DEPARTMENT OF SOLID STATE PHYSICS F-5

Our research program is focused on the study of the structure and dynamics of disordered and partially ordered condensed matter at the atomic and molecular levels with a special emphasis on phase transitions. The purpose of these investigations is to discover the basic laws of physics governing the behaviour of these systems, which represent the link between perfectly ordered crystals, on the one hand, and amorphous matter, soft condensed matter and living systems, on the other. Such knowledge provides the key to our understanding of the macroscopic properties of these systems and is an important condition for the discovery and development of new multifunctional materials, nanomaterials and biomaterials for new applications. An important part of the research program is devoted to the development of new experimental methods and techniques in the field of magnetic resonance, magnetic resonance imaging, fluorescence microspectroscopy, scanning tunnelling, electronic and atomic force microscopy, as well as dielectric relaxation spectroscopy and dynamic specific heat measurements.

Head:
Prof. Igor Muševič

The experimental techniques used are:

- One (1D) and two (2D) dimensional nuclear magnetic resonance (NMR) and relaxation, as well as quadrupole (NQR) resonance and relaxation,
- Multi-frequency NMR in superconducting magnets of 2T, 6T and 9T, as well as the dispersion of the spin–lattice relaxation time T_1 via field cycling,
- Nuclear double resonance and quadrupole double resonance such as ^{17}O–H and ^{14}N-H,
- Fast field cycling NMR relaxometry,
- Frequency-dependent electron paramagnetic resonance (EPR) and 1D and 2D pulsed EPR and relaxation
- MR imaging and micro-imaging
- Measurement of the electronic transport properties
- Magnetic measurements.
- Fluorescence microscopy and microspectroscopy
- Linear and non-linear dielectric spectroscopy in the range 10^{-2} Hz to 10^{9} Hz,
- Electron microscopy and scanning tunnelling microscopy,
- Atomic force microscopy and force spectroscopy,
- Dynamic specific heat measurements.

The research program of the Department of Solid State Physics at the "Jožef Stefan Institute" is performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics and the Jožef Stefan International Postgraduate School. In 2013, the research was performed within three research programs:

- Magnetic resonance and dielectric spectroscopy of smart new materials
- Physics of Soft Matter, Surfaces and Nanostructures
- Experimental Biophysics of Complex Systems

I. Research programme "Magnetic resonance and dielectric spectroscopy of smart new materials"

The research of the program group *Magnetic Resonance and Dielectric Spectroscopy of Smart New Materials* has focused on a study of physical phenomena in condensed matter at the atomic and molecular levels. The purpose of the investigations was to discover the basic laws of physics governing the behaviour of the investigated systems. The obtained knowledge provides the key to the understanding of microscopic and mac-

The group has discovered the first superconducting, high-entropy alloy, quantum magnetism in low-dimensional spin systems, physical properties of nanostructures, materials with giant electrocaloric and thermomechanical effects, and multiferroic and relaxor phases. The research included pharmaceutical and biological substances, where an NQR-based portable sensor for distinguishing bring original and forged drugs was developed.

roscopic properties of various types of solids and is an important condition for the discovery and development of new multifunctional materials and nanomaterials for novel technological applications.

In our research, we used the following experimental techniques:

- Nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR) and nuclear quadrupole resonance (NQR),
- Nuclear double resonance ^{17}O–H and ^{14}N–H,
- Fast field cycling NMR relaxometry,
- Linear and non-linear dielectric spectroscopy in the range 10^{-2} Hz to 10^{9} Hz,
- Frequency-dependent ac calorimetry,
- Measurement of electrical and thermal transport coefficients,
- Magnetic measurements.

The research program was performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics, and the Jožef Stefan International Postgraduate School. The investigations were focused on the following research fields:

Discovery of a superconducting high-entropy alloy

Traditionally, metallic alloy systems have been based mainly on one principal chemical element as the matrix, even though a substantial number of other elements were incorporated for property/processing enhancement. Within the past several years, a new approach to metallic alloy design with multiple principal elements in equimolar or near-equimolar ratios, termed high-entropy alloys (HEAs), has been proposed. According to this concept, the high entropy of mixing can stabilize disordered solid-solution phases with simple structures like a body-centred cubic (bcc) or a face-centred cubic (fcc) with small unit cells, in competition with ordered crystalline intermetallic phases that often contain structurally complex giant unit cells. The HEA structure is characterized by a topologically ordered lattice with an exceedingly high chemical (substitutional) disorder, so that a HEA can be conveniently termed as a "***metallic glass on an ordered lattice***". The physical properties of HEAs remain largely unexplored. In 2014, the group of prof. Janez Dolinšek discovered the first superconducting HEA within the Ta-Nb-Hf-Zr-Ti system (Koželj et al. Phys. Rev. Lett. 113, 107001 (2014)), showing a high superconducting transition temperature (for a metallic system) of 7.3 K and a large upper critical field of 8.2 T. The temperature-dependent electrical resistivity of the Ta-Nb-Hf-Zr-Ti HEA is shown in Fig. 1.

