

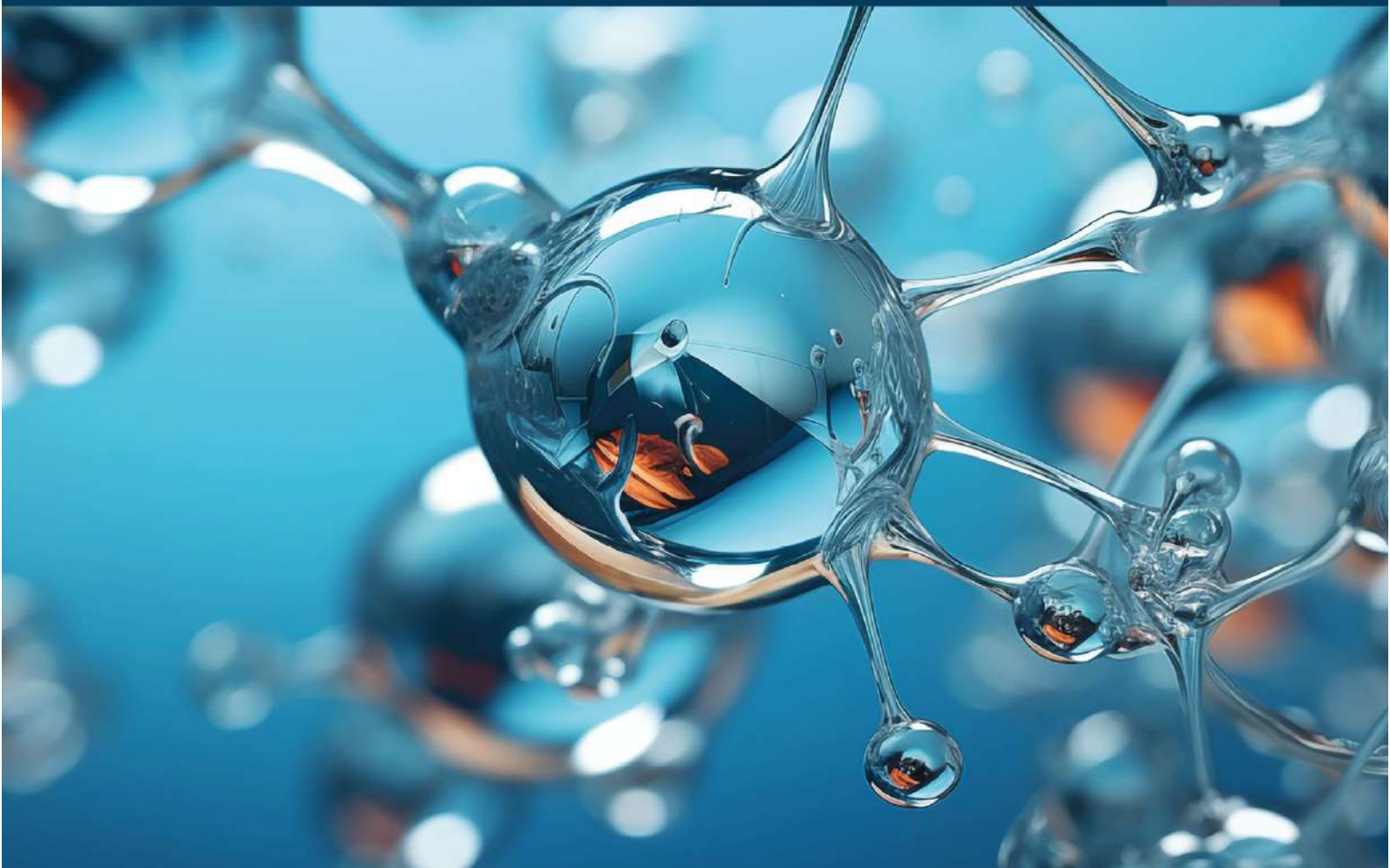
EMLG-JMLG Annual Meeting 2024

Structure and Dynamics of
Hydrogen-Bonded Systems

Trieste, 8-13 September 2024



Programme



Detailed Day-by-day Schedule/Program

Sunday 8th September

17:00 - 20:00	Registration + Welcome Cocktail
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Monday 9th September

