ESF Exploratory Workshop on

Defect-assembled soft matter for nanoscience and biotechnology

Rogaška Slatina (Slovenia), 14-16 September 2013

Convened by:
Samo KRALJ, Epifanio G. VIRGA

SCIENTIFIC REPORT
1. Executive summary

The workshop “Defect-assembled soft matter for nanoscience and biotechnology” was held at Rogaška Slatina in Slovenia in the period 14-16 of September, 2013. Rogaška Slatina is one of the oldest tourist places in Slovenia. It is a popular European Health Spa resort, in particular due to the unique composition of the natural mineral water Donat Mg. Activities took place at the hotel Slovenija (http://www.hotel-slovenija.net/) where all participants were accommodated. The hotel was built by the famous historical architect Jože Plečnik. It has been recently renovated in line with the most recent trends and has a nice location along the promenade leading to the touristic centre of Rogaška Slatina. The environment contributed to a relaxing general atmosphere of workshop participants. Convenors of the workshop were Samo Kralj and Epifanio G. Virga. Members of local organizing committee were Mitja Slavinec and Maja Fras.

The central theme of the workshop were functional soft materials. Recent studies have revealed that by combining unique properties of soft materials (SMs) and nanoparticles (NPs) new hybrid materials with exceptional properties could be developed. Furthermore, there is a strong evidence that topological defects (TDs) in soft materials could be exploited to assemble and to control positions of appropriate NPs. It is of interest to find robust synthesis strategies enabling to produce new soft complex nanocomposites with tunable functionality and/or exceptional material properties. One promising avenue is to exploit interactions between NPs and TDs. There is also a need to develop appropriate modeling of such complex systems and to propose new devices and applications.

The corresponding main goal of the workshop was to i) assemble in one place leading experts in the field of soft materials, soft nanocomposites and topological defects, ii) to identify new directions and key open problems by combining these fields of research, and iii) to synchronize future activities in order to make breakthrough discoveries. The meeting enabled interactive exchanges of ideas, discussion of new approaches merging the above mentioned fields of research and nucleated further organized activities.

As basic working material, we considered various soft materials, mostly liquid crystals (LCs), and nanoparticles. The latter could be trapped within tunable configurations of topological defects in SMs. Added NPs either permit the construction of materials with an otherwise inaccessible combination of properties, or enable self-assembling of SM units into complex hierarchical structures. Possible applications are new stimuli responsive, phase change memory storage, and photonic band gap devices and controlled biological cell shape manipulations.

At the meeting were present 28 researchers, including experimentalists, mathematicians, physicists, chemists, computer scientists. All invited scientists are experts either in the field of topological defects, soft materials, nanocomposites or a combination thereof. The participants were invited on the basis of their scientific excellence and covered a wide range of countries. Care was given to gender balance (10 female and 18 male participants). In addition to leading scientists in the listed topics, also several outstanding early stage researchers participated in the workshop.

The main subtopics of the workshop were as follows.

- **Complex structures and phases – theory and experiment**
  We discussed i) fundamental concepts of defect-driven self-assembly at different levels of hierarchy, ii) complex self-assembling in soft matter on a nano-scale level, iii) proposals for new assembling strategies.

- **Complexity and giant response**
  Ways to obtain giant responses in multiferroic materials and “soft crystals” were considered.

- **Synthesis**
  Design and synthesis of complex systems with high functionality and multiferroic properties were presented and discussed. Furthermore, robust and simple concepts,
general strategies for the synthesis of appropriate NPs with specific magnetic, electric, photonic, or thermal conducting properties were demonstrated.

- **Applications in biology and in technology**
  Possible applications of the new materials for stimuli responsive devices, e.g., actuators, transducers, sensors, artificial muscles, recognition, etc. and photonic band gap devices were presented and discussed.

The program was structured so as to encourage discussion and full participation of all delegates. For this purpose, each completed session was closed by a discussion, where open problems were identified and possible solutions presented.

The main conclusions of the workshop are the following.

Current numerical approaches allow efficient and surprisingly accurate predictions of material behavior, including surface interaction and self assembling properties of mixtures of NPs and SMs. Numerical simulations and also experiments demonstrate that combinations of geometry, kinetics and external fields can be readily exploited for stabilization of different templates of NPs in SM matrices. Complex combinations of SM and NPs with giant mechanical, thermal or electromagnetic responses were experimentally demonstrated. In particular, it was shown that synthesis of ferronematics with a relatively large magnetization response is finally possible. It was demonstrated that methods established in other fields of science (e.g., the parallel transport in relativity theory) could be applied to predict regions favoring topological defects, at least in effectively two-dimensional systems. Different NPs, which can be employed as carriers of desired supplementary material properties, could be efficiently trapped within cores of topological defects if they are adequately surface decorated. They should relatively weakly disrupt the bulk SM structure to enable dominance of the universal Defect Core Replacement mechanism. The latter enables condensation free energy gain driven stabilization of structures exhibiting TDs. Nevertheless, NPs outside cores of TDs should at least weakly disrupt a gauge field of relevant SM order to be efficiently driven to TDs. Possible directions were proposed to form crystals at µm scale exploiting LC shells. It was demonstrated that the valence of LC shells could be sensitively controlled via various parameters. Furthermore, current technology allows that particles of different topology could be synthesized. If immersed in LCs, they could enforce a rich variety of different TDs with complex structures. It was also demonstrated how various entities could be efficiently transported within SMs using the distorted gauge-field levitation. It was also demonstrated that nanoparticle driven stabilization of structures exhibiting TDs could be extremely efficient for specific NP microstructures. For example, it was shown that even ppm concentrations of endotoxin are sufficient to stabilize LC structures with TDs. Furthermore, it was also shown that interactions between NPs and membranes could trigger diverse membrane transformations of vital biological importance.