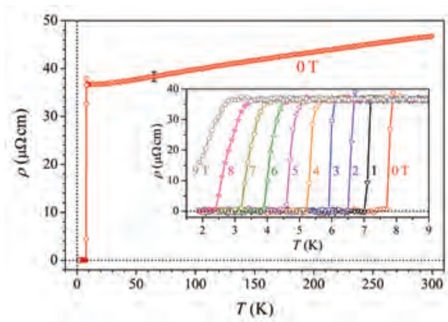

Figure 1: Electrical resistivity of a Ta-Nb-Hf-Zr-Ti high-entropy alloy in the region of the phase transition to the superconducting state.

Quantum magnetism

Andrej Zorko, Denis Arčon and collaborators discovered the first realization of phase separation in a pure spin system. Phase separation breaking the translational symmetry of a Hamiltonian on a local scale is particularly intriguing, as it regularly appears in chemically homogeneous systems and is related to some fundamental functional properties of materials, such as the colossal magnetoresistance of manganites, the giant electrostriction of relaxors, and possibly even high-T_c superconductivity. The conventional paradigm where electronic charge plays the leading role in promoting phase-separated states when competing phases are present in the solid state has been proven wrong in the case of α-$NaMnO_2$. Here, a novel kind of a phase-separated state was identified and suggested to be due to the interplay of geometrical frustration and a structural instability of the lattice, leading to a magnetostructural inhomogeneity at the nanoscale. The results were published in the paper A. Zorko ***et al***., "Frustration-induced nanometre-scale inhomogeneity in a triangular antiferromagnet", Nat. Commun. 5, 3222 (2014).

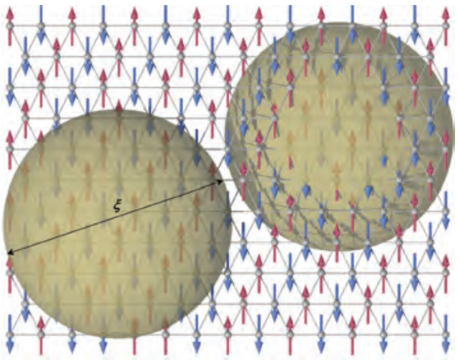

Figure 2: Illustration of the magnetostructurally inhomogeneous ground state of α-$NaMnO_2$, with the monoclinic antiferromagnetic phase being randomly disturbed by defect triclinic regions (spheres).

Andrej Zorko and collaborators investigated spin dynamics and disorder effects in a spin-liquid phase of the quantum antiferromagnetic known as the mineral kapellasite. The authors have found that despite a variety of magnetic environments due to a severe random depletion of the magnetic kagome lattice by 27%, the system remains homogeneous with a unique spin susceptibility at high temperatures. Moreover, in the low-temperature, correlated, spin-liquid regime, a broad distribution of spin-lattice NMR relaxation times was observed and ascribed to the presence of local low-energy modes. The findings were published in the paper E. Kermarrec ***et al***., "Spin dynamics and disorder effects in the $S = 1/2$ kagome Heisenberg spin-liquid phase of kapellasite", Phys. Rev. B. 90, 205103 (2014).

Martin Klanjšek was invited by the editors of the Physics journal to write a review paper about quantum criticality in spin systems. The journal publishes review papers about the works published in Phys. Rev. Lett. and Phys. Rev. X. In the paper, he generally described an interesting and topical phenomenon of quantum criticality (Figure 3), which leads to the most complicated currently known quantum states in nature. To understand them, it is worth studying the systems with a few degrees of freedom, like one-dimensional quantum spin systems. The paper describes a recent interesting NMR experiment on $CoNb_2O_6$, which is a realization of the transverse field Ising ferromagnet. This is the simplest quantum-mechanical many-body model featuring even the analytical predictions, fully confirmed by the experiment for the first time. The results are placed in the context of other recent works on quantum criticality, where the author also took part. The paper was published in M. Klanjšek, "A Critical Test of Quantum Criticality", Physics 7, 74 (2014).

