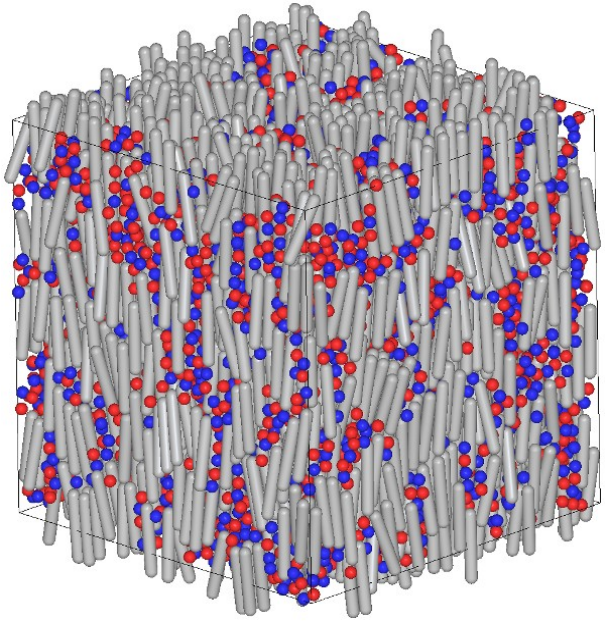
H2020-MSCA-RISE-2016 CONIN

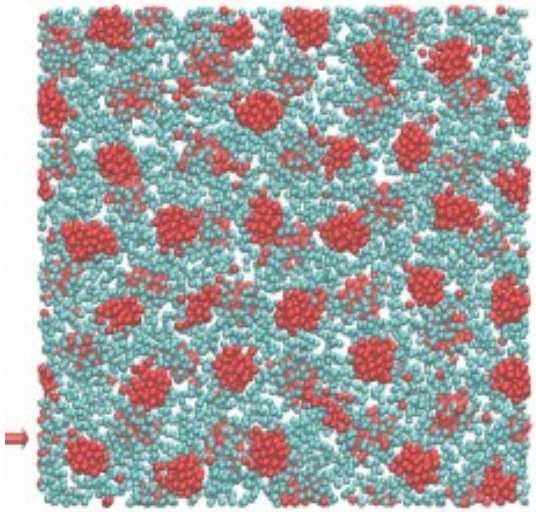
”**Effects of confinement on inhomogeneous systems**”

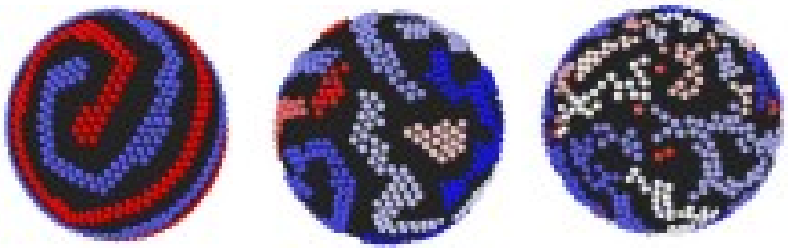
Grant agreement No 734276



MID-TERM MEETING

Coordinator's report





Madrid, March 2018

OUTLINE

1. **General status of the project and the WP implementation**
- main research objectives of the network
- scientific progress and success achieved

2**.Training, Transfer of Knowledge & Networking**
- Events organised within the network and beyond
- Secondment implementation
- Secondments - new knowledge acquisition, training activities

3**. Management**
- Institutions reorganization
- Proposed seecondment changes

4. **Dissemination of results and publications**

General status of the project and the WP implementation

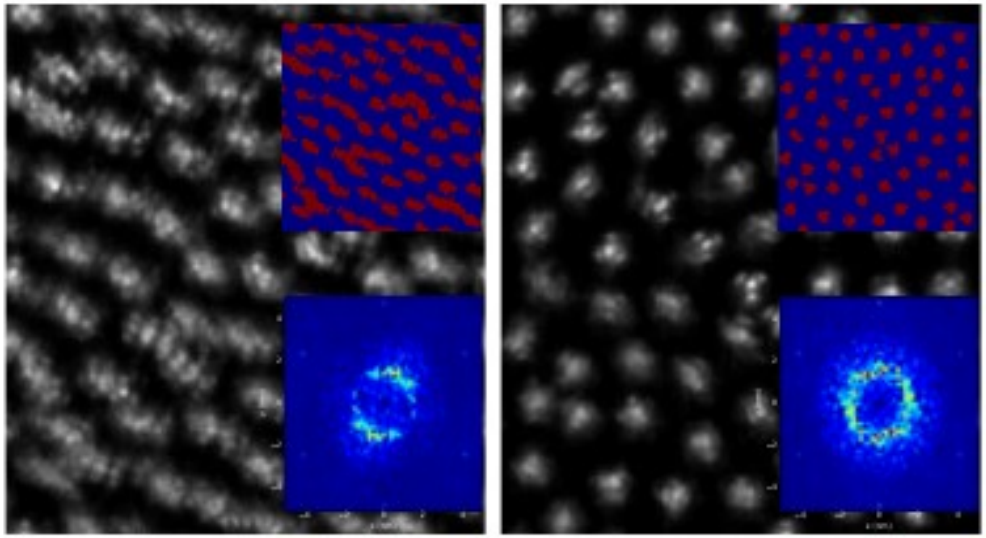
Main research objectives of the network

The general scientific objective of the project is determination of universal features and specific properties of various systems **spontaneously** ordering into spatially **inhomogeneous structures** (mobile ions in solids, ionic liquid mixtures, soft matter and biological systems), with special focus on effects of **confinement**.

Spontaneous formation of spacial inhomogeneities on various length scales is often induced by competing interactions. Competing interactions or tendencies are present in variety of systems across length scales from Angstroms to meters, as shown in the next slide.

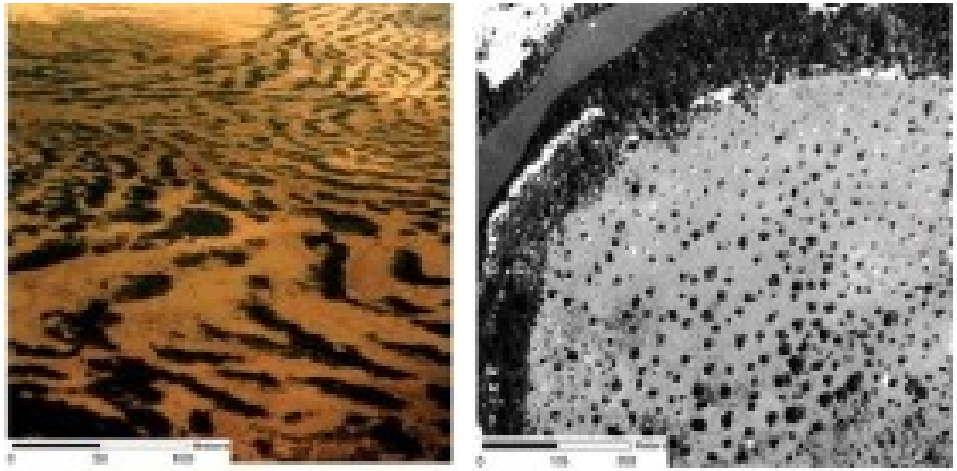
Despite importance of the systems with mesoscopic inhomogeneities and similarities of patterns formed at different length scales, a **unified theory of such systems is still missing.**

Another goal of the project is to intensify existing collaboration and to establish new collaboration between 3 groups form EU MS, 1 group from AC and 2 groups from TC.

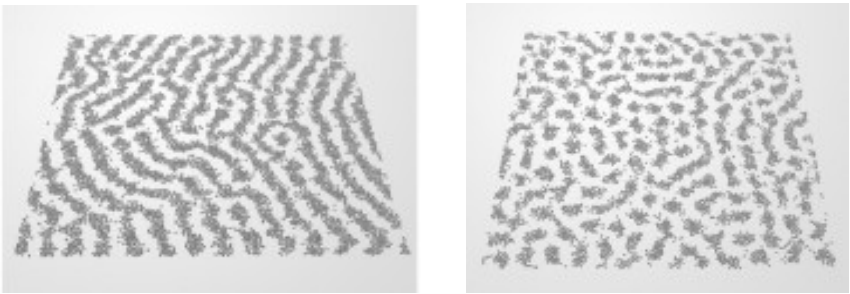


Density of a mixture of [BMIM][BF_4] with a 10% of Li[BF4] next to a graphene cathode with 5% (left) and 8% (right) of vacancy defects. The left image shows a striped phase while the right one an hexagonal phase.

H. Montes-Campos et. al.,*Universal 2D Pattern Formation in Confined Ionic Liquids,* PCCP, **19**, 24505 (2017)



Left: Striped pattern of bushy vegetation in Niger. Right: Tree patches in Ivory Coast.



Monte Carlo simulations on SALR interacting individuals in stressed ecosystems. Views are in perspective. La Plata group result.

Pattern formation in both cases can be described by a functional **of the same general form.** What is different is the nature of the order parameter, and the relation with measurable quantities. Mathematical structure of models is similar, and tranfer of knowledge is important.

Work packages:

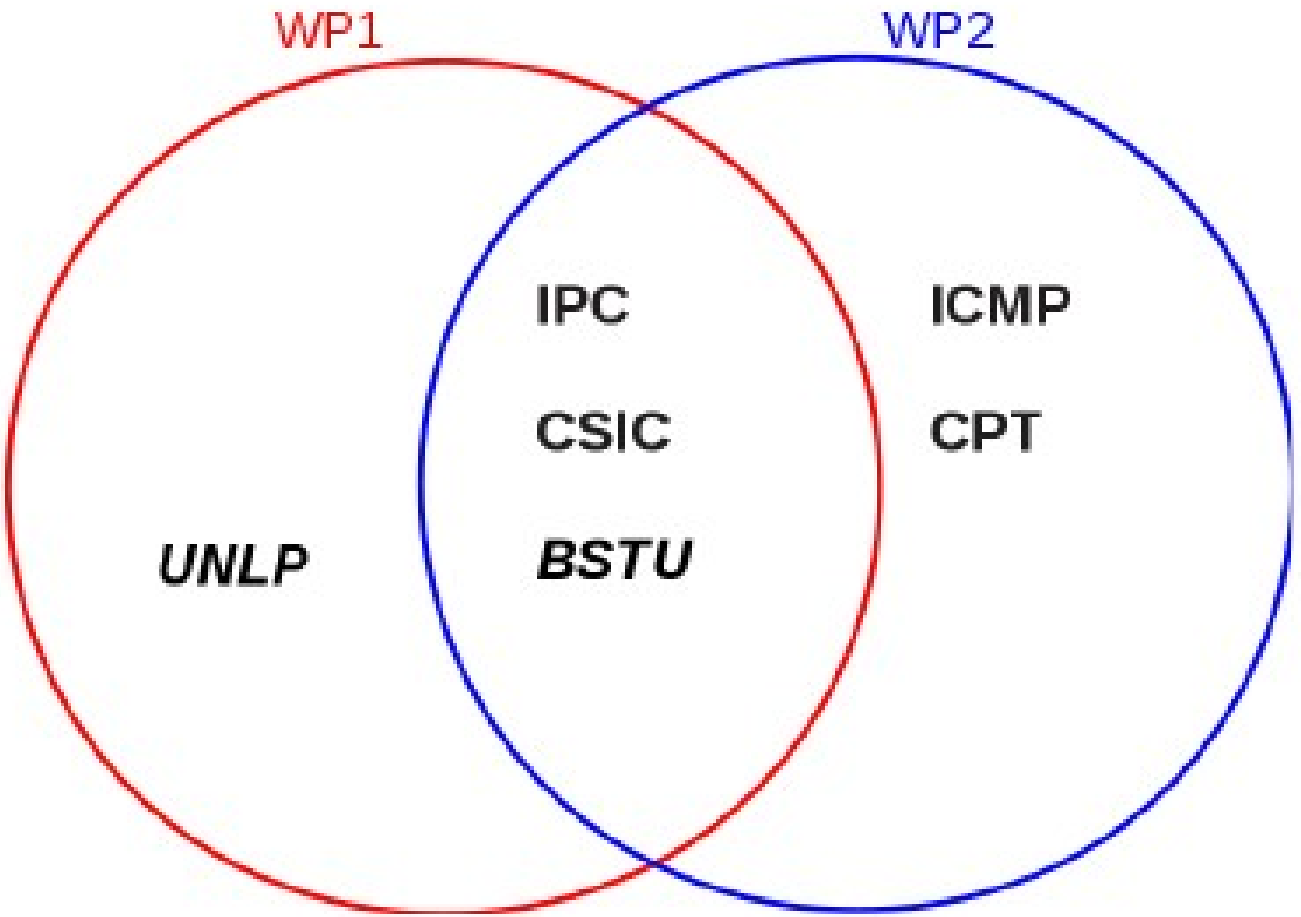
WP1:
Modelling of self-assembly in systems with competing interactions

