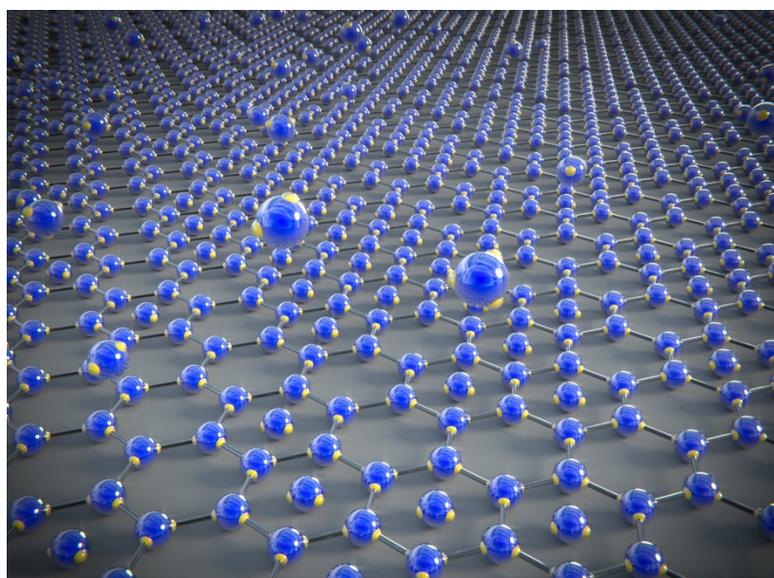


II CONIN Workshop: Systems with competing electrostatic and short-range interactions

Book of abstracts



Madrid, 7th-8th March 2018

Instituto de Química-Física Rocasolano

Consejo Superior de Investigaciones Científicas (CSIC)

<http://conin.iqfr.csic.es>



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March 7

14:30-15:00- Registration (IQFR main entrance)

Chair: Enrique Lomba

15:00-15:10 – Workshop opening

15:10-15:50 – **Willem Kegel**: *“Structure formation in colloids with competing interactions”*

15:50-16:30 – **Alexei Kornyshev**: *“New Horizons in Ionics: Electrochemical ‘Metamaterials’”*

16:30-17:00: *Coffee break*

Chair: Vyacheslav Vikhrenko

17:00-17:30 – **Abdelhafed Taleb**: *“New preparation approach of nanodiamond and poly pyrrole nanocomposite coating for anti-corrosion applications”*

17:30-18:00 – **Enrique Lomba**: *“Effective SARL interactions and hyperuniformity”*

18:00-18:30 – **Taras Patsahan**: *“Phase behaviour of ionic solutions: the restricted primitive model of ionic liquid in an explicit neutral solvent”*

March 8

Chair: Guillermo Zarragoicoechea

09:00-09:40 - **Martin Sweatman**: *“The SALR fluid at low concentrations: giant clusters and their reproduction”*

09:40-10:20 - **John Griffin**: *“Understanding the behaviour of ions in carbon micropores by NMR spectroscopy”*

10:20-10:40 - **Wojciech Gozdz**: *“Monocrystals, thin films, and cubosomes made from lyotropic liquid crystals”*

10:40-11:00- *Coffee break*

Chair: Wojciech Gozdz

11:00-11:30- **Svyatoslav Kondrat**: *“Accelerating charge/discharge in nanoporous supercapacitors”*

11:30-12:00 – **Vyacheslav Vikhrenko**: *“Charge screening of mobile ions in lattice models”*

II CONIN Workshop program (March 7th-8th, 2018)

12:00-12:30 – **Oksana Patsahan**: *“Vapour-liquid phase behaviour of an asymmetric primitive model of ionic fluids confined in a disordered matrix”*

12:30- 14:30- *Lunch*

Chair: Dung Di-Caprio

14:30 –15:10 - **Jose Nuno Canongia Lopes**: *“Ionic Liquids as Cnidaria or Mollusca: From bulk to surface structuration”*

15:10-15:40 - **Jakub Pekalski**: *“Stripes under confinement”*

15:40-16:00 – **Ihor Mryglod**: *“A simple ansatz for memory functions evaluation: single particle dynamics as a case study”*

16:00-16:30: *Coffee break*

Chair: Oksana Patsahan

16:30-17:00-**Yaroslav Groda**: *“Lattice fluid with SALR interaction potential on simple square lattice”*

17:00-17:30-**Guillermo Zarragoicoechea**: *“Self-organization, self-assembly and SARL potential”*

17:30-18:00- **Myroslav Holovko**: *“Primitive models of room temperature ionic liquids. Vapour-liquid phase coexistence”*

Structure formation in colloids with competing interactions.

Willem K. Kegel

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In this presentation I will provide an overview of experiments and theory on structure formation in colloidal particles that interact via short-range attraction and 'competing' long-range electrostatic repulsion. Next to thermodynamically stable finite aggregates, these systems may form non-equilibrium clusters as well as other states that depend on the formation pathway, such as polycrystalline gels and low-density gels. I will discuss recent experimental observations in colloidal model systems as well as in proteins, and end up with a discussion of the possible stability of periodic structures.

New Horizons in Ionics: Electrochemical 'Metamaterials'

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Term *metamaterials* stands for materials with unusual properties and functionalities. These, mainly photonic metamaterials, were enabled by progress in nanotechnology. Highly demanded now is their tuneability, ideally in real time. Physical chemistry responded to it with the idea of chemically tuneable self-assembly of nanostructures, however, without real-time control, but electrochemistry could be the game changer here. At electrochemical interfaces one can create electric fields, controlled by potentiostat that may not only affect the structural changes in real time, but could literally turn them on and off.

Typical examples of such systems are:

- (1) self-assembling **electro-tuneable/switchable nanoplasmonic devices such as**
 - mirror-windows
 - reflectors with tuneable spectra
 - optical cavities
 - nano-columnar displays
- (2) **variable-focus electrowetting-based lenses and mirrors**
- (3) **supercapacitors** for energy storage and backup
- (4) polymer-electrolyte-based **electroactuators** for converting voltage in mechanical motion for robotics
- (5) **reverse actuators** for generating AC current from mechanical motion, e.g. walking
- (6) **voltage-controlled lubricity** for tuning or turning friction on and off

What unites all these topics from the physical point of view is the key role of ionic structures controlled by applied potential at the nanoscale. Noteworthy new scenarios for *electrochemical metamaterials* were almost always navigated by theory, some realised, some in the stage of development. Altogether, this emerging directions of research open new horizons in *ionics*, interesting both from fundamental and applied points of view.

Electric-field control at the nanoscale is based on ionic screening. Although for this we can use ordinary electrolytes, for many reasons it is interesting and appropriate to employ room-temperature ionic liquids and their mixtures with solvents.

In my talk I will show few selected examples of electrochemical metamaterials, with a primary focus on photonic ones, as well as smart structures for robotics and current generating shoes.

With intention to overview in the allocated time just a small part of this emerging research area, my talk will be majorly based on a series of joint works of Imperial College theoretical chemical physics team at (Dr. D.Sikdar, Z.Goodwin, C.Zagar, A.Bucher) with experimental groups of Prof. J.Edel and Prof. A. Kucernak, as well as with our partners at the University of Tel Aviv (Professor Urbakh) and University of Iowa (Professor M.Flatte), Rice University (Prof. A. Kolomeisky), Duesseldorf University (Prof. H. Loewen and Prof. M.Eikerling), and few other groups, to be highlighted and acknowledged in the talk.

New preparation approach of nanodiamond and poly pyrrole nanocomposite coating for anti-corrosion applications

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Materials in aggressive environment are usually subjected to degradations, whose severity level depends on the properties of both materials and the mediums with which they are in contact. Usually these degradations are of electrochemical and/or mechanical natures and induce materials weight loss [1]. Furthermore, other material properties could be weakened by these degradations, such as the mechanical properties [2]. Corrosion, through electrochemical dissolution is one of the processes, which induces materials degradation and limit their sustainability and usefulness.

Different approaches were developed to limit the corrosion deleterious effect, among which the anticorrosion coating is the most popular. Furthermore, among these coatings, those based on nanocomposites improve considerably the material properties in terms of performances and lifespan [3]. For a given material and its surface properties in terms of roughness and wetting behavior, adequate coating must be used to optimize its anticorrosion efficiency.

In the present work, some results are reported regarding the use of nanocomposite coating based on nanodiamond and polypyrrole, as efficient anticorrosion coating for steel. The properties of prepared coating were characterized by different methods, such as DLS, FEGSEM, profilometer and electrochemical measurements. A plotted Tafel curves show clearly that the anticorrosion efficiency of prepared coatings depends on both the metal surface properties and the coating properties in terms of structure, composition and design.

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Effective SALR interactions and hyperuniformity

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Long ranged interactions (either effective or bare) are a key element in the presence of disordered hyperuniformity [1]. This property, which is connected with the suppression of long range density fluctuations, is reflected in the presence of structural long range order (as in crystals) and short range disorder (as in fluids). It has been shown to occur in a wide number of man-made and natural materials, such as wide gap disordered semiconductors, some stealth materials, and bird retina [2]. We will show how some simple multicomponent systems display a variety of patterns as a result of self-organisation due to the interplay of short range effective attractive interactions and long range Coulomb-like repulsions, while preserving a disordered multi-hyperuniform structure [3].

References

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- [3] Lomba, E., Weis, J.J., and Torquato, S. *Phys. Rev. E*, 97, 010102(R) , **2018**

Phase behaviour of ionic solutions: the restricted primitive model of ionic liquid in an explicit neutral solvent

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We report recent theoretical results on a study of the phase behaviour of ionic solutions, where a neutral solvent is treated explicitly. For this aim, we consider a restricted primitive model (RPM) of ionic fluid in a mixture with uncharged particles of solvent. We applied the well known approaches such as the random phase approximation (RPA), mean spherical approximation (MSA) and associative mean spherical approximation (AMSA), and observed some qualitative differences between their results. In particular, in the RPA we obtained an evidence of the closed solubility loop and lower critical solution temperature (LCST)-type of phase transition for a mixture of RPM fluid and hard sphere solvent, while in the MSA and AMSA they were not found. Also the phase diagrams calculated in the RPA indicate the transition to an ordered phase at higher densities and at low solvent concentrations. On the other hand, the AMSA provides much better quantitative agreement with computer simulations data for the upper critical point. Besides, we extend the mentioned approaches to take into account an attraction between ions and solvent in the form of square-well pair potential. It was shown that this attraction makes the phase diagram much broader and the second critical point can appear in the region of higher densities. Finally, we propose an approach for the description of thermodynamic properties of ionic solutions, where solvent molecules are of an elongated shape and can be presented, for instance, as hard spherocylinders. For sufficiently long spherocylinders the phase diagram alters significantly due to the isotropic-nematic phase transition occurring in such a system.

Understanding the behaviour of ions in carbon micropores by NMR spectroscopy

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Ion adsorption in porous carbons underpins many important devices and processes in areas such as energy storage, filtration and purification. In order to optimise and fully exploit these technologies, we need to have a detailed picture of the ion behaviour at the electrolyte-carbon interface; however, this is difficult to do experimentally due to the highly complex and dynamic nature of the system. In this talk I will show how NMR spectroscopy can be used as a probe of ion behaviour in these complex systems, and how in situ experiments can reveal how ions populate the pores in charged electrodes. This has relevance to the design of electrodes and electrolytes for supercapacitors as well as considerations for capacitive water desalination.

The SALR fluid at low concentrations: giant clusters and their reproduction

M.B. Sweatman

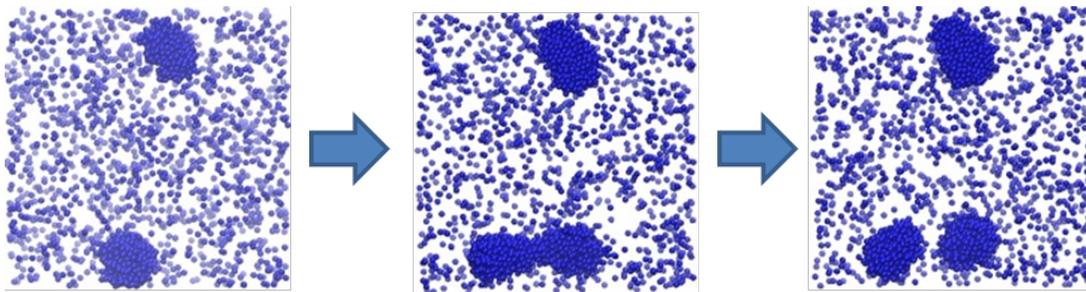
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Particles with SALR (short-range attraction and long-range repulsion) interactions are common to many physical systems, especially biological and soft matter, yet their behaviour is still not completely understood. Here, I will provide a survey of my recent work concerning theory and simulation of the equilibrium behaviour of SALR fluids at low concentrations. These fluids display micelle-like phase behaviour, forming giant clusters above a critical cluster concentration. This 'cluster fluid' can itself undergo novel phase transitions. I will also show that giant SALR clusters can grow and reproduce in these fluids, potentially leading to chemical evolution of giant SALR clusters (life?) in suitable systems

M.B. Sweatman, Molecular Physics, published online 2017

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Monocrystals, thin films, and cubosomes made from lyotropic liquid crystals

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Bicontinuous cubic phases are composed of two disjoint water channels separated by a lipid bilayer. Examples of a unit cell of the cubic phases are shown in Fig. 1, where the surface represents the location of the bilayer. When a liquid crystal phase is in equilibrium with an isotropic phase an interface is formed. The structure of such an interface is presented in Fig. 1. Liquid crystals are anisotropic and the structure of the interface depends on the orientation of the unit cell with respect to the surface of the interface. Such interfaces are formed in monocrystals [3,4], thin films [2], and nanoparticles [1] formed from bicontinuous phases. We have determined the structure and stability of the interfaces for different phases and different orientations of the unit cell with respect to the interface surface. The calculations were performed within the framework of the Landau-Brazovskii functional [1-3]. The results of the calculations were compared with the results of available experiments. Good agreement between the theoretical calculations and the experimental results was obtained. It has been shown that different phases have the stable interfaces for different orientations of the unit cell with respect to the interface. Such behavior influences the orientation of the lyotropic liquid crystals in thin films and the stability of different facets in monocrystals.

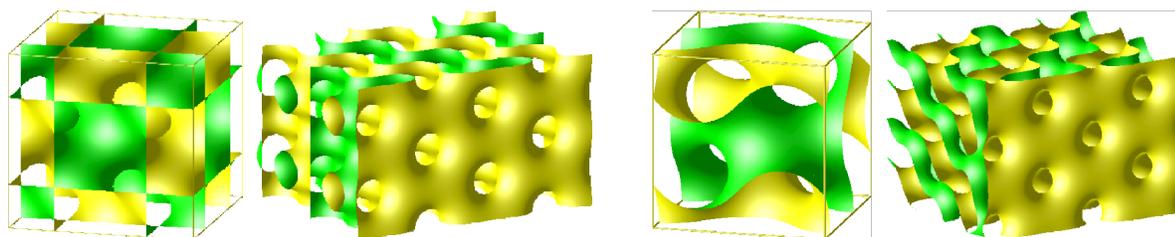


Fig1. The unit cell of diamond and gyroid phases with the most stable interfaces. The interfaces are perpendicular to the [111] and [110] directions for the diamond and gyroid phase respectively. The colors represent different sides of the surface.

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Accelerating charge/discharge in nanoporous supercapacitors

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Nanoporous supercapacitors attract considerable attention as green energy storage devices with remarkable cyclability and high power and energy densities. However, their use in high frequency devices is limited by relatively slow charging processes. In this talk I focus on the physics and optimization of charge/discharge cycles. We will see that the frequently used step-voltage charging is slow because the co-ions become trapped inside narrow pores of supercapacitor electrodes. To avoid co-ion trapping, a slow voltage sweep is applied, which allows to accelerate the overall charging process substantially if the sweep rate is properly optimized. We shall see, however, that the step-voltage, rather than sweeping, is best for fast discharging. Based on our findings we propose an optimal charge/discharge cycle and discuss optimization strategies.

Charge screening of mobile ions in lattice models

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The system of mobile ions with long range Coulomb and additional short range interactions on the background of fixed counterions is considered. The lattice fluid model of the system is suggested. In the framework of the collective variables method, the screening of the Coulomb interactions in the bulk and at the plane boundary is considered and it is shown that the Debye length includes additional concentration dependence inversely proportional to the square root of the mean concentration of vacant sites. The Coulomb interaction contribution to the free energy of the system is calculated in the approach close to the mean spherical approximation and is given in an analytical form.

The influence of the variation of the crystal field near the system boundary on the structure and characteristics of the electric double layer in the mean field approximation is investigated. In this approximation the Fermi-Dirac type of concentration distribution is deduced. In a more general case when interparticle correlations are taken into account the Fermi-Dirac type distribution cannot be analytically solved with respect to concentration and includes additional concentration dependent term.

As compared to the system with equal crystal potentials at the lattice sites throughout the system, the pronounced difference for the electric capacitance appears at low absolute values of the surface potential and for positive ions it is more pronounced for negative electric potentials. In the mean field approximation the capacitance diverges at the potential values at which the surface electric field tends to zero, and attains negative values in regions of the surface potentials depending on their polarity and the difference between the surface and bulk crystal potentials. Negative values of the capacitance may indicate the thermodynamic instability of the system although more consistent accounting of the short range interaction contribution and interparticle correlations can considerably change the behavior of the system at low absolute values of the surface potential.

Vapour-liquid phase behaviour of an asymmetric primitive model of ionic fluids confined in a disordered matrix

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I will present our recent results [1,2] for the vapour-liquid phase behaviour of ionic fluids in a disordered porous medium obtained by using the theoretical approach which combines the collective variable-based theory [3] with a recent extension of the scaled particle theory (SPT) [4]. The ionic fluid is described as a two-component asymmetric primitive model (PM) and a porous medium is modelled as a disordered matrix formed by hard-sphere obstacles. In addition to a size- and charge-asymmetry of ions we consider different size-ratios between the ion particles and the matrix obstacles. The approach proposed allows one to formulate the perturbation theory using the SPT for the description of the thermodynamics of the reference system. We derive an explicit expression for the chemical potential conjugate to the order parameter which takes into account the third-order correlations between ions. Using this expression, the vapour-liquid phase diagrams depending on the characteristics of an ionic fluid and a hard-sphere matrix are calculated-. We analyse how variations in the parameters of size- and charge-asymmetry and in the matrix porosity affect the critical parameters of a confined ionic model.

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Ionic Liquids as Cnidaria or Mollusca: From bulk to surface structuration

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The title of this presentation is based on the notion that ionic liquids will adapt their electrostatic and nano-structured nature to different two-dimensional boundary conditions. Two types of situation will be considered: hydrotrophy¹ and surface effects^{2,3}. The analogy between ionic liquids and animals from the Cnidaria or Mollusca animal phyla will be apparent throughout the presentation.

Hydrotropes are compounds able to enhance the solubility of hydrophobic substances in aqueous media and therefore are widely used in the formulation of drugs, cleaning and personal care products. In this presentation, it is shown that ionic liquids are a new class of powerful catanionic hydrotropes where both the cation and the anion synergistically contribute to increase the solubility of biomolecules in water. Molecular Dynamics simulations are used to explain the molecular mechanisms responsible for the strong hydrotrope effects exhibited by the studied ionic liquids.

Those mechanisms can also explain the surfactant or tribological behavior of ionic liquids at interfaces, as films or in confined conditions. Numerical density profiles obtained from the MD simulation trajectories and other MD data-farming tools are able to emphasize the very unusual packing of different IL systems under diverse confined situations.

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Stripes under confinement

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When short range attraction competes with long range repulsion variety of inhomogeneous structures can self-assemble. On quasi two-dimensional interfaces with increasing density clusters, stripes or bubbles are predicted by theoretical studies and computer simulations. The periodic boundary conditions which are typically used to model the bulk enhance periodic ordering of the structures. It is then of interest, what happens to the ordering when different type of boundary conditions are used. In this talk, I will review results obtained with A. Ciach and N. G. Almarza on the properties of the stripe phase in systems with different boundary conditions. In particular, I will present the influence of semi-infinite slit confinement [1] and of closed and curved surface of spherical shape [2], as well as some preliminary results for the closed and flat surface of hexagonal shape.

[1] N. G. Almarza, J. Pękalski, A. Ciach "Effects of confinement on pattern formation in two dimensional systems with competing interactions" *Soft Matter* 12, 7551-7563 (2016)

[2] J. Pękalski, A. Ciach, "Orientational ordering of lamellar structures on closed surfaces" (2018) (under revision)

A simple ansatz for memory functions evaluation: single particle dynamics as a case study

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A simple ansatz for the memory functions evaluation at different timescales is developed. This ansatz is based on an effective summation of the infinite continued fraction at a reasonable assumption about convergence of relaxation times of the higher order memory functions, which have purely kinetic origin. As a case study single particle dynamics is considered. The results obtained within our approach for velocity autocorrelation function (VAF) are compared with computer simulation data for the liquid Ne at different densities as well as with the theoretical results found for VAFs with different approximations for memory functions. It is shown that in all the thermodynamic points and at the chosen level of the hierarchy, our results agree much better with the MD data. The density dependence of the long tail amplitude and the transition time, needed for the fluid to attain the hydrodynamic stage of evolution, are evaluated. The common and distinctive features of our approach and the predictions of the generalized collective mode theory and the mode coupling theory are discussed.

Lattice fluid with SALR interaction potential on simple square lattice

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At present, there is a great interest in studying the processes of self-organization and self-assembly in nanoscale systems. The interaction between elements of such systems is very complex. In many cases it can be characterized as the competing interaction: along with a hard core repulsion when the distance between particles is close to their geometric dimension there are the Van der Waals type attraction on small distances and the electrostatic repulsion on a longer separation. For such interactions the SALR (short-range attraction and long-range repulsion) abbreviation is frequently used.

In [1] the Monte Carlo simulation was used for investigating the phase behavior of the SALR system on a triangular lattice. This report presents the results of a computer simulation study of a similar model on a square lattice.

We adopted, by analogy with [1], that $J_3/|J_1| = 3$, where J_1 and J_3 are the interaction energies of the particles occupying the nearest lattice sites and the nodes that are neighbors of the third order, respectively. In the case of SALR system $J_1 < 0$ and $J_3 > 0$ where taken that correspond to the attraction of the nearest neighbors and the repulsion of the next-next nearest neighbors. The Monte Carlo modeling of the equilibrium properties of the system was realized in the framework of the standard Metropolis algorithm. For simulation we used a lattice containing 2^{14} lattice sites with periodic boundary conditions. A preliminary simulation on a lattice containing 2^{10} lattice sites showed that two different types of ordered phases are formed in the system at sufficiently low temperatures. The specific type of the phase depends on the selected values of the chemical potential $\mu/k_B T$ and the interaction parameter $|J_1|/k_B T$.

For describing the ordered phases, the initial square lattice was divided into a system of 8 identical sublattices with the spacing $2a\sqrt{2}$, where a is the lattice spacing of the initial lattice. In the case of complete ordering of the system at the lattice concentration $c=0.5$ four sublattices are completely filled and four sublattices are completely vacant. This makes it possible to determine the system order parameter δc as the difference between the maximal and minimal concentrations on the sublattices.

With the introduced order parameter, it was established that the critical parameter of the model is equal to $|J_1|/k_B T = 0.655 \pm 0.005$ and the phase diagram of the system was constructed. In addition, the influence of the interaction energies of the nearest and the third neighbors on the critical parameter of the system was studied.

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Self-organization, self-assembly and SARL potential.

Guillermo J. Zarragoicoechea

Universidad de La Plata (Argentina)

Some applications of the short-range attraction/long-range repulsion (SARL) potential are shown in this presentation. This kind of interaction is used to represent self-assembly or self-organization in various systems. First, it is shown an application in ecology. When an ecosystem is under hydric stress, individuals self-organize forming different but very interesting spatial patterns. In this case, attractions are associated with collaboration between individuals while repulsion is associated with the competition for resources between them. Monte Carlo simulations are done in the Grand Canonical ensemble. External resources injected into the systems are, for instance, precipitations or nutrients in the soil. Results show a qualitative agreement between the simulated and the observed patterns on different semi-arid ecosystems on Earth. Another system is a coarse-grained representation of nanoparticles that interact through a SARL potential over a surface of a sphere of different radii. Simulations run over a NVT ensemble at different temperatures (parallel tempering technique). The system self-assembles forming very distinct patterns, as a function of the concentration and temperature. Finally, we use this kind of potential to represent cellular interaction and differentiation, or the reproduction and death of individuals in a growing system. The system model consists of an initial configuration where two components are distributed in different zones of the simulation cell, without mixing. This system is allowed to evolve using Monte Carlo simulation in the Grand Canonical ensemble. Results show that the patterns and behavior obtained (connection of isolated areas of the same characteristics) represent, for example, the vascularization of tissues, where cells with a certain functionality try to connect with each other.

Primitive models of room temperature ionic liquids. Vapour-liquid phase coexistence

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Several versions of primitive models of room temperature ionic liquids (RTILs) are proposed. RTIL is modeled as a two-component mixture of hard-sphere anions and flexible linear chain cations, represented by tangentially bonded hard spheres with the charge located on one of the terminal bonds. The theoretical description of the model is carried out using the solution of the appropriately modified associative mean spherical approximation (AMSA) with the ideal chain approximation for cations. The solution reduces to solving one nonlinear algebraic equation for the Blum's screening parameter Γ , which in turn is used to express all thermodynamic properties of the models of interest. We calculate liquid-gas phase diagrams using theoretical and computer simulation methods for two versions of the model represented by the dimer and chain models. Theoretical predictions for the phase diagrams appear to be in a reasonably good agreement with the computer simulation results. It is demonstrated that the models and the theory are able to qualitatively reproduce experimentally observed phase behavior of RTILs, in particular the decrease of the critical temperature and critical density with increasing asymmetry of the model in its shape and position of the charge.

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