Basic information (principal goal of the workshop, participants, abstracts of participants, programme, venue) on the workshop are also available on the web page http://softnano.fnm.um.si/.
2. Scientific content of the event

The workshop consisted of 28 lectures, presented in sessions i) Selfassembling, ii) Complexity, iii) Soft Nanocomposites, iv) Topological Defects, v) Interactions between Nanoparticles, Topological Defects and Confinement, vi) Colloids and Topological Defects, vii) Biological Systems. Abstracts of presentations are available at http://softnano.fnm.um.si/lecturers. Note that initially 30 lecturers were invited to attend the workshop. However, Prof. Dr. Fodor-Csorba Katalin and Prof. Dr. Andre Sonnet cancelled their participation two days before the beginning of the workshop due to unexpected events. In addition lecture of Prof. Dr. Ivan Smylukh (he could not arrive due to floods in Boulder) was presented by Dr. Paul Ackerman.

i) Complexity

In her talk “Hybrid models for liquid crystals and their applications” A. Majumdar focused on the development, analysis and numerical implementation of mathematical models for a planar bistable nematic device. She presented simulations using different approaches (lattice-based Landau-de Gennes interaction potential and Lebwohl-Lasher lattice-based approach). Multistability was investigated by means of Monte Carlo methods. She discussed a multiscale modelling approach wherein a lattice-based interaction potential is coupled to a conventional continuum model.

N. Vaupotič presented in the talk “Faraday and Cotton-Mouton effect in ferrofluids” a combination of experimental measurements and theoretical modelling of ferrofluids, which enables determination of the magnetic moment of a single nanoparticle, its plasma frequency and the effect of particle chain formation on optical properties. She focused on induced optical activity and induced birefringence in a composite material made of cobalt nanoparticles embedded in a dielectric liquid host. To analyse experimental results, an effective dielectric tensor of a composite material was constructed, taking into account the orientational distribution of nanoparticle magnetic moments in external magnetic field. The proposed approach enables quantitative determination of the magnetic moment and plasma frequency of a single nanoparticle.

In the talk “Unusual optical properties of liquid crystal elastomers” I. Drevenšek considered photoactive components (azobenzene) added to liquid-crystalline elastomer (LCE) which opens up different possibilities for optical manipulation of mechanical, thermal, electrical and optical properties of the material. Optical properties in these samples depend on the isomerization state of the azobenzene molecules. She demonstrated that optical irradiation can trigger in LCE their size and shape, flips between different shapes, oscillations, or even moving on supporting surfaces, which makes them very promising materials for various micro- and nano-size devices.

T. Tóth-Katona in the lecture “Photo-induced effects in some methylhydrosiloxane-based side chain liquid crystalline polymers” presented a new azo-benzene group containing monomer and several respective functional side-chain polymers grafted on methylhydrosiloxane backbone. These materials show self-assembling behaviour and exhibit a broad temperature range of nematic liquid crystalline phase even below the room temperature. Besides the considerable chromatic dispersion, a substantial dichroism is detected which together with the photo-induced reorientation demonstrates the potential applicability of these materials for optical storage.

ii) Soft Nanocomposites

In the lecture “Dielectric spectroscopy in nanoparticle - liquid crystal pressurized composites” S. J. Rzoska presented temperature and high pressure studies in composites (5CB, hydrophilic silica spheres) and (5CB, BaTiO₃) using broad band dielectric spectroscopy. The
research was focused on the influence of nanoparticles on pretransitional effects and clearly non-Arrhenius and non-Debye dynamics. The significant influence of the concentration of nanoparticles on phase transition temperatures/pressures as well as on the form of pretransitional effects was observed. For the analysis of subtle effects, he presented their original derivative-based analysis.

In her lecture “Interplay between liquid crystal and nanoparticles for functional composites” G. Scalia presented alignment of CNT by liquid crystalline hosts. She showed that both classes of liquid crystals, thermotropics as well as lytropics, are capable of transferring their inherent long-range orientational order to CNTs over areas easily reaching square centimetre. She also demonstrated that lyotropic LC phases can be also formed by CNTs or by graphene oxide in water. Because of the highly anisotropic shape the threshold for the formation of LC phases can be very low. Several factors influence the LC phase formation like the anisotropic ratio and the polidispersity but also the presence of defects in the nanoparticles are expected to have an important role.