WP2:
Modelling of systems with dominant electrostatic interactions

WP3:
Communication, Dissemination and transfer of knowledge

WP4:
Coordination and Management

Groups involved in scientific work packages:



WP1:
Modelling of self-assembly in systems with competing interactions

Objective:

To gain fundamental knowledge about universal and specific properties of self-assembling systems, with a special focus on the effects of confinement. In particular, structure, thermodynamic and mechanical properties of various model systems with competing interactions in single compartments with different types of walls and in porous media will be described. Younger researchers will learn advanced theoretical and simulation methods during long-term visits to IPC and CSIC

Deliverable 1.1.: Characterization of ordered structures in selected models with competing interactions

Task 1.1:

Pattern formation on surfaces or interfaces - theoretical and simulation study.

New methods of distinguishing patterns with long- and short-range order formed by aggregates in systems with competing interactions will be developed. Theoretical and simulation studies of several model systems with competing interactions confined to a surface, interface or a membrane will be performed. Flat and curved surfaces will be considered for one and two-component systems with various interaction ranges and strengths. The ordered structures and the defects will be characterized for a range of densities and temperature. Mechanical and thermal properties will be determined for different structures and degree of order.

Lead Participant: IPC (W. T. Gozdz)

Secondments (11):

from **BSTU to IPC** (6): N. Akulich (ESR, 3), V. Zhylinsky (ER, 1), I. Narkevych (ER, 1), E. Blidanau (ESR, 1+2)

from **BSTU to CSIC** (2) Y. Lasovsky (ER 1), Y. Groda (ER 1)

from **CSIC to UNLP** (1): E. Lomba (ER, 1)

from **UNLP to CSIC** (2) G. Zarragoicoechea (ER,1), A. Meyra (ER, 1+5)

Results

1. System composed of amphiphilic molecules in a solvent, exposed to a flat confining surface W.T. Gozdz (IPC)

2. Thermodynamic and Kinetic Properties of the System with Competing Interactions on a Triangular and Square Lattices,
Y. Groda, E. Bildanov, and V. Vikhrenko, (BSTU)

3. Colloidal particles interacting with short-range attraction and long-range repulsion (SALR) potential on a surface of a sphere,
J. Pękalski, A. Ciach (IPC)

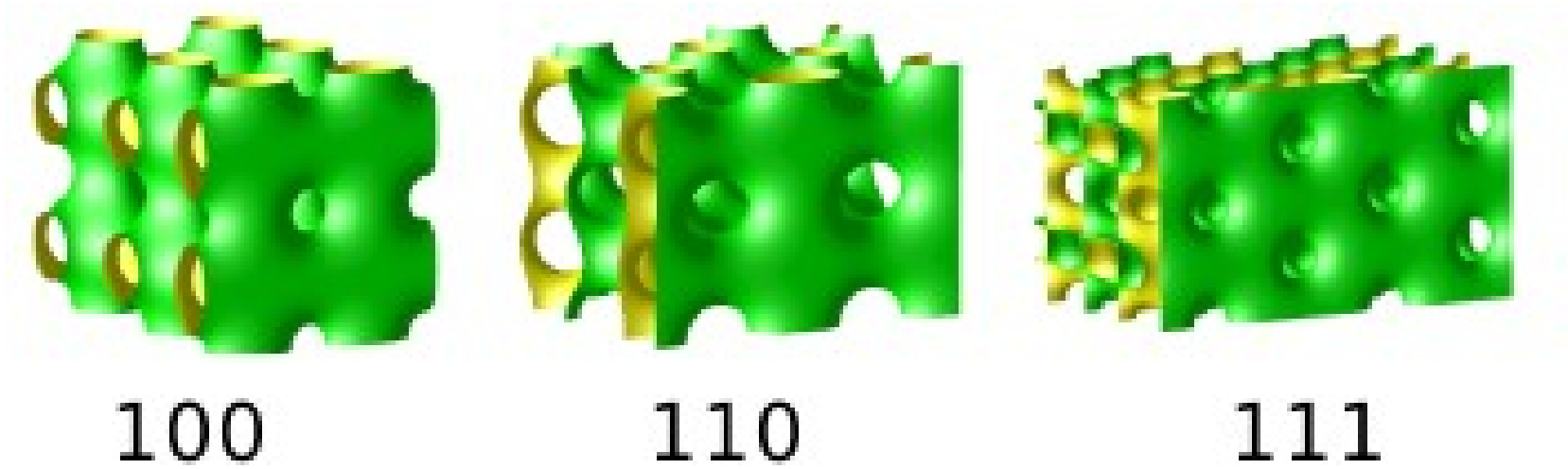
4. Pattern formation at ionic liquid-electrode interfaces, A. Ciach (IPC)

5. Influence of Obstacles on Equilibrium Properties of the Lattice Fluid on a Surface, Y. G. Groda, V. Vikhrenko (BSTU)

6. Growth and connection of colonies of cells or individuals in ecosystems. Monte Carlo standard and bias Monte Carlo,
G. J Zarragoicoechea and A. G. Meyra (UNLP)

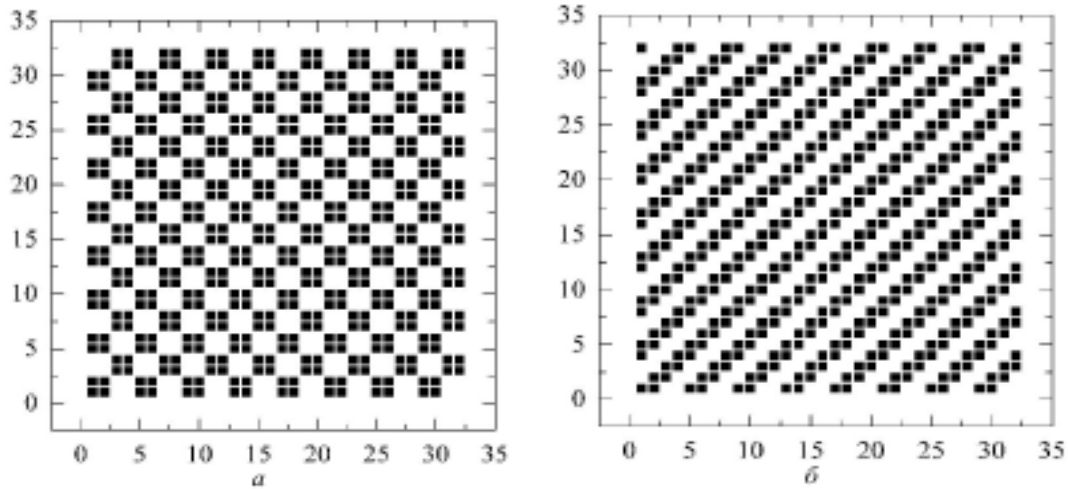
7. Dynamics and structure of nanoconfined water and decane mixtures,
A. G. Meyra (UNLP)

1. System composed of amphiphilic molecules in a solvent, exposed to a flat confining surface



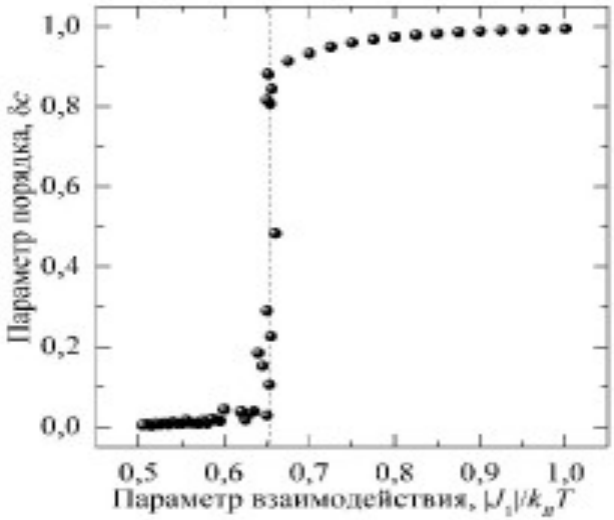
Structure of the bilayer near the confining surface for indicated orientations of the unit-cell wrt the confining surface. Different colours correspond to the two sides of the bilayer.

2. Thermodynamic Properties of the System with Competing Interactions on a Square Lattice

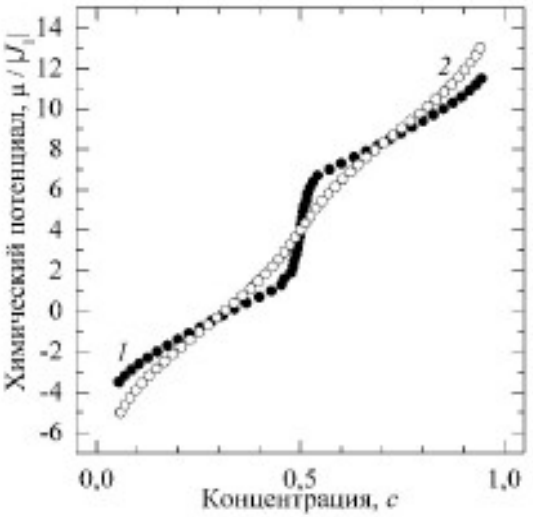


Two ordered structures of the SALR model on the square lattice. Ground state.

