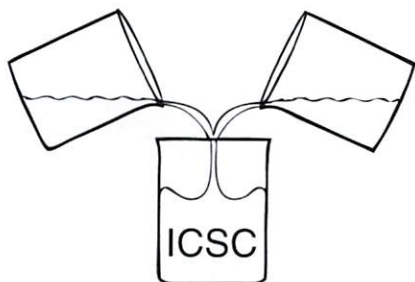


34th International Conference on Solution Chemistry 2015

30th August - 3rd September 2015, Prague, Czech Republic



PROGRAM AND LIST OF PARTICIPANTS



34th International Conference on Solution Chemistry 2015

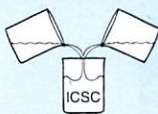
30th August - 3rd September 2015, Prague, Czech Republic

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Welcome to Prague!



It is my pleasure to welcome you to the 34th International Conference on Solution Chemistry, held 30 August-September 4, 2015, in Prague, Czech Republic.

This conference is a continuation of the successful series of conferences on solution chemistry and related topics held in alternate years, and most recently in Innsbruck (2009), La Grand Motte (2011), and Kyoto (2013). It brings together scientists from both academia and industry from all over the world to discuss the latest developments in all aspects of solution chemistry, including theoretical, experimental, computational, and practical applications. Session topics of the conference will include: analytical chemistry, spectroscopy of solutions, electrochemistry, solutions at extreme conditions, molecular simulations, and interfaces.

I am pleased that you came and I hope that you will enjoy the conference!

Sincerely,

Ivo Nezbeda
Chairman



SUNDAY

14.00-18.45	REGISTRATION
19.00-19.10	Opening address
19.10-20.00	A. Luzar
20.05-22.00	SOCIAL MIXER

SCIENTIFIC

MONDAY

SESSION I

chair: C. Vega

9.00- 9.40	A. A. Chialvo
9.40-10.00	A. Melchior
10.00-10.20	I. Persson
10.20-10.40	S. Pinho
10.40-11.20	coffee

SESSION II

chair: F. Moucka

11.20-12.00	A. Perera
12.00-12.20	M. Duvail
12.20-12.40	A. Gacsi
12.40-13.00	J.L. Gómez-Estévez
13.10	lunch

SESSION III

chair: T. Yamaguchi

14.30-15.10	A. Kovalenko
15.10-15.30	J. Dobnikar
15.30-15.50	G. Meriguet
16.00-18.00	POSTER SESSION with refreshment

TUESDAY

SESSION IV

chair: I. Persson

9.00- 9.40	N. Matubayashi
9.40-10.00	T. Yamaguchi
10.00-10.20	D. Fellhauer
10.20-10.40	P. Sipos
10.40-11.20	coffee

SESSION V

chair: A. Luzar

11.20-12.00	C. Vega
12.00-12.20	J. Kolafa
12.20-12.40	E. Waghorne
12.40-13.00	Y. Ishii
13.10	lunch

CONFERENCE

EXCURSION:

14.30	Prague sightseeing
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PROGRAM SCHEDULE

WEDNESDAY		THURSDAY	
SESSION VI chair: L. S. Romsted		SESSION IX chair: A. Kovalenko	
9.00- 9.40	Y. Umebayashi	9.00- 9.40	G. Grazziano
9.40-10.00	S. Tsuzuki	9.40-10.00	V. Vlachy
10.00-10.20	T. Makino	10.00-10.20	Y. Marcus
10.20-10.40	G. Hefter	10.20-10.40	R. Buchner
10.40-11.20	coffee	10.40-11.20	coffee
SESSION VII chair: A. A. Chialvo		SESSION X chair: A. Perera	
11.20-12.00	F. Moucka	11.20-12.00	L. S. Romsted
12.00-12.20	B. Salamanca	12.00-12.20	F. Sokolic
12.20-12.40	M. Borowko	12.20-12.40	A. Wakisaka
12.40-13.00	I. Sedov	12.40-13.00	L. Turi
13.10	lunch	13.10	lunch
SESSION III chair: G. Grazziano		SESSION XI chair: W. R. Smith	
14.30-15.10	W. R. SMITH	14.30-15.10	J. F. Dufreche
15.10-15.30	A. Carof	15.10-15.30	W. Schroer
15.30-15.50	A. Apelblat	15.30-15.50	I. Sanchez
15.50-16.10	B. Kutus	15.50-16.10	D. Rowland
		16.10-16.25	closing remarks
		19.00-22.30	BANQUET





Welcome mixer

Sunday, 30th August 2015

at the premises of NTK (National technical library)

20:00 - 22:00

Dresscode: casual

All invited - including accompanying persons

Prague sightseeing tour

Tuesday, 1st September 2015

Meeting point: in front of NTK (National technical library) at 14:30

Dresscode: informal, comfortable shoes recommended

The excursion is especially made for tourists who want to see the main Prague monuments. The tour begin by bus transfer at 14:30 from the National technical library to the Prague Castle. With an English speaking guide you will see Prague Castle, St. Vitus Cathedral, Neruda street, Lesser Town Square, Charles Bridge, Jewish Town and Old Town with Old Town square, which is the end of sightseeing tour.