In the lecture “Shape driven ferromagnetic ordering in suspensions of magnetic nanoplatelets in nematic liquid crystal” A. Mertelj demonstrated that in ordered nematic liquid-crystalline phase of the suspension of BaHF nanoplatelets doped with Sc in liquid crystal 5CB ferromagnetic ordering appears. The magnetization is along the nematic director and comes from the ferromagnetic ordering of the nanoplatelets. When the sample is prepared in the absence of an external magnetic field, two types of magnetic domains appear with magnetizations in opposite directions. If during the preparation an external magnetic field is applied along the director, a monodomain sample is obtained. Magnetization curves show that a small magnetic field is needed to switch the domains.

M. Slavinec in the lecture “Slave-master mechanism in soft composites” showed that LC structures are soft and consequently could be efficiently controlled via various mechanisms. He presented a homogeneous binary mixtures of LCs and appropriate nanoparticles with “slave-master” type of behaviour. In such systems, a change of a relevant control parameter has strong impact on the “slave” while the “master” is only weakly affected.

In the lecture “Impact of Curvature on Topological Defects in Liquid Crystals” S. Kralj presented the impact of Gaussian curvature $K$ and NPs on both stability and position of TDs. He demonstrated how $K$ affects number and position of TDs in nematic shells, emphasising an analogy with electrostatics. He also consider NP and $K$ driven stabilization of lattices of TDs in blue phases in and twist grain phases of chiral LCs.

W. Haase demonstrated in his lecture “Subhertz dielectric processes in SmC* and SmA* phases of FLC gold and silver nanocomposites” that besides molecular reorientation around short and long molecular axes and collective relaxation processes like Goldstone, domain or soft mode, some more processes appear at low frequencies in the SmC* and SmA* phases. There are hints for the appearance of such processes already in the nematic phase. The physical origin of the subhertz process was investigated in various mixtures of silver nanospheres dispersed in FLC mixtures.

In the lecture “Structural phase transition in ferronematics - nematic liquid crystals doped with magnetic nanoparticles” N. Tomasovicova studied field-induced reorientational effect of liquid crystals. The preparation of magnetic particles of different shapes (spherical, rod-like and chain-like) were described. An overview was given of the experimental results obtained on the behaviour of ferronematics depending on the host liquid crystal, on the type, shape, size and concentration of the magnetic particles. A mechanism to explain how magnetic particles may affect the magnetic response was presented. The obtained experimental results were explained in terms of the Burylov-Raikher theory.

Discussion sections (i), (ii) and (iii): lectures were dominantly experimental. They proposed avenues to several new applications, particularly in the field of optics and self-organisation. In particular, combination of holographic optic properties and elastomers have great potential for breakthrough applications. Furthermore, for the first time ferronematics
with relatively large magnetization were synthesized, what promises to open ways to magnetic phenomena in applications based on soft matrices. Lectures also clearly revealed, that new applications need new materials with exotic properties, and combinations of NPs and soft matrices seems to be ideal for such purpose. Again, the importance of ions was emphasized which need to be put under control for competitive applications. A new catch word was “slave-master” mechanism, suggesting different paths of controlling “slave” via “master”, which depend on the structure of the coupling between "slave" and "master" order parameters.

iii) Topological Defects

J. Ball in his talk “Some mathematical questions related to the modelling of liquid crystals” described some mathematical issues related to the description of liquid crystals, such as the role of function spaces in the mathematical model, the description of defects and the relationship between different models such as the Oseen-Frank, Landau – de Gennes and Onsager/Maier-Saupe theories.

In the presentation “Curvature potentials on nematic shells” G. E. Virga introduced the two-dimensional order tensor that describes the local organization of liquid crystal molecules, which tend to lie parallel to the colloids' surface, this tensor vanishes wherever no orientation is prevailing on average. In the lecture he reviewed recent work concerned with the interaction between defects and the underlying surface. In particular, arguments were offered that identify appropriate geometric potentials, depending on the shell's shape, which either promote or hamper defects, attract or repel them.

iv) Interactions between Nanoparticles, Topological Defects and Confinement,

In his talk L. Longa “Landau-de Gennes theory of blue phases - an analytical approach” discussed the generic Landau-deGennes theory of blue phases that allows us to understand these chiral structures. The theory explains correctly the structure of the body-centered cubic blue phase I and the simple cubic blue phase II, but encounters difficulties in describing properties of BPIII. This theory introduces higher order elastic terms. Their influence on the phase diagrams of the chiral nematic phases was discussed. Also, a general question concerning the applicability of the Landau-deGennes theory in describing the chiral phases, especially BPIII, was addressed.

In her talk “Oriented liquid crystal defects for the control of nanoparticles optical properties in hybrid systems” E. Lacaze presented trapping of NPS within smectic dislocations in oily streaks patterns. By increasing the nanoparticles concentration, the trapping efficiency of different kinds of smectic dislocations was probed combining optical measurement (UV-Vis spectroscopy, ellipsometry, Raman spectroscopy) and X-rays diffraction under synchrotron radiation. The interplay between the dislocations structure and the nanoparticles organization is observed when the nanoparticles concentration is increased. The structure of the dislocations varies in the presence of NPs, highly compressing the NPs assemblies perpendicular to the oily streaks at high concentration. Results reveal the importance of the knowledge of dislocation structure at the nanoparticle scale, to control the induced optical properties.