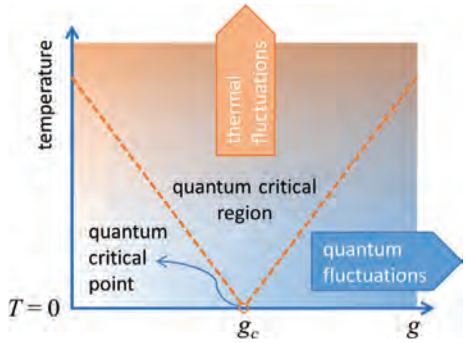

Figure 3: Quantum fluctuations controlled by the non-thermal parameter g lead to the phase transition at a critical value gc, the so-called quantum-critical point, already at zero temperature, T = 0. Their interplay with thermal fluctuations opens up a characteristic V-shaped quantum-critical region.

Diluted magnetic oxides

Andrej Zorko, Denis Arčon and collaborators addressed the pending question of the intrinsic/extrinsic nature of the Mn-induced magnetism of the wide-band-gap perovskite $SrTiO_3$. They showed that this diluted magnetic oxide remains paramagnetic down to low temperatures, in contrast to previous suggestions of intrinsic magnetic freezing. Moreover, using local-probe magnetic-characterization techniques of muon spin relaxation and electron spin resonance they demonstrated that that the dopants partially aggregate into nanosized clusters. Their findings were published in the paper A. Zorko ***et al***., "Intrinsic paramagnetism and aggregation of manganese dopants in $SrTiO_3$", Phys. Rev. B. 89, 094418 (2014).

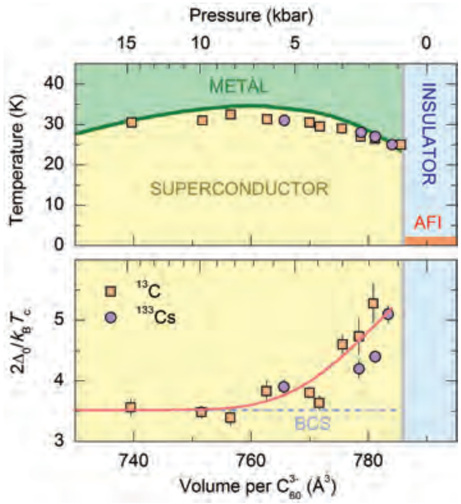

Figure 4: The low-temperature phase diagram and the superconducting gap of face-centred-cubic Cs_3C_{60} as derived from the NMR measurements in the superconducting state.

Unconventional molecular superconductors

Anton Potočnik, Peter Jeglič, Denis Arčon and collaborators from the UK, Estonia and Japan studied unconventional superconductivity in expanded fullerides and rare-earth carbides. First they reported a nuclear magnetic resonance (NMR) study of face-centred-cubic Cs_3C_{60}, which can be tuned continuously through the insulator-to-metal transition by pressure. For large inter-fullerene separations they observed a large non-BCS but s-wave gap in a superconductor, which upon further pressurization approaches the weak-coupling BCS value (Figure 4). These results indicate the importance of the electronic correlations for the pairing interaction and were published in the paper A. Potočnik ***et al***., "Size and symmetry of the superconducting gap in the f.c.c. Cs_3C_{60} polymorph close to the metal-Mott insulator boundary", Sci. Rep. 4, 4265 (2014).

In their second study they observed the freezing of the dynamic Jahn-Teller effect in the Mott insulating state of the metrically cubic but merohedrally disordered Cs_3C_{60} by low-temperature magic-angle spinning NMR. These results were published in the paper A. Potočnik ***et al***., "Jahn–Teller orbital glass state in the expanded fcc Cs_3C_{60} fulleride", Chem. Sci. 5, 3008 (2014). Finally, they investigated the rare-earth carbide, La_2C_3, which showed abnormal behaviour that dramatically deviated from the conventional s-wave superconductors. Such an unconventional response in the local static and dynamic spin susceptibilities was discussed in terms of a possible mixture of spin-singlet and spin-triplet Cooper pairs, which may be promoted by the asymmetric spin-orbit coupling in the system without the centre of inversion. Their findings were published in the paper A. Potočnik ***et al***., "Anomalous local spin susceptibilities in noncentrosymmetric La_2C_3 superconductor", Phys. Rev. B 90, 104507 (2014).

