

**Preliminary program of the
Trilateral Scientific Seminar
"Solvation in Complex Liquids: Bridging Length Scales by Theory and Experiment"**

DAY 1: Wednesday, June 23rd, 2010

		Title	Speaker	Affiliation
9:00	13:50	Reception, installation of posters, lunch, discussions etc		
13:50	14:00	Introductory speech (Maxim Fedorov)		
Thermodynamics of solution				
14:00	14:40	Statistical thermodynamics of structure, dynamics and critical properties of ionic fluids	Wolfram Schröer	University of Bremen
14:40	15:00	<i>Coffee break</i>		
Computational methods for prediction properties of solutions				
15:00	15:40	Combining classical and ab initio molecular dynamics. Application to the liquid-liquid transition and related problems	Noël Jakse	Grenoble Institute of Technology
		<i>5 min break</i>		
15:45	16:15	Computer simulations and theory of spatially confined charged and dipolar systems	Sabine Klapp	TU Berlin
16:15	16:25	<i>10 min break</i>		
16:25	17:05	Simulations Studies of Fluctuations: From Supercritical Fluids to Interfaces	Philippe Anthony Bopp	University of Bordeaux
17:05	17:15	Prediction of hydration free energy by the Structural Descriptor method	Ekaterina Ratkova	MPI for Mathematics in the Sciences, Leipzig
17:15	17:30	<i>Coffee break</i>		
Structure in Super Critical and Non-Aqueous Fluids				
17:30	17:50	<i>To be confirmed</i>		
17:50	17:55	<i>5 min break</i>		
17:55	18:15	Structure of hydrogen bonded clusters from IR spectroscopy	Roman Oparin	Institute of Solution Chemistry RAS, Ivanovo
18:15	18:25	Inhomogeneity in Ar in supercritical conditions: A combined molecular simulations and density based clustering approaches	Ivan Vyalov	University of Lille
18:25	18:35	Potential of mean force for ion pairs in aprotic organic solvents and their binary mixtures.	Alexey Odinkov	Photochemistry Center RAS, Moscow
18:35	19:30	Poster Session		

DAY 2.Thursday, June 24th 2010

		Title	Speaker	Affiliation
Polyelectrolytes				
9:00	9:40	Hydration measurement of salt ions, polyelectrolytes, and proteins in dilute solutions by high resolution dielectric relaxation spectroscopy	Makoto Suzuki	Tohoku University
<i>10 min break</i>				
9:50	10:30	The Impact of Specifically Interacting Metal Cations on the Solution Behaviour of Long Chain Anionic Polyacrylates	Klaus Huber	University of Paderborn
10:30	10:35	<i>5 min break</i>		
10:35	10:55	Thermodynamic Modelling of Polyelectrolyte Systems	Shahbaz Naeem	TU Dortmund
10:55	11:10	<i>To be confirmed</i>	Evgeny Nogovitsyn	Institute of Solution Chemistry RAS, Ivanovo
11:10	11:25	<i>Coffee break</i>		
Solvation effects on molecular level: Theoretical and experimental studies				
11:25	12:05	Ion solvation versus association: Insights from dielectric spectroscopy on competing processes in solutions	Richard Buchner	University of Regensburg
12:05	12:30	Local structure in aqueous solutions	Abdenacer Idrissi	University of Lille
12:30	14:00	lunch		
Ionic liquids				
14:00	14:40	Interplay between local hydrogen bonding and long-range Coulomb interactions in Ionic Liquids	Ralf Ludwig	University of Rostock
14:40	14:45	<i>5 min break</i>		
14:45	15:05	In silico studies of ionic liquids at electrified interfaces	Nikolaj Georgi	MPI for Mathematics in the Sciences, Leipzig
15:05	15:20	<i>Coffee break</i>		
Solvation at interfaces				
15:20	16:00	Molecular Dynamics of the Discharge of Solvated Protons at the Aqueous/Metallic Interface	Eckhard Spohr	University of Duisburg-Essen
16:00	16:10	<i>10 min break</i>		
16:10	16:50	Solvent dynamics effects in electron transfer across electrochemical interfaces	Renat Nazmutdinov	Kazan State Technological University
16:50	17:00	<i>Coffee break</i>		
Modeling techniques: Towards Applications				
17:00	17:25	Investigation of the bioprotective properties of disaccharide/water mixtures from Molecular Dynamics simulations	Frederic Affouard	University of Lille
17:25	17:50	Dressed molecule theory: screening and charge renormalization for ionic and molecular interactions in solution	Rosa Ramirez	University of Évry
17:50	18:00	<i>10 min break</i>		
18:00	18:10	<i>To be confirmed</i>	Anastasia Romanova	MPI for Mathematics in the Sciences, Leipzig
18:10	18:30	Self-assembly in aqueous solutions treated by integral equations methods of molecular liquids	Gennady Chuev	MPI for Mathematics in the Sciences, Leipzig
18:30	19:00	Poster Session		
19:15	21:00	Conference Dinner		

DAY 3. Friday, June 25th 2010

		Title	Speaker	Affiliation
New computational methods for liquid systems				
9:00	9:40	Free-Energy Analysis of Solvation in the Energetic Perspective	Nobuyuki Matubayasi	Kyoto University
<i>10 min break</i>				
9:50	10:20	Simulations of molecular liquids: simulation approaches, fast algorithms, parallelization and coarse graining	Godehard Sutmann	Jülich Supercomputing Center
10:20	10:30	Numerical solution of the molecular liquids theory integral equations	Volodymyr Sergiievskyi	MPI for Mathematics in the Sciences, Leipzig
10:30	10:45	<i>Coffee break</i>		
10:45	11:25	The implicit electrostatic solvent model with continuous dielectric permittivity function	Michael Basilevsky	Photochemistry Center RAS, Moscow
11:25	11:35	<i>10 min break</i>		
Solvation in Super Critical Fluids				
11:35	12:05	Solvation of organic molecules in supercritical CO ₂	Thierry Tassaing	University of Bordeaux
12:05	12:10	<i>5 min break</i>		
12:10	12:35	Solvation and association of polar molecules at ambient and supercritical conditions	Michael Kiselev	Institute of Solution Chemistry RAS, Ivanovo
12:35	14:00	<i>lunch</i>		
14:00	16:00	Round Table Discussion: Solvation Sciences, present, and future.		