In the lecture “Nanoparticle-mediated stabilization of modulated structures with topological effects” G. Cordoyiannis presented the impact of different surface-functionalized NPs on various defect lattices in chiral LCs. The resulting soft nano-composites have been studied by means of high-resolution calorimetry, small-angle X-ray scattering and polarizing optical microscopy. As NPs, spherical CdSe and CdSS, MoS$_2$ and graphene nanosheets were used, surface functionalized with flexible molecules. It was demonstrated that by choosing different NPs one could stabilize different defect lattices.

G. Nounesis in his lecture “Nanoparticle-assisted functional targeting in soft materials” presented CdSe quantum dots mediated transport of polyvinylpyrrolidone (PVP) chains to specific, orientationally disordered locations, created in an aligned nematic liquid-crystal sample, by the implantation of colloidal particles. Driven by phase separation at the isotropic – nematic transition, the site-specific condensation of nanoparticle-decorated PVP chains triggers the extraordinarily fast self-assembly of PVP along disclination lines, and
nematic domain interfaces leading to the formation of hollow fibrous superstructures extending in all directions for several hundreds of microns.

In the talk “Topological defects of nematics in bicontinuous media with controlled geometry” F. Serra presented memory effects in a porous material with a cubic symmetry and micron-sized pores inside a liquid crystal cell, by using laser microfabrication techniques. When NLCs are incorporated within the cubic scaffold and a homeotropic alignment is imposed on all the surfaces, the onset of an electric field induces a complete alignment of the LC in the direction of the field. The removal of the field leads to elastic response to the initial (random) state if the field is below a certain threshold, while memory effects can be easily detected if the field is above this threshold, when the alignment induced by the field is partially retained even when the field is turned off.

**Discussion section (iii) and (iv):** There was illuminating discussion about how a defined theoretical frame might hide phenomena inherent to real systems. Questions about stability of blue phases were raised, because several researchers claim they might be glasses, and consequently not useful for desired display applications. Therefore, it could be perhaps better to reorient theoretical endeavours towards other, more promising directions. It was asked whether nematic shells are really effectively two-dimensional. The latter assumption might suppress some mechanisms playing important roles in real systems. The importance of different kinetics paths on self-assembling was again emphasized. Furthermore, lectures gave clear evidence that combination of TDs and geometry could be exploited to store and retrieve efficiently information. Furthermore, potential of smectic dislocations to enforce linear assembly of NPs was emphasized for future nano-engineering technologies.

**v) Colloids and Topological Defects**

In the lecture “Towards an optical nano-laboratory in a liquid crystal defect” P. Ackerman presents varous LC structures and defects stabilized by chirality, confinement, and/or the presence of colloidal microparticles. He demonstrates that they enable efficient trapping and well-defined alignment of anisotropic semiconductor, plasmonic, and other nanoparticles.

J. Lagerwall in “Defect configurations and textural developments during phase transitions in colloidal liquid crystal shells with varying boundary conditions” presented a study of nematic, smectic-A and smectic-C phases as well as transitions between the phases in shells with varying characteristics. In their experiments they can tune the alignment of the director at each interface by choosing the composition of the inner and outer phases. A smectic-A shell can exhibit a defect-free director field in case of radial alignment, a spherical lune texture in case of uniform planar alignment, and a regular patterning of toric focal conics in case of hybrid alignment. If a dopant particle that itself seeds a defect is present in the shell, also negative-valued disclinations may occur. If the liquid crystal is polymerized into an elastomer, the potential of actuating the shell mechanically allows it to be used as a self-assembled micropump.

O. Lavrentovich in “Liquid-crystal-enabled colloidal transport” presented mechanisms of particle transport enabled by liquid crystal environment. Among them are the motion of particles caused by gradients of the director, director fluctuations, and effects in the electric field: backflow powered by director reorientations, dielectrophoresis in a liquid crystal with varying dielectric permittivity and liquid crystal-enabled nonlinear electrophoresis with velocity that depends on the square of the applied electric field and can be directed differently from the field direction.

**Discussion section (v):** Discussion revealed that Nelson’s dream of forming scaled crystals might not be close to a real application. In particular, recent experimental methods allow the formation of a rich variety of “atoms” (LC shells exhibiting different valences), which have the potential to form crystals exhibiting different symmetries. The latter could lead to tunable band-gap applications. Furthermore, it was revealed that non-equilibrium phenomena can be well controlled in various submicron-scale transports. Richness in transport mechanism is enabled by the interplay between gradients of order parameters, backflow, and Brownian motion. Therefore, LCs have the potential to mimic to some extent various dynamic
mechanisms at the molecular level in living systems. Furthermore, optical generation of complex defect structures on demand has the potential for several applications.

**vi) Biological Systems**

In his lecture “Defect-Assembled Soft Matter from Wisconsin” N. Abbott showed that polymerizable, micrometer-sized liquid crystalline droplets (dispersed in water) provide the basis of general and facile methods leading to the synthesis of spherical or non-spherically polymeric particles with well-defined chemical patches. He demonstrated that such particles are exciting building blocks for studies of self-assembly. Defects in thermotropic liquid crystals were also described along with principles leading to highly sensitive methods for detection of biological lipids (such as endotoxin).

