Time	Mon 31 August
9:00 - 10:15	Registration and Coffee
10:15 - 10:50	Opening Address Dr Miguel Jorge – Conference Chair Prof Ralf Ludwig – EMLG Chair
Session 1	*Chair: Ralf Ludwig*
10:50 - 11:30	Colin Bain: "Surfactant Assembly and Disassembly far from Equilibrium"
11:30 - 11:50	Doug Cleaver: "Computer simulations of complex self-assembly – and obstinate agglomeration"
11:50 - 12:10	Martin Sweatman: "Integral Equations and Density Functional Theory for the cluster fluid phase of fluids with competing interactions"
12:10 - 12:30	Hirofumi Sato: "Comprehensive Theoretical Approaches to the Self-Assembly Process at the Molecular Level"
12:30 - 13:50	Lunch – TIC foyer
Session 2	*Chair: Abdenacer Idrissi*
13:50 - 14:30	Ellen Backus: "2D Network of PDMS and PEO-PPO-PEO at the air-water interface"
14:30 - 14:50	Pál Jedlovszky: "Structure and Single Particle Dynamics at the Free Surface of Imidazolium-Based Ionic Liquids"
14:50 - 15:10	Hisashi Okumura: "Flow-enhanced self-assembly of amyloid-β peptides studied by nonequilibrium molecular dynamics simulations"
15:10 - 15:30	Judith Mihály: "Molecular Structure and Lipid Ordering at Vesicle–Gold Nanoparticle Interfaces Revealed by SEIRS Spectroscopy"
15:30 - 16:00	Coffee Break – TIC foyer
Session 3	*Chair: Toshiyuki Takamuku*
16:00 - 16:20	Klaas Wynne: "A metastable phase of amorphous aggregates governs solution structure"
16:20 - 16:40	Giancarlo Franzese: "Protein sequestration into biomolecular condensates and hydration water"
16:40 - 17:00	Martina Požar: "Structure-Making Solvation of Ferulic Acid in Protic and Aprotic Solvents: Experiments, Molecular Simulations, and Perspectives on Viscosity"
17:00 - 18:00	EMLG/JMLG Board Meeting: auditorium and Early-Career Networking Session: foyer
18:30 - 20:00	Civic Reception (drinks and nibbles) – Glasgow City Chambers

Time	Tue 1 September
EMLG/JMLG School	*Chair: Giancarlo Franzese* In memoriam Prof. Ruth Lynden-Bell
8:45 - 9:35	Paola Carbone: "Characterizing the electrolyte/graphene interface: an integrated approach with modelling and experiments"
9:35 - 10:25	Barbara Rossi: "What can UV Resonance Raman tell us about molecular liquids? From solutions to self-assembly"
10:25 - 10:50	Coffee Break – TIC foyer
Session 4	*Chair: Martina Požar*
10:50 - 11:10	Dietmar Paschek: "When Theory Meets Experiment: What Does it Take to Accurately Predict ^{1}H NMR Dipolar Relaxation Rates in Neat Liquid Water from Theory?"
11:10 - 11:30	Shinya Hosokawa: "Generalised Langevin Data Analysis for Phonon Dynamics in Liquid Water"
11:30 - 11:50	Ioannis Skarmoutsos: "Structural transitions in liquid water at high temperatures and pressures: A molecular dynamics approach"
11:50 - 12:10	Marcel Brandt: "OrthoBoXY: A Simpler Way to Compute True Self-Diffusion Coefficients and Viscosities from MD Simulations"
12:10 - 12:30	Tom Frömbgen: "A Multifidelity Monte Carlo Approach for Simulating the Diffusion Coefficient of Water"
12:30 - 13:50	Lunch – TIC foyer
Session 5	*Chair: Judith Mihály*
13:50 - 14:30	João Coutinho: "On the Aggregation of Amphiphiles in Water: Hydrotropy as the missing link between salts and surfactants"
14:30 - 14:50	Jule Kristin Philipp-Taube: "How Much Water Is Too Much? Structural and Dynamical Transitions in Solvate Ionic Liquid Electrolytes"
14:50 - 15:10	Pamella da Silva: "Stability and affinity of Plasmodium falciparum proteins in ionic liquids"
15:10 - 15:30	Hideshi Maki: "Relationship between ion pair formation in aqueous solutions and anomalous decrease in NMR signal intensity of solvent"
15:30 - 15:50	Maham Azhar: "Structural and Spectroscopic Evidence of Hydrogen Bonded Anionic Wires in Protic Ionic Liquids"
15:50 - 16:10	Katsura Nishiyama: "Hierarchical Self-Assembly and Sound Attenuation in the Audible-Frequency Region in Phenol–AOT Organogels"
16:10 - 17:00	Coffee Break – TIC foyer
16:30 - 18:00	Poster Session: TIC foyer

