Conference Program

Wednesday, 5 September

17.40-18.00: Conference opening

Session 1 (chair: Pál Jedlovszky):

18.00-19.00: **Gábor Pálinkás** (Budapest, Hungary): *Characterization of supramolecular associations in solution*

19.00-21.00: Welcome reception

Thursday, 6 September

Session 2 (chair: Hajime Torii):

08.30-09.30: **Colin Bain** (Durham, UK): *Micelle processes at surfaces and in solution*

09.30-09.50: **Martin Lísal** (Prague, Czech Republic): *Chiral room-temperature ionic liquids: insight from molecular dynamics simulations*

09.50-10.10: **Ralf Ludwig** (Rostock, Germany): *Low-frequency modes of protic molten salts and ionic liquids: detecting and quantifying hydrogen bonding*

10.10-10.30: **Bogdan Marekha** (Kiev, Ukraine): *Microscopic structure of ion pairs formed by [$Bmim^+BF_4^-$] and [$Bmim^+TfO^-$]*

10.30-11.00: Coffee break

Session 3 (chair: Philippe Bopp):

11.00-12.00: **Miguel Jorge** (Porto, Portugal): *Ionic liquid interfaces: new insights from molecular simulation*

12.00-12.20: **Hideaki Shirota** (Chiba, Japan): *Microscopic aspect of ionic liquid and water mixtures probed by femtosecond raman-induced kerr effect spectroscopy*

12.20-12.40: **Eliane Schmidt** (Rostock, Germany): *The influence of the cation and the anion on the diffusion coefficients of ionic liquids in different solvents*

12.40-13.00: **Toshiyuki Takamuku** (Saga, Japan): *Substituent effects on mixing of ionic liquid with benzene derivatives*

13.00-14.30: Lunch

Session 4 (chair: Mauro Rovere):

14.30-15.30: **Ilan Benjamin** (Santa Cruz, USA): *Fluid interface fluctuations and chemical reactivity*

15.30-15.50: **George Horvai** (Budapest, Hungary): *Experiences with the ITIM model in simulating liquid surfaces and interfaces*

15.50-16.10: **Marcello Sega** (Rome, Italy): *Interfacial properties of water: an atomistic perspective on hydrodynamic problems*

16.10-16.30: **Mária Darvas** (Budapest, Hungary): *Computer simulation study of the transfer of simple and composite ions through water/organic interface – an intrinsic approach*

16.30-17.00: Coffee break

Session 5 (chair: Myroslav Holovko):

17.00-18.00: **Geraldine Richmond** (Eugene, USA): *Line 'em all up: Assembly of surfactants, macromolecules and nanoparticles at liquid-liquid interfaces*

18.00-18.20: **Milan Předota** (Ceske Budejovice, Czech Republic): *Molecular dynamics determination of the dynamic properties of the solid–liquid interface*

18.20-18.40: **Dung di Caprio** (Paris, France): *Fluctuations effects at confining interfaces. Depletion density profiles*

18.40-19.00: **Takayoshi Kimura** (Osaka, Japan): *Enthalpic interactions of chiral limonenes in some aliphatic alcohols*

19.00-22.00: Wine tasting (optional event)

Friday, 7 September

Session 6 (chair: Renzo Vallauri):

08.30-09.30: **Marie-Paule Pileni** (Paris, France): *Nanocrystallinity and supracrystallinity: a real challenge*

09.30-09.50: **Mikhail Kiselev** (Ivanovo, Russia): *The conformational manifolds of drug-like molecules as studied in combination of experimental and computational techniques*

09.50-10.10: **Dominik Horinek** (Regensburg, Germany): *Stability of peptides in urea/water mixtures*

10.10-10.30: **Dezső Boda** (Veszprém, Hungary): *Selectivity and conduction of a model calcium channel studied by the NP+LEMC method*

10.30-11.00: Coffee break

Session 7 (chair: Abdenacer Idrissi):

11.00-12.00: **Miklós Zrínyi** (Budapest, Hungary): *Complex fluids and polymer networks: a fascinating alliance*

12.00-12.20: **Sofia Kantorovich** (Rome, Italy): *Structure factor of the self-assembling short DNA duplexes: theory and coarse-grained simulations*

12.20-12.40: **Koji Yoshida** (Fukuoka, Japan): *Alcohol effect on structure, dynamics, and aggregation of peptide and protein*

12.40-13.00: **Zuzana Benková** (Porto, Portugal): *Molecular dynamics study of water interacting with siloxane surface modified by poly(ethylene oxide) chains*

13.00-14.30: Lunch

Session 8 (chair: Toshio Yamaguchi):

14.30-15.30: **Mikhail Avdeev** (Dubna, Russia): *Particle interaction in polydisperse magnetic fluids: experimental aspects*