Simulation results

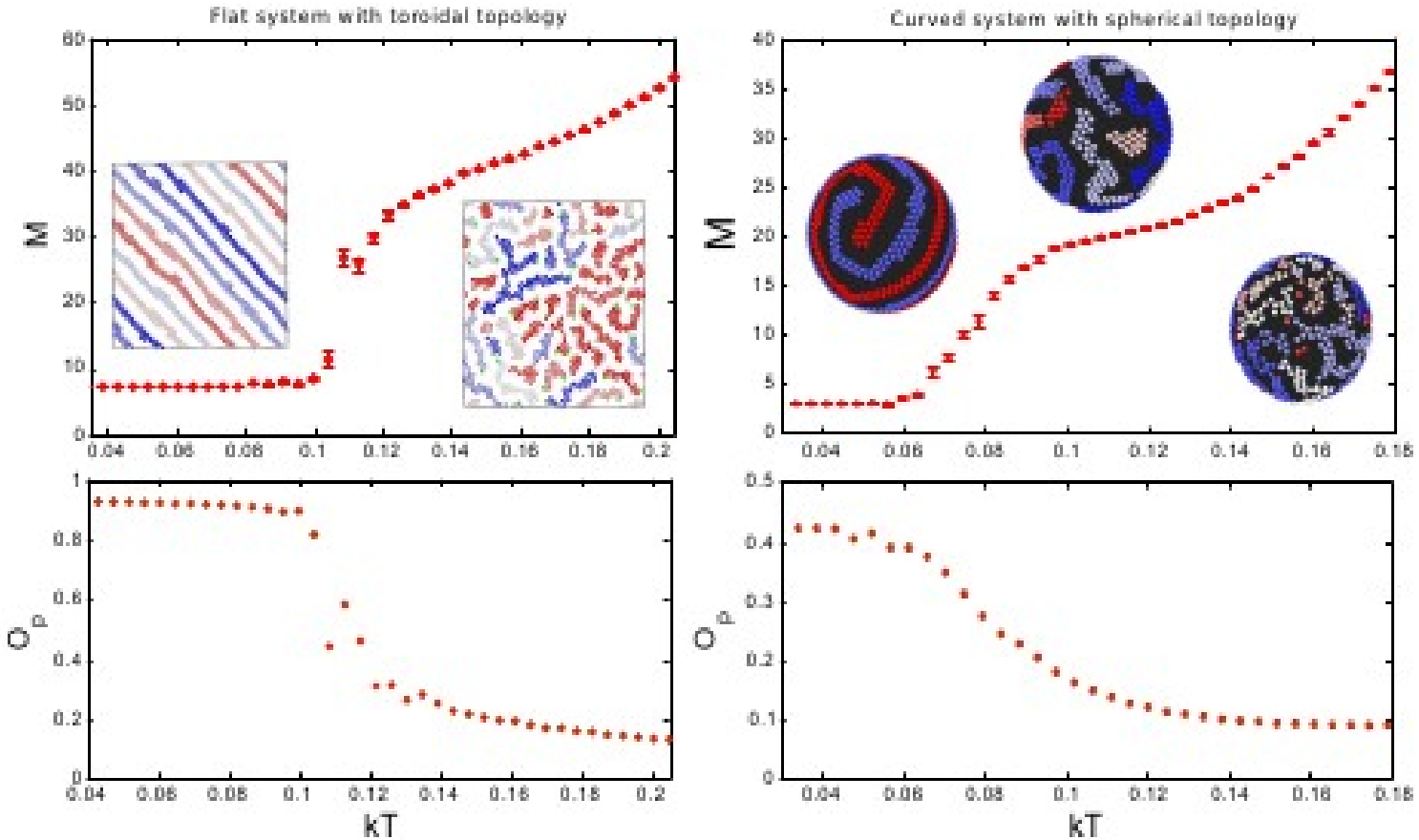


Order parameter as a function of inverse temperature



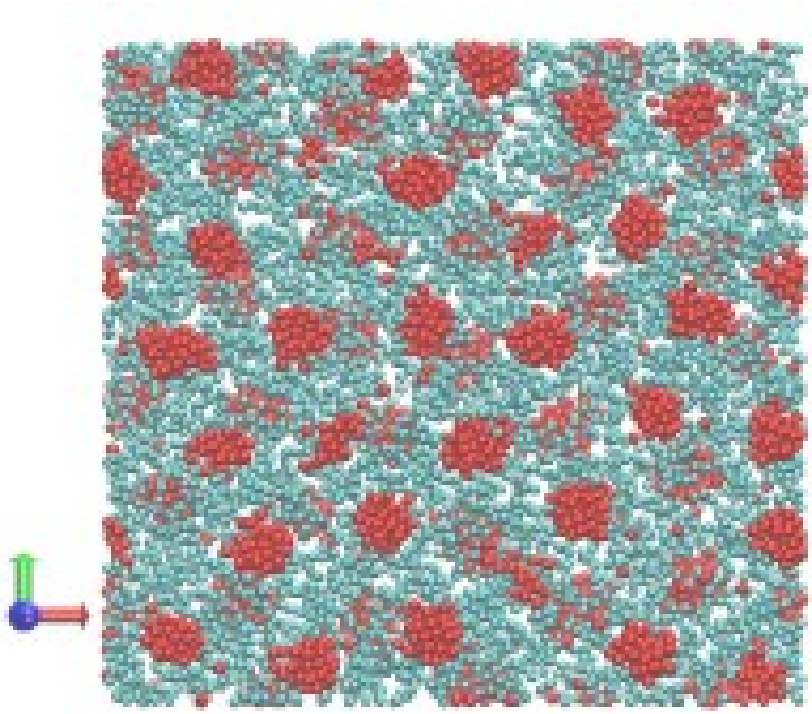
Chemical potential as a function of concentration. Open circles- high T, full circles – low T

3. Colloidal particles interacting with short-range attraction and long-range repulsion (SALR) potential on a surface of a sphere,



The number of aggregates, M (T), and the orientational order parameter Op as a function of temperature in the case of a flat system (left column) and particles adsorbed at the surface of a sphere (right column). The insets show representative configurations at different temperatures. Different aggregates are marked with different colors

6. Growth and connection of colonies of cells or individuals in ecosystems. Monte Carlo standard and bias Monte Carlo



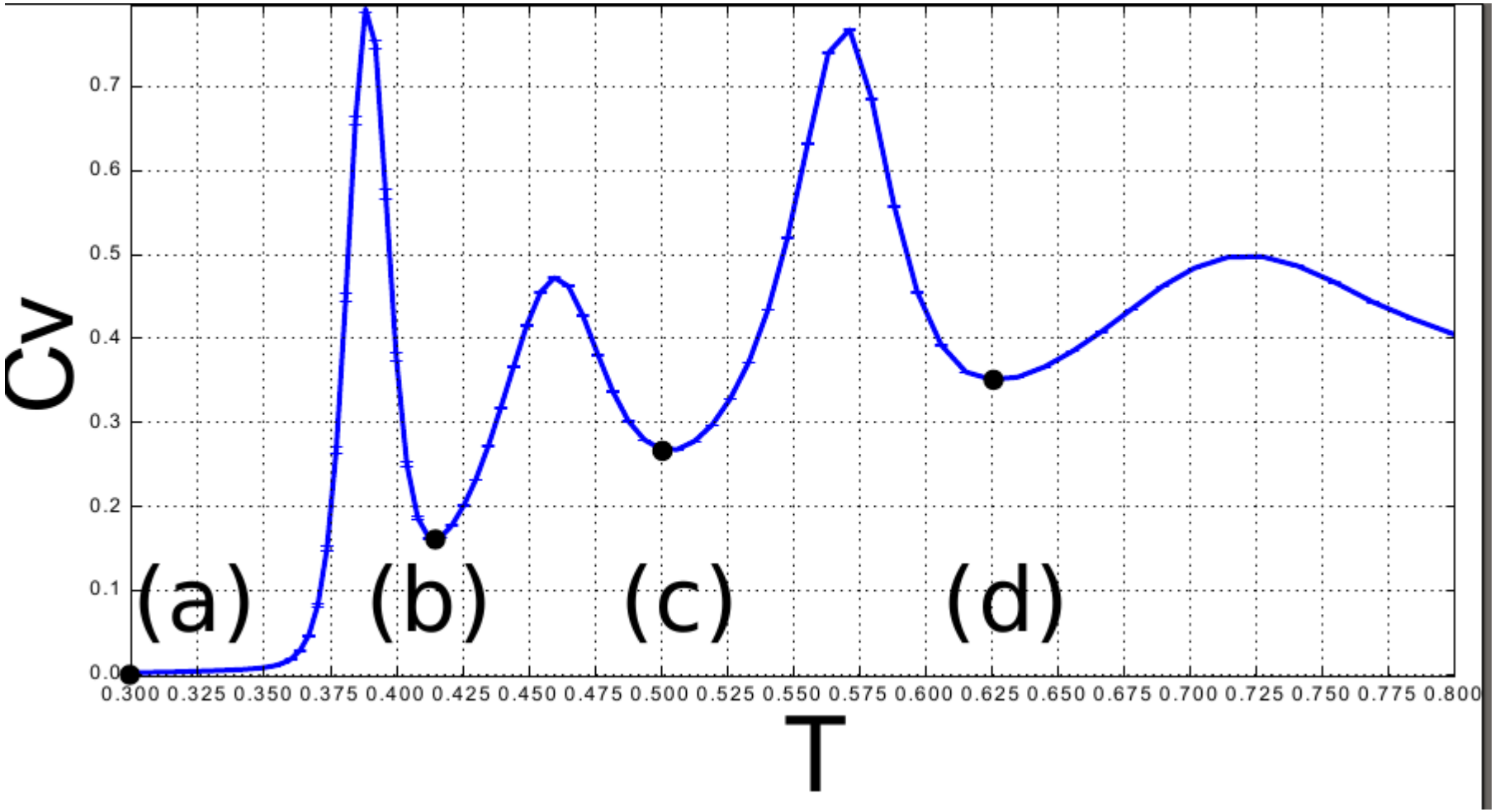
The system evolves in such a way that individuals with the same functionality (the same component) connect and form clusters or colonies. And this is independent of the starting configuration.

