONS**
Oral	**Phillip Choi**, University of Regina, Canada
17h30 – 17h55	**MOLECULAR THERMODYNAMICS OF PHASE EQUILIBRIA FOR COMPLEX SYSTEMS WITH APPLICATIONS**
Oral	**Nicolas von Solms**, Technical University of Denmark, Denmark
17h55 – 18h20	**LIQUID-LIQUID EQUILIBRIUM ISLANDS IN TERNARY SYSTEMS COMPRISING AN IONIC LIQUID**
Oral	**Héctor Rodriguez**, Universidade de Santiago de Compostela, Spain

PARALLEL SESSIONS JOHN M. PRAUSNITZ II – Modelling & General

Room: Arrábida III
Chair: Justin Salminen and Oscar Rodríguez

16h40 – 17h05	**THERMODYNAMIC CONTRIBUTIONS OF MOBILE AND STATIONARY PHASES TO RETENTION IN DIFFERENT MODES OF CHROMATOGRAPHY**
Oral	**J. Ilja Siepmann**, University of Minnesota, USA
17h05 – 17h30	**INFERENCE OF VIRIAL COEFFICIENTS FROM EXPERIMENTAL DATA**
Oral	**David Kofke**, University at Buffalo, USA
17h30 – 17h55	**MODELLING THE STRUCTURE AND DYNAMICS OF IONIC LIQUID MEDIA**
Oral	**José Nuno Canongia Lopes**, Universidade de Lisboa, Portugal
17h55 – 18h20	**A DENSITY GRADIENT THEORY OF SURFACTANT SOLUTIONS**
Oral	**Leo Lue**, University of Strathclyde, Scotland

18h20 – 18h45	**RECENT ADVANCEMENTS IN THE FUNDAMENTAL UNDERSTANDING IN THE ROLE OF ADDITIVES IN MODULATING CLATHRATE HYDRATES**
Oral	**Alberto Striolo**, University of Oklahoma, USA

ROUND TABLE DISCUSSION – IUT

Room: Arrábida IV
Chair: Jean-Charles de Hemptinne and Antoon ten Kate

16h35 – 16h40	**PRESENT OBJECTIVE AND TOOLS**
	Jean-Charles de Hemptinne, IFPEN, France
16h40 – 16h55	**INTRODUCTION AND THERMOCHEMICAL PERSPECTIVE ON A TRANSIENT WORLD**
Oral	**Antoon ten Kate**, Chemspiration, Netherlands
16h55 – 17h10	**EXPERIMENTAL AND MODELLING INSIGHTS INTO ANION EXCHANGE MEMBRANES FOR MOISTURE-DRIVEN DIRECT AIR CAPTURE**
Oral	**Maria Grazia de Angelis**, University of Edinburgh, Scotland
17h10 – 17h25	**THERMODYNAMICS AND PROCESS MODELLING FOR A (MORE) SUSTAINABLE CHEMICAL INDUSTRY**
Oral	**José M. S. Fonseca**, AVEVA, England
17h25 – 17h40	**THERSAURUS: TOWARDS A THERMODYNAMICS OF SUSTAINABILITY**
Oral	**Alicia Valero**, Universidad de Zaragoza, Spain
17h40 – 17h55	**ENERGY IS CONSERVED – ENERGY IS DESTROYED: RETHINKING EFFICIENCY FOR CIRCULAR INDUSTRIAL PROCESSES**
Oral	**Jean-Noël Jaubert**, Université de Lorraine, France
17h55 – 18h10	**PROCESS ENGINEERING AND THERMODYNAMICS CHALLENGES IN PLASTICS CIRCULARITY: CLOSING THE LOOP WITH INDUSTRIAL RECYCLING TECHNOLOGIES**
Oral	**Bernhard von Vacano**, BASF SE, Germany
18h10 – 18h25	**ROLE OF THERMODYNAMICS IN BATTERY RECYCLING AND CRITICAL RAW MATERIAL RECOVERY**
Oral	**Daniele Marchisio**, Politecnico di Torino, Italy
18h25 – 18h30	**HOW IS THERMODYNAMICS USED TODAY IN SHAPING THE DEVELOPMENT OF SUSTAINABLE TECHNOLOGIES?**
	The Current Role
18h30 – 18h45	**HOW IS THERMODYNAMICS USED TODAY IN SHAPING THE DEVELOPMENT OF SUSTAINABLE TECHNOLOGIES?**
	Discussion
18h45 – 18h50	**WHAT PRINCIPLES ARE NOT SUFFICIENTLY UNDERSTOOD OR KNOWN FOR SUPPORTING CIRCULARITY?**
	Expanding the Role
18h50 – 19h05	**WHAT PRINCIPLES ARE NOT SUFFICIENTLY UNDERSTOOD OR KNOWN FOR SUPPORTING CIRCULARITY?**
	Discussion
19h05 – 19h10	**FINAL COMMENTS**
	Jean-Charles de Hemptinne, IFPEN, France

Scientific programme: Talks

Tuesday, May 12th

PLENARY SESSION – Hans Hasse

Room: Arrábida I-II
Chair: Jean-Noël Jaubert

08h30 – 09h30	**REALIZING THE DREAM OF THERMODYNAMIC MODELING**
PS	**Hans Hasse**, RPTU Kaiserslautern, Germany