Duration: approx. 3 hours

All invited - including accompanying persons

Conference banquet

Thursday, 3rd September 2015

Meeting point: in front of the NTK (National technical library) at 18:30, or directly at the Novoměstský pivovar at 19:00. No transport back to NTK is provided.

Dresscode: casual

The Conference banquet will be held at the Novoměstský pivovar (New Town Brewery), Vodičkova 20, Prague 1.

You will have a buffet dinner with 5 drinks per person included (beer or non alcoholic drinks).

All invited - including accompanying persons

Ladies program

We will be happy to arrange for you any trip (to Karlovy Vary - Carlsbad, Cesky Krumlov, Karlstejn Castle...etc.), just please visit us at the registration desk and we will assist you.





MENU SERVED during the conference

ICSC
2015

SOCIAL MIXER

Sunday, from 20:00

WELCOME DRINK

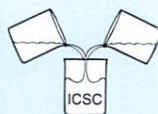
Prosecco del Veneto Ca di Rajo
Orange & Apple Juice
Still & Sparkling water

COLD BUFFET

Baby caprese salad with mozzarella, tomatoes & fresh basil
Mexican salad with chicken, corn and BBQ dressing
Greek salad with olives & feta cheese
Vegetable crudité's with beetroot dressing
(carrot, celery, cucumber, bell peppers)

Slowly roasted beef flank in garlic crust with Dijon dip
Whole poached salmon with pineapple-dill dressing
Chicken roll with dried apricots and nut stuffing
Pork tenderloin with marinated shitake mushrooms
Marinated duck breast with balsammico and arugula salad
Roastbeef in pepper crust with chili mayo
Chicken breast with arugula
Chicken Teriyaki skewers
Vegetable wraps with dressing
Pork schnitzels with pickled vegetable
Czech cheeses selection with nuts & fruit

Pizza bread
Homemade leavened bread
White & wholegrain baguette
Olive Focaccia



MONDAY 31. 8. 2015

MORNING COFFEE BREAK

Cookies selection
Platter with whole fruit
Platter with sliced fruit

LUNCH

Goulash soup

Capresse baguette
White French baguette with mozzarella, tomatoes, lettuce and basil pesto
Parma foccacia
Italian foccacia with parma ham, arugula, dried tomatoes and pesto

AFTERNOON COFFEE BREAK

Brownies
Mini raisin pastry

Chicken sandwich
White baguette with shaved chicken breast and avocado dressing
Mortadela baguette with mortadela, tomatoes and herb dressing
Platter with sliced fruit

BEVERAGES

9:00 – 17:00

Filtered coffee
Tea selection
Still & Sparkling water
Orange & Apple juice



MENU SERVED during the conference

**ICSC
2015**

TUESDAY 1. 9. 2015

MORNING COFFEE BREAK

Cookies selection
Platter with whole fruit
Platter with sliced fruit

LUNCH

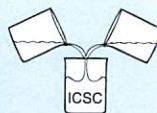
Homemade potato soup

Chicken Baguette
Wholegrain french baguette with shaved chicken,
lettuce, tomatoes and avocado dressing
Ham & Cheese baguette
White baguette with ham & cheese, tomatoes and horseradish dressing

BEVERAGES

9:00 – 13:00

Filtered coffee
Tea selection
Still & Sparkling water
Orange & Apple juice



WEDNESDAY 2. 9. 2015

MORNING COFFEE BREAK

Cookies selection
Platter with whole fruit
Platter with sliced fruit

LUNCH

Mixes lettuce, arugula, cherry tomatoes, cucumber, bell pepper, olives ad
Feta cheese
Mozzarella capresse
Dressings: olive oil, pesto, balsamico, herb

Broccoli cream soup

Roasted boneless chicken legs with cherry tomatoes
Penne pasta with porcini sauce and parmesan cheese
Gratinated potatoes
Selection of home made bread and pastry

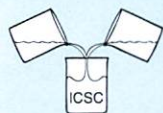
AFTERNOON COFFEE BREAK

Cookies selection
Platter with whole fruit
Platter with sliced fruit

BEVERAGES

9:00 – 17:00

Filtered coffee
Tea selection
Still & Sparkling water
Orange & Apple juice



MENU SERVED during the conference

**ICSC
2015**

THURSDAY 3. 9. 2015

MORNING COFFEE BREAK

Cookies selection
Platter with whole fruit
Platter with sliced fruit

LUNCH

Mixes lettuce, arugula, cherry tomatoes, cucumber, bell pepper, olives ad Feta cheese
Grilled bell pepers carpaccio with herb dresing
Dressings: olive oil, pesto, balsamic, herb

Tomato soup

Stuffed chicken breast with spinach and ricotta, basil sauce
Vegetable lasagne with aubergine, zucchini, tomato sauce and herb
Roasted Grenaille potatoes with coarse salt
Selection of home made bread and pastry