8:00 - 8:30	Registration
8:30 - 9:00	Opening
9:00 - 9:40	Paul S. Cremer "Exploring Water Structure at Charged Interfaces"
9:40 - 10:00	Ivo Nezbeda "Structure of water at planar and curved hydrophobic and hydrophilic surfaces: Direct comparison using the α -shape analysis"
10:00 - 10:20	Toshio Yamaguchi "Violation of the structure-making/breaking concept of aqueous alkali metal chloride solutions in the gigapascal pressure range"
10:20 - 10:40	Pal Jedlovsky "Surface affinity of simple ions in aqueous solutions"
10:40 - 11:10	Coffee
11:10 - 11:40	Abdenacer Idrissi "Widom Line in Supercritical Water in Terms of Changes in Local Structure"
11:40 - 12:00	Zoe Macpherson "Hydrogen-Bonding Contributions to the Dipole Moment of Supercritical Water"
12:00 - 12:20	Zahra Tohidi Nafe "Theoretical investigation of dielectric properties of ice"
12:20 - 12:40	François-Alexandre Miannay "Picosecond time-resolved spectroscopic investigations of the Morin and morin-cation complexes fluorescence: towards new techniques for detecting metal pollutants in water"
12:40 - 13:00	Nicolas R de Souza "Emu neutron backscattering spectrometer: capabilities and applications"
13:00 - 14:30	Lunch
14:30 - 14:50	Damien Laage "On the mechanism of excess proton transport in water"
14:50 - 15:10	Pierre Çarçabal "Hydrogen bonding between water molecules and sugars probed in the gas phase"
15:10 - 15:30	Katalin Bere "Effects of Fluorocarbon Chain Length on the Adsorption of Perfluoroalkyl Substances on Nanoplastic Particles"
15:30 - 15:50	Masahiro Higashi "Theoretical study on solvent dependency of photophysical properties"
15:50 - 16:10	Artem Shagurin "Molecular dynamics investigation of interfacial properties of pharmaceutical molecules: curcumin on vacuo and sCO ₂ interfaces"

16:10 - 16:40 **Coffee**

16:40 - 17:00	Luis Miguel Varela Cabo "Hydrogen absorption in ionic liquids"
17:00 - 17:20	Brenda Bracco "Water structures in BMIMBF ₄ aqueous solutions: an insight on H-bond interactions"
17:20 - 17:40	Ioannis Skarmoutsos "Pillared graphene oxide frameworks for the adsorption and separation of dimethylsulfoxide-water mixtures"
17:40 - 18:00	Giancarlo Franzese "The mutual interplay between structure and dynamics of hydrogen bonds at organic and inorganic interfaces"
18:00 - 19:00	EMLG Board Meeting

Tuesday 10th September

9:00 - 9:40	Dmitry Kurouski "Raman and Infrared Imaging of Biological Systems at the Nanoscale"
9:40 - 10:00	Sara Catalini "Aggregation of whey proteins in mixed solutions"
10:00 - 10:20	Dmitry Nerukh "Viruses in aqueous media as colloidal systems: particle's hydrodynamic diameter and zeta-potential, surface charge, and solution stability"
10:20 - 10:40	Denis Rajnovic "Deep UV Raman spectroscopy for probing active eukaryotic viruses"
10:40 - 11:10	Coffee
11:10 - 11:40	Hadrián Montes Campos "Computational Modelling of Hydrogen Bonds in Ionic Liquids"
11:40 - 12:00	Ralf Ludwig "Spectroscopic evidence for doubly hydrogen-bonded cationic dimers in the solid, liquid and the gaseous phases of carboxyl-functionalized ionic liquids"
12:00 - 12:20	Stefano Nejrotti "Non-vehicular proton transport mechanism through rational design of a fluorine-free protic ionic liquid"
12:20 - 12:40	Martín Otero-Lema "Ionic transport mechanism in mixtures of protic ionic liquids"
12:40 - 13:00	Jule Kristin Philipp "Influence of Water on the Transport Properties of Ternary Mixtures with Triglyme and [Li][NTf ₂]"
13:00 - 14:30	Lunch
14:30 - 15:10	Anna Martinelli "Hydrogen bonding in ionic liquids and derivated materials"
15:10 - 16:10	Poster session
16:10 - 16:40	Coffee
16:40 - 19:30	Elettra Visit to Elettra

Wednesday 11th September

9:00 - 9:40	Sylvie Roke "Aqueous Nanoscale Systems"
9:40 - 10:00	Dezső Boda "How to model divalent ions?"
10:00 - 10:20	Filip Moučka "Molecular modeling of alkali halides using phase-transferable models: aqueous solutions, crystalline hydrates, molten salts, and noncovalent bonds"
10:20 - 10:40	Li Zhang "Interfacial Inversion, Interference and IR Absorption in Vibrational Sum Frequency Scattering Experiments"
10:40 - 11:10	Coffee
11:10 - 11:40	Hideaki Shirota "Highly Conductive Deep Eutectic Solvents Using Iodine"
11:40 - 12:00	Lennart Kruse "Hydrogen bonding in ionic liquids: A ¹ H and ¹⁹ F NMR relaxometry study"
12:00 - 12:20	Toshiyuki Takamuku "Extraction of Ni(II) Ion from an Aqueous Solution by Functionalized Ionic Liquids"
12:20 - 12:40	Angel Mary Chiramel Tony "The bottom up approach: frequency dependent relaxation rates from md simulations"
12:40 - 13:00	Olga Russina "Sustainable PET solvation in eutectic solvents"
13:00 - 14:00	Lunch
14:00 - 14:40	Paola D'Angelo "The role of hydrogen-bonds in the formation and structural properties of deep eutectic solvents"
14:40 - 15:40	Poster session + Coffee
15:40 - 19:00	Social Excursion