PARALLEL SESSIONS IV – Equations of state

Room: Arrábida I-II
Chair: Epaminondas Voutsas

09h30 – 09h50	**SOME RECENT DEVELOPMENTS IN ELECTROLYTE THERMODYNAMICS**
Oral	**Georgios M. Kontogeorgis**, Technical University of Denmark, Denmark
09h50 – 10h10	**MIXING RULES FOR CUBIC EQUATIONS OF STATE: WHAT WORKS, WHAT FAILS, AND WHAT REMAINS TO BE INVESTIGATED**
Oral	**Romain Privat**, University of Lorraine, France
10h10 – 10h30	**SPECIATION IN SAFT-γ MIE: FORMULATION AND APPLICATION FOR LOADED AQUEOUS MONOAMINE SOLUTIONS**
Oral	**Evangelos Tsochantaris**, Technical University of Denmark, Denmark

PARALLEL SESSIONS IV – Absorption and adsorption

Room: Arrábida III
Chair: Antonio Marcilla

09h30 – 09h50	**ADSORPTION OF PARACETAMOL ON GRAPHITE: A THERMODYNAMIC STUDY COMBINING ISOTHERMAL TITRATION CALORIMETRY AND SPECTROSCOPY**
Oral	**Jean Duprat**, Institut de Chimie de Clermont-Ferrand, France
09h50 – 10h10	**MOLECULAR INVESTIGATION OF CO_2 EFFECTS ON FKM ELASTOMERS FOR CO_2 TRANSPORT APPLICATIONS**
Oral	**Matteo Minelli**, University of Bologna, Italy
10h10 – 10h30	**SOLUBILITY, DISSOLUTION AND MIXING ENTHALPIES OF METALLIC SALTS IN IONIC LIQUIDS**
Oral	**Margarida Costa Gomes**, CNRS, France

PARALLEL SESSIONS IV – Sustainable processes

Room: Arrábida IV
Chair: Amparo Galindo

09h30 – 09h50	**ELECTROCHEMICALLY DRIVEN RECOVERY OF CADMIUM AND TELLURIUM FROM CDTE SOLAR CELLS: A THERMODYNAMIC MODELING AND SIMULATION STUDY**
Oral	**Gaurav Das**, OLI Systems Inc, USA
09h50 – 10h10	**GREEN SOLVENT MIXTURES FOR BIOMASS VALORIZATION: A SYNERGISTIC APPROACH COMBINING EXPERIMENTS AND MOLECULAR DYNAMICS SIMULATIONS**
Oral	**Vojtěch Jeřábek**, Univ. of Chemistry and Technology Prague, Czech Republic
10h10 – 10h30	**INTEGRATED MOLECULAR AND PROCESS DESIGN FOR SOLVENT-BASED PLASTIC RECYCLING: EXPERIMENTS, THERMODYNAMIC MODELLING AND PROCESS DESIGN**
Oral	**Riccardo Standish**, Imperial College London, United Kingdom

PARALLEL SESSIONS V – Phase equilibria

Room: Arrábida I-II
Chair: Joachim Groß

10h50 – 11h10	**THERMODYNAMIC CONSISTENCY OF DATA FOR ELECTROLYTE MODEL PARAMETERIZATION: A CASE STUDY PROPOSED BY ELETHER JIP**
Oral	**Jean-Charles de Hemptinne**, IFPEN, France
11h10 – 11h30	**THERMODYNAMIC EXPERIMENTS AND MODELLING OF CYCLOPENTANE HYDRATES IN PRESENCE OF PURE AND MIXED SALTS FROM NABR, KBR, NaCl, KCl, Na_2SO_4, K_2SO_4 AND $CaCl_2$**
Oral	**Baptiste Bouillot**, Ecole des Mines de Saint-Etienne, France
11h30 – 11h50	**A NEW METHOD FOR MULTIPHASE ISENTHALPIC FLASH CALCULATIONS BY DIRECT MAXIMIZATION OF ENTROPY**
Oral	**Dan V. Nichita**, Université de Pau et des Pays de l'Adour, France
11h50 – 12h10	**INVESTIGATION OF THE HSA SOLVATION IN DIVERSE SOLVENTS AT HIGH CONCENTRATIONS**
Oral	**Abtin R. Shirazi**, Ecole des Mines de Saint-Etienne, France

PARALLEL SESSIONS V – Carbon capture, utilisation and storage

Room: Arrábida III
Chair: Clare McCabe

10h50 – 11h10	**A UNIVERSAL ACTIVITY COEFFICIENT MODEL WITH FIRST-PRINCIPLES/ATOMISTIC-SIMULATION-DRIVEN GIBBS ENERGY MINIMIZATION FOR PREDICTING CO_2 REACTIVE ABSORPTION**
Oral	**William R. Smith**, University of Guelph, Canada
11h10 – 11h30	**PREDICTIVE THERMODYNAMIC MODELLING OF GAS SORPTION AND PERMEATION IN POLYMERS FOR HIGH-PRESSURE GAS HANDLING APPLICATIONS**
Oral	**Gaia Lazzari**, Alma Mater Studiorum - University of Bologna, Italy