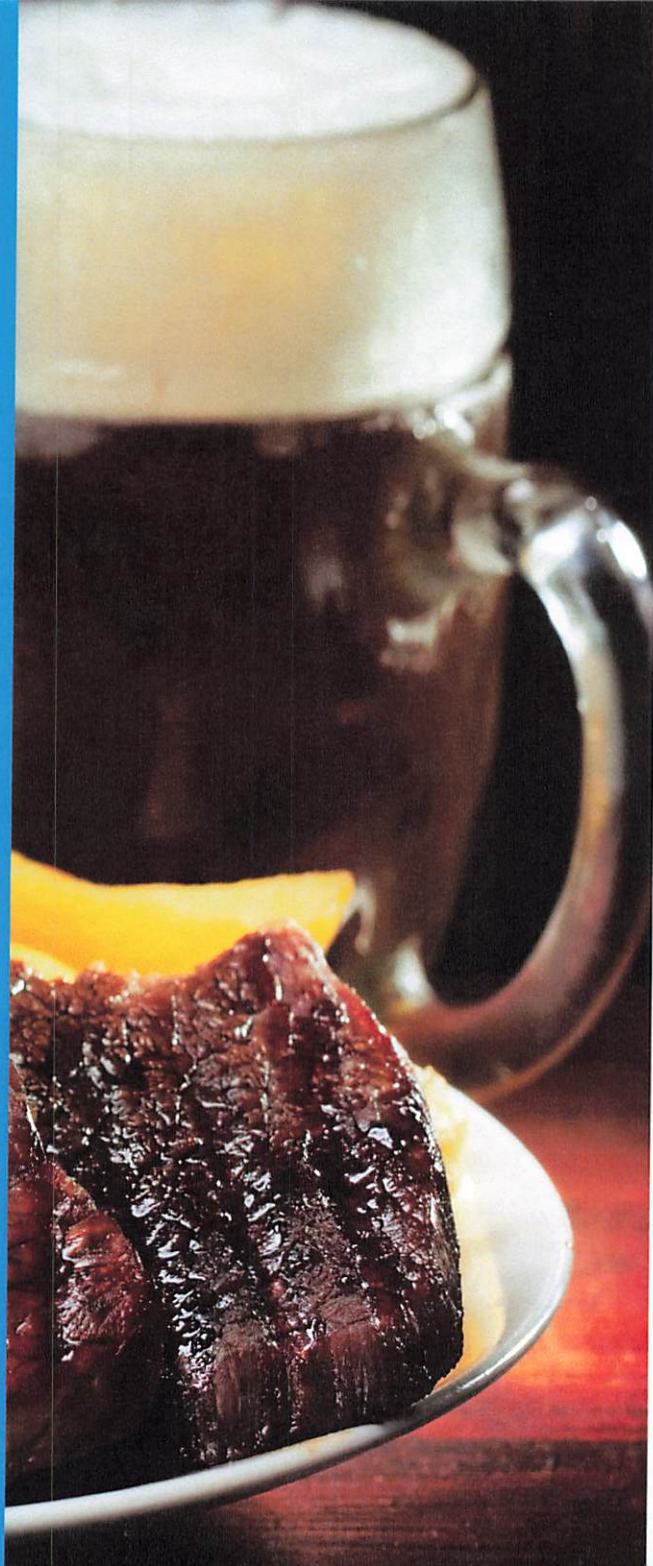
AFTERNOON COFFEE BREAK

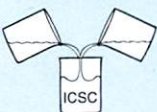
Cookies selection
Platter with whole fruit
Platter with sliced fruit

BEVERAGES

9:00 – 17:00

Filtered coffee
Tea selection
Still & Sparkling water
Orange & Apple juice





Conference banquet

at the Novoměstský pivovar (*brewery*)

Thursday, from 19:00

Appetizer

Cold buffet

- Bowl garnished with ham, salami and smoked poultry Hercules ham
- Mini pickled herring with pickled cucumber
- Sausages with onion soup
- Meat croquettes stuffed with spinach
- Prague bun filling with smoked meat
- Šumava jelly

Salad buffet

- Cabbage coleslaw with carrot
- Homemade slaw with dill
- Sliced tomatoes and cucumbers
- Austrian potato salad
- Pasta salad with basil
- Iceberg lettuce with peppers, French dressing

Hot buffet

- Fried pork cutlets
- Roasted chicken drumsticks
- Homemade meatloaf
- Brewery goulash
- Boiled Parisian potatoes
- Steamed vegetables

Cheese

- selection of Czech cheeses

Desserts

- Apple strudel
- Selection of mini desserts

Fruit bowl

Drinks incl.: beer, non-alcoholic drinks



The background of the entire page is a light blue color with a faint, abstract pattern of overlapping circles and lines, resembling a molecular or network structure. The circles vary in size and are connected by thin lines, creating a sense of interconnectedness. The overall aesthetic is clean and modern, typical of scientific or academic publications.