Work in progress

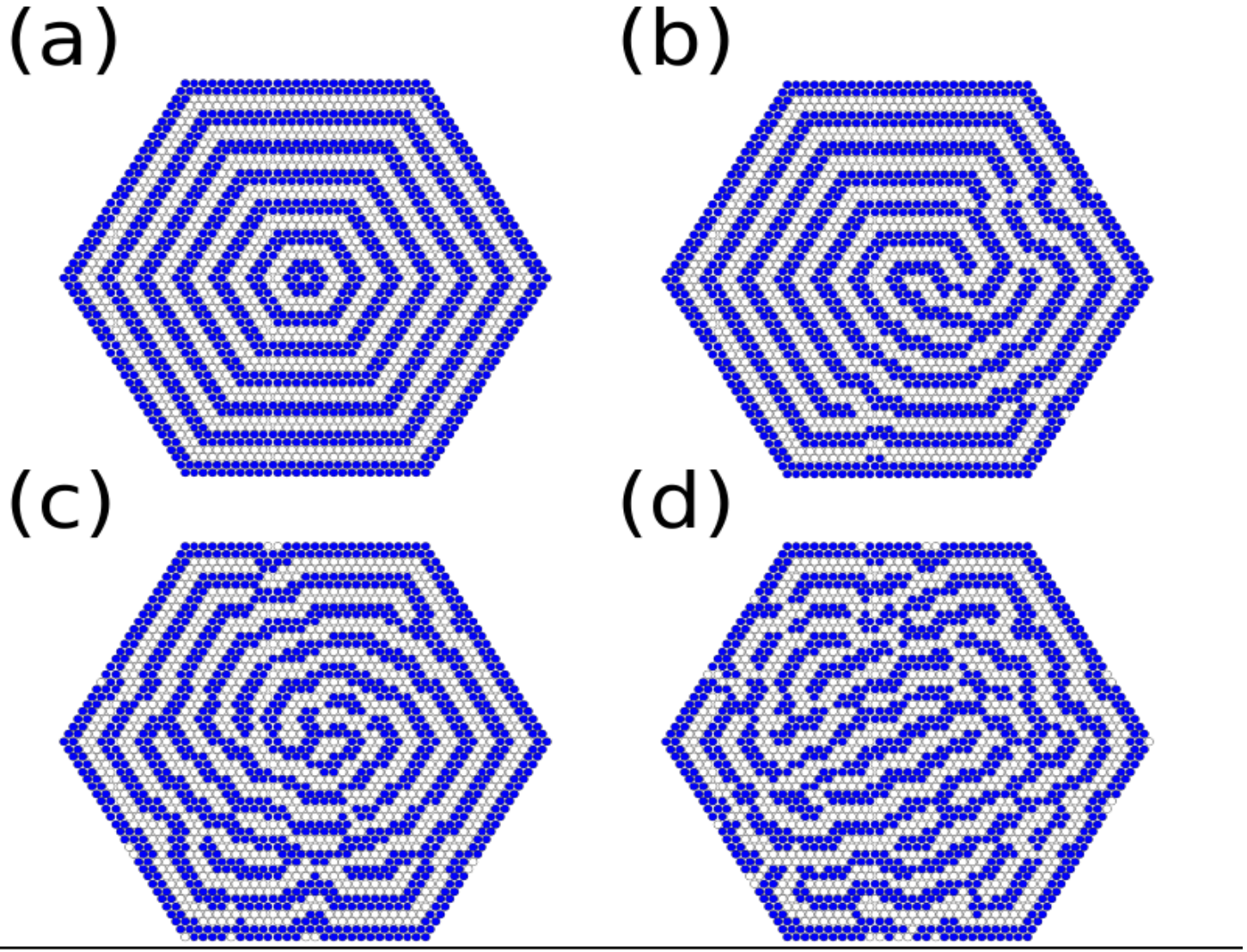
Collaboration between **IPC** and **BSTU**

A SALR model on a triangular lattice in a confinement of a hexagonal shape.

Preliminary results:



Specific heat obtained in MC simulations



Snapshots corresponding to the minima of the spceific heat

work in progres
CSIC-UNLP collaboration

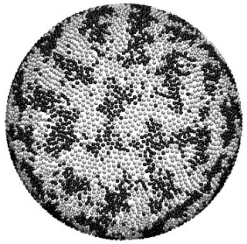


Fig. 9a - Moyano et al.

Fig. 9c - Moyano et al.

Fig. 9b - Moyano et al.

We have been developing a model of **dipolar particles anchored on a spherical surface**

- Interparticle interactions become long ranged
- Due to competition of the long range vs volume effects we have patterns
- The long ranged interactions induce hyperuniformity (the fluctuation of the number of particles grows in a given surface with the perimeter).
- This has important implications for the design of optical materials

$$\left\langle N^2 \right\rangle_R - \left\langle N \right\rangle_R^2 \mu R$$

WP2:

Modelling of systems with dominant electrostatic interactions

Objectives:

to describe ionic systems in bulk and at an interface. A special attention will be paid to ionic liquids in disordered porous media and to mobile ions in the areas of large concentration gradients. Various models and confinements will be considered within this study.

D2.1 Structural and thermodynamic properties of ionic liquids in the bulk and near the wall

Task 2.1: **Structural and thermodynamic properties of ionic liquids near a hard wall**

The FT method will be applied in order to study ionic liquids next to a hard wall. We will provide an extension of this approach to the case of a complex interaction potential between molecules, which besides a short-range interaction involves a long-range electrostatic potential and takes into account the fluctuation effects. In order to describe complex ionic molecules the developed approach will be combined with the concepts of the theory of associating liquids. The correlation functions of the considered liquids will be obtained in the bulk as well as the density profiles of ionic liquid near the wall will be calculated. The main thermodynamic quantities such as chemical potential and pressure will be obtained. We will also provide the corresponding computer simulation results in order to verify the theory. Lead participant **ICMP**

Task 2.5: **Experimental study of nanostructured surfaces by electrochemistry methods.**

We plan experimental study of deposited nanostructured thin films based on nanoparticles as building units on solid surfaces. In particular, nanoparticles production and their assembly during film formation processes will be investigated and the role of different interactions will be pointed out. The relationship between the film architecture and different interactions will be established. Lead Participant: **CPT**

Secondments (21):

BSTU to ICMP (6): V. Vikhrenko (ER, 1), R. Lasovsky (2), G. Bokun (3),

BSTU to CPT (7): V. Yaskelchyk (ESR, 6), V. Vikhrenko (ER, 1)

ICMP to BSTU (6): M. Holovko (ER, 1), T. Patsahan (ER, 2),
I. Kravtsiv (ER, 1), M. Hvozd (ESR, 2)

CPT to BSTU (1): D. Di Caprio (ER, 1)

UPMC to BSTU (1): A. Taleb (ER, 1)

Results:

1. Distribution of ions and electrostatic potential in ionic liquids and ionic liquid mixtures near a charged surface, A. Ciach (IPC)

2. The effect of finite pore length on ion structure and charging, S. Kondrat (IPC)

3. Free energy and chemical potential distribution for inhomogeneous charged systems,
M. Holovko (ICMP), G. Bokun, V. Vikhrenko (BSTU), D. Di Caprio (CPT)

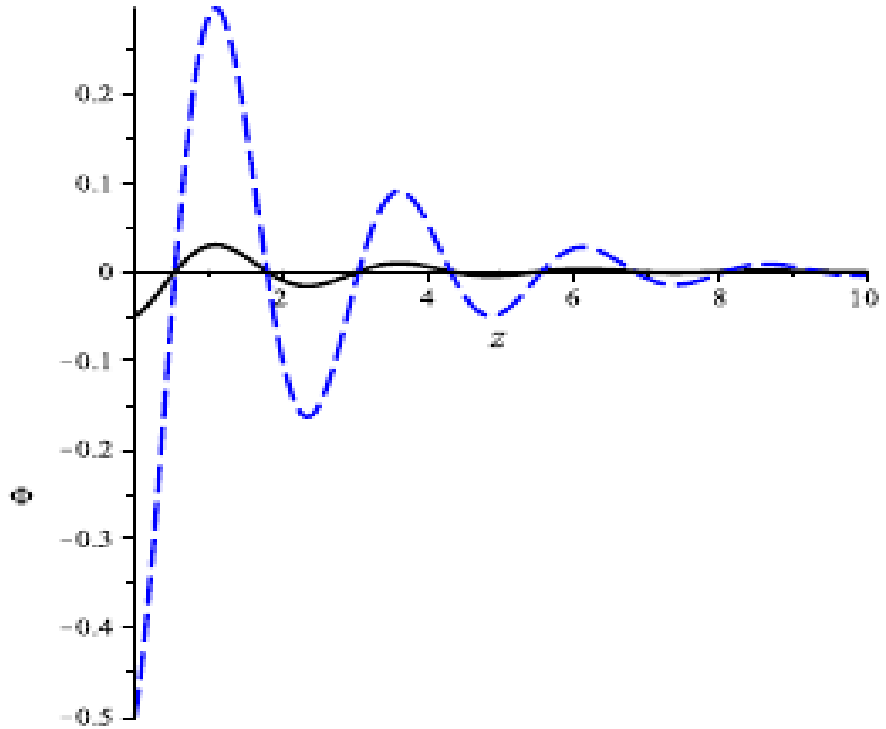
4. Phase transitions in mixtures of a model ionic liquid and neutral solvents,
M. Holovko and M.V. Hvozd (ICMP)

5. Vapor-liquid phase behavior of model ionic liquids confined in disordered hard-sphere matrices, O. Patsahan T. M. Patsahan, and M. F. Holovko (ICMP)

6.Charge screening for mobile ions in lattice fluid models, M. Holovko (ICMP), G. S. Bokun, V. Vikhrenko (BSTU), D. Di Caprio (CPT)

7. Nanodiamond coating for anti-corrosion applications, V. Yaskelchyk (BSTU), A. Taleb (CPT+UPMC)

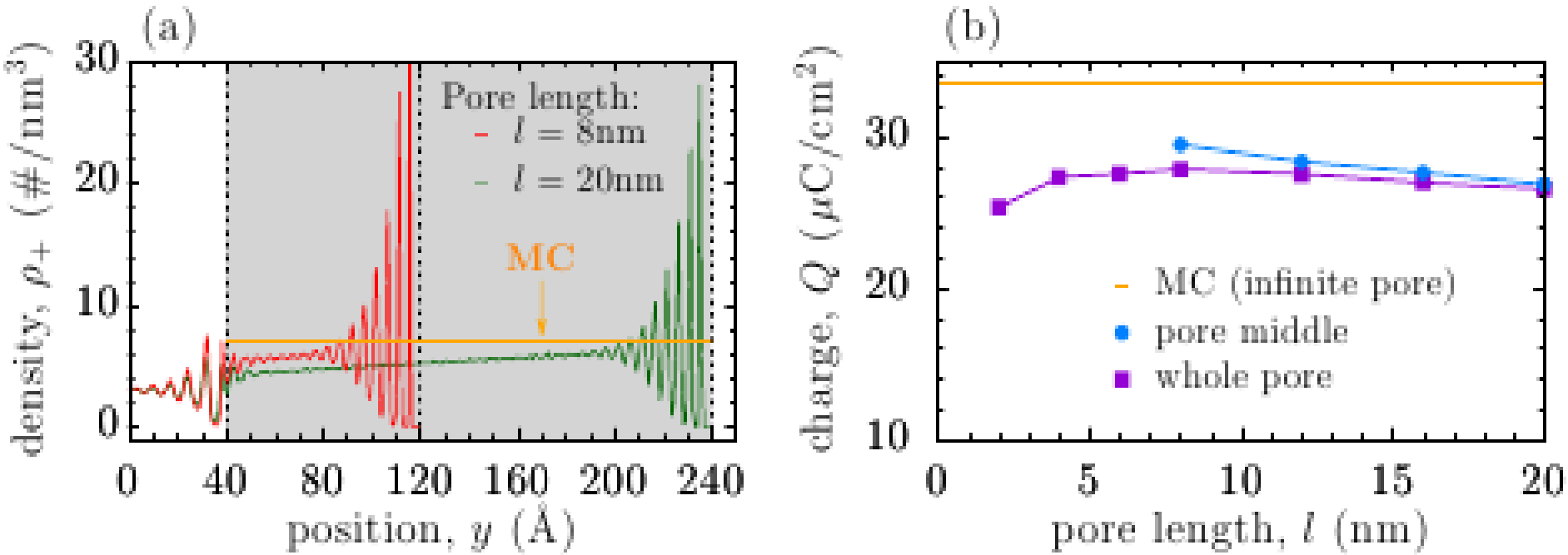
1. Distribution of ions in ionic liquids near a charged surface



Local charge-density Φ(z) in IL at a distance z from a negatively charged surface located at z = 0 for small (solid line) and large (dahed line) surface charge.