11h30 – 11h50	**THERMOPHYSICAL PROPERTIES OF BINARY MIXTURES AMINE + CARBON DIOXIDE FOR THE DEPLOYMENT OF CARBON CAPTURE**
Oral	**Xavier Paredes**, University of Valladolid, Spain
11h50 – 12h10	**EXTENSION OF RAND-BASED CHEMICAL EQUILIBRIUM CALCULATION TO MULTIPLE ELECTROLYTE-CONTAINING PHASES IN CO_2 CAPTURE MODELING**
Oral	**Antonio C. L. Neto**, Technical University of Denmark, Denmark

PARALLEL SESSIONS V – Mesoscale methods and COSMO-RS

Room: Arrábida IV
Chair: Sabrina Reartes

10h50 – 11h10	**COSMOTHERM PREDICTION OF CARBON DIOXIDE SOLUBILITY IN BIO-BASED SOLVENTS**
Oral	**Filippo Marchelli**, University of Genova, Italy
11h10 – 11h30	**CALCULATION METHODS FOR COSMO-BASED ACTIVITY COEFFICIENT MODELS**
Oral	**Wei Yan**, Technical University of Denmark, Denmark
11h30 – 11h50	**THERMODYNAMIC MODELING OF PFAS PHYSICOCHEMICAL PROPERTIES WITH COSMO-RS**
Oral	**Daria Grigorash**, Technical University of Denmark, Denmark
11h50 – 12h10	**BOOSTING THERMOPHYSICAL PROPERTY PREDICTIONS WITH GRAPH NEURAL NETWORKS**
Oral	**Martin Richter**, Dassault Systèmes, Germany

PARALLEL SESSIONS VI – Equations of state & Distillation

Room: Arrábida I-II
Chair: Eleonora Ricci

13h30 – 13h50	**ENHANCING THE PR EQUATION OF STATE FOR THE HYDROGEN ECONOMY WITH A NOVEL HYBRID NEURAL NETWORK FRAMEWORK**
Oral	**Elahe Rostaminikoo**, University of Lancashire, United Kingdom
13h50 – 14h10	**PROCESS INTENSIFICATION AND OPTIMIZATION OF AROMA COMPOUNDS PRESERVATION IN THERMAL DEALCOHOLISATION OF BEER**
Oral	**Mariangela Falconieri**, Technical University of Munich, Germany
14h10 – 14h30	**ONE EOS TO RULE THEM ALL? SYSTEMATIC REVIEW OF EQUATIONS OF STATE FOR PURE COMPONENT PREDICTION**
Oral	**Simon Müller**, Hamburg University of Tehcnology, Germany

PARALLEL SESSIONS VI – New fuels and refrigerants & Interfaces

Room: Arrábida III
Chair: Helena Passos

13h30 – 13h50	**COMPARATIVE 3D VISUALIZATION OF PROCESSES IN POWER-TO-HEAT AND HEAT-TO-POWER CYCLES USING VARIOUS TYPES OF WORKING FLUIDS**
Oral	**Réka Kustán**, Budapest University of Technology and Economics, Hungary
13h50 – 14h10	**A HYBRID COMPUTATIONAL FRAMEWORK FOR THE DISCOVERY AND THERMODYNAMIC CHARACTERISATION OF NEW WORKING FLUIDS**
Oral	**Tiago Mendonça Eusébio**, Universitat Ramon Llull, Spain
14h10 – 14h30	**ROLE OF ACIDS IN STABILIZING REVERSE MICELLES: CASE OF DODECY SULFATE**
Oral	**Qixuan Li**, Ruhr-University Bochum, Germany

PARALLEL SESSIONS VI – Separation processes & General

Room: Arrábida IV
Chair: Hector Rodríguez

13h30 – 13h50	**FIRST APPLICATION OF MEMBRANE-ABSORPTION INTEGRATION FOR THE SEPARATION OF AZEOTROPIC REFRIGERANT BLENDS**
Oral	**Miguel Viar Fernández**, Universidad de Cantabria, Spain
13h50 – 14h10	**LIQUID-LIQUID EQUILIBRIA FOR THE BINARY SYSTEMS γ-VALEROLACTONE + HYDROCARBON: EXPERIMENTAL DATA AND MODELLING**
Oral	**Hiroyuki Matsuda**, Nihon University, Japan
14h10 – 14h30	**ADVANCING THERMODYNAMIC APPROACHES TO MODEL THE PHASE BEHAVIOUR OF PEPTIDES IN AQUEOUS AND MIXED SOLVENTS**
Oral	**Shubhani Paliwal**, Imperial College London, UK

PARALLEL SESSIONS VII – Molecular modelling and simulation

Room: Arrábida I-II
Chair: Matteo Minelli

14h30 – 14h50	**INSIGHTS INTO THE MOLECULAR MECHANISMS UNDERLYING DIFFERENCES IN PROPERTIES OF STRUCTURALLY SIMILAR COMPOUNDS**
Oral	**Maria Fontenele**, Roquette Frères, Carbohydrate & Advanced Process Tech., France
14h50 – 15h10	**PREDICTIVE METHODS FOR ESTIMATING THE THERMAL CONDUCTIVITY OF PURE SUBSTANCES AND MIXTURES USING ENTROPY SCALING**
Oral	**Julia Burkhardt**, University of Stuttgart, Germany
15h10 – 15h30	**SURFACTANT-BASED REMEDIATION OF CONTAMINANTS ON SOLID SURFACES AND IN AQUEOUS ENVIRONMENTS: A MOLECULAR DYNAMICS STUDY**
Oral	**Hector Dominguez**, Universidad Nacional Autónoma de México, México