A. Iglič considered in “Orientational ordering of water in a thin layer near a highly charged surfaces in saturation regime” electrolyte-charged surface interface, described within the Langevin Poisson-Boltzmann and Langevin-Bikerman models. He demonstrated that in the saturation regime close to a charged surface, water dipole ordering and depletion of water molecules may result in a strong local decrease of permittivity. Analytical expressions for the space dependence of relative permittivity for both models were presented.

S. Perukova presented in “Nanoparticles induced interactions between like-charged membrane surfaces” a possible mechanism which can lead to attractive interaction between two like-charged biological surfaces based on average orientation of charged nanoparticles. In this study they used analytical as well as numerical methods: modifications of Poisson-Boltzmann equation and Monte Carlo simulations. She demonstrated that under certain conditions an attractive force appears between like-charged surfaces.

**Discussion section (vi):** Lectures emphasized the role of anchoring in biological systems. At interfaces they lead to renormalization of electrostatic interactions. It is clear that the chemistry of the mechanisms at work is far from being completely understood and further investigations are needed. Furthermore, in case of endotoxin driven structural changes, where the structure with a topological defect was stabilised, it is obvious that the Defect Core Mechanism is nevertheless not so dominant. Other mechanisms, most probably saddle-splay elasticity, also play a significant role. Furthermore, experimental pioneering studies reveal that appropriate soft matter configurations could be efficiently exploited for a very sensitive detection of appropriate NPs or toxins.
3. Assessment of the results, contribution to the future direction of the field, outcome

The near future is expected to be dominated by nano and biotechnology. To develop these technologies it is of interest

- to dope various condensed matter phases with appropriate nanoparticles in order to obtain new effective materials with either anomalously enhanced, qualitatively new material properties, or controlled functionality;
- to determine and understand the relationship between structures or super-structures of complex hybrid materials or nano-composites and the resulting macroscopic behaviour;
- to master precise targeting and controlled partitioning of specific NPs to desired specific locations;
- to detect sensitively concentration of specific NPs in an environment because their presence is becoming ubiquitous in new materials and technologies.

These issues were presented and discussed within the workshop. As working materials we considered various anisotropic soft materials and different NPs. In several cases we exploited topological defects to control position of NPs within soft matrices.

During the workshop the current state in the fields of interest was enlightened, open problems were identified, possible solutions to them were proposed and future activities were planned. Special emphasis was put on possible applications. In the following we outline the main conclusions of the workshop and the corresponding suggestions for further activities.

The most important conclusions that we reached are as follows:

- It is clear that new applications require new materials with exotic properties. Combining SMs and appropriate NPs is certainly an adequate and competitive avenue towards this goal. SM matrices contribute sensitive responses to various parameters, some responses could be relatively easily observed mainly due to optical transparency of most SM phases. An additional required quality could be introduced by adequate NPs. For example, NPS exhibiting plasmonic excitations, ferromagnetic or ferroelectric properties, photoluminescence with predetermined wavelength were presented. For the first time a stable ferronematic phase with relatively large magnetic response was presented. The latter was primarily achieved by appropriate shape of magnetic NPs. From most lectures it was evident that shape, size and surface treatment of NPs play often a dominant role. Consequently, systematic investigations of the impact of these parameters to optimize the resulting nanocomposites and soft hybrid systems is necessary.

- Localised non-singular or singular (i.e. with Topological Defects) distortions in SM matrices could be readily exploited as assembling sites for NPs. It was experimentally shown that different regular patterns of NP organisations could be achieved. Chirality and imposed geometrical constraints are in particular adequate to impose controlled localised elastic distortions. It was shown that a strong enough chirality stabilises various blue phases (BPs) and the twist grain boundary (TGB) smectic A phase. These phases exhibit regular lattices of line disclinations and line dislocations, corresponding to TDs in orientational and translational degrees of ordering, respectively. Straight edge dislocations and regular patterns of grain boundary were obtained via geometrical constraint. Combination of chirality and geometry open ways to even more complex scenarios. It was shown that all these distortions are efficient traps for appropriately surface decorates NPs. Furthermore, trapped NPs could significantly (even by orders of magnitude) enhance the stability range of BPs and TGB A phases. The latter can be
even nucleated by NPs. Experiments demonstrate, that even graphene nano-sheets, the characteristic length of which is much larger than the core size of dislocations, could be efficiently trapped by TDs. Nevertheless, it seems that the geometry of NPs and their characteristic linear size play an important role. It is evident that the recently proposed Defect Core Replacement mechanism is not sufficient to explain all the observed features related to the efficient trapping of NPs to TDs. There are clear suggestions that Gaussian curvature and related saddle splay elasticity also play a significant role. Further synchronized experimental and theoretical activities are needed to answer these questions.