PLENARY LECTURES SUMMARIES

VISCOSITY OF ELECTROLYTE SOLUTIONS

Jean-François Dufrêche^a, John Jairo Molina^b, Pierre Turq^c, Biman Bagchi^d

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^bFukui Institute for Fundamental Chemistry, Kyoto, Japan

^cUniversité P. M. Curie – Paris 6, Sorbonne Universités, 4 place Jussieu 75005 Paris, France

^dSSCU, Indian Institute of Science, Bangalore 560012, India

In the last decades, the description of dynamical properties of electrolyte solutions made tremendous progresses. The original limiting laws by Debye, Hückel, Fuoss, Falkenhagen and Onsager that are valid only for dilute dissociated solutions have been extended¹ up to molar concentrations. The original concepts based on the relaxation of the ionic atmosphere and hydrodynamic interactions have been clarified in view of molecular simulations² and modern Brownian motion theory³. This works have especially been a success in the domain of ion transport in water. A Smoluchowski equation based approach coupled to a MSA description of the solution structure can quantitatively predict the various ionic equilibrium and transport properties up to molar⁴ concentrations. In accordance with this approach, the time dependency of the transport coefficients can be analysed from mode-coupling⁵ theories.

Nevertheless, these improvements had not been possible for all the transport coefficients: despite its significance, there have been no comparable progresses for viscosity. More precisely we know since 1929 that the viscosity η of a relatively dilute electrolyte solution is related to the viscosity η^0 of the pure solvent thanks to the relation

$$\frac{\eta}{\eta^0} = 1 + Ac^{1/2} + Bc$$

with c the concentration of the solution. The calculation of the A is due to Falkenhagen and Onsager but despite numerous efforts in the last decades, there was no real predictive microscopic theory of the following term proportional to the concentration (Bc). The coefficient B is experimentally additive so that it is possible to add the various ionic contributions. Mode-coupling⁶ theories (MCT), which take into account ion modes, had been able to recover the limiting laws ($Ac^{1/2}$ term), but to our knowledge no predicting formula for B emerged. For example, the coefficient is generally found positive whereas it is negative for numerous electrolytes (such as KCl in water).

We propose a new approach based on mode-coupling theory where the solvent is explicitly considered. Taking into account the relaxation effects of all the species (ions and solvent), we obtain a general expression of the viscosity, which is related to the change of solvent structure due to the presence of ionic solutes. The resulting Jones-Dole coefficient B corresponds to the sum of several effects: electrostatic relaxation, Einstein mechanism, and breaking structure effects. With the help of molecular simulations, we show that for simple (relatively) spherical ions, the effect on the solvent can be simplified since it appears to be relatively independent on the ion. The corresponding simplified MCT that emerges is able to predict the Jones-Dole coefficients of simple electrolytes for the first time thanks to a microscopic model and it allows the complex dependence of viscosity with the concentration to be understood.

¹ See e.g. J.-F. Dufrêche, O. Bernard, S. Durand-Vidal, P. Turq, *J. Phys. Chem. B* **109**, 9873-9884 (2005)

² J. Molina J.-F. Dufrêche M. Salanne P. Turq, *Phys. Rev. E* **80**, 065103 (2009),

J.-F. Dufrêche, M. Duvail, B. Siboulet, M. Jardat and O. Bernard *Mol. Phys.* **112**, 1405 – 1417 (2014)

³ W. Ebeling, R. Feistel, G. Kelbg, R. Sändig, *J. Non-Equilib Thermodyn.* **3**, 11, (1978)

⁴ G. Allaire, R. Brizzi, J.-F. Dufrêche, A. Mikellie and A. Piatnitski *Physica D: Non linear Phenomena* **282**, 39 (2014)

J.-F. Dufrêche, M. Jardat, P. Turq, B. Bagchi *J. Phys. Chem. B* **112**, 10264 (2008)

⁵ A. Chandra B. Bagchi *J. Chem. Phys.* **110**, 10024 (1999)

A. Chandra B. Bagchi *J. Chem. Phys.* **112**, 1876 (2000)

J.-F. Dufrêche, O. Bernard, P. Turq, A. Mukherjee, B. Bagchi, *Phys. Rev. Lett.* **88**, 095902 (2002)

C. Contreras Aburto G. Nägele *J. Chem. Phys.* **139**, 134109 (2013)

⁶ A. Chandra B. Bagchi *J. Chem. Phys.* **113**, 3226 (2000)

C. Contreras Aburto G. Nägele *J. Phys. Cond. Matt.* **24**, 464108 (2012)

“Thought experiments” as dry-runs for “tough experiments”

Novel approaches to the hydration behavior of aqueous electrolytes

Ariel A. Chialvo,^{1*} and Lukas Vlcek^{1,2}

¹Chemical Sciences Division, Geochemistry & Interfacial Sciences Group
Oak Ridge National Laboratory, Oak Ridge, TN 37831-6110, U. S. A.

²Joint Institute for Computational Sciences
Oak Ridge National Laboratory, Oak Ridge, TN 37831-6173, U. S. A.

In this presentation we will discuss the microstructural analysis of aqueous electrolytes and present a detailed account of crucial issues underlying the interpretation of neutron scattering with isotopic substitution (NDIS) for the experimental determination of accurate ion coordination numbers in ionic systems involving both halides anions and oxyanions. In particular, we will emphasize the issues associated with the frequently overlooked ion-pairing phenomenon in the context of the determination of coordination numbers, and will examine novel techniques to deal with the degree of ion-pairing and the correction of its effects on the experimentally measured quantities. Finally, we will provide examples for representative aqueous halides (single isotopic substitution) and oxyanions (single and double isotopic substitutions) via molecular simulation, as convenient dry runs for the challenging NDIS experiments involving heavy- and null-aqueous environments, to illustrate our new developments for the interpretation of ion coordination.