15h30 – 15h50	**THERMODYNAMICS AND STRUCTURES IN SELF-ASSEMBLY PROCESSES OF SOFT MATTER**
Oral	**Giuseppe Milano**, Università di Napoli Federico II, Italy
15h50 – 16h10	**EXTENDING THE SAFT-γ MIE APPROACH: FROM POLYCYCLIC AROMATIC COMPOUNDS TO ASPIRIN**
Oral	**Amparo Galindo**, Imperial College London, UK

PARALLEL SESSIONS VII – Novel solvents and equations of state

Room: Arrábida III
Chair: Catinca Secuianu

14h30 – 14h50	**FROM AI TO THERMODYNAMICS: PREDICTING PURE-COMPONENT EOS INPUTS WITH ENSEMBLE LEARNING**
Oral	**Jean-Noël Jaubert**, University of Lorraine, France
14h50 – 15h10	**COSMO-NET: EFFICIENT GRAPH NEURAL NETWORK SURROGATES FOR COSMO-BASED MOLECULARDESCRIPTORS**
Oral	**Saman N. Boroujeni**, Imperial College London, United Kingdom
15h10 – 15h30	**PREDICTION OF THE SURFACE TENSION OF AMINE-BASED SOLVENTS WITH A NEW GROUP-CONTRIBUTION MACHINE-LEARNING MODEL: GriTo**
Oral	**Thomas Bernet**, Imperial College London, United Kingdom
15h30 – 15h50	**THERMOPHYSICAL PROPERTIES OF SUSTAINABLE LIQUID FUELS**
Oral	**Lillian R. T. Ladu**, Imperial College London, United Kingdom

PARALLEL SESSIONS VII – Machine learning and data-driven methods

Room: Arrábida IV
Chair: Wei Yang

14h30 – 14h50	**CONFIDENTIALITY-PRESERVING TRAINING OF THERMODYNAMIC MODELS WITH FEDERATED LEARNING**
Oral	**Pascal Zittlau**, RPTU Kaiserslautern, Germany
14h50 – 15h10	**TERPENE-BASED EUTECTIC MIXTURES AS GREENSOLVENTS FOR CO_2 CAPTURE: EXPERIMENTALCHARACTERIZATION AND MOLECULAR INSIGHTS**
Oral	**Esteban Cea-Klapp**, Pontificia Universidad Católica de Chile, Chile
15h10 – 15h30	**TWENTY YEARS OF DEEP EUTECTIC SOLVENTS: ARE THERMODYNAMIC MODELS READY FOR INDUSTRY?**
Oral	**Reza Haghbakhsh**, Universidade Nova de Lisboa, Portugal
15h30 – 15h50	**A THERMODYNAMIC FRAMEWORK TO DESIGN GREENHOUSE GAS CAPTURE UNITS USING PHOSPHONIUM-BASED IONIC LIQUIDS**
Oral	**Sabrina B. R. Reartes**, Universitat Rovira i Virgili, Spain

SPECIAL SESSION – Maurizio Fermeglia

Room: Arrábida I-II

Chair: Eugénia A. Macedo and Andrea Mio

16h30 – 16h45	**PRESENTATION IN HONOUR OF MAURIZIO FERMEGLIA** **Andrea Mio**, University of Trieste, Italy
16h45 – 17h45	**DEVELOPMENT OF MACHINE LEARNING MODELS FOR THERMOPHYSICAL PROPERTIES REQUIRED FOR PROCESS MODELING AND OPTIMIZATION OF CARBON CAPTURE PROCESSES** PS **Peter T. Cummings**, Heriot-Watt University, Scotland
17h45 – 18h45	**USING MOLECULAR SIMULATION TO PROVIDE INSIGHTS INTO SKIN BARRIER FUNCTION** PS **Clare McCabe**, Heriot-Watt University, Scotland

Scientific programme: Talks

Wednesday, May 13th

SPECIAL SESSION – Karel Aim

Room: Arrábida I-II
Chair: Ana Soto and Martin Lisal

08h30 – 08h45	**PRESENTATION IN HONOUR OF KAREL AIM**
	Martin Lisal, Institute of Chemical Process Fundamentals, Czech Republic
08h45 – 09h45	**EXPERIMENTS AND MODELLING AT MODERATE AND HIGH PRESSURES: CHALLENGES AND PERSPECTIVES**
PS	**Catinca Secuianu,** Nat. Univ. of Sci. and Tech. Politehnica Bucharest, Romania
09h45 – 10h45	**NEW EQUATIONS OF STATE: FROM NON-SPHERICAL TO CONFINED PARTICLES**
PS	**Luís F. M. Franco**, Universidade Estadual de Campinas, Brazil