- Various applications aiming at anomalous responses require realizing of percolation threshold of NPs. It was demonstrated that, in addition to NP geometry, interactions might also play a significant role. There is a need for systematic investigations of different ways to control and manipulate percolation threshold of different NPs.
- Simulations and experiments indicate that non-equilibrium phenomena could be readily exploited to realize different patterns of assembled NPs and to transport them. Therefore, controlled kinetics and imposed biases could lead to diverse new patterns. In particular, nonlinear defects and conditions, which push systems towards edge of chaos are of particular interest. This field of research intersects soft matter physics and physics of complex systems, promising to open an unexpected variety of new patterns and related applications.
- The workshop demonstrated that topological defects could be, among others, exploited for efficient trapping of NPs. Current simulations can relatively well determine cores of various defects and different regular organisations of them. In particular, it was demonstrated that diverse patterns of TDs could be realized in relatively thin SM films by playing with geometry. Mathematical approaches borrowed from general relativity could be exploited to predict efficiently sites in planar nematic LC films, where TDs are favoured. The workshop demonstrated that the Nelson's dream to form scaled soft crystals seems to become a reality. However, to this purpose further activities are needed. In particular, it is important to find out i) how effective material properties change when the characteristic LC film thickness size is reduced, ii) which nano-linkers would be most efficient to bind nearby LC shells, iii) how to transport efficiently nano-linker to the desired sites.
- It was demonstrated in several lectures that adequate NPs could stabilise LC structures exhibiting a single or even a lattice of topological defects. Structures possessing TDs are relatively easily observed because of characteristic distortions in a relevant gauge field. It was shown that geometrical details or flexibility of NPs might also play a role. Trapping efficiency of TD depends on adaptiveness of NPs with defect cores. A variety of different defect core structures could be realized by appropriate conditions. Results clearly indicate that adequate configurations of SMs could be exploited for sensitive detections of various NPs or toxins. There is need for further systematic investigations to identify competing LC structures which could be adequate for sensitive detection of specific NPs. Furthermore, combination with photosensitive LCs in which structural transition could be imposed by UV irradiation promises ways to determine different concentration of NPs.
- It was demonstrated that interactions between NP and biological membranes might trigger several phenomena of vital biological importance. In case of in-plane membrane order TDs almost unavoidably appear which in general breaks the system's symmetry. Preliminary theoretical studies show that TDs could play an important role in various biological processes. For example, they could trigger membrane fission processes. There is a need for further systematic theoretical and experimental studies to clarify the role of TDs in membranes and their interaction of NPs. Understanding of such
interactions could lead us to control the transport of various NPs via membranes, opening avenues to various applications in biology and medicine.

At the workshop we decided to synchronise our future activities to tackle open problems at the intersections of the following research fields: i) soft condensed materials, ii) topological defects, iii) complex systems, iv) nanoscience, iv) chemistry, v) biology, and vi) medicine.

At a first step, we intend to propose to Soft Matter or a similar journal to publish a special issue covering the topics addressed at the workshop. In addition to the workshop participants we intend to invite also other leading researchers in these fields to submit an article.

As a further step, we intend to continue our activity within the COST-frame. Continuous COST calls invite researchers throughout Europe to submit proposals for research networks to exchange knowledge and to embark on new European perspectives. We intend to submit a proposal at the first possible collection date in 2014 (i.e. in March). The proposal will contain all open issues raised above; all European participants are interested to participate. Within the COST programme we intend to organize regular annual workshops to exchange the new knowledge gained and to exchange (in particular young) researchers.

Furthermore, appropriate complementary groups tend to apply for different future adequate calls at European or other levels. Of particular interest will be the future Marie Curie programme calls which enable exchange of PhD students and postdoctoral researchers among participants.

In addition, we intend to collaborate via existing and newly planned PhD educational programmes. For example, at the University of Maribor (main organiser of the workshop) there is strong initiative to create high quality international PhD programme covering the topics of the workshop. Several workshop participants will be invited to participate.
4. Final programme

Saturday 14 September 2013

09.00-09.10  Opening of the workshop

09.10-09.30  Presentation of the European Science Foundation (ESF)
Ana-Maria Ciubotaru
(Standing Committee for Physical and Engineering Sciences)

09.30-12.30  Morning Session: Selfassembling

09.30-10.00 “Modelling and computer simulations of soft complex materials: from liquid crystals to actuators”
C. Zannoni (University of Bologna, Bologna, Italy)

10.00-10.30 “Emergent Length-Scales in Self-Assembling Soft Matter”
D. Cleaver (Sheffield Hallam University, Sheffield, United Kingdom)

10.30-11.00 Coffee / Tea break / Informal discussions

11.00-11.30 “Liquid crystals form hybrid inorganic/organic particles”
E. Gorecka (University of Warsaw, Warsaw, Poland)

11.30-12.00 “Structured assemblies of nanocarbons in complex fluids”
P. Poulin (University of Bordeaux, Pessac, France)

12.00-12.30 Discussion, open problems

12.30-13.30 Lunch

13.30-16.00 Afternoon Session I: Complexity

13.30-14.00 “Hybrid models for liquid crystals and their applications”
A. Majumdar (University of Bath, Bath, United Kingdom)

14.00-14.30 “Faraday and Cotton-Mouton effect in ferrofluids”
N. Vaupotič (University of Maribor, Maribor, Slovenia)