Cocrystals

Cocrystals are often used in crystal engineering. A cocrystal is a nonionic supramolecular complex that is constructed through several types of interaction, including hydrogen bonding and van der Waals forces. ^{14}N NQR represents a very sensitive tool for the study of crystal structure and intermolecular interactions in hydrogen bonded cocrystals. Cocrystals of 2,3,5,6-tetramethyl-pyrazine and several carboxylic acids have been studied with complete ^{14}N NQR. The ^{14}N nuclear quadrupole resonance spectra have been used to check whether the cocrystals are indeed formed and to investigate the hydrogen-bonding scheme of 2,3,5,6-tetramethylpyrazine molecules. Published in J. Seliger et al., J. Phys. Chem. B 118, 996–1002 (2014), J. Seliger, V. Žagar, Phys.Chem. Chem.Phys. 16, 18141-18147 (2014).

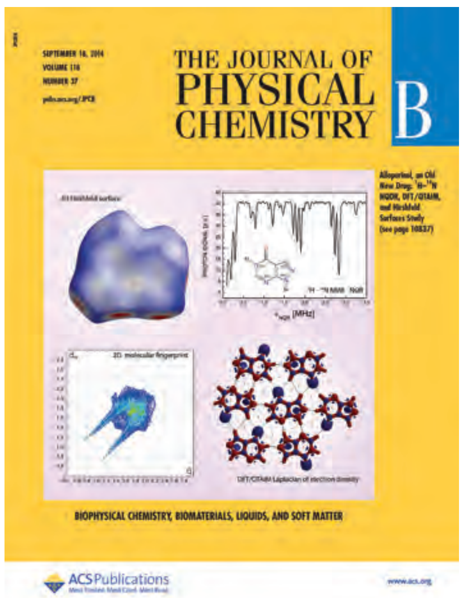

Figure 5: The figure from our paper J. N. Latosinska, et al., was selected for the cover of J. Phys. Chem. B.

Pharmaceutical substances

^{14}N NQR represents a useful tool to characterize pharmaceutical substances and the method of their preparation. In combination with a quantum chemical calculation the electron structure of these molecules and the properties of functional groups can be determined. ^{14}N nuclear quadrupole resonance (NQR) in two known polymorphs of famotidine was measured. At room temperature, seven quadrupolar sets of transition frequencies corresponding to seven different nitrogen sites in the crystal structure of each of the two polymorphs were found. The NQR frequencies, line shapes, and tentative assignation to all seven molecular ^{14}N atoms were obtained. Published in J. Lužnik, et al., J. Pharm. Sci. 103, 2704-2709 (2014). Allopurinol (1,5-dihydro-4H-pyrazolo [3,4-d]pyrimidin-4-one), is an active pharmaceutical ingredient of the drugs, applied for the treatment of gout and tumour lysis syndrome. It was recently discovered to have multifaceted therapeutic potential, and hypoxanthine, which is a naturally occurring purine, has been studied experimentally in the solid state by ^{1}H−^{14}N NMR-NQR double resonance by J. N. Latosinska, et al., J. Phys. Chem. B 118, 10837−10853 (2014). This study demonstrated the advantages of combining NQR, DFT/QTAIM, and Hirshfeld surface analysis to extract detailed information on electron density distribution and complex H-bonding networks in crystals of purinic type heterocycles, relevant in pharmacological processes. Figure 5 shows cover of J. Phys. Chem. B featuring a figure from our paper in this number.

Three anhydrous methylxanthines, i.e., caffeine, theophylline and theobromine, have been studied by the same group experimentally in solid state by ^{1}H−^{14}N NMR-NQR (nuclear magnetic resonance−nuclear quadrupole resonance) double resonance (NQDR). Published in J. N. Latosinska, et al., J. Chem. Inf. Model. 54, 2570−2584 (2014).

Liquid crystals

In a paper A. Gradišek et al., J. Phys. Chem. B 118, 5600−5607 (2014), a detailed study of the cross-relaxation effects between the ^{1}H and ^{2}H spin systems is presented in the nematic phase of a 5-cyanobiphenyl (5CB) liquid crystal, partially deuterated at α position (5CB-αd2). In the low-frequency domain, the spin−lattice relaxation rate (T_1^{-1}) dispersion clearly differs from that of the fully protonated 5CB homologue, as it shows two local maxima at distinct frequencies, T_1^{-1} presents two distinct local maxima and for low frequencies T_1^{-1} presents stronger frequency dependence when compared with what is observed for 5CB. The T_1^{-1} dispersion obtained for 5CB-αd2 for frequencies above 60 kHz was interpreted in terms of the relaxation mechanisms usually accepted to interpret the spin−lattice relaxation in nematic phases in general and 5CB in particular. For lower frequencies it was necessary to consider cross-relaxation contributions between the proton and deuterium reservoirs. The analysis of the quadrupolar relaxation independently confirms that the order director fluctuations are the dominant mechanism of proton relaxation in the low-frequency domain.