Shedding light on the hydrophobicity puzzle

Giuseppe Graziano

Department of Science and Technology, University of Sannio,
Benevento, Italy; graziano@unisannio.it

The hydrophobic effect is still considered to be the main driving and stabilizing interaction of protein folding and micelle formation. It is usually divided into two arms: the so-called hydrophobic hydration and hydrophobic interaction. The first one has peculiar thermodynamic features, the most famous of which is the large and negative entropy change associated with the hydration of nonpolar species around room temperature. In addition, a large positive heat capacity change affects both the hydration enthalpy and entropy changes, but has little effect on the hydration Gibbs energy change due to enthalpy-entropy compensation. The hydration entropy change of several compounds proved to reach a common value at an entropy convergence temperature. The occurrence of a crossover from small to large length-scales hydration of cavities (the prototype of nonpolar solutes) has been emphasized. All these features can be rationalized by means of a single theoretical approach. The fundamental ingredient is the solvent-excluded volume effect associated with cavity creation, whose magnitude is amplified in water by the small size of water molecules in comparison to that of the other common liquids. It leads to a decrease in the accessible configurational space, and so to a large decrease in the translational entropy of water molecules. The solvent-excluded volume effect is correlated to the water accessible surface area of the solute molecule. This fact allows a simple rationalization of hydrophobic interaction. The association of two or more nonpolar objects is entropically favoured around room temperature due to the large WASA decrease associated with the formation of the “complex”.

G. Graziano, J.Phys.Chem.B. 109 (2005) 12160; J.Phys.Chem.B 110 (2006) 11421; J.Phys.Chem.B 113 (2009) 11232; J.Chem.Phys. 140 (2014) 094503.

Spatial-Decomposition Analysis of Electrical Conductivity in Concentrated Ionic Systems

Nobuyuki Matubayasi

Division of Chemical Engineering, Graduate School of Engineering Science
Osaka University, Toyonaka, Osaka 560-8531 Japan

The electrical conductivity is a key quantity of ionic systems, especially in the development of electric cell. It quantifies how easily the electric current is induced in the system, and is governed by the dynamics of ionic species. At low concentration, the movement of each ion may be considered uncorrelated; the electrical conductivity is determined by the Nernst-Einstein equation. At medium to high concentrations, the cross correlation between ions can become significant and the formation and decay of aggregated ions play influential roles in the transport phenomena in electrolyte solution. In the present work, we formulate a new analysis framework to incorporate the concept of ion aggregation and the correlated motions between ions to the electrical conductivity. On the basis of the Green-Kubo formula, the conductivity is decomposed into the contributions from the ionic species in the system to enable the determination of the transport number, and is further expressed as a sum of the autocorrelation term of the Nernst-Einstein form and the cross-correlation term describing the two-body motions of ions. The spatial decomposition is then conducted for the cross-correlation term by formulating an integral expression over the ion-pair distance to bridge the static picture of ion pairing and the dynamic picture of correlated motions. With the spatially decomposed Green-Kubo formula, the extent of localization of the ion-pair contribution to the conductivity can be examined by introducing a cutoff to the spatial integration in the formula. The analysis framework described above is applied, in combination with molecular dynamics simulation, to 1 *m* NaCl aqueous solution and [C₄mim][NTf₂] (1-*n*-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide) ionic liquid. It is found that the ion-pair contribution to the electrical conductivity is localized within the first coordination shell for the NaCl system and is not localized with an oscillation extending over nanometers for the ionic liquid system.

Molecular theory of solvation: A mental microscope into structure and effective interactions in multiscale description of chemical and biomolecular nanosystems

Andriy Kovalenko^{1,2}

¹ National Institute for Nanotechnology, 11421 Saskatchewan Drive, Edmonton, AB, T6G 2M9, Canada

² Department of Mechanical Engineering, University of Alberta, Edmonton, AB, T6G 2G8, Canada