14.30-15.00 “Unusual optical properties of liquid crystal elastomers”
I. Drevenšek (University of Ljubljana, Ljubljana, Slovenia)

15.00-15.30 “Photo-induced effects in some methylhydrosiloxane-based side chain liquid crystalline polymers”
T. Tóth-Katona (Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary)

15.30-16.00 Coffee / Tea break / Informal discussions

16.00-19.00 Afternoon Session II: Soft Nanocomposites

16.00-16.30 “Dielectric spectroscopy in nanoparticle - liquid crystal pressurized composites”
S. J. Rzoska (University of Silesia, Katowice, Poland)

16.30-17.00 “Interplay between liquid crystal and nanoparticles for functional composites”
G. Scalia (Seoul National University, Seoul, South Korea)

17.00-17.30 “Shape driven ferromagnetic ordering in suspensions of magnetic nanoplatelets in nematic liquid crystal”
A. Mertelj (Jožef Stefan Institute, Ljubljana, Slovenia)

17.30-18.00 “Slave-master mechanism in soft composites”
M. Slavinec (University of Maribor, Maribor, Slovenia)

18.00-18.30 “Impact of Curvature on Topological Defects in Liquid Crystals”
S. Kralj (University of Maribor, Maribor, Slovenia)
18.30-19.00 Discussion, open problems

19.00 Dinner

Sunday 15 September 2013

09.00-10.00 Morning Session I: Soft nanocomposites
09.00-09.30 “Subhertz dielectric processes in SmC* and SmA* phases of FLC gold and silver nanocomposites”
W. Haase (Darmstadt University of Technology, Darmstadt, Germany)
09.30-10.00 “Structural phase transition in ferronematics - nematic liquid crystals doped with magnetic nanoparticles”
N. Tomasovicova (Institute of Experimental Physics of Slovak Academy of Sciences, Košice, Slovakia)

10.00-12.30 Morning Session II: Topological Defects
10.00-10.30 “Some mathematical questions related to the modelling of liquid crystals”
J. Ball (University of Oxford, Oxford, United Kingdom)
10.30-11.00 “Curvature potentials on nematic shells”
G. E. Virga (Universtita di Pavia, Pavia, Italy)

11.00-11.30 Coffee / Tea break / Informal discussions

11.30-13.30 Morning Session III: Interactions between Nanoparticles, Topological Defects and Confinement
11.30-12.00 “Landau-de Gennes theory of blue phases - an analytical approach”
L. Longa (Jagiellonian University, Krakow, Poland)
12.00-12.30 “Oriented liquid crystal defects for the control of nanoparticles optical properties in hybrid systems”
E. Lacaze (Université Pierre et Marie Curie-Paris 6, Paris, France)
12.30-13.00 “Nanoparticle-mediated stabilization of modulated structures with topological effects”
G. Cordoyiannis (National and Kapodistrian University of Athens, Athens, Greece)

13.30-14.30 Lunch

14.30-15.30 Afternoon Session : Interactions between Nanoparticles, Topological Defects and Confinement
14.30-15.00 “Nanoparticle-assisted functional targeting in soft materials”
G. Nounesis (National Centre for Scientific Research Demokritos, Athens, Greece)
15.00-15.30 “Topological defects of nematics in bicontinuous media with controlled geometry”
F. Serra (Università degli studi di Milano, Milano, Italy)

15.30-16.00 Discussion, open problems
16.30-20.00 Excursion to Olimije

20.00-21.00 Dinner
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Speaker</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>09.00-11.00</td>
<td>Morning Session I: Colloids and Topological Defects</td>
<td>“Towards an optical nano-laboratory in a liquid crystal defect”</td>
<td>P. Ackerman (University of Colorado at Boulder, Boulder, USA)</td>
<td></td>
</tr>
<tr>
<td>09.00-09.30</td>
<td></td>
<td>“Defect configurations and textural developments during phase transitions in colloidal liquid crystal shells with varying boundary conditions”</td>
<td>J. Lagerwall (Seoul National University, Seoul, South Korea)</td>
<td></td>
</tr>
<tr>
<td>09.30-10.00</td>
<td></td>
<td>“Liquid-crystal-enabled colloidal transport”</td>
<td>O. Lavrentovich (Kent State University, Kent, USA)</td>
<td></td>
</tr>
<tr>
<td>10.00-10.30</td>
<td></td>
<td>“Defect configurations and textural developments during phase transitions in colloidal liquid crystal shells with varying boundary conditions”</td>
<td>J. Lagerwall (Seoul National University, Seoul, South Korea)</td>
<td></td>
</tr>
<tr>
<td>10.30-11.00</td>
<td></td>
<td>Discussion, Open Problems</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11.00-11.30</td>
<td></td>
<td>Coffee / Tea break/ Informal discussions</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11.30-13.30</td>
<td>Morning Session II: Biological Systems</td>
<td>“Defect-Assembled Soft Matter from Wisconsin”</td>
<td>N. Abbott (University of Wisconsin, Wisconsin, USA)</td>
<td></td>
</tr>
<tr>
<td>11.30-12.00</td>
<td></td>
<td>“Orientational ordering of water in a thin layer near a highly charged surface in saturation regime”</td>
<td>A. Iglič (University of Ljubljana, Ljubljana, Slovenia)</td>
<td></td>
</tr>
<tr>
<td>12.00-12.30</td>
<td></td>
<td>“Nanoparticles induced interactions between like-charged membrane surfaces”</td>
<td>S. Perutkova (Czech Technical University in Prague, Prague, Czech Republic)</td>
<td></td>
</tr>
<tr>
<td>12.30-13.00</td>
<td></td>
<td>Discussion, open problems</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13.00-13.30</td>
<td></td>
<td>Lunch</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13.30-14.30</td>
<td></td>
<td>Discussion on follow-up activities/networking/collaboration</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14.30-16.00</td>
<td></td>
<td>End of Workshop and departure</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### 5. Final list of participants

