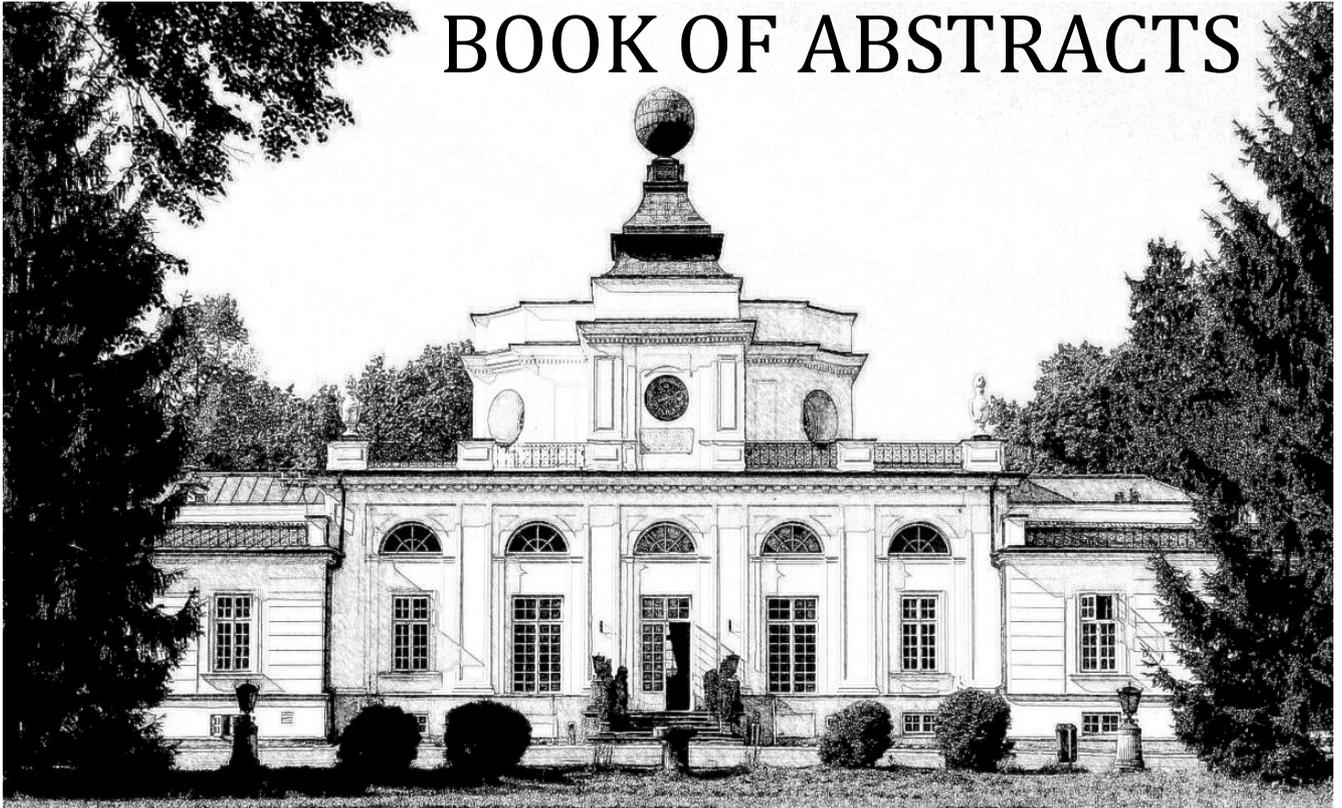


BOOK OF ABSTRACTS



Systems with competing electrostatic and short-range interactions

February 17-20 2017
Jablonna Palace, Poland

Jablonna 2017 - Conference Agenda

February 17

Registration
Dinner

February 18

7:30	Breakfast
	chair: A. Ciach
8:30	R. Lynden-Bell: <i>Modelling CS2 solutions in ionic liquids</i>
9:10	S. Kondrat: <i>Physics of nanoporous supercapacitors with ionic liquids</i>
9:50	L. Varela: <i>Structure of the electric double layer in ionic liquid mixtures</i>
10:30	<i>Coffe break / poster session</i>
	Chair: R. Lynden-Bell
11:00	A. Iglic: <i>Electrostatic and steric interactions of particles with internal charge distribution</i>
11:40	M. Turmine: <i>Experimental study of transport and electronic transfer in pure ionic liquid and their mixtures with molecular solvent</i>
12:20	Di Caprio: <i>Particle indiscernibility in a classical field theory. Application to ionic systems at interfaces</i>
12:50	<i>Lunch / poster session</i>
	chair: L. Varela
14:00	M. Holovko: <i>Effects of disordered porous media on the vapour-liquid phase equilibrium in ionic fluids: Application of the association concept.</i>
14:30	V. Vikhrenko: <i>Charge distribution and ion transfer across the intergrain region in a model of solid state ionics</i>
15:00	I. Mryglod: <i>Some rigorous relations for transport coefficients in theory of fluids: the case of model ionic liquids</i>
15:30	O. Patsahan: <i>Vapour-liquid phase behaviour of ionic fluids in the bulk and under confinement from the collective variable based theory</i>
16:00	<i>Coffe break in the restaurant / kick-off meeting (CONIN members)</i>
18:00	<i>Dinner</i>

February 19

8:00	Breakfast
	chair: O. Patsahan
9:00	G. Kahl: <i>Tunability and order: the plethora of polymorphism of Wigner bilayer systems</i>
9:40	N. Wilding: <i>Computer simulation studies of short-ranged attractive and long-ranged repulsive (SALR) potentials</i>
10:20	Coffe break / poster session
	chair: G. Kahl
11:00	P. Charbonneau: <i>Equilibrium phase behavior and self-assembly dynamics of microphase forming models</i>
11:40	R. Roth: <i>Phase Diagram of a System with Competing Interactions</i>
12:20	Lunch / poster session / concert
	chair: D. di Caprio
14:30	P. Royall: <i>Hunting Mermaids in Real Space</i>
15:10	E. Lomba: <i>Inhomogeneous integral equation approaches to describe confinement</i>
15:40	A. Taleb: <i>Nanoparticles interactions tailoring toward nanomaterial design for targeted application</i>
16:10	Coffe break / poster session
	chair: V. Vikhrenko
16:30	E. Noya: <i>Phase behaviour and assembly of colloids with heterogeneously charged surfaces</i>
17:00	Y. Groda: <i>Thermodynamic and diffusion characteristics of lattice models with obstacles and competing interactions</i>
17:30	A. Ciach: <i>Comparison of the amphiphilic and the colloidal self-assembly</i>
18:30	Dinner

February 20

7:30	Breakfast
	Round table discussion

Modelling CS₂ solutions in ionic liquids

R. M. Lynden-Bell and A. J. Stone

Department of Chemistry, University of Cambridge, UK.
rmlb@cam.ac.uk

Ionic Liquids, with rather large ions, provide a good example of materials where electrostatic and short range interactions are in competition. The molecule CS₂, which is both quadrupolar and polarizable, provides a possible probe of the intermolecular environment and is soluble in the Ionic Liquid [dmim][NTf₂]. Quitevis and co-workers [1] have carried out optical Kerr spectroscopy on CS₂/[dmim][NTf₂] solutions while Lynden-Bell and Quitevis [2] performed complementary simulations using an isotropically polarizable model for CS₂.

Here we present an improved model for CS₂ which uses point charges on 7 sites and anisotropic polarizabilities on three atomic sites [3]. We monitor the induced dipoles in an 8 molar % solutions of CS₂ in [dmim][NTf₂] and investigate the local structure of the liquid near the solute. The distributions of induced dipoles on the atomic sites provide insight into the fluctuations of the local fields in the ionic liquid.

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Physics of nanoporous supercapacitors with ionic liquids

S. Kondrat

Forschungszentrum Jülich, IBG-1: Biotechnology, 52425 Jülich, Germany

Room temperature ionic liquids (RTILs), owing to their unique properties, have recently attracted much attention in various fields and found numerous industrial applications, ranging from lubricants to energy storage devices. RTILs have wide electrochemical window and are almost non-volatile, what makes them a promising ‘green’ alternative to conventional electrolytes [1]. On the other side, recent advances in fabrication of porous carbon-based materials [2] have stimulated the development of electric double-layer capacitors (EDLCs, or supercapacitors) with nano- and subnano-porous [3] carbon electrodes. These supercapacitors make use of the high surface-to-volume ratio, which is due to porosity, and thus increase the stored energy-density significantly. In this lecture I present a brief overview of the recent developments in this research area. We will discuss various issues related to the nanoscale size of the pores, specifically the nature of the electrical double layer in nanoconfinement and the emergence of a ‘superionic state’ [4]; optimization of the structure of the nanoporous electrodes [5]; and how phobicity of ions towards pores can help simultaneously maximize the energy storage [6] and power delivery [7].

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Structure of the electric double layer in ionic liquid mixtures

L. Varela

Departamentos de Física de Partículas y de Física Aplicada, Facultad de Física,
Universidade de Santiago de Compostela, Campus Vida s/n E-15782, Santiago de
Compostela, Spain
luismiguel.varela@usc.es

The electric double layer (edl), i.e. the strongly inhomogeneous interface region formed at a surface immersed into a media with mobile charge carriers, crucially determines the interfacial properties. Understanding the relation between the edl structure and the interfacial properties is critically important in the fields of electrochemistry and colloid science, among others. The edl exhibits a rich structure when the density of charge carriers is low and exponential charge and potential profiles are registered (Stern model), but the situation becomes even more complex and fascinating as the concentration of charges increases up to typical ionic liquid values, where screening and edl 2D and 3D structures are still under intense scrutiny [1,2].

In this contribution we review the current state of the art of edl structure in ionic liquids, and we report some of our recent activity in the field for pure ionic liquids and their mixtures with cosolvents (water [3], alcohols [4]), monovalent [5] and divalent [6] salts close to graphene walls in the absence and presence of random vacancies [7]. Typical oscillations of charge are observed in all cases in the direction normal to the wall, and the effect of the additives on the edl structure is thoroughly analyzed. Moreover, the lateral 2D structure of the layer closest to the wall (adlayer) is characterized, and different mesomorphic structures are observed induced by the adsorption of the ionic liquid on the walls which extend to layers further away from the wall (3D structure). Transitions between different patterns (stripes, hexagons) induced by additives, voltage [1] and also by vacancies in the electrode are seen, in what resembles a quite universal organizational pattern which could open the door to fine tuning of the edl.

We acknowledge the supercomputing support from the EPSRC funded ARCHIE-WeSt High-Performance Computer Centre (www.archie-west.ac.uk, EPSRC grant no. EP/K000586/1) and the Galician Supercomputing Centre (CESGA). The financial support of the Estonian Personal Research Project PUT1107 is highly appreciated. The financial support of the Spanish Ministry of Economy and Innovation MAT2014-57943-C3-1-P and MAT2014- 57943-C3-3-P is gratefully acknowledged. Moreover, this work was funded by the Spanish Ministry of Economy and Competitiveness and by the Xunta de Galicia (AGRUP2015/11). All these research projects were partially supported by FEDER. Funding from the European Union (COST Action CM 1206) and by the Galician Network on Ionic Liquids, REGALIS (CN 2014/015) is also acknowledged.

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Electrostatic and steric interactions of particles with internal charge distribution in electric double layer

A. Iglič and V. Kralj-Iglič

Faculty of Electrical Engineering and Faculty of Health Studies,
University of Ljubljana, Slovenia
ales.iglic@fe.uni-lj.si

Here we present the generalization of electric double layer (EDL) mean-field theory of electrolyte solution in contact with a charged surface based on lattice statistics [1-3]. The dipole and quadrupole moments of water are described within triangular atomic model while considering orientational ordering of water molecules near the highly charged surface. Analytical expressions for the spatial distribution of ions and water dipoles are given [1-3]. The effects of asymmetric finite size of monovalent cations and anions on accumulation of counterions [2], depletion of water molecules in EDL, spatial dependence of relative permittivity and on differential capacitance of electric double layer are described.

The orientational ordering of water molecules is also considered in the region of planar lipid bilayer where the rotational degree of freedom of lipid headgroups is taken into account. The results were tested by using molecular dynamic (MD) simulations [3,4].

At the end, the generalization of the mean-field theory of EDL for the case of multivalent charged nanoparticles is presented by taking into account the internal space charge distribution of a single multivalent nanoparticle [3,5,6]. It is shown that orientational ordering (intra-ionic correlation) of charged nanoparticles with internal quadrupolar charge distribution may lead to attractive forces between like-charged surfaces [3,5,6]. The predicted results are in remarkably good agreement with corresponding Monte Carlo (MC) simulations which include also direct interactions between multivalent nanoparticles [3,5,6]. We therefore concluded that the bridging effect arising from the orientational ordering of nanoparticles with quadrupolar internal charge distribution is sufficient for the existence of attractive interaction between two like-charged surfaces as is revealed within the mean-field approach and MC simulations and also confirmed in experiments [3,5].

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Experimental study of transport and electronic transfer in pure ionic liquid and their mixtures with molecular solvent

Mireille Turmine

Sorbonne Universités, UPMC Univ Paris 06, CNRS, Laboratoire Interfaces et Systèmes Electrochimiques, 4 place Jussieu, F-75005, Paris, France
mireille.turmine@upmc.fr

For many years, chemists have become increasingly interested in ionic liquids (or room-temperature molten salts) as reaction media. But their physicochemical properties are not well described probably because ionic liquids (ILs) do not consist on one class of compounds. Indeed, one of the main advantages of ionic liquids is the possibility of modulating and adjusting their physicochemical properties (viscosity, conductivity, solvation power towards molecules or electrolytes...) by changing the nature of the associated anion or cation. These salts are ionic conductors by nature and this is why they are considered as potential new electrolytes for electrochemical devices. In a first step, we examined the electrochemical behavior of ferrocene (Fc) by cyclic voltammetry and electrochemical impedance spectroscopy, at 298 K, in various pure ILs. We chose two ammonium salts which are protic ionic liquids: ethylammonium nitrate [EAN] and propylammonium nitrate [PAN]; and two aprotic imidazolium salts: 1-butyl-3-methylimidazolium tetrafluoroborate [bmim][BF₄] and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [bmim][NTf₂]. [NEA], [PAN] and [bmim][BF₄] are miscible in water in all proportions whereas [bmim][NTf₂] is insoluble in water. All these ILs are very viscous compared to water. So, in order to decrease the viscosity, it could be interesting to add some quantity of molecular solvent in the IL. Thus, in a second part, we studied the behavior of ferrocenemethanol (FcMeOH) in IL mixed with molecular solvent. We chose three systems: EAN + water; EAN + γ -butyrolactone and [emim][NTf₂] + γ -butyrolactone. Diffusion coefficients of FcMeOH are determined in all these mixtures and plotted against the reverse of the viscosity..

Particle indiscernibility in a classical field theory. Application to ionic systems at interfaces.

Dung di Caprio

Laboratory of Energetic and Reactivity at Interfaces, University Pierre et Marie Curie, Paris,
France

dung.di-caprio@chimie-paristech.fr

A simple field theory description of classical liquids is presented [1,2]. The formalism is distinct from the standard density functional theory (DFT). The partition function is a functional integral. The Hamiltonian of the system includes the standard interaction potential between particles as well as the ideal gas free energy functional. This well known term, often viewed as a trivial contribution, has in this context an important role when calculating the functional integral. It couples the fields and accounts for the principle of indiscernability.

The approach is applied to systems at interfaces. Emphasis is put on the validity of the contact theorem to verify the consistency of the different approximations. A new contact theorem for the charge will be given [3]. Analytic expressions for the density profiles have been derived for the mean field as well as the fluctuation contributions. The above mentioned ideal entropic coupling is shown to be essential to ensure the contact theorem for mean field and fluctuation contributions introducing a coupling between charge and total density fields. This is in contrast with the Mean Spherical Approximation MSA where total density and charge profiles are set by two independent relations and contact theorem is not verified. Ionic profiles show a depletion at the interface [4], in relation with the so called anomalous behaviour of the electric capacitance [5]. Asymmetric in valence systems can also well described in this formalism and exclusion volume taken into account [4,6].

Prospective application to ionic liquids combining association theory and field theory will be discussed.

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Effects of disordered porous media on the vapour-liquid phase equilibrium in ionic fluids: application of the association concept

Myroslav Holovko, Taras Patsahan, Oksana Patsahan

Institute for Condensed Matter Physics of the Academy of Sciences of Ukraine, 1 Svientsitskii Str., Lviv 79011, Ukraine
holovko@icmp.lviv.ua

We study the vapour-liquid phase behaviour of two-component size-symmetric and size-asymmetric primitive models of ionic fluids confined in disordered porous matrix formed by uncharged hard spheres (HS) or overlapping hard spheres (OHS). The proposed theoretical approach combines the scaled particle theory and the associative mean-spherical approximation based on the simplified mean-spherical approximation. The theory correctly reproduces the basic effects of porous media on the vapour-liquid phase diagram, i.e. with a decrease of porosity the critical point shifts toward lower fluid densities and lower temperatures and the coexistence region is getting narrower. An analysis of the ion-association along the vapour-liquid coexistence curves demonstrates that it strongly depends on a matrix porosity by causing an increase of ionic pairing degree in the ionic system when the porosity is lowering. At the critical point it is observed that the association degree reaches its minimum in the gas phase and the maximum in the liquid phase. It is also shown that the critical parameters of both the symmetrical and asymmetric ionic fluids confined in the OHS matrix are higher than in the HS matrix if the porosity is fixed.

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Charge distribution and ion transfer across the intergrain region in a model of solid state ionics

Vyacheslav Vikhrenko

Belarusian State Technological University, 13a Sverdlova str., 220006 Minsk, Belarus
vvikhre@gmail.com

A simple model of an intergrain region of an oxide ceramic electrolyte is used for kinetic Monte Carlo (KMC) simulations of the charge and electric field distribution in the system consisted of the grain bulks and intergrain region. The activation energies of thermally activated particle transitions in the grain bulk and intergrain region alongside the medium dielectric constant were the parameters of the model. The influence of the charge distribution on the grain boundary resistance is discussed. The density gradient contribution to the free energy was taken into account; the modified Nernst-Planck-Poisson (NPP) equation was formulated and used for the analysis of the charge distribution in the vicinity of the intergrain region. The analytical solutions of the modified NPP equation are compared with the results of the KMC simulations. The parameters of yttria stabilized zirconia are used as reference values while the model is of a more general nature. The model discloses a significant contribution of Coulomb interion interactions into the electric conductivity activation energy that at low values of the dielectric constant can reach 0.5 eV or even larger values.

The intergrain region is characterized by bigger activation energy for thermally activated particle transitions between neighboring lattice cells as compared to the grain bulk that have to result in its bigger electrical resistance. The simulations reveal the appearance of electric double layers at the boundaries of the intergrain region. At equilibrium conditions or at a weak external electric field the double layers appear at both sides of the intergrain region, while at a stronger field the only double layer is formed by excess charges of opposite signs at the boundaries of the intergrain region. These local deviations from electroneutrality appear due to hindered transitions from the grain bulk to the intergrain region and Coulomb interion interactions. In turn, these double layers produce quite a strong electric field that pushes the ions through the intergrain region and in fact suppress the intergrain region resistance. All the ions that come to the region of the double layers are rapidly transferred through the intergrain region in the direction of the external applied field so that the total resistance of the system is almost completely determined by the grain bulk resistance. These charge distributions are compared with the analytical solutions of the modified Nernst-Planck-Poisson equation that accounts for large density gradients in the vicinity of the intergrain region, and a complete qualitative agreement of the results is observed.

Some rigorous relations for transport coefficients in theory of fluids: the case of model ionic liquids

Ihor Mryglod

Institute for Condensed Matter Physics of National Academy of Sciences of Ukraine, 1
Svientsitskii Street, 79011 Lviv, Ukraine,
mryglod@icmp.lviv.ua

Some aspects of transport phenomena in fluids are discussed on the basis of non-equilibrium statistical theory. In particular, it is shown that so-called “universal golden rule”, formulated empirically by Sundheim for partial conductivities of binary charge-symmetric molten salts more than 60 years ago, can be derived rigorously. Furthermore, it is demonstrated that this relation has to consider as an example of a wider class of explicit identities for generalized transport coefficients valid for a multi-component mixture.

Phase Behaviour and Criticality in Primitive Models of Ionic Fluids

Oksana V. Patsahan

Institute for Condensed Matter Physics of NASU, Lviv, Ukraine

oksana@icmp.lviv.ua

Over the past several decades, the phase diagrams and the critical behaviour of ionic fluids with dominant Coulomb interactions have been intensively studied by using experimental and theoretical methods. A major part of theoretical and numerical works has been focused on the phase diagram of primitive models (PMs) consisting of an electroneutral mixture of charged hard spheres immersed in a structureless dielectric continuum. Considerable efforts have been made in order to develop theories for the description of vapour-liquid phase behaviour in these systems. In particular, the theoretical approaches have been proposed in which ion association is explicitly taken into account. The main of them are the generalized Debye-Hückel theory and the associative mean-spherical approximation. On the other hand, the theories have been developed that use functional integration methods and allow one to take into account the effects of higher-order correlations. In particular, a number of important results have been obtained by using the mesoscopic field theory and the approach that exploits the collective variable (CV) method. In contrast to the bulk case, the phase behaviour of ionic fluids in disordered confinements has not been studied well.

In this talk, we present the results obtained within the framework of the CV based theory. First, we present a brief overview of the main results for the phase and critical behaviour of PMs in the bulk. Then, the recent progress in studying the vapour-liquid equilibrium of a simple ionic model confined in a disordered porous medium is reported.

Tunability and order: the plethora of polymorphism of Wigner bilayer systems

Gerhard Kahl

Institut für Theoretische Physik and CMS, TU Wien, Vienna, Austria

gerhard.kahl@tuwien.ac.at

Self-assembly into target structures is an efficient strategy of materials design. In our problem we consider an ensemble of mobile point charges (carrying nominal charges $-e$) that are confined between two parallel plates; these plates are separated by a distance η and bear uniform charge densities $\sigma_1 e$ and $\sigma_2 e$, with $A = \sigma_2/\sigma_1$. Combining complementary theoretical approaches (i.e., analytical calculations, computational techniques based on evolutionary algorithms, and Monte Carlo simulations) we provide a comprehensive diagram of ordered ground state configurations of the charges as we systematically vary the asymmetry parameter A and the plate separation η [1]. The complex interplay between structural commensurability requirements and charge neutralization leads to a plethora of exotic Wigner bilayer ground state configurations (among those Archimedean tilings or pentagonal structures). Further we observe long-range attractions between the plates, the appearance of macroscopic charges, and the emergence of non-conventional phase transitions, pertaining to different universality classes. The simplicity of the system offers the possibility to conveniently and precisely control these features via the two external parameters, A and η .

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Simulation studies of short-ranged attractive and long-ranged repulsive (SALR) potentials

Nigel Wilding
University of Bath, UK

A SALR potential can be used as a simplified representation of the effective interaction between like charged colloids (in a sea of counter-ions) when they are mixed with polymer. In such a system a short ranged attractive depletion interaction between the colloids competes with a longer ranged (eg. screened coulomb) repulsion. Theory and computer simulation have revealed that such models exhibit rich phase diagrams that differ qualitatively from those of systems having solely attractive or repulsive interactions. For instance, as the degree of repulsion is increased from zero the standard liquid-vapor critical point may transform into a Lifshitz point heralding entry to a microphase separated state. In this talk I will review some of the principal simulation and theoretical findings to date before focusing on the results of simulation studies for continuous and lattice based models of a two-Yukawa fluid.

Equilibrium phase behavior and self-assembly dynamics of microphase forming models

Patrick Charbonneau

Trinity College of Arts and Sciences, Duke University, Durham, USA

patrick.charbonneau@duke.edu

Colloidal models with short-range attraction and long-range repulsion (SALR) assemble into a rich set of equilibrium periodic microphases, including cylindrical, double gyroid and lamellar phases. We present the phase diagram of such an SALR system obtained using specialized Monte Carlo methods. Remarkably, we also find that the disordered phase displays rich structural crossovers that give rise to a complex sequence of dynamical regimes. The dynamics notably depends on the formation and percolation of mesoscale cavities. We finally consider how easily periodic microphases can self-assemble. This analysis provides guidance for the design of colloidal experiments that should reliably obtain periodic mesophases.

Phase Diagram of a System with Competing Interactions

Roland Roth, Markus Edelmann, and Daniel Stopper
Institut für Theoretische Physik, Eberhard Karls Universität Tübingen
Tübingen, Germany
Roland.Roth@uni-tuebingen.de

Classical density functional theory (DFT) is a powerful tool to study the equilibrium structures and corresponding thermodynamics of a system with competing interactions. It also provides a framework to study the influence of various theoretical approximations. Here we study a system with competing interactions consisting of two Yukawa potentials and study its phase diagram. As a first step we derive a Landau-like theory to connect to previous work by A. Ciach et al [1,2] by expanding a local density approximation (LDA) functional into a Taylor series. The predictions of this approach are compared to numerically more demanding full minimizations of a DFT within the so-called fundamental measure theory (FMT), the state of the art functional for hard-sphere repulsion. We study the structures and their thermodynamical stability of different inhomogeneous bulk structures and verify the existence of the gyroid phase for systems with spherically symmetric interaction potentials [3,4]. Some extensions of the model are discussed.

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Hunting Mermaids in Real Space

Patrick C. Royall

HH Wills Physics Laboratory, Tyndall Avenue, Bristol, BS8 1TL, United Kingdom
The School of Chemistry, University of Bristol, Bristol, BS8 1TS, United Kingdom

Paddy.Royall@bristol.ac.uk

We report studies of model colloidal system tuned to exhibit a so-called mermaid type potential with a short-ranged attraction and long-ranged repulsion. We consider a very well-characterised experimental system, in which both attractions and repulsions are well-characterised individually, by the Asakura-Oosawa and Derjagun-Landau Verwey and Overbeek models respectively [1,2,3]. Remarkably, by comparing with expectations [4,5,6], we show that bringing both interactions together leads to a fundamental breakdown in a spherically-symmetric one-component description of the colloid-colloid interactions. This broken spherical symmetry is replaced by a complex, many-body interaction in which the energy landscape of the colloidal clusters formed is profoundly altered. We present evidence that this complex energy landscape may be related to coupling of the dynamics of the colloids and small ions [7].

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Inhomogeneous integral equation approaches to describe confinement

E. Lomba

Institute of Physical Chemistry ROCASOLANO, CSIC, Madrid, Spain

Enrique.Lomba@csic.es

We explore a series of full N-dimensional integral equation approaches based on the Ornstein-Zernike relation, following the prescriptions both of Beglov and Roux (3DOZ) and Kjellander and Sarman (IOZ) to describe the explicit density distribution of simple and molecular fluids confined in geometries ranging from the simple slit pore to extreme confinement in disordered media.

Nanoparticles interactions tailoring toward nanomaterial design for targeted applications

Abdelhafed Taleb

PSL Research University, Chimie ParisTech - CNRS, Institut de Recherche de Chimie Paris,
75005, Paris, France

Université Pierre et Marie Curie, 4 place Jussieu, 75231 - Paris France
abdelhafed.taleb@upmc.fr

Over the past few years, nanoscience and nanotechnology have been the focus of significant research interest, from scientists in academia and industry. Nanomaterials play an important role in the development of new materials with new properties or enhanced existing properties. Material design based on nanoparticles as building units appear as a new approach with an unprecedented opportunity to prepare material with desired properties for targeted applications. This approach present the advantage to be flexible by offering a wide range of possibilities to assemble nanoparticles in various architectures. Additionally, it offers new possibilities to combine nanoparticles of different chemical compositions, sizes, shapes, and surface modifications with a myriad of molecules. All these possibilities allow to tune the properties of the designed material; and in turn to target a given application. To develop such approach of material design, a comprehensive knowledge of how nanoparticles interact with each other is a crucial parameter of paramount importance. We will present how the interactions between nanoparticles can guide their design for targeted applications. A general overview of the interactions involved in nanoparticles assembly design is provided with an emphasis to targeted applications.

Phase behaviour and assembly of colloids with heterogeneously charged surfaces

Eva G. Noya¹, Ismene Kolovos², Günther Doppelbauer², Emanuela Bianchi² and Gerhard Kahl²

¹ Instituto de Química Física Rocasolano, Consejo Superior de Investigaciones Científicas (CSIC), C/ Serrano 119, 28006 Madrid, Spain

² Institut für Theoretische Physik and Center for Computational Materials Science (CMS), Technische Universität Wien, Wiedner Hauptstraße 8-10, A-1040 Vienna, Austria
eva.noya@iqfr.csic.es

In the last few years the theoretical investigation of the phase behaviour of particles either with anisotropic shapes or interactions has been a very active field of research. Initially this work was motivated by advances in colloidal science that allowed the synthesis of those particles and that lead to the suggestion of building new materials with the desired properties using a "bottom-up" approach, i.e. by designing the particles that would self-assemble into the target structure [1, 2]. However it soon became evident that the theoretical study of those particles was interesting also from a fundamental point of view. Anisotropic particles can exhibit an amazingly rich and unusual phase behaviour [3]. Here we investigate the phase behaviour of Inverse Patchy Particles (IPC), a model representative of negatively charged particles with two positively charged patches at the poles [4]. As a consequence regions with opposite charge attract each other but regions with like charge repel each other. The equilibrium phase diagram was evaluated using a combination of two well established techniques: first, an efficient optimization tool based on ideas of evolutionary algorithm is used to identify the stable structures at zero temperature and, second, the stability of those phases at finite temperature is investigated by free energy calculations [5]. We found that the competition between the attractive and repulsive interactions leads to a wealth of ordered structures, including a laminar structure that is stable over a quite broad region of the phase diagram. The effect of the model parameters on the stability of the ordered phases will also be discussed.

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Thermodynamic and diffusion characteristics of lattice models with obstacles and competing interactions

Ya. G. Groda

Belarusian State Technological University, 13a, Sverdlova str., 220006, Minsk, Belarus
groda@belstu.by

The models of a lattice fluid with nearest neighbor interactions on a square lattice (SQ) with blocked sites and lattice fluid with SALR-potential on a triangular lattice (TR) is considered. For calculating equilibrium properties the reference lattice system that is defined by the one-particle mean potentials is introduced. The free energy of the initial lattice system is represented as a sum of the free energy of the reference system and the diagram part. The free energy of the reference system is represented in a closed form through elementary functions, whereas the diagram part of the free energy is represented by the diagram expansion in Mayer-like functions renormalized by the mean potentials with averaging over the states of the reference system.

As a first step in the free energy expansion we considered the free energy of the reference system and the two-vertex irreducible diagram contributions only. For the system with nearest neighbor interactions such an approximation corresponds to the ordinary quasi-chemical approximation (QChA). For more distant interactions the mean potentials are determined by the same expressions with the interaction energies of the corresponding neighbors only. In this QChA all the equilibrium properties are represented through the mean potentials that in turn are selfconsistently calculated with the extremity principle.

Based on the proposed approximation the expression for the chemical potential, the thermodynamic factor and the distribution functions are obtained in a closed form. The QChA predicts the appearance of the ordered phase in the system with repulsive nearest neighbor interactions.

The results of Monte Carlo simulation of equilibrium properties and diffusion characteristics are compared with the results of QChA. It is shown that QChA offers reasonable semiquantitative results for the studied systems and can be used as a basis for the next order approximations. It has been established that in the case of systems with repulsive interaction the blocked sites destroy a global chess board order on the lattice.

Diffusion of a lattice fluid on a simple square lattice with blocked sites is considered. The dependences of the jump diffusion coefficient versus concentration of blocked sites and concentration of particles are investigated. It has been established that at $k_B T > |J|$ the jump diffusion coefficient can be estimated by Zhdanov's expression through equilibrium characteristics of the system. The new expression for the jump diffusion coefficient at low temperature and high concentration of blocked sites is proposed.

The Monte Carlo simulation results for equilibrium properties of the lattice fluid with SALR-potential are compared with the results of QChA. The GQChA reasonably reproduce the equilibrium thermodynamic quantities (chemical potential, thermodynamical factor) and structural (the two-particle distribution functions for the nearest neighbors). However, it fails to reproduce more distant correlations in the system.

Comparison of the amphiphilic and the colloidal self-assembly

A. Ciach

Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland
aciach@ichf.edu.pl

In this talk amphiphilic systems are compared with systems containing spherical particles attracting each other at small-, and repelling each other at large distances (SALR interactions). We show that close similarity between phase diagrams in these systems follows from the fact that both of them can be described by the Landau-Brazovskii (LB) functional. Key steps of the coarse-graining procedure applied to the SALR system and leading to the LB functional are presented. In the second part of the talk equation of state, correlation function and specific heat obtained by the exact transfer matrix method for one-dimensional models of various inhomogeneous systems are compared.