PARALLEL SESSIONS VIII – Molecular modelling and simulation

Room: Arrábida I-II
Chair: Margarida Costa Gomes

11h05 – 11h25	**INCLUSION COMPLEXATION OF NATIVEAND FUNCTIONALIZED α-, β-, AND γ-CYCLODEXTRINS WITH PFAS**
Oral	**Bowen Sha**, Delft University of Technology, the Netherlands
11h25 – 11h45	**SUSTAINABLE EPOXY NETWORK DESIGN BY MULTISCALE SIMULATION: TOWARDS HIGH PERFORMANCE MEMBRANES FOR GAS SEPARATION**
Oral	**Amro Mohamed**, Heriot-Watt University, Scotland
11h45 – 12h05	**FROM SMALL MOLECULES TO COLLOIDAL ASSEMBLIES - TOWARDS A UNIFYING THEORY OF NANOSCALE MATTER**
Oral	**Thi Vo**, Johns Hopkins University, USA
12h05 – 12h25	**MECHANICAL BEHAVIOR OF POLYMERS UNDER SHOCK LOADING: A MOLECULAR DYNAMICS STUDY**
Oral	**Claire Lemarchand**, Université Paris-Saclay, France
12h25 – 12h45	**READY-TO-USE DURVILLAEA INCURVATE EXTRACT USING EDIBLE DEEP EUTECTIC SOLVENTS**
Oral	**Nicolás F. Gajardo Parra**, Pontificia Universidad Católica de Chile, Chile

PARALLEL SESSIONS VIII – Phase equilibria & LOHC

Room: Arrábida III
Chair: Eva Rodil

11h05 – 11h25	**FROM MOLECULAR SIMULATION TO EQUATION OF STATE: CO2 ADSORPTION ENTHALPIES ON CALF-20**
Oral	**Ana Paula de Barros Barreto Mazó**, Univ. Estadual de Campinas, Brazil

11h25 – 11h45	**THERMODYNAMIC AND DYNAMIC ASPECTS OF GLASS TRANSITION OF WATER AND AQUEOUS SYSTEMS**
Oral	**Vitaly Kocherbitov**, Malmö University, Sweden
11h45 – 12h05	**HOW RENEWABLE CAN GREEN AMMONIA BE? HOW EXERGY COSTS AFFECT NATURAL RESOURCES AVAILABILITY AND IMPACT PLANETARY BOUNDARIES**
Oral	**Alessandro J. T. B. de Lima**, Universidad de Zaragoza, Spain
12h05 – 12h25	**THIRD VIRIAL COEFFICIENT OF HYDROGEN FROM FIRST PRINCIPLES**
Oral	**Philipp Marienhagen**, Universität der Bundeswehr Hamburg, Germany

PARALLEL SESSIONS VIII – Molecular modelling and simulation

Room: Arrábida IV
Chair: Begoña Gonzalez

11h05 – 11h25	**NOVEL COMPUTATION OF THE CO_2 HYDRATE PHASE DIAGRAM: IDENTIFYING THE HYDRATE-LIQUID-VAPOR COEXISTENCE AND QUADRUPLE POINT Q_2**
Oral	**Jesús A. Fernández**, Universidad de Huelva, Spain
11h25 – 11h45	**MONTE-CARLO SIMULATIONS OF VAPOR-LIQUID PHASE EQUILIBRIA OF THE ARGON-XENON BINARY SYSTEM IN THE CONTEXT OF NOBLE GASES DETECTORS**
Oral	**Quentin Berger**, Laboratoire Interdisciplinaire Carnot de Bourgogne, France
11h45 – 12h05	**CONFINED ACTIVE COLLOIDS: WALL ACCUMULATION AND MOTILITY-INDUCED PHASE SEPARATION**
Oral	**Martin Lisal**, Institute of Chemical Process Fundamentals, Czech Republic
12h05 – 12h25	**PREDICTING EQUILIBRIUM AND KINETICS OF ESTERIFICATION REACTIONS USING ELECTROLYTE THERMODYNAMICS AND THE IMPORTANCE OF H_3O^+ ACTIVITY**
Oral	**Paul Figiel**, TU Dortmund, Germany

CLOSING SESSION

Room: Arrábida I-II

12h45 – 13h15	**CLOSING SESSION**

Scientific programme: Posters

Monday, May 11th: 19h10-19h55

Tuesday, May 12th: 18h45-19h30

Room: Conference centre

PHASE EQUILIBRIA

P01	**BUBBLE POINT PRESSURE MEASUREMENTS AND PREDICTIONS FOR DIMETHYL ETHER-CHLOROFORM-ETHANOL AND PROPANE-CHLOROFORM-ETHANOL AT 313.15 K** **Tomoya Tsuji**, Universiti Teknologi Malaysia, Malaysia
P02	**SURFACE TENSION OF n-ALKANE MIXTURES: MODEL COMPARISION AND PERFORMANCE ANALYSIS** **Virginia Vadillo-Rodríguez**, Universidad de Extremadura, Spain
P03	**Fives ProSim, A RANGE OF PROCESS ENGINEERING SOFTWARE DEDICATED TO INDUSTRIALS AND MODEL DEVELOPERS** **Edouard Moine**, Fives ProSim, France
P04	**IMPACT OF NANOSTRUCTURING ON THE CHEMICAL AND PHASE EQUILIBRIA OF SWITCHABLE HYDROPHOBICITY SOLVENTS** **Tanja Traini**, Technical University of Munich, Germany
P05	**A NOVEL METHOD FOR MULTIPHASE EQUILIBRIUM CALCULATIONS FOR CO_2-WATER-HYDROCARBON MIXTURES** **Juan Heringer**, University of Pau, France
P06	**THERMODYNAMIC MODELLING OF CARBON DIOXIDE, WATER AND SODIUM CHLORIDE SYSTEMS AT MODERATE PRESSURES** **Renato M. M. Barcellos**, Federal University of Rio de Janeiro, Brazil
P07	**CHARACTERISATION AND MODELLING OF LIQUID-LIQUID EQUILIBRIA FOR NOVEL TERNARY SYSTEMS CONTAINING WATER AND ETHYL ACETATE** **Pedro Velho**, University of Porto, Portugal
P08	**POLYMER-BASED AQUEOUS TWO-PHASE SYSTEMS AS A SUSTAINABLE SEPARATION STRATEGY FOR THE TEXTILE INDUSTRY: DYE PARTITIONING** **Afonso M. Madaleno**, University of Porto, Portugal
P09	**AQUEOUS TWO-PHASE SYSTEMS BASED ON GREENER SOLVENTS: PHASE EQUILIBRIA, THERMODYNAMIC MODELLING AND AMOXICILLIN REMOVAL** **Eduardo Sousa**, Faculdade de Engenharia da Universidade do Porto, Portugal
P10	**SOLUBILITY OF BIOACTIVE COMPOUNDS CONTAINED IN SPENT COFFEE GROUND: COMPUTATIONAL SCREENING AND EXPERIMENTAL DATA** **Emilio J. González**, Universidad Politécnica de Madrid, Spain
P11	**DENSITY GRADIENT THEORY FOR INTERFACIAL TENSION: CUBIC EoS AND FLORY-HUGGINS APPROACHES** **Anna Šmídová**, University of Chemistry and Technology Prague, Czech Republic

P12	**PHASE EQUILIBRIA, eNRTL MODELLING AND QUANTUM-INFORMED FORCE-FIELDS: AQUEOUS BIPHASIC SYSTEMS BASED ON SODIUM FORMATE** **Eugénia A. Macedo**, University of Porto, Portugal
P13	**DETERMINATION OF HENRY'S LAW COEFFICIENTS OF CO_2 IN CYRENE** **Valentina Schiattarella**, Politecnico di Milano, Italy
P14	**MODELING THE COMPLETE PEG/CITRATE AQUEOUS TWO-PHASE SYSTEM PHASE DIAGRAM** **René Gómez-Pineda**, Universidade de Santiago de Compostela, Spain
P15	**DETERMINATION AND PREDICTION OF EXCESS MOLAR ENTHALPIES AT HIGH PRESSURE OF THE BINARY SYSTEMS CARBON DIOXIDE + BIO-BASED SOLVENT** **Taichi Izawa**, Nihon University, Japan
P16	**SURFACE TENSION FOR 27 ALKENES. SELECTION OF DATA AND CORRELATION WITH THE TEMPERATURE** **Ángel A. Mulero.**, Universidad de Extremadura, Spain
P17	**SCREENING OF AQUEOUS TWO-PHASE SYSTEMS FOR FISH PROTEIN RECOVERY** **Eva Rodil**, Universidade de Santiago de Compostela, Spain
P18	**PHASE TRANSITIONS OF POLYMER NETWORKS UNDER TENSION** **Michele Valsecchi**, Columbia University, USA
P19	**MOFs AS POTENT ICE RECRYSTALLIZATION INHIBITORS: MECHANISTIC INSIGHTS FROM MACHINE LEARNING AND MOLECULAR SIMULATIONS** **Jayant K. Singh**, Indian Institute of Technology, India

MOLECULAR MODELLING AND SIMULATION

P20	**EVALUATION OF EXCESS SURFACE TENSIONS AT NORMAL AND HIGH PRESSURE FOR BINARY AND TERNARY SYSTEMS USING WILSON- AND ASOG-SURTENSION MODELS** **Katsumi Tochigi**, Nihon University, Japan
P21	**MOLECULAR DYNAMICS SIMULATIONS OF THE DIELECTRIC CONSTANT OF R410A** **Estefânia P. Canzian**, Universidade Estadual de Campinas, Brazil
P22	**THERMODYNAMIC BEHAVIOUR OF 2-(2-ETHOXYETHOXY)ETHANOL + 1-ALKANOL MIXTURES: EXCESS MOLAR ENTHALPIES AND MOLECULAR INTERACTIONS** **Fernando Aguilar Romero**, University of Burgos, Spain
P23	**SIMULATION OF THE N_2 HYDRATE-WATER INTERFACIAL FREE ENERGY FROM COMPUTER SIMULATION ALONG THE DISSOCIATION LINE OF THE N_2 HYDRATE** **Miguel J. T. Ríos**, Universidad de Huelva, Spain
P24	**MOLECULAR DYNAMICS INSIGHTS INTO SOLVENT-BIOMASS INTERACTIONS IN GREEN SOLVENT MIXTURES** **Vojtěch Jeřábek**, University of Chemistry and Technology Prague, Czech Republic
P25	**EFFECTS OF FORCE FIELDS ON THE MECHANICAL PROPERTIES OF CALF-20 VIA MOLECULAR DYNAMICS SIMULATIONS** **Gabriel Pereira da Silva**, Universidade Estadual de Campinas, Brazil

P26	**REQUIREMENTS AND LIMITATIONS FOR OPTIMISED PROPERTY PACKAGES IN PROCESS SIMULATION - A CASE STUDY ON AROMATICS EXTRACTION** **António J. Queimada**, KBC, United Kingdom