Counterfeit pharmaceuticals interception using nuclear quadrupole resonance

In cooperation with the EU project CONPHIRMER partners from King's College London, Franco-German Research Institute St. Louis, Institute of Mathematics, Physics and Mechanics, Post-graduate School of the J. Stefan Institute, Lund University, industrial partners, and end-users, we have developed a prototype of a medicines authentication device. A prototype portable N-14 nuclear quadrupole resonance based easy-to-use device was developed, which made it possible to distinguish an original and a forged drug. The advantage of the method is that during the scan medicines can remain in original, unopened package and can be later used as intended. The prototype of the device was successfully tested at the end user's location – at the post customs service at Warsaw airport.

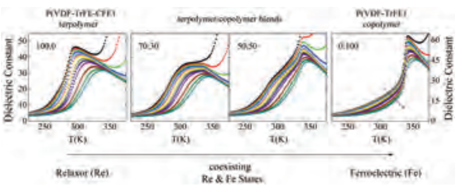

Figure 6: Blending a relaxor terpolymer with a ferroelectric copolymer resulted in a system with coexisting ferroelectric and relaxor states, thus our polymer-blend approach could be suggested as a model method for tailoring various properties of relaxor polymers.

Relaxor ferroelectrics

Investigations of electroactive polymers have so far mainly focused on either normal ferroelectric polymers or systems that are completely transformed into a relaxor. Only recently properties of the P(VDF-TrFE) copolymer, irradiated with low doses of high-energy electrons, have been reported. Clear evidence that ferroelectric and relaxor states coexist has been provided and it has furthermore been shown that such a coexistence strongly influences various material properties. Since irradiation also creates undesirable side effects, we have, in collaboration with researchers from Pennsylvania State University, developed a polymer system where a similar coexistence of states could be expected: blends of relaxor P(VDF-TrFE-CFE) terpolymer and ferroelectric P(VDF-TrFE) copolymer. We showed that blends entirely exhibit a relaxor dielectric response at a low copolymer content, while in samples with 20-50 wt. % of P(VDF-TrFE) the ferroelectric and relaxor states coexist. DSC data clearly revealed that both components form separate crystalline phases and also the influence of blending on the crystallinity and melting points of both components. Moreover, the relative crystallinity data, obtained from the normalized enthalpy changes at melting, excellently explain the variation of the dielectric constant in developed blends. Published in Casar et al., J. Appl. Phys. 115, 104101 (2014).

Liquid-crystalline elastomers

A new series of composite liquid-crystalline elastomers was developed, containing both nematogenic and smectogenic molecules. By varying the ratio of the two mesogen species, the width of the temperature interval of the nematic phase, intermediate between the high temperature isotropic and the low temperature smectic A phase, can be controlled. A temperature-concentration phase diagram of this system has been determined via DSC and X-ray diffraction, as well as independently via stress vs. strain measurements. These indicate a possible re-entrant nematic phase for higher values of the mechanical load. Moreover, a soft-elasticitylike behaviour has been detected at low temperatures for systems in the vicinity of the characteristic concentration of the nematogen, below which the nematic phase vanishes.

Published in Domenici et al., RSC Advances 4, 44056-44064 (2014).

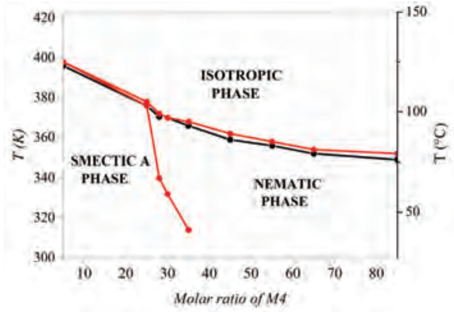

Figure 7: Phase diagram of a composite liquid single-crystal elastomer.

Nanomaterials

An ***in-situ*** doping approach was successfully employed for the synthesis of Mn^{2+}-doped sodium titanate nanoribbons, which were used as a precursor for the preparation of TiO_2 nanoribbons with a homogenous distribution of Mn^{2+} ions. The comprehensive structural characterization using powder X-ray diffraction and electron paramagnetic resonance provided evidence that the Mn^{2+} ion predominantly substitutes for the Ti^{4+} ion at octahedral coordination sites in a bulk. Measurements performed on individual nanoribbons using near-edge X-ray absorption fine structure spectromicroscopy revealed that the strong alkaline environment required for the formation of sodium titanate nanoribbons did not affect the manganese oxidation state. In the next two steps, