EQUIFASE 2024
Program

	9th September (Monday)
11.00 15.00	**Registration**
15.00 15.10	**Opening Session**
15.10 15.20	
15.20 15.30	
15.30 15.40	**IL1 - Walter Chapman** *Towards Linking Engineering Workflows: Phase Behavior, Self-Assembly, and Fluctuations from Thermodynamic Perturbation Theory and Molecular Simulation*
15.40 15.50	
15.50 16.00	
16.00 16.10	
16.10 16.20	**O1.1 - Velisa Vesovic** Predicting the Viscosity of Liquid Mixtures
16.20 16.30	
16.30 16.40	**O1.2 - Gustavo Chaparro** Multiphase parametrization of quasi-spherical Mie particles
16.40 16.50	
16.50 17.00	**O1.3 - Andrés Mejía** Reliable prediction of VLE in mixtures using the SAFT VR Mie EoS
17.00 17.10	
17.10 18.00	
18.00 20.00	**Welcome Reception**

EQUIFASE 2024
Program

		10th September (Tuesday)
9.00	9.10	**IL2 - Carlos Vega**
9.10	9.20	*Simulations of water and electrolyte solutions: where are we?*
9.20	9.30	
9.30	9.40	
9.40	9.50	**O2.1 - German Perez-Sanchez**
9.50	10.00	Interactions between phospholipid membranes and drug nanocarriers through CG sims.
10.00	10.10	**O2.2 - Leslie V. Woodcock**
10.10	10.20	Physical-constant Fluid EoSs Using Boyle and Rigidity-Symmetry Lines: Water-Steam Example
10.20	10.30	**O2.3 - Mariana Hoyer Moreira**
10.30	10.40	Characterizing K+-Based Conductive Hydrogels through Exp. and Comput. Analysis
10.40	11.10	**coffee break**
11.10	11.20	**IL3 - Frederico W. Tavares**
11.20	11.30	*Thermodynamics of Confined Fluids via EoS, DFT, and Molecular Simulation*
11.30	11.40	
11.40	11.50	
11.50	12.00	**O3.1 - Felipe Mourão Coelho**
12.00	12.10	Dielectric Constant Tensor of Electrolyte Solutions Confined by Quartz Crystals via MD
12.10	12.20	**O3.2 - David A. Kofke**
12.20	12.30	Virial Equation of State Using Volume-Dependent Coefficient
12.30	12.40	**O3.3 - Luís Franco**
12.40	12.50	H and S of Mixing of Hydrocarbon Mixtures: Insights from Molecular Simulations
12.50	14.30	**Lunch**
14.30	14.40	**IL4 - José Palomar**
14.40	14.50	*Carbon Capture and Conversion Thermodynamics:*
14.50	15.00	*How to Promote Process Efficiency*
15.00	15.10	
15.10	15.20	**O4.1 - Arthur B. Weidmann**
15.20	15.30	Nucleation and growth of mixed CO2 and C3H8 hydrates through MD simulations
15.30	15.40	**O4.2 - Rafael de P. Soares**
15.40	15.50	Addressing Hydrogen Bond Cooperativity in Modern Quasi-Chemical Methods
15.50	16.00	**O4.3 - Martín Cismondi Duarte**
16.00	16.10	yaeos: Yet Another Equation of State Library
16.10	16.40	**coffee break**
16.40	18.00	**Poster Session**

EQUIFASE 2024
Program

		11th September (Wednesday)
9.00	9.10	**IL5 - Clare McCabe** *Understanding the Self-Assembly of Skin Lipids from* *Molecular Dynamics Simulations: A Multiscale Perspective*
9.10	9.20	
9.20	9.30	
9.30	9.40	
9.40	9.50	**O5.1 - Eugénia A. Macedo** The impact of the nonrandomness factor on biomolecule partitioning in green ATPS
9.50	10.00	
10.00	10.10	**O5.2 - Jorge F. B. Pereira** New insights into the molecular interactions governing PEG/PPG ATPS formation
10.10	10.20	
10.20	10.30	**O5.3 - Oscar Rodríguez** PEG/sodium citrate ATPS: phase diagrams & fish protein partitioning
10.30	10.40	
10.40	11.10	**coffee break**
11.10	11.20	**IL6 - Carlos M. Silva** *Advancements in Supercritical Fluid Extraction:* *Research-Based Strategies for Effective Scale-Up and Design*
11.20	11.30	
11.30	11.40	
11.40	11.50	
11.50	12.00	**O6.1 - Murilo L. Alcantara** Thermodynamic Insights into Thiocyanate-Enhanced ATPS for Redox Flow Batteries
12.00	12.10	
12.10	12.20	**O6.2 - Mariana Pereira** FPE modelling to enhance downstream processes in the pharmaceutical industry
12.20	12.30	
12.30	12.40	**O6.3 - Antonio Marcilla** On the quality of exp. phase equilib. data at moderate pressure. Determination and correlation
12.40	12.50	
12.50	14.30	**Lunch**
14.30	14.40	**IV E. Brignole Lecture:** **IL7 - Fèlix Llovell** *The Key Role of Computational Thermodynamics in Developing* *Sustainable Solutions for the Mitigation of Greenhouse Gases*
14.40	14.50	
14.50	15.00	
15.00	15.10	
15.10	15.20	
15.20	15.30	
15.30	15.40	**O7.1 - Pedro Morgado** PFAS Surfactants – Molecular Modelling and Simulation for Environmental Remediation
15.40	15.50	
15.50	16.00	**O7.2 - Tiago M. Eusébio** Novel Fluorinated Surfactant-Free Microemulsions: Bulk and Interface Behaviour
16.00	16.10	
16.10	16.20	**coffee break**
16.20	16.30	
16.30	16.40	
16.40	18.00	**Poster Session**
18.00	19.00	
19.00	21.00	**Conference Dinner**

EQUIFASE 2024
Program

		12th September (Thursday)
9.00	9.10	**IL8 - Aaron M. Scurto** *Ionic Liquid Mixtures with Compressed Hydrofluorocarbon Gases: Thermophysical Properties, Spectroscopy, and X-ray Scattering*
9.10	9.20	
9.20	9.30	
9.30	9.40	
9.40	9.50	**O8.1 - Silvana Mattedi** Thermodynamic and micellization behavior of protic ILs in aqueous medium
9.50	10.00	
10.00	10.10	**O8.2 - Dinis O. Abranches** Combining High Throughput Experiments and Active Learning to Characterize DESs
10.10	10.20	
10.20	10.30	**O8.3 - Neeraj Rai** Thermal and Coverage Effects in Heterogeneous Catalysis using ML Interatomic Potentials
10.30	10.40	
10.40	11.10	**coffee break**
11.10	11.20	**IL9 - Margarida Bastos** *Isothermal Titration Calorimetry as a Tool in Phase Transfer Studies*
11.20	11.30	
11.30	11.40	
11.40	11.50	
11.50	12.00	**O9.1 - Simão P. Pinho** An Overview of the Salt Effect on the Solubility of Biomolecules
12.00	12.10	
12.10	12.20	**O9.2 - Sofia C. Aparício** Natural solvent systems for plastic recycling: dissolution-precipitation
12.20	12.30	
12.30	12.40	**Closing Session**
12.40	12.50	
13.00	13.10	
13.10	14.30	**Lunch**