A. Ciach, Simple theory for oscillatory charge profile in ionic liquids near a charged wall, J. Mol. Liq. doi.org/10.1016/j.molliq.2017.10.002. arXiv:1705.10551 [cond-mat.soft]

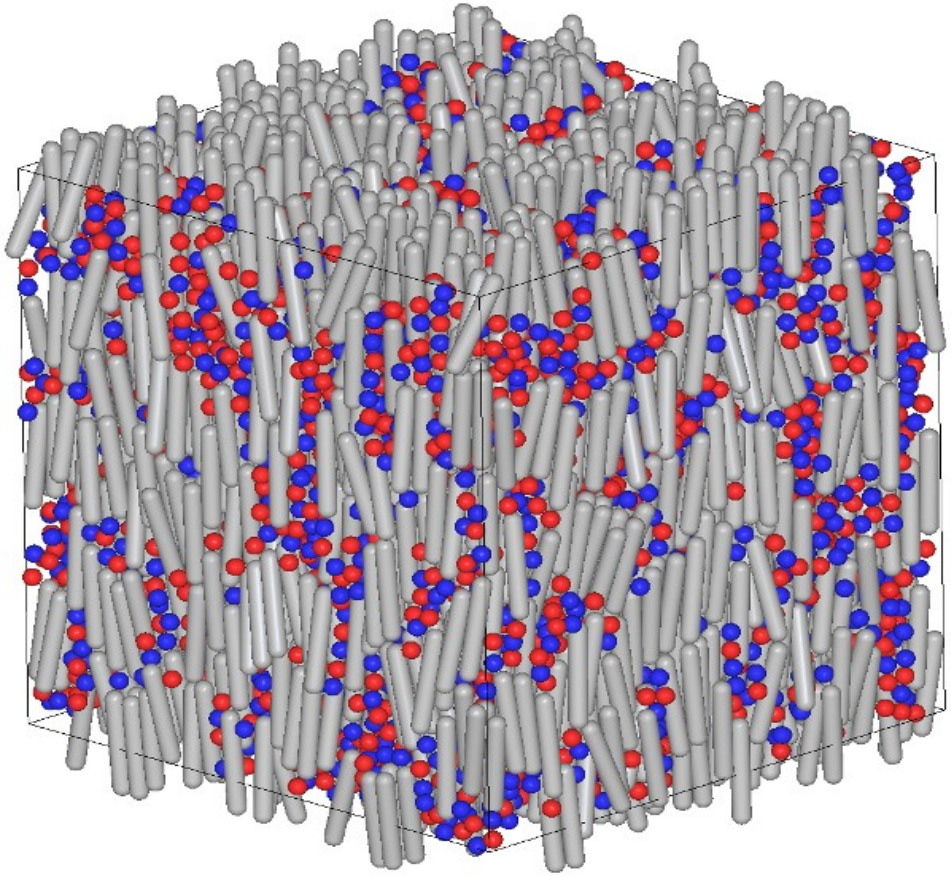
2. The effect of finite pore length on ion structure and charging



(a) Counter-ion densities from MD simulations. The horizontal orange line shows the corresponding MC result for an infinitely long pore. The vertical dash lines show the pore entrance and closings. Only half of a supercapacitor is shown. (b) Accumulated charge per surface area as a function of pore length.

K. Breitsprecher, M. Abele, **S. Kondrat**, and Ch. Holm, The effect of finite pore length on ion structure and charging, J. Chem. Phys. **147**, 104708 (2017).

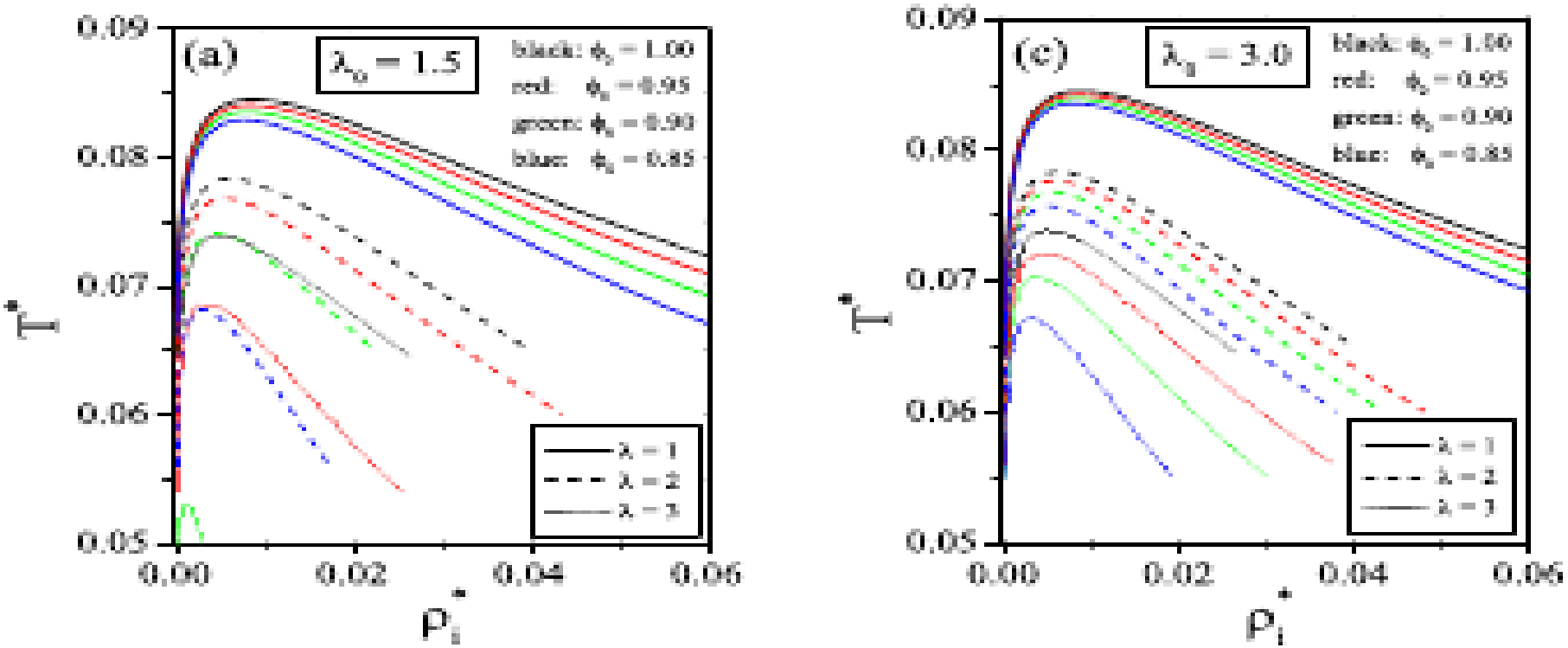
4. Phase transitions in mixtures of a model ionic liquid and neutral solvents



Mixture of a model ionic fluid and neutral spherocylinder solvent. Blue and red particles denote posively and negatively charged ions, grey spherocylinders denote neutral solvent.

M.F. Holovko and M.V. Hvozd, Isotropic-nematic mixture of hard spheres and hard spherocylinders: scaled particle theory description, Condens. Matter Phys. **20** 43501 (2017)

5. Vapor-liquid phase behavior of model ionic liquids confined in disordered hard-sphere matrices



Vapor-liquid phase diagrams at the fixed size ratios between the matrix obstacles and the negatively charged ions, λ0 = 1.5 (a), and λ0 = 3.0 (c). In each case, data are shown for different matrix porosities φ0 and for different ratios of ion size asymmetry λ, as indicated in the legends. The bulk case (φ0 = 1) is presented for comparison.

O. V. Patsahan, T. M. Patsahan, and M. F. Holovko, Vapour-liquid critical parameters of a 2:1 primitive model of ionic fluids confined in disordered porous media, J. Mol. Liq., doi.org/10.1016/j.molliq.2017.12.033

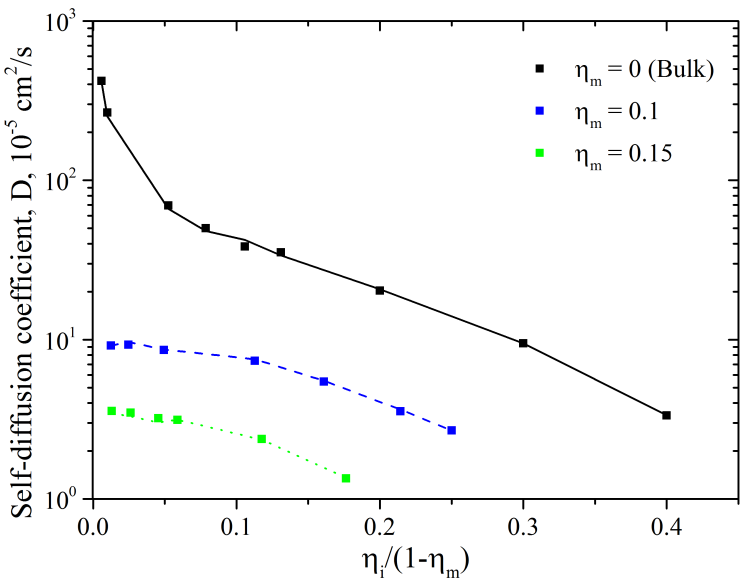
Work in progress

Collaboration between **ICMP** and **BSTU**

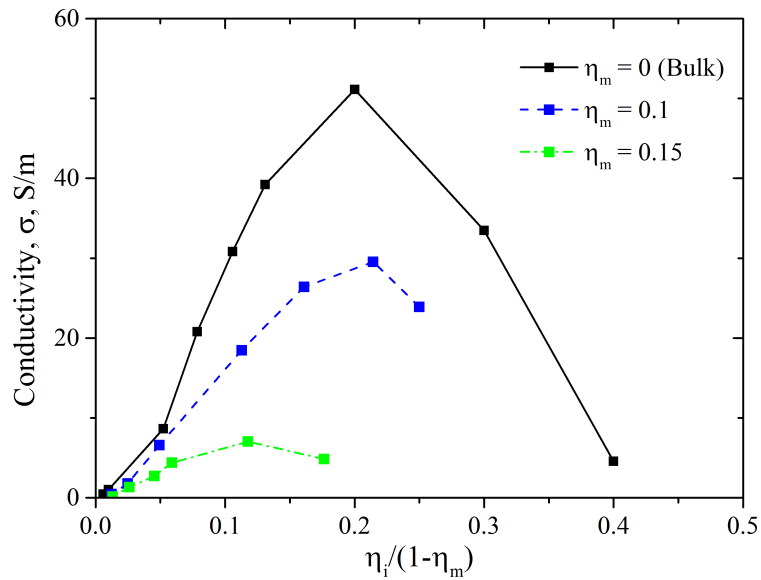
A. Structural and dynamic properties of ionic fluid in disordered porous matrix

Molecular dynamics simulation of RPM fluid in disordered matrix.