15.30-15.50: **Elena Pyanzina** (Ekaterinburg, Russia): *Ground state of magnetic particles with shape anisotropy*

15.50-16.10: **István Szalai** (Veszprém, Hungary): *Nonlinear magnetic properties of ferrofluids*

16.10-16.30: **Elena Minina** (Stuttgart, Germany): *Various methods of pressure calculation for polydisperse ferrofluids in bulk and confinement*

16.30-17.00: Coffee break

17.00-19.00: POSTER SESSION

19.00-20.00: EMLG/JMLG Board Meeting

Saturday, 8 September

Session 9 (chair: Ivo Nezbeda):

08.30-09.30: **Akihiro Wakisaka** (Tsukuba, Japan): *Molecular clustering inherent in the liquid state: Effect of relativity in the intermolecular interaction energies*

09.30-09.50: **Toshio Yamaguchi** (Fukuoka, Japan): *Thermal behaviour, structure and dynamics of low temperature water confined in periodic mesoporous organosilica*

09.50-10.10: **Mauro Rovere** (Roma, Italy): *Do ions affect the structure of water? Ion hydration and structure of water in supercooled aqueous solutions: a test of the structure making and breaking concept*

10.10-10.30: **Myroslav Holovko** (Lviv, Ukraine): *The scaled particle theory for fluids in random porous media*

10.30-11.00: Coffee break

Session 10 (chair: Wojciech Gadomski):

11.00-12.00: **Maria Antonietta Ricci** (Roma, Italy): *Proton momentum distribution and kinetic energy in water*

12.00-12.20: **Ari Seitsonen** (Zürich, Switzerland): *Solvation of flavonoids in organic solvents: Study using ab initio molecular dynamics*

12.20-12.40: **Hajime Torii** (Shizuoka, Japan): *Electronic reorganizations induced by intra- and intermolecular vibrational dynamics and spectral intensities in liquid water*

12.40-13.00: **Shinya Hosokawa** (Kumamoto, Japan): *Collective dynamics of molecular liquids*

13.00-14.30: Lunch

14.30-19.00: Conference Excursion (to the Miskolctapolca cave bath)

19.00-23.00: Conference Banquet

Sunday, 9 September

Session 11 (chair: Toshiyuki Takamuku):

08.30-09.30: **Nobuyuki Matubayasi** (Kyoto, Japan): *Effects of water and cosolvent on functional molecules in solution*

09.30-09.50: **Ivo Nezbeda** (Prague, Czech Republic): *Excluded volume versus hydrogen bonding: Complementary or incompatible concepts?*

09.50-10.10: **Nikolai Medvedev** (Novosibirsk, Russia): *Calculation of the volumetric characteristics on molecular dynamics models of solutions. Ability and pitfalls*

10.10-10.30: **Alexander Kaiser** (Innsbruck, Austria): *Visualization of long- and short-lived hydrogen-bonded clusters in liquid ethylene-glycole*

10.30-11.00: Coffee break

Session 12 (chair: Richard Buchner):

11.00-11.40: **Yoshihito Osada** (Wako, Japan): *Artificial muscle - soft and wet nano-biomachine of the next era*

11.40-12.00: **Koichiro Sadakane** (Tokai, Japan): *Do ions affect the structure of water? Ion hydration and structure of water in supercooled aqueous solutions: a test of the structure making and breaking concept*

12.00-12.20: **Imre Bakó** (Budapest, Hungary): *Electronic structure of liquid water*

12.20-12.40: **Péter Kiss** (Budapest, Hungary): *From high pressure ice to gas clusters of water*

12.40-13.00 EMLG/JMLG General Assembly

13.00-14.30: Lunch

List of Posters

Szabolcs Bálint (Budapest, Hungary): *The structure of aqueous sodium and gallium hydroxide solutions – a combined solution X-ray diffraction and simulation study*

Marina Fedotova (Ivanovo, Russia): *3D-RISM study of ion-molecular complex formation of glycine zwitterion with inorganic ions in biologically relevant aqueous electrolyte solutions*

Marina Fedotova (Ivanovo, Russia): *The hydration of aniline and benzoic acid: Analysis of radial and spatial distribution functions*

György Hantal (Cambridge, USA): *Locality and energetics of charge transfer effects in ionic liquids*

Zoltán Ható (Veszprém, Hungary): *Direct simulation of steady-state diffusion by classical Monte Carlo methodologies*

Silke Heckhausen (Rostock, Germany): *Computer simulation study of molecular processes in ice and supercooled solutions*

Myroslav Holovko (Lviv, Ukraine): *Maier-Saupe nematogenic fluid in contact with a hard wall: bulk and surface properties*

Myroslav Holovko (Lviv, Ukraine): *Thermodynamics for a fluid of hard spherocylindrical rods in random porous media*

Yuka Horikawa (Tokyo, Japan): *Electronic state of liquid molecules observed by soft X-ray emission spectroscopy*

Shinya Imura (Fukuoka, Japan): *Molecular dynamic simulation of 10 residues peptide in fluoroalcohol - water mixtures*

Yutaro Inada (Kusatsu, Japan): *High-pressure solubility of benzene in water at temperatures between 288.2 K and 318.2 K*

Angéla Jedlovszky-Hajdú (Budapest, Hungary): *Magnetoresponsive 2D and 3D electrospun scaffold for tissue engineering*

Angéla Jedlovszky-Hajdú (Budapest, Hungary): *The effect of adsorbed carboxyl groups on magnetite nanoparticles in water relaxation*

Jan Jirsák (Ústí nad Labem, Czech Republic): *Hydration thermodynamics of nonpolar solutes by simple molecular models*

Yasuo Kameda (Yamagata, Japan): *Solvation structure of Li^+ in concentrated $LiPF_6$-DMC solutions studied by neutron diffraction with $^6Li/^7Li$ isotopic substitution method*

Alexandra Kim (Novosibirsk, Russia): *MD-study of volumetric and hydrophobic properties of the amphipile molecule C_8E_6*

Ekaterina Krutikova (Ekaterinburg, Russia): *Anisotropy of a structure factor of polydisperse magnetic nanofluids under an external field*

Elena Minina (Stuttgart, Germany): *Virial coefficients for the systems of magnetic dipolar spheres: the influence of confinement*

Maurizio Musso (Salzburg, Austria): *The noncoincidence effect of the overtone of the C=O stretching mode of acetone*

Bernd Mühldorf (Regensburg, Germany): *Dynamics, hydration and ion association in aqueous solutions of ionic liquids based on oligoether carboxylates*

Saidmuhamad Odinaev (Dushanbe, Tajikistan): *Investigation of the law of corresponding states for the viscous properties of classical liquids*

Saidmuhamad Odinaev (Dushanbe, Tajikistan): *On the determination of the range of frequency dispersion of dynamical coefficients of viscosity of aqueous solutions of electrolytes*

Stanislav Pařez (Prague, Czech Republic): *Determination of distance-dependent viscosity of mixtures in parallel slabs using non-equilibrium molecular dynamics*

Stanislav Pařez (Prague, Czech Republic): *Mutual diffusion in the ternary mixture water + methanol + ethanol and its binary subsystems*

Dietmar Paschek (Rostock, Germany): *Computer simulation of the OH/D stretching band of liquid water as a function of temperature and pressure*

Kamil Polok (Warsaw, Poland): *Dynamics in ethanol/water mixtures: Optical Kerr Effect and simulation study*

Milan Předota (Ceske Budejovice, Czech Republic): *Electrokinetic properties of the rutile/water interface: Zeta-potential prediction from computer simulations*

Elena Pyanzina (Ekaterinburg, Russia): *Pressure and correlations in systems of anisotropic dipolar particles*

Dimitriy Rozhkov (Ekaterinburg, Russia): *The effect of a wedge on the ionic distribution of an electrolyte solution*

Marcin Rybicki (Lodz, Poland): *Solvation of biologically important ions in water-acetonitrile mixtures: MD simulation studies*

Seiji Sawamura (Kusatsu, Japan): *Compressibility phenomena of the partial molar volume of L-valine in water*

Volodymyr Sergiievskyi (Glasgow, UK): *The optimal closure for 3DRISM calculations*

Jiří Škvor (Ústí nad Labem, Czech Republic): *Morphological analysis of self-assembled diblock copolymer structures in dissipative particle dynamics simulations*

Jiří Škvor (Ústí nad Labem, Czech Republic): *Simulations of hard/pseudo-hard body mixtures*

Thomas Sonnleitner (Regensburg, Germany): *Dynamics of ethylammonium nitrate and its mixtures with acetonitrile*

Joanna Szala-Bilnik (Lodz, Poland): *Hydration mechanisms and vibrational spectrum of $^{\bullet}OH$ radical in liquid and supercritical water*

Elena Tsurko (Kharkiv, Ukraine): *Thermodynamic functions of dissociation and solvation of aliphatic amino acids in H_2O-MeOH, H_2O-EtOH, H_2O-PrOH-2*

Ivan Vyalov (Leipzig, Germany): *Extracting bridge functions from molecular simulations*

Ryoichi Wada (Kusatsu, Japan): *Solvent and pressure effects on conformational equilibria of 1,2-dimethoxyethane and dimethoxymethane: A Raman spectroscopic study*

Norio Yoshida (Fukuoka, Japan): *Developments of molecular Ornstein-Zernike self-consistent field theory and its applications*

Miklós Zrínyi (Budapest, Hungary): *Heat conduction in microgels*