e-mail: andriy.kovalenko@ualberta.ca

It is widely recognized that solvation is critical for a broad range of chemistry, pharmacology, and molecular biology. At present, there is a need of theoretical models of solvation that adequately include molecular structure of solvent. This becomes of particular importance for the emerging areas of molecular biology and nanotechnology which involve solvation effects in local confinement of chemical and biomolecular nanosystems and nanomaterials. Such theoretical models are of great demand to extend the capabilities of molecular simulations which are by far not sufficient to address complex phenomena and processes on the whole spectrum of scales from fast to very slow in large nanosystems of interest. Statistical mechanics based, Ornstein-Zernike type integral equation theory of liquids is promising as an essential part of multiscale methods for chemical and biomolecular nanosystems in solution. One molecular version of this formalism is the three-dimensional reference interaction site model (3D-RISM) integral equation complemented with the Kovalenko-Hirata (KH) closure approximation. It yields solvation structure in terms of 3D maps of correlation functions (including density distributions) of solvent interaction sites around a solute (supra)molecule, and the solvation free energy (and subsequent thermodynamics, including mean force potentials) at once analytically as a simple integral of the correlation functions obtained. This allows analytical differentiation and self-consistent field coupling of the 3D-RISM-KH integral equations in multiscale approaches. The 3D-RISM-KH molecular theory of solvation consistently accounts for all effects of chemical specificities on solvation properties in complex chemical and biomolecular systems, problematic for molecular simulations and continuum solvation models. This talk will review the recent developments of molecular theory of solvation, including its multiscale couplings with KS-DFT, CASSCF, and FMO methods of quantum chemistry, molecular mechanics (MM), molecular dynamics (MD) and dissipative particle dynamics (DPD) simulations, protein-ligand docking protocols, structural water detection and placing, prediction of the octanol-water partition coefficient used in pharmacology and environmental studies to characterize hydrophobic (lipophilic) / hydrophilic properties of chemical compounds and to predict drug distribution of within the body, as well as its other numerous applications to chemical nanosystems in solution, soft matter, fragment-based drug design, biomolecular systems, and bionanomaterials.

Small is Beautiful, and Smart: Reversible Control of Nanoscale Hydration

Alenka Luzar, VCU

As accessible experimental length scales become shorter, the modification of interfacial properties of water due to nanopatterned surface topography, functionalization, or electric field, must come to grips with novel effects existing at the nanoscale. The talk will review our theoretical and molecular simulation works that predict and elucidate thermodynamic driving forces and kinetic factors pertinent to nanoconfined water. Examples will range from changes in hydration and water-mediated interactions in response to surface texture, to nanoelectrowetting. A picture emerges in which molecular modeling can dissect nanoscale phenomena in ways that surprise. Applying this knowledge, we will show how to tailor wetting properties in a reversible manner, to make smart or responsive surfaces for dynamical tunable devices.

Speaker's website: <http://chemistry.vcu.edu/bios/alenka-luzar/>

Osmotic Ensemble Monte Carlo Molecular Simulations for Solubility, Chemical Potentials and Activity Coefficients in Aqueous Alkali-Halide Electrolyte Solutions

Filip Moučka

*Faculty of Science, Jan Evangelista Purkyně University, 400 96 Usti nad Labem, Czech Republic
filip.moucka@ujep.cz*

Aqueous solutions of alkali-halide electrolytes are the most abundant liquids on the Earth. They are important both for their biological functions and their industrial use. There is a great knowledge of their thermodynamics, however, this does not apply to their microscopic properties. Current understanding of these solutions at the molecular scale is very limited. This is evident from the number of different intermolecular interaction models commonly used in molecular simulation studies.

Among the most important properties of an electrolyte solution are its solubility and chemical potentials of its components. Until recently, calculations of these properties based on molecular models were almost impossible, and results obtained by different research groups were contradictory. We developed a novel Osmotic Ensemble Monte Carlo (OEMC) method which provides results of solubility and dependence of chemical potentials of the individual components as functions of electrolyte concentration.

Using the OEMC method, we discovered a great scatter in results obtained from simulations of different commonly employed pairwise additive intermolecular interaction models of NaCl compatible with typically used models of water (SPC/E, TIP4P, TIP3P). Solubility values of some models are virtually equal to zero. Consequently, these models exhibit homogeneous nucleation, followed by precipitation, at low concentrations. It is hard to imagine any reasonable use of such interaction models. Even the best performing pairwise additive models of NaCl compatible with SPC/E water are not able to reproduce solubility well, e.g., Joung-Cheatham model (I. S. Joung, T. E. Cheatham III., *J. Phys. Chem.* **112** (2008) 9020) yields a value of solubility 3.6 mol/kg whereas the experimental value is 6.144 mol/kg. We tried to reparametrize a new pairwise additive model for Na⁺ and Cl⁻ ions compatible with SPC/E water so as to yield simultaneously correct concentration dependence of the electrolyte chemical potential, density of the solution, and solubility. It proved to be impossible. Thus, we extended our OEMC simulation codes to polarizable interaction models AH/SWM4-DP (G. Lamoureux, B. Roux, *J. Phys. Chem. B* **110** (2006), 3308) and state-of-the-art gaussian charge on spring AH/BK3 models (P. T. Kiss, A. Baranyai, *J. Chem. Phys.* **141** (2014), 114501). Resulting AH/BK3 concentration dependence of chemical potentials of NaCl and of H₂O are closer to experiments, however, solubility of the model is 1.0 mol/kg, which is too low. As a byproduct, we obtained approximate concentration dependence of electrolyte activity coefficient, and we showed that our chemical potential results are very consistent with experimental activity coefficients. After all, our results were confirmed by independent simulations of another research group based on different methods (Z. Mester and A. Z. Panagiotopoulos, *J. Chem. Phys.* **142** (2015), 044507).

From solutions to molecular emulsions

Aurélien Perera

Laboratoire de Physique Théorique de la Matière Condensée

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Concentration fluctuations play an important role in the statistical description of liquids, particularly in the neighbourhood of phase transitions. Classical Thermodynamics is blind to fluctuations, and it is Statistical Thermodynamics that gives the relevant meaning to quantities such as the isothermal compressibility, by linking them to fluctuations and showing that they are response functions. This is illustrated by the seminal Kirkwood-Buff theory of solutions. However, the existence of micro-heterogeneous structures, particularly in aqueous mixtures, poses the problem of whether the statistical thermodynamics approach is sufficient to describe these systems. The problem comes from the fact that such mixtures exhibit large Kirkwood-Buff integrals, suggesting that micro-heterogeneity is a form of concentration fluctuation. This interpretation becomes difficult to accept when extrapolated to micellar aggregates and micro-emulsions. By analyzing the different methods of measure, namely thermodynamical methods such as calorimetry, scattering (neutron, x-ray) and computer simulations, we show how the usual statistical approach needs to be reconsidered in order to describe complex forms of disorder. This new approach allows the description of emergent “objects”, such as the micro-heterogeneous structures from a molecular point of view, and shows that fluctuations are related to how such objects “interact” between them. The concept of “molecular emulsion” allows to describe in a unified way all type of disordered liquids, from solutions to the organized liquids of soft matter.

To Model Chemical Reactivity in Heterogeneous Emulsions: Think Homogeneous Microemulsions

Laurence Stuart Romsted, Carlos Bravo-Díaz

We have demonstrated that pseudophase kinetic models that work in association colloids also describe observed rate constants and reactant distributions in kinetically stable emulsions just as they do in homogeneous microemulsions. Over 20 years ago, William Porter aptly characterized then current knowledge about antioxidant efficiencies in aqueous organized media and non polar oils as the *polar paradox*: i.e., nonpolar or amphiphilic antioxidants tend to function better in organized media, e.g., emulsions or membranes of high surface to volume ratios while polar antioxidants are more efficient in bulk lipids. This apparent paradox and the difficulty in determining antioxidant distributions in emulsions made the selection of the best antioxidant for a particular application for scientific reasons is difficult. Here we show our solution to this problem.

Pseudophase kinetic models work in homogeneous microemulsions and emulsions for two reasons: the totality of each region—oil, interfacial and aqueous—in microemulsions can be treated as separate reaction regions without considering microemulsion or emulsion droplet size. The diffusivity of the reactants are near the diffusion controlled limit such that after bulk mixing their distributions are in dynamic equilibrium between the oil, interfacial and aqueous regions in homogeneous microemulsions or in kinetically stable or stirred emulsions throughout the time of the reaction being studied.

This talk will include: (a) the basic assumptions of the pseudophase kinetic model as applied to microemulsions and emulsions; (b) the important properties of the hydrophobic arenediazonium ion probe; and (c) two methods for monitoring reactions in opaque, fluid emulsions, dye derivatization and linear sweep voltammetry, and example results, e.g., antioxidant partition constants between the oil and interfacial and aqueous and interfacial regions of the emulsions and the rate constant for reaction in the interfacial region. Together the results demonstrate that the chemical kinetic method provides a unique, versatile, and robust approach for determining the effect of emulsion properties such as oil hydrophobicity, emulsifier structure, temperature, droplet size, surfactant charge, and pH on partition constants. The chemical kinetic method also provides a natural explanation for the, until now, unexplained “cut-off” effect, a sharp drop in antioxidant efficiency with increasing alkyl chain length of a particular antioxidant.

Interconnections Among Solvent and Solute Chemical Potentials, Osmotic Pressure and Vapour Pressure Lowering of Aqueous Electrolyte Solutions and Exploitation in Molecular Simulations

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The chemical potential of the water solvent, μ_w , and of an electrolyte solute, μ_s , are arguably the most important properties of aqueous electrolyte solutions. In the first half of the last century, much effort was expended on designing ways to determine them experimentally. Two of the most often used methods involved measuring the osmotic pressure, Π , and the lowering of the water vapour pressure above the salt solution, (P^*/P^0) , where P^0 is the vapour pressure of pure water. Both are thermodynamically connected to μ_w and via the Gibbs-Duhem equation to μ_s , and are also quantities of interest in their own right.

The existing molecular simulation method for calculating Π in aqueous electrolyte solutions in the context of discrete water force fields (FFs) involves a special-purpose molecular dynamics approach using virtual semi-permeable membranes separating the solution and water solvent phases (Luo *et al.*, J. Phys. Chem. Letters 1(2010), 183; Faraday Disc. 160 (2013), 135; Saxena *et al.*, J. Phys. Chem. B 119 (2015), 219). The vapour pressure of aqueous NaCl solutions as a function of concentration has recently been calculated using Gibbs Ensemble Monte Carlo (GEMC) methodology for a range of non-polarizable FFs (Orozco *et al.*, J. Chem. Phys. 141 (2014), 234505).

Here, we exploit the thermodynamic interconnections among Π , P , μ_w and μ_s in the context of molecular simulations to calculate the remaining quantities from one of them and/or to test the thermodynamic consistency of separately calculated quantities. We demonstrate the methodology for aqueous NaCl solutions over the entire experimentally accessible concentration range at ambient conditions. We consider the predictions of two polarizable FFs and a commonly used non-polarizable force field, and show comparisons with the experimental results.