- Structural and dynamic properties
- Comparison with theoretical predictions
- Clustering phenomena
- Effect of quenched disorder



The self-diffusion coefficient of ions depending on their density in matrices of different packing fractions



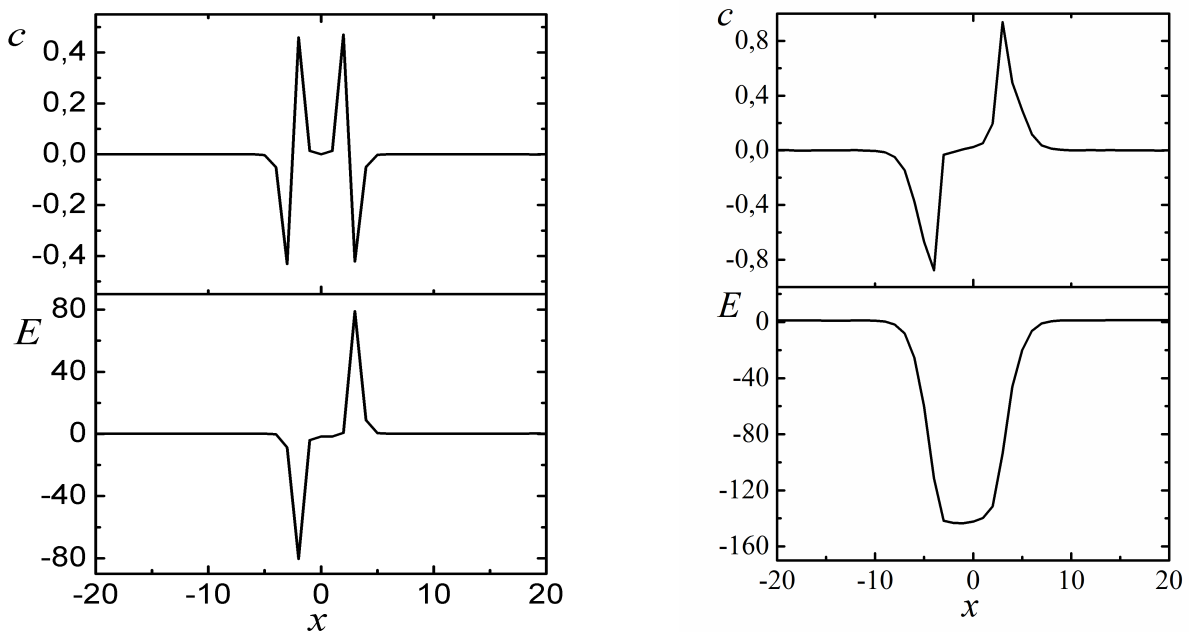
Electric conductivity of RPM fluid depending of its density in matrices of different packing fractions

B. Distribution of charge density and electric potential in solid electrolytes

Monte-Carlo simulation of ceramic electrolytes in the presence of external field

An intergrain region of oxide ceramic electrolyte is described with a simple lattice model of yttria stabilized zirconia.

G.S. Bokun, Y.G. Groda, R.N. Lasovsky, V.S. Vikhrenko, Solid State Ionics, 302 (2017) 25.



The concentration distribution and the local electric field. Left panel: at E = 106 V/m, ε = 200, T = 1000 K, E_{gb} = 0.3 eV, L = 128, l = 5. Right panel: at E = 107 V/m, ε = 500. The electric field is given in units V/μm.

2. Training, Transfer of Knowledge & Networking

WP3:

Communication, Dissemination and transfer of knowledge

Objective:

1.Dissemination of the project results and transfer of knowledge between the participants from different groups and to students in the visited cities, through:
(i) organization of the open project workshops (4),
(ii) coordination of participation at conferences,
(iii) seminars and courses for graduate students delivered by senior seconded scientists in visited cities.

2. Communication through press news, participation in science festivals and picnics, etc.

D 3.1 Report on the workshop and kick-off meeting organized in Warsaw

Task 3.1:
Organization of an open 3 days workshop
“Competing electrostatic and short-range interactions"
in February 2017 in Warsaw.

Review lectures by invited outstanding scientists and by senior researchers participating in the project will be given.

The aim is to summarize the recent progress in colloidal and amphiphilic selfassembly and in the RTIL and MIIC, both in the bulk and in confinement, and to present the recent advances in theoretical and simulation methods.

Important open questions will be discussed during the round-table discussion closing the workshop.

Project Management Board will meet just after the workshop.

Lead Participant: IPC.

I CONIN Workshop:

“Competing electrostatic and short-range interactions"

Jablonna Palace, February 17-20 2017

Invited speakers:

Patrick Charbonneau, Duke University, USA

Ales Iglic, University of Lublana, Slovenia

Gerhard Kahl, Technical University, Vienna , Austria

Svatoslav Kondrat, Forschungzentrum Juelich, Germany

Ruth M. Lynden-Bell, Cambridge University, UK

Roland Roth, Tuebingen University, Germany

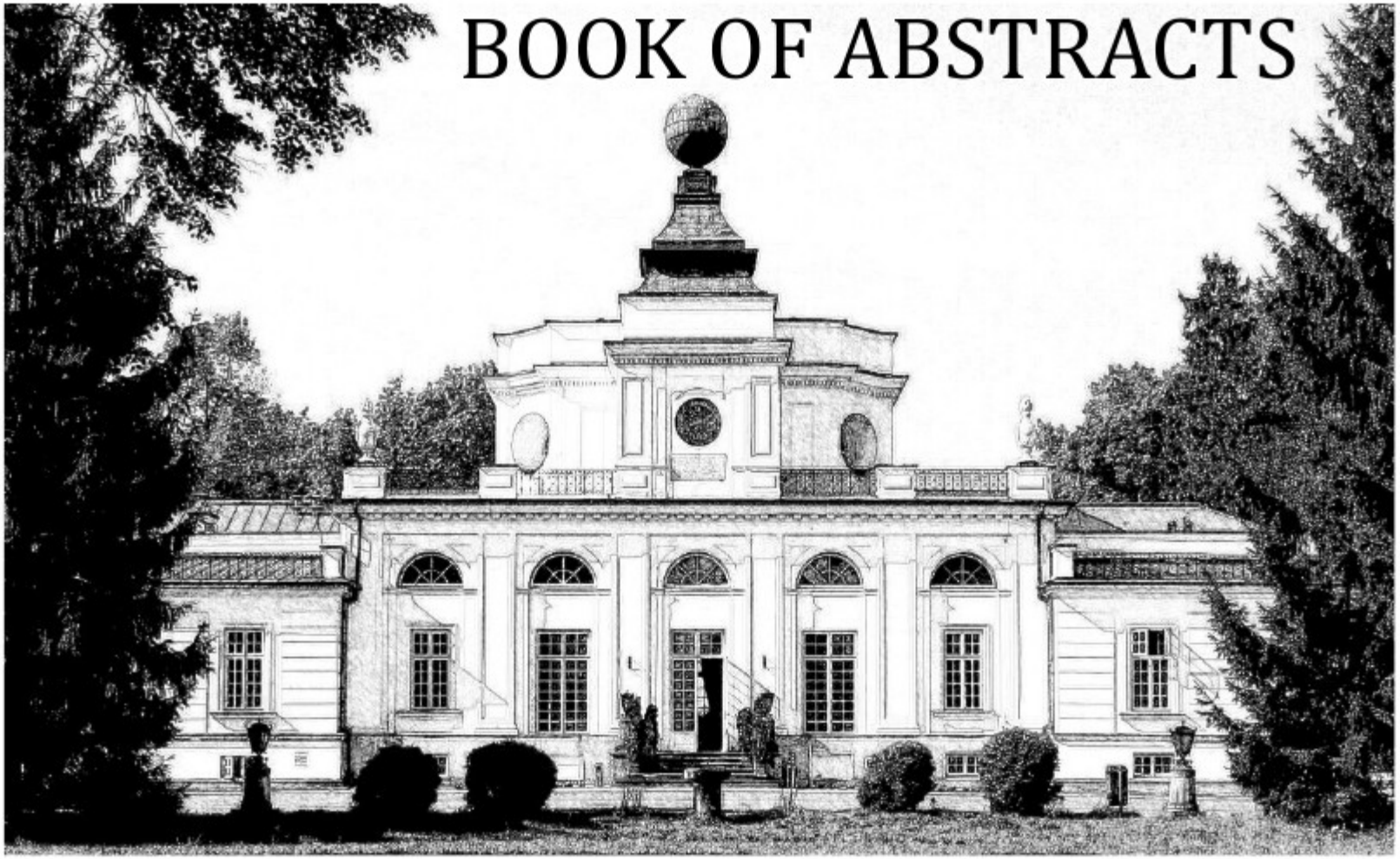
Paddy Royall, Bristol University, UK

Mireille Turmine, P&M Curie University, Paris, France

Luis M. Varela, Santiago de Compostella, Spain

Nigel Wilding, University of Bath, UK

Web page http://ichf.edu.pl/conin



Systems with competing electrostatic and short-range interactions

February 18

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

Febuary 19	
8:00	Breakfast
	chair: O. Patsahan
9:00	**G. Kahl**: *Tunability and order: the plethora of polymorphism of Wigner bilayer systems*
9:40	**N. Wilding:** *Computer simulation studies of short-ranged attractive and long-ranged repulsive (SALR) potentials*
10:20	Coffe break / poster session
	chair: G. Kahl
11:00	**P. Charbonneau**: *Equilibrium phase behavior and self-assembly dynamics of microphase forming models*
11:40	**R. Roth**: *Phase Diagram of a System with Competing Interactions*
12:20	Lunch / poster session / concert
	chair: D. di Caprio
14:30	**P. Royall**: *Hunting Mermaids in Real Space*
15:10	**E. Lomba**: *Inhomogeneous integral equation approaches to describe confinement*
15:40	**A. Taleb**: *Nanoparticles interactions tailoring toward nanomaterial design for targeted application*
16:10	*Coffe break / poster session*
	chair: V. Vikhrenko
16:30	**E. Noya**: *Phase behaviour and assembly of colloids with heterogeneously charged surfaces*
17:00	**Y. Groda:** *Thermodynamic and diffusion characteristics of lattice models with obstacles and competing interactions*
17:30	**A. Ciach***: Comparison of the amphiphilic and the colloidal self-assembly*
18:30	Dinner

Task 3.2:

organization of an open 2 1/2 days **workshop "Effects of confinement on systems with competing interactions"** in the second year in Madrid.

Planned topics:

Novel theoretical approximations: Integral Equation Theories, DFT, CV, SPT etc. Advances in simulation methodology.

Applications: Colloids, charged nanoparticles and proteins, lipid bilayers, etc.

Experiments: We invite experimentalists working in colloids, diblock copolymers or other systems with competing interactions.

Project Management Board will meet just after the workshop.

Lead Participant: CSIC.

II CONIN Workshop:
Systems with competing electrostatic and short-range interactions
Madrid, 7-8 March 2018

Invited speakers:

Willem Kegel, Utrecht University, Netherlands

Alexei Kornyshev, Imperial Colleage, London, UK

John Griffin, Lancaster University, UK

Martin Sweatman, University of Edinburgh, Scotland, UK

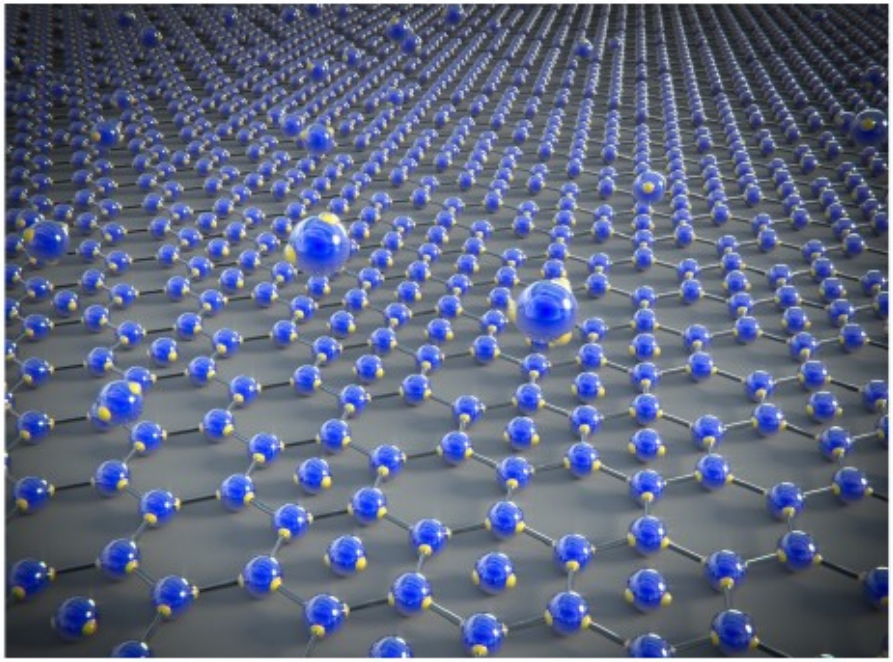
Jose Nuno Canongia Lopes, Instituto Superior Técnico, U Lisboa, Portugal

Web page: http://conin.iqfr.csic.es

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)

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 anto-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 **- John Griffin**: *"Understanding the behaviour of ions in carbon micropores by NMR spectroscopy"*

09:40-10:20 - **Martin Sweatman**: *"The SALR fluid at low concentrations: giant clusters and their reproduction"*

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"*

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

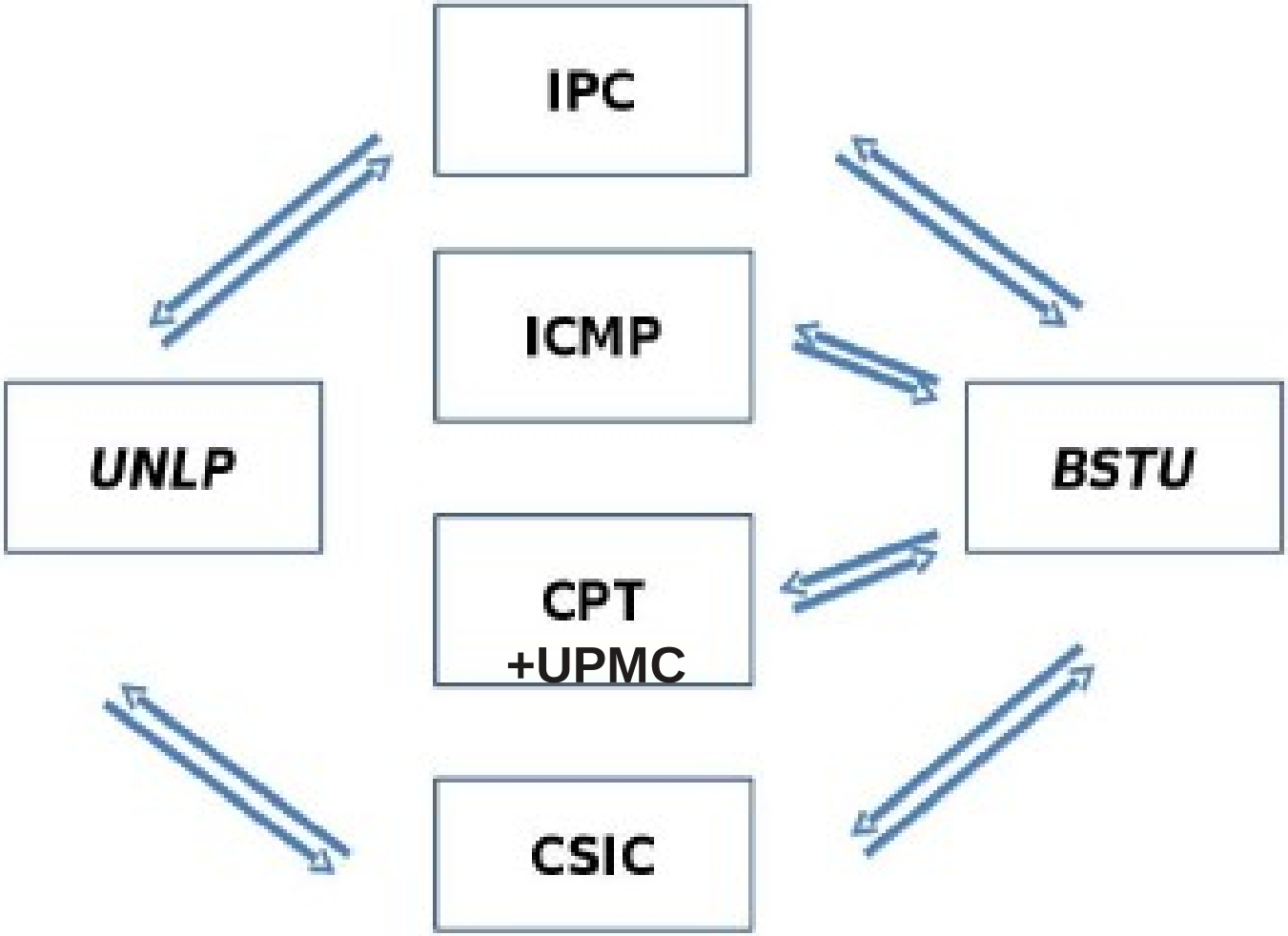
16:30-17:00-**Yaroslav Groda:** *"Lattice fluid with SALR interaction potential on simple square lattice"*

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"*

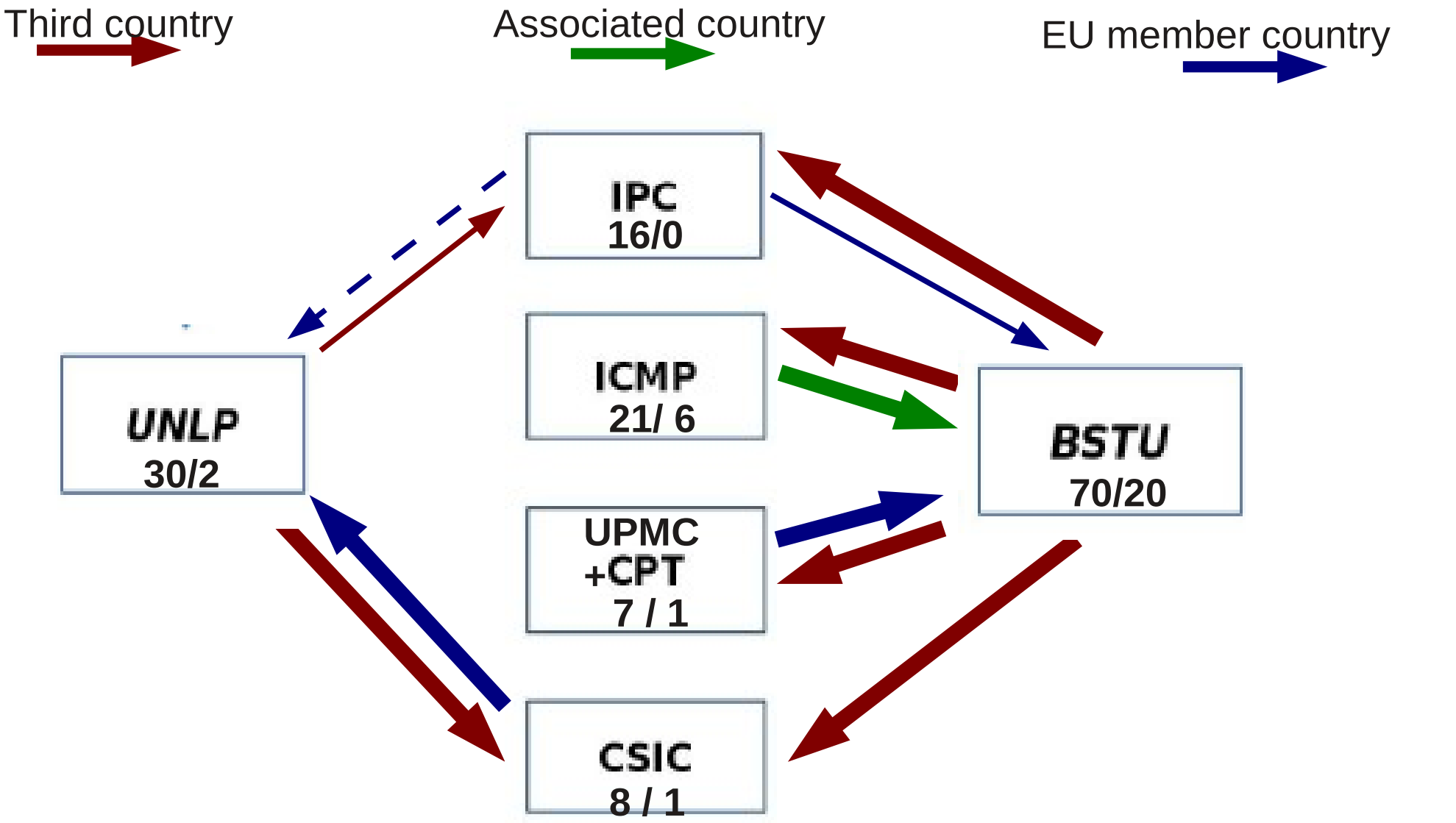
Secondment implementation

Secondments were planned between the institutions:



Thick arrows show secondments that took place already.
Thin arrows: secondments planned for 2018

Planned (till the end of the project)/realized (till March 2018) secondment months from:



Secondment implementation

planned/realized secondments (person/month) per beneficiary institution

IPC 52/6+2

CSIC 45/5+5

ICMP 31/12

CPT+UPMC 24/9

All **152 / 32 + 7**

Task 3.5: Coordination of seminars and specialized courses for graduate and PhD students and coordination of participation at conferences and communication activities associated with WP1. Lead Participant: CSIC

Task 3.6: Coordination of seminars and specialized courses for graduate and PhD students and coordination of participation at conferences and communication activities associated with WP2. Lead Participant: CPT

Secondmens
new knowledge acquisition, training activities

Training:

Valiantsin Yaskelchyk, a PhD student from BSTU, was trained in using the equipment of CPT: Dektak 6 M stylus profiler, centrifugal technique for thin film deposition, Autolab potentiostat and high-resolution Zeiss Ultra 55 CDS field emission gun scanning electron microscope (FEGSEM).

Different experiments were conducted mainly dealing with the design of nanodiamond and polypyrrole nanocomposite coatings for anticorrosion application. His results show that the anticorrosion efficiency of prepared coating is connected to the interaction of nanoparticles and their assembly into a thin coating with controlled porosity. Mr. Yaskelchyk is continuing these experiments in his department using the samples prepared in CPT.

Secondmens
new knowledge acquisition, training activities

Training:

Nadejda Akulich, a PhD student from BSTU, was trained in using the equipment of IPC: the electron scanning electron microscope Nova NanoSEM 450, Autolab PGSTAT302N, the optical microscope MicroXAM-1200 and the PHI 5000 VersaProbe scanning microanalyzer. The measurements concerned the subject of her PhD thesis "Anticorrosive modified zinc coatings on carbon steel".

V. Zhylinski, an experimentalist from BSTU visited several experimental departments with modern equipment at IPC and discussed possibilities of joint work.

Secondmens
new knowledge acquisition, training activities

Informal meetings, networking:

June 2017, Informal meetings of CPT, ICMP and BSTU teems in Minsk

June 5-9, 2017, Oksana Patsahan from ICMP visited IPC

Courses:

November 2017, E. Lomba (CSIC) delivered a one-week course at UNLP "General Purpose GPU programming with CUDA®"

Seminars:

The members of our teams delivered 6 seminars concerning the subject of the CONIN project, mainly (but not only) at the visited institutions.

WP4:
Coordination and Management

Objective:

Coordination of the project activities according to the project research objectives and time schedule concerning the secondments and the deliverable reports, and the administrative and financial management of the project.

D4.1 Progress report 1

Task 4.1: **Coordination and management of the project.**
Prof. Alina Ciach will be the Project Coordinator (PC) responsible for strategic and scientific management of the project. She will be also the Chair of the Project Management Board. PMB will participate in planning of the activities, in decision making and in monitoring the progress of the tasks associated with WP 1-3. The PC and the the PMB will be responsible for risk management and the decision making. PMB meetings are planned once a year during workshops. In addition, contacts by email, skype or phone are planned. Leaders of all the groups in the Beneficiary and Partner Institutions will participate in the Project Management Board.

There were 2 PMB meetings, February 2017 and March 2018

Task 4.2**: The administration of the project.**
The Project Support Office (PSO) will coordinate and manage all technical and administrative management components of the project. PSO will monitor the dates of secondments and deliverables and inform the PC and PMB about any risk of delay of the project activities.

PSO monitors the dates of secondments and deliverables.
We have no serious delays so far

Issues:

1. From January, 1st 2018, the “Université Pierre et Marie Curie” (PIC number : 999986193) and « Paris Sorbonne » (PIC number: 998096051) have merged and became a new entity « Sorbonne Université ». The rights of the two universities will accordingly be assigned to the new institution, therefore, a Universal Transfer of Right and Obligations (UTRO) has been done in order to implement the transfer of all the ongoing projects.

Question: is an amandmet to the Grant Agreement necessary?

2. We planned that a PhD student from BSTU would spend 3+9 months at CSIC, starting from 2019. However, there are no suitable candidates that speak English sufficiently fluently, but there are candidates that can communicate in Belorussian or Russian with the IPC team.

Question: Is it possible to change the host institution from CSIC to IPC?

Could the two changes be included in a single amendment or annex?

4. Dissemination of results

Articles published:

[1] H. Montes-Campos, J. M. Otero-Mato, T. Mendez-Morales O. Cabeza, L.J. Gallego, A. Ciach, and L. M. Varela, Universal 2D Pattern Formation in Confined Ionic Liquids, PCCP **19**, 24505 (2017)
[2] A. Ciach, Simple theory for oscillatory charge profile in ionic liquids near a charged wall, J. Mol. Liq. doi.org/10.1016/j.molliq.2017.10.002
[3] K. Breitsprecher, M. Abele, S. Kondrat, and Ch. Holm, The effect of finite pore length on ion structure and charging, J. Chem. Phys. **146** 104708 (2017)
[4] M. Holovko, T. Patsahan, and W. Dong, On the improvement of SPT2 approach in the theory of a hard sphere fluid in disordered porous media, Condens. Matter Phys. **20** 33602 (2017)
[5] M.F. Holovko and M.V. Hvozd, Isotropic-nematic mixture of hard spheres and hard spherocylinders: scaled particle theory description, Condens. Matter Phys. **20** 43501 (2017)
[6] O. V. Patsahan, T. M. Patsahan, and M. F. Holovko, Vapor-liquid phase behavior of a size-asymmetric model of ionic fluids confined in a disordered matrix: the collective-variables-based approach, Phys. Rev. E **97**, 022109 (2018)
[7] O. V. Patsahan, T. M. Patsahan, and M. F. Holovko, Vapour-liquid critical parameters of a 2:1 primitive model of ionic fluids confined in disordered porous media, J. Mol. Liq., doi.org/10.1016/j.molliq.2017.12.033
[8] Y .V. Kalyuzhnyi, J. Reščič, M. F. Holovko, and P. T. Cummings, “Primitive models of the room temperature ionic liquids. Liquid-gas coexistence”. J. Mol. Liq. doi.org/10.1016/j.molliq.2018.01.109

Articles submitted:

- G. S. Bokun, D. di Caprio, M. Holovko and V. Vikhrenko “Charge screening for mobile ions in lattice fluid models”, J. Mol. Phys.
- J. Pękalski and A. Ciach “Self-assembly of lamellar structures on spherical surfaces” J. Chem. Phys.

Articles in preparation:

E. Parsons, E. Mason, W. T. Góźdź, A. M. Squires, A. Tyler, “A square nano-array formed by surface alignment of Primitive bicontinuous lipid cubic phase adopting lowest energy (100) facet.”

Conference Proceedings:

- Y. Groda, E. Bildanov, and V. Vikhrenko, Thermodynamic Properties of the System with Competing Interactions on a Triangular Lattice. Proceedings of the 2017 IEEE 7th International Conference on Nanomaterials: Applications & Properties (NAP-2017). Part 3. Paper 03NNSA31 (5 p.)
- G. Bokun, V. Vikhrenko, D. Di Caprio, M. Holovko, Chemical Potential Distribution of Nonhomogeneous Solid Electrolyte. Proceedings of the 2017 IEEE 7th International Conference on Nanomaterials: Applications & Properties (NAP-2017). Part 3. Paper 03NE16 (4 p.)
- P. Argyrakis, P. Giazitzidis, L. Skarpalezos, Y. G. Groda, V. S. Vikhrenko, Influence of Obstacles on Equilibrium Properties of the Lattice Fluid on a Surface. Proceedings of the 2017 IEEE 7th International Conference on Nanomaterials: Applications & Properties (NAP-2017). Part 1. Paper 01PCSI15 (5 p.)

Conference Presentations:

- T. Patsahan, O. Patsahan, M. Holovko, Phase behaviour of primitive models of ionic fluids confined in disordered matrices: collective variables approach", 10th Liquid Matter Conference, Ljubljana, 17-21.07.2017 , poster

- M. Holovko, T. Patsahan, O. Patsahan, Vapour-liquid phase behaviour of ionic fluids in disordered porous media: application of the scaled particle theory and the ion-association concept, 10th Liquid Matter Conference, Ljubljana, 17-21.07.2017, poster

- M. Holovko, An application of the scaled particle theory and the ion association concept to the description of vapour-liquid phase equilibrium of ionic fluids in disordered porous matrices, at at EMLG/JMLG joint meeting, Vienna, 10-14 September, 2017, oral presentation

- G. J Zarragoicoechea and A. G. Meyra, Growth and connection of colonies of cells or individuals in ecosystems. Monte Carlo standard and bias Monte Carlo, XV Congreso Regional de Física Estadística y Aplicaciones a la Materia Condensada TREFEMAC 2017, May 2017, Santa Rosa, La Pampa, Argentina, poster.

- G. Ferrara and A. Meyra, Dynamics and structure of nanoconfined water and decane mixtures, Reunión de la Asociación Física Argentina, September 2017, La Plata, Argentina, oral presentation

Conference Presentations:

- Y. G. Groda, E. E. Bildanov, The order parameter and critical temperature of the lattice fluid with SALR potential on a square lattice. VI-th Congress of the Physicists of Belarus, Minsk, 20-23 November, oral presentation

- Y. G. Groda, V. S. Vikhrenko, Kinetic diffusion coefficient of the lattice fluid on the simple cubic lattice with blocked sites VI-th Congress of the Physicists of Belarus, , Minsk, 20-23 November, oral presentation

- K. Bretsprecher, C. Holm, S. Kondrat, "Charge me slowly, I am in a hurry: Accelerating charge/discharge in nanoporous supercapacitors" ILMAT 4. International Conference on Ionic Liquid-based Materials, Oct 24-27, 2017, Santiago de Comostella, Invited presentation

- Abdelhafed Taleb, New scientific and nanotechnological opportunities of nanomaterials in the field of electrochemistry, Conference Modern electrochemical technologies and installations. Minsk 28 - 30 November 2017, oral presentation.

- Valiantsin Yaskelchyk and Abdelhafed Taleb, “Nanodiamond coating for anti-corrosion applications”, NANOSMAT conference , Paris 11 - 13 September 2017, poster.

Seminars:

- IPC, March 2017, V. Zhylinski, “Summary of Recent Activities of the Electrochemistry Laboratory of the Belarusian State Technological University”
- ICMP, March 2017, G. Bokun, “Description of long-range and short-range interactions in crystalline nonhomogeneous medium”
- ICMP, March 2017, I. Kravtsiv, “Density field theory of fluids”
- BSTU, May 2017, T. Patsahan, “Ionic liquids in a disordered matrix: equilibrium and dynamic properties”
- ICMP, September 2017, V. Vikhrenko “Statistical description of solid electrolytes”
- Statistical Physics Seminar at the Faculty of Physics, University of Warsaw, Jan 2018 , S. Kondrat, "Physics, modelling and optimization of nanoporous supercapacitor"