Thursday 12th September

9:00 - 9:40	Yusuke Morisawa "Investigation of Hydrogen Bonding using the Attenuated Total Reflectance Spectroscopy in the Ultraviolet Region"
9:40 - 10:00	Mischa Flór "Multiscale probing of interactions in aqueous ionic solutions"
10:00 - 10:20	Fabio Novelli "The birth and evolution of solvated electrons in water"
10:20 - 10:40	Marta Monti "Structure and optical properties of water: a study on aqueous solutions and ice"
10:40 - 11:10	Coffee
11:10 - 11:40	Ana Vila Verde "Molecular basis for acidic proteomes in halophilic proteins"
11:40 - 12:00	Valeria Libera "Solvent Vibrations Reflecting Telomere G-Quadruplex Rearrangements during Thermal Unfolding"
12:00 - 12:20	Germaine Neza Hozana "Data Driven Discovery of the Origins of UV-Absorption in Alpha-3C Protein"
12:20 - 12:40	Imre Bakó "Hydration shell structure of ordered and disordered proteins"
12:40 - 13:00	Keisuke Tominaga "Dynamics of Hydrated Soft Matters Studied by Broadband Dielectric Spectroscopy and Molecular Dynamics Simulations"
13:00 - 14:30	Lunch
14:30 - 14:50	Kamil Polok "Exploring 2-propanol and its fluorinated derivatives using femtosecond optical Kerr effect spectroscopy and theoretical chemistry methods"
14:50 - 15:10	Bernarda Lovrinevic "Microscopic dynamics of liquid glycerol in ambient conditions: new insights"
15:10 - 15:30	Thierry Tassaing "Co-localized infrared/Raman spectroscopic investigation of water/H ₂ /N ₂ /CO ₂ mixtures at high pressure and temperature"
15:30 - 16:10	Poster session
16:10 - 16:40	Coffee
16:40 - 17:00	Tetsuro Nagai "Dynamic Monte Carlo method enhanced by machine learning model to understand mass transport in heterogeneous medium"
17:00 - 17:20	Mikel Loizate "Understanding the Molecular Structure of Choline Geranate (CAGE): Insights from Molecular Dynamics Simulations"
17:20 - 17:40	Katsura Nishiyama "Properties of binary organogels comprising phenol and anionic surfactant investigated by sound damping and dielectric relaxation measurements"
17:40 - 18:00	Laszlo Almasy "Small-angle neutron scattering and Raman spectroscopy studies of solvation behavior in aqueous solutions of alcohols, amines and ionic liquids"
18:00 - 19:00	EMLG General Assembly
20:30	Social Dinner

Friday 13th September

9:00 - 9:40	Ali A Hassanali "Chemical Continuum: Overcoming Discrete Notions Underlying Fluctuations in Water"
9:40 - 10:00	Andrij Trokhymchuk "Thermodynamics of hydrogen bonding liquids using the van der Waals concept"
10:00 - 10:20	Matteo Busato "Ag ⁺ ion coordination in molecular solvents: a complex case study"
10:20 - 10:40	Cesare Malosso "Evidence of ferroelectric features in low-density supercooled water from ab initio deep neural-network simulations"
10:40 - 11:10	Coffee
11:10 - 11:40	Letizia Tavagnacco "Investigation of polymer networks using atomistic simulations"
11:40 - 12:00	Miguel Jorge "Sticky-MARTINI – A Reactive Coarse-Grained Model for Self-Assembly"
12:00 - 12:20	Vitalii Bardyk "Multiscale Hybrid Model for Liquids: Coupling Molecular Dynamics with Hydrodynamics in Simulations"
12:20 - 12:40	Ari Paavo Seitsonen "Stress fluctuations and adiabatic speed of sound in liquids: A simple way to estimate Cs from simulations"
12:40 - 13:00	Edward Danquah Donkor "Beyond Local Structures in Critical Supercooled Water through Unsupervised Learning"
13:00 - 14:30	Lunch
14:30 - 14:50	Martina Pozar "Charge order and the absence of scattering pre-peak in alkylamines"
14:50 - 15:10	Abdulkareem Ummer "Exploring the Complexity of Hydrogen-Bonded Liquids Through Voronoi Entropy"
15:10 - 15:30	Fatima Matroodi "Exploring Hydrogen Bonding structures in Aqueous Solutions of Imidazolium-based Protic Ionic Liquids through UV Resonance Raman Spectroscopy"
15:30 - 15:50	Ana Licia Gomes "Photophysics of the indoline derivative photosensitizer D205: investigation on the influence of the binary mixture 1-butanol/acetonitrile"
15:50 - 16:10	Closure
16:10 - 16:40	Coffee