Time	Wed 2 September
Session 6	*Chair: Pál Jedlovszky* In memoriam Prof. Pavel Jungwirth
8:45 - 9:25	Venkat Kapil: "Machine learning-based first-principles simulations of nanoconfined water"
9:25 - 9:45	Toshiyuki Takamuku: "LCST-type Phase Separation of Phosphonium-based Ionic Liquid-Water Mixed Solutions"
9:45 - 10:05	Abdenacer Idrissi: "Free energy of mixing of BmimBF4 and water mixtures"
10:05 - 10:25	Jun-Ho Choi: "Mixing, De-mixing and Molecular Aggregation in Aqueous Solutions: Molecular Dynamics Simulation and Graph Theoretical Analysis"
10:25 - 10:45	Marco Paolantoni: "Revisiting the State of Water in [BMIM][BF4] Aqueous Solutions"
10:45 - 11:10	Coffee Break – TIC foyer
Session 7	*Chair: Dietmar Paschek*
11:10 - 11:30	Elixabete Rezabal: "Resolving Oligomeric Anions in Carboxylic Acid–Carboxylate Systems: the case of Choline–Geranate"
11:30 - 11:50	Hideaki Shirota: "Intermolecular Vibrational Band of Deep Eutectic Solvents Composed of Lithium Salt and Amide: Composition Dependence"
11:50 - 12:10	Andrew Mawbey: "Harnessing machine learning for the design and structural classification of periodic mesoporous silica"
12:10 - 12:30	Katrin Jonas: "A Graph-based approach for the structural characterization of macromolecules and their interactions with the environment"
12:30 - 12:50	Oldamur Hollóczki: "Nanoplastics from theoretical chemistry"
12:50 - 13:50	Lunch – TIC foyer
14:00 - 18:00	Conference Excursion New Lanark World Heritage Site
18:00 - 22:00	Gala Dinner: House for an Art Lover

Time	Thu 3 September
Session 8	*Chair: Marco Paolantoni*
8:45 - 9:25	Ed Maginn: "Machine-learning-tuned force fields for refrigerants: transferability across thermophysical properties, state points, and liquid interfaces"
9:25 - 9:45	Dinis Abranches: "AI-Enabled Discovery of Deep Eutectic Solvents and Their Chemical Space"
9:45 - 10:05	Gaopeng Ren: "AI-Driven Discovery of Novel Low-Melting-Point Ionic Liquids"
10:05 - 10:25	Margarida Pinhão: "Predicting Partition Coefficients of Biomolecules in Aqueous Biphasic Systems"
10:25 - 10:45	Fausto Martelli: "The role of interfacial water in stabilizing biological membranes"

Time	Thu 3 September (cont.)
10:45 - 11:10	Coffee Break – TIC foyer
Session 9	*Chair: Ioannis Skarmoutsos*
11:10 - 11:30	Mónika Valiskó: "Cation/anion and monovalent/divalent selectivity in negatively charged nanopores: reduced models versus experiments and molecular dynamics simulations"
11:30 - 11:50	Tetsuro Nagai: "Toward large-scale coarse-grained dynamics simulations of gas diffusion aided by machine-learning in realistic systems"
11:50 - 12:10	Nobuaki Kikkawa: "Oxygen Diffusion in Water- and Ionomer-filled Carbon Mesopores"
12:10 - 12:30	Sergi Ruiz-Barragan: "Water self-dissociation in slit pores displays non-monotonic behavior as a function of water filling"
12:30 - 12:50	Karel Šindelka: "Confined Binary Active Brownian Particles: Preferential Wall Accumulation and Correspondence with Equilibrium Fluid Mixtures"
12:50 - 14:10	Lunch – TIC foyer
Session 10	*Chair: Katsura Nishiyama*
14:10 - 14:50	Nobuyuki Matubayasi: "Cosolvent Effects on Peptide Aggregation Studied with All-Atom MD and a Solvation Theory"
14:50 - 15:10	Norio Yoshida: "Software development and application for material design based on the statistical mechanics theory of liquids"
15:10 - 15:30	Volodymyr Farafonov: "Electrical properties of the inner space of infectious bacteriophage MS2"
15:30 - 15:50	Agaya Johnson: "Coarse-grained model to study the effects of electric fields on protein interactions"
15:50 - 16:10	Coffee Break – TIC foyer
Session 11	*Chair: Mónika Valiskó*
16:10 - 16:30	Toshifumi Mori: "Tuning the water models to elucidate the effect of ATP to disordered proteins in high ATP concentration"
16:30 - 16:50	Myroslav Holovko: "Application of the modern theory of associated fluids for the description of self-assembly phenomena of surfactant molecules. Solubilization of biomolecules in reverse micelles"
16:50 - 17:10	Francisca Benítez: "Deep Eutectic Solvents for Biocatalysis: Advanced Materials and Enzymatic Modulation"
17:10 - 18:00	EMLG/JMLG General Assembly and Closing Session Dr Miguel Jorge – Conference Chair Prof Toshiyuki Takamuku – JMLG Chair