IONIC LIQUIDS / EUTECTIC SOLVENTS / SUPERCRITICAL FLUIDS

P27	**DENSITY AND SURFACE-TENSION MODELING OF BINARY MIXTURES CONTAINING A DEEP EUTECTIC SOLVENT** **Ricardo Macías-Salinas,** Instituto Politécnico Nacional, Mexico
P28	**DEEP EUTECTIC SOLVENTS AS GREEN AGENTS FOR DYE REMOVAL AND TEXTILE RECYCLING** **Begoña González,** Universidad de Vigo, Spain
P29	**FROM SOLUBILITY TO EXTRACTION PROCESSES: GELATINE FROM FISH SKIN** **Alexandra Cáceres**, Universidade de Santiago de Compostela, Spain
P30	**SYNTHESIS AND THERMOPHYSICAL CHARACTERISATION OF BINARY MIXTURES CONTAINING BIO-BASED IONIC LIQUIDS: CHOLINE L-THREONINATE** **Pedro Velho**, University of Porto, Portugal
P31	**APPLICATION OF HYDROPHILIC AND HYDROPHOBIC DEEP EUTECTIC SOLVENTS FOR THE EXTRACTION OF CAFFEINE AND PIPERINE** **Aleksandra Sander,** University of Zagreb, Croatia
P32	**PHASE EQUILIBRIA AND THERMAL DECOMPOSITION OF BINARY EUTECTIC SYSTEMS: QUATERNARY AMMONIUM SALTS AND FATTY ACIDS** **Sérgio A. M. Vilas-Boas,** Universidade de Santiago de Compostela, Spain
P33	**CARBON DIOXIDE ABSORPTION IN AN EQUIMOLAR MIXTURE OF TWO ACETATE-BASED IONIC LIQUIDS** **Ana Soto**, Universidade de Santiago de Compostela, Spain
P34	**THE IONIC LIQUID 1-ETHYL-3-METHYLIMIDAZOLIUMPROPIONATE AS ENTRAINER FOR THE DETERPENATION OF CITRUS ESSENTIAL OIL BY SOLVENT EXTRACTION** **Héctor Rodríguez**, Universidade de Santiago de Compostela, Spain
P35	**RATIONAL SCREENING AND PRE-DESIGN OF DEEP EUTECTIC SOLVENTS FOR BIOMASS FRACTIONATION VIA COSMO-RS AND soft-SAFT** **Fèlix Llovell,** Universitat Rovira i Virgili, Spain

CARBON CAPTURE, UTILISATION AND STORAGE

P36	**MODELLING OF LIGHT-DRIVEN CO_2 CAPTURE USING THE ePC-SAFT EQUATION OF STATE** **Gustavo Chaparro**, ETH Zurich, Switzerland
P37	**FLUE GAS AND DESALINATION FROM SEAWATER WITH CYCLOPENTANE HYDRATES: THERMODYNAMIC EXPERIMENTS AND MODELLING, KINETIC INFLUENCE** **Baptiste Bouillot**, École des Mines Saint-Etienne, France
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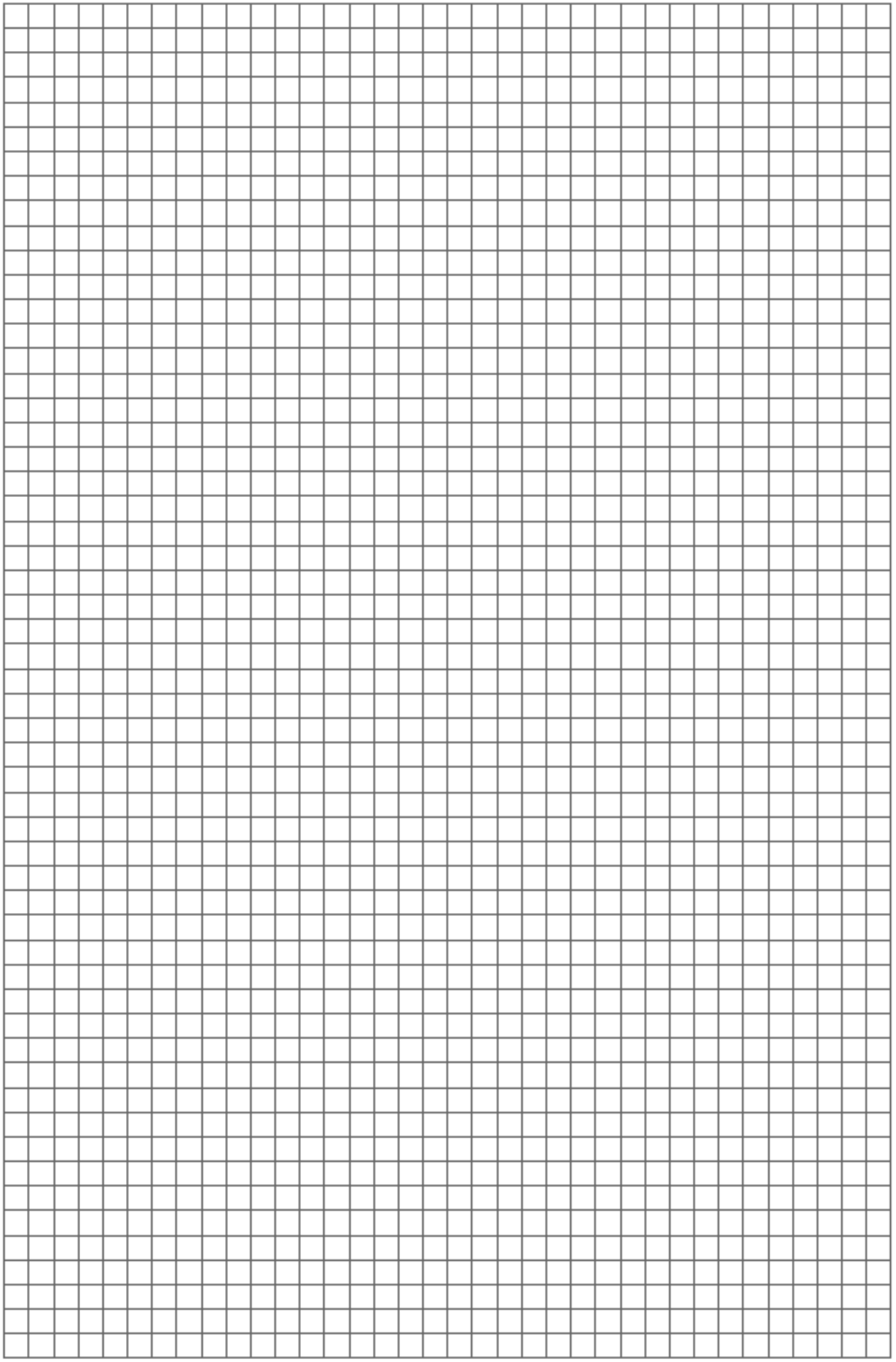

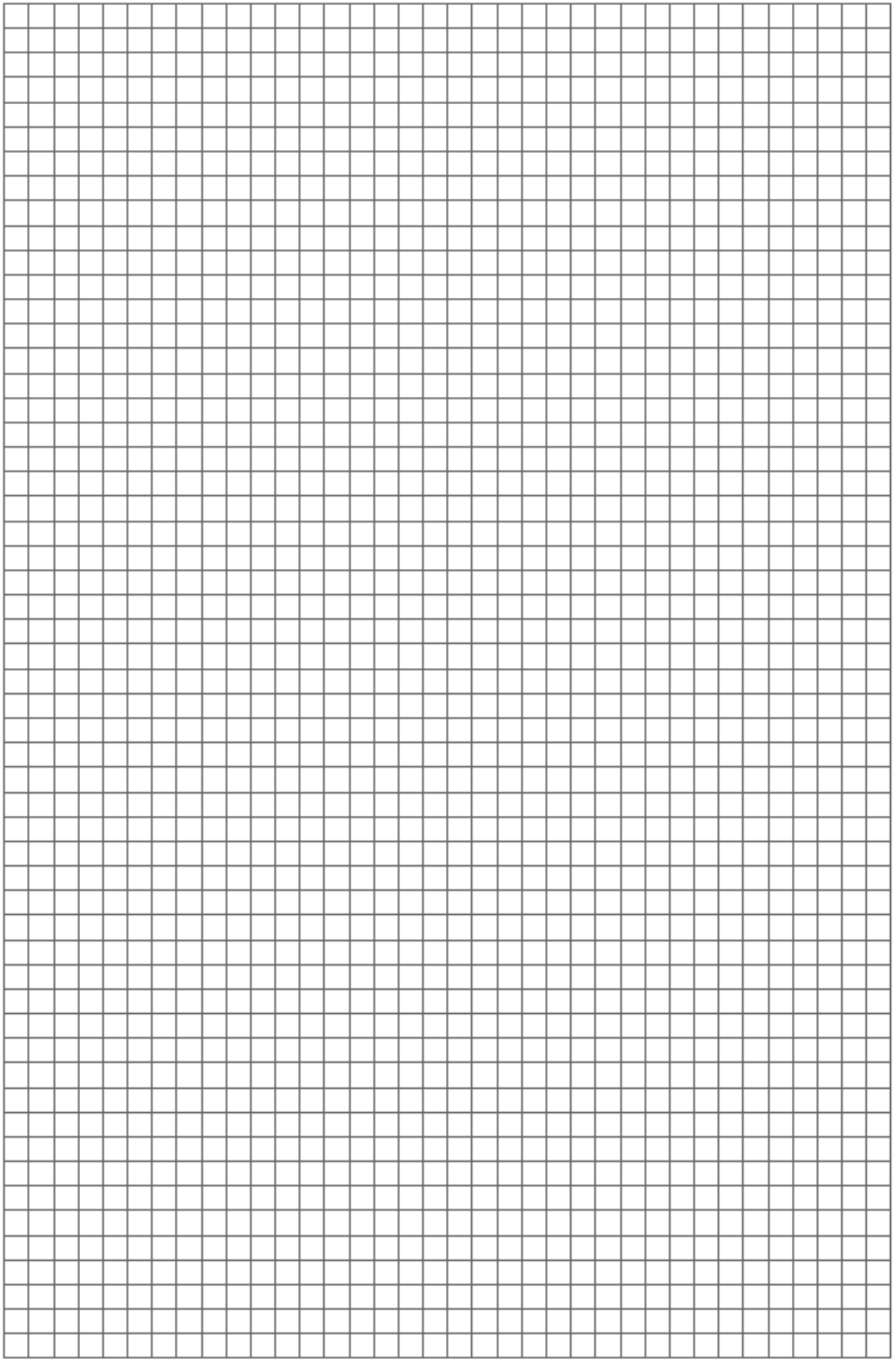

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