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** *Simulations of water and electrolyte solutions: where are we?*
9.10 – 9.20	
9.20 – 9.30	
9.30 – 9.40	
9.40 – 9.50	**O2.1 - German Perez-Sanchez** Interactions between phospholipid membranes and drug nanocarriers through CG sims.
9.50 – 10.00	
10.00 – 10.10	**O2.2 - Leslie V. Woodcock** Physical-constant Fluid EoSs Using Boyle and Rigidity-Symmetry Lines: Water-Steam Example
10.10 – 10.20	
10.20 – 10.30	**O2.3 - Mariana Hoyer Moreira** Characterizing K+-Based Conductive Hydrogels through Exp. and Comput. Analysis
10.30 – 10.40	
10.40 – 11.10	**coffee break**
11.10 – 11.20	**IL3 - Frederico W. Tavares** *Thermodynamics of Confined Fluids via EoS, DFT, and Molecular Simulation*
11.20 – 11.30	
11.30 – 11.40	
11.40 – 11.50	
11.50 – 12.00	**O3.1 - Felipe Mourão Coelho** Dielectric Constant Tensor of Electrolyte Solutions Confined by Quartz Crystals via MD
12.00 – 12.10	
12.10 – 12.20	**O3.2 - David A. Kofke** Virial Equation of State Using Volume-Dependent Coefficient
12.20 – 12.30	
12.30 – 12.40	**O3.3 - Luís Franco** H and S of Mixing of Hydrocarbon Mixtures: Insights from Molecular Simulations
12.40 – 12.50	
12.50 – 14.30	**Lunch**
14.30 – 14.40	**IL4 - José Palomar** *Carbon Capture and Conversion Thermodynamics: How to Promote Process Efficiency*
14.40 – 14.50	
14.50 – 15.00	
15.00 – 15.10	
15.10 – 15.20	**O4.1 - Arthur B. Weidmann** Nucleation and growth of mixed CO2 and C3H8 hydrates through MD simulations
15.20 – 15.30	
15.30 – 15.40	**O4.2 - Rafael de P. Soares** Addressing Hydrogen Bond Cooperativity in Modern Quasi-Chemical Methods
15.40 – 15.50	
15.50 – 16.00	**O4.3 - Martín Cismondi Duarte** yaeos: Yet Another Equation of State Library
16.00 – 16.10	
16.10 – 16.20	**coffee break**
16.20 – 16.30	
16.30 – 16.40	
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**