Lithium Ion Solvation in Room-temperature Ionic Liquids toward Next Generation Batteries Based on Spectrothermodynamics

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Among the last decade, room-temperature ionic liquids (RTILs) have been attracted much attention as electrolytes towards next generation lithium batteries. For the purpose, bis-(trifluoromethanesulfonyl) amide (TFSA) and bis-(fluoromethanesulfonyl) amide (FAS) based RTILs are widely used. From the viewpoint of electrolyte solution chemistry, lithium ion solvation has been understood based on the huge accumulated experimental and theoretical studies on ions both in aqueous and non-aqueous solvent solutions, in which the electrostatic charge-dipole interaction predominantly operates between Li^+ -solvents. However, in RTILs, dominant interaction should be the charge-charge one even among the solvent ions. Thus, it can be expected unique and noble ion solvation mechanism could be operate in RTILs.

On the other hand, speciation analysis is defined as identifying and/or measuring the quantities of one or more individual chemical species in a sample, and also contains evaluation of the species distribution and molecular structure of the species even their conformers. Raman/IR vibration spectroscopy and neutron/X-ray scattering experiments can reveal not only molecular and/or liquid structures but also species formation equilibria thermodynamically. We propose such techniques can be called *Spectrothermodynamics*. In this contribution, we show the speciation analysis applied for the lithium ion solvation in RTILs based on the spectrothermodynamics, and propose specific lithium ion stabilization in the RTILs.

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Modelling water in computer simulations

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In computer simulations, water is often described by simple models using partial charges and Lennard Jones centers.

In 2004 we obtained the phase diagram for two water models:

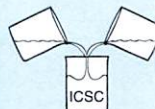
SPC/E and TIP4P. TIP4P was better, and there was room for improvement so that in 2005 we proposed a modified version denoted as TIP4P/2005. Since then we have calculated a number of properties for this model and proposed a test to evaluate the performance of water models. The model obtained an score of 7 out of 10 points. The model probably represents the limit of what can be done with a simple non-polarizable potential. TIP4P/2005 has been quite useful in providing some hints on different problems of water and several examples will be discussed in this talk: the origin of the re-entrant behavior in the melting curve, the existence of a quasi-liquid layer on the surface of ice, the possibility of plastic crystal phases at high temperatures, the impact of an electric field on phase transitions, the behavior of supercooled water, the nucleation rate for the formation of ice and the study of hydrates.

However the model has some limitations and the key question now is how to go beyond that. We shall discuss several possibilities, including polarizability and electronic structure calculations.



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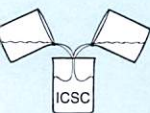
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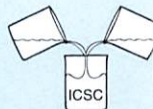
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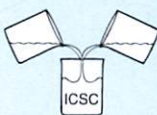




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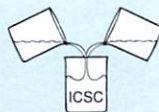
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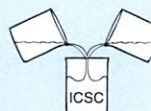


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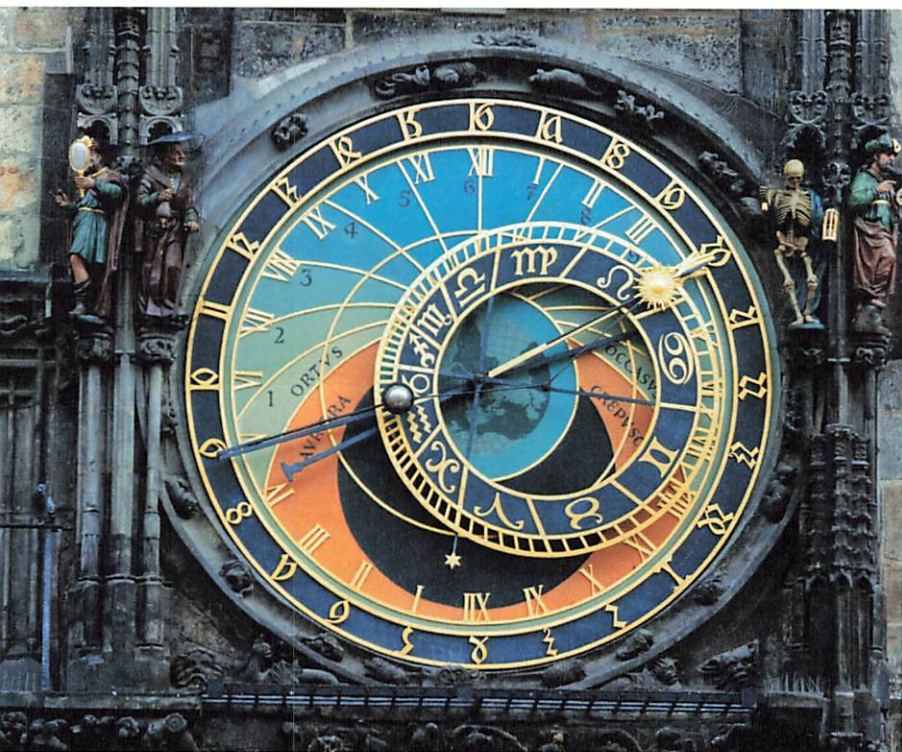


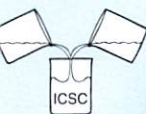
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