<table>
<thead>
<tr>
<th>Name and surname</th>
<th>Affiliation</th>
<th>Country</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nicholas Abbott</td>
<td>University of Wisconsin</td>
<td>USA</td>
</tr>
<tr>
<td>Paul Ackerman</td>
<td>University of Colorado at Boulder</td>
<td>USA</td>
</tr>
<tr>
<td>John Ball</td>
<td>University of Oxford</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Doug Cleaver</td>
<td>Sheffield Hallam University</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>George Cordoyiannis</td>
<td>National and Kapodistrian University of Athens</td>
<td>Greece</td>
</tr>
<tr>
<td>Irena Drevenšek</td>
<td>University of Ljubljana</td>
<td>Slovenia</td>
</tr>
<tr>
<td>Ewa Gorecka</td>
<td>University of Warsaw</td>
<td>Poland</td>
</tr>
<tr>
<td>Wolfgang Haase</td>
<td>Darmstadt University of Technology</td>
<td>Germany</td>
</tr>
<tr>
<td>Aleš Iglič</td>
<td>University of Ljubljana</td>
<td>Slovenia</td>
</tr>
<tr>
<td>Samo Kralj</td>
<td>University of Maribor</td>
<td>Slovenia</td>
</tr>
<tr>
<td>Emmanuelle Lacaze</td>
<td>Université Pierre et Marie Curie-Paris</td>
<td>France</td>
</tr>
<tr>
<td>Jan Lagerwall</td>
<td>Seoul National University</td>
<td>South Korea</td>
</tr>
<tr>
<td>Oleg Lavrentovich</td>
<td>Kent State University</td>
<td>USA</td>
</tr>
<tr>
<td>Lech Longa</td>
<td>Jagiellonian University</td>
<td>Poland</td>
</tr>
<tr>
<td>Apala Majumdar</td>
<td>University of Bath</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Alenka Mertelj</td>
<td>Jožef Stefan Institute</td>
<td>Slovenia</td>
</tr>
<tr>
<td>George Nounesis</td>
<td>National Centre for Scientific Research Demokritos</td>
<td>Greece</td>
</tr>
<tr>
<td>Šarka Perutkova</td>
<td>Czech Technical University in Prague</td>
<td>Czech Republic</td>
</tr>
<tr>
<td>Philippe Poulin</td>
<td>University of Bordeaux</td>
<td>France</td>
</tr>
<tr>
<td>Sylwester J.Rzoska</td>
<td>University of Silesia</td>
<td>Poland</td>
</tr>
<tr>
<td>Giusy Scalia</td>
<td>Seoul National University</td>
<td>South Korea</td>
</tr>
<tr>
<td>Francesca Serra</td>
<td>Universita degli studi di Milano</td>
<td>Italy</td>
</tr>
<tr>
<td>Mitja Slavinec</td>
<td>University of Maribor</td>
<td>Slovenia</td>
</tr>
<tr>
<td>Natalia Tomasovicova</td>
<td>Institute of Experimental Physics of Slovak Academy of Sciences</td>
<td>Slovakia</td>
</tr>
<tr>
<td>Tibor Tóth-Katona</td>
<td>Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian</td>
<td>Hungary</td>
</tr>
</tbody>
</table>
6. Statistical information on participants

**Table 1**: Number of participants per country and M/F repartition

<table>
<thead>
<tr>
<th>Country</th>
<th>Males</th>
<th>Females</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Czech Republic</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>France</td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Germany</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Greece</td>
<td>2</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>Hungary</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Italy</td>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Poland</td>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Slovakia</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Slovenia</td>
<td>3</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>South Korea</td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>United Kingdom</td>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>USA</td>
<td>3</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td><strong>Sum</strong></td>
<td><strong>18</strong></td>
<td><strong>10</strong></td>
<td><strong>28</strong></td>
</tr>
</tbody>
</table>

**Table 2**: Age distribution of participants

<table>
<thead>
<tr>
<th>Age interval</th>
<th>20-29</th>
<th>30-39</th>
<th>40-49</th>
<th>50-59</th>
<th>Older</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number or participants</td>
<td>2</td>
<td>5</td>
<td>10</td>
<td>7</td>
<td>4</td>
</tr>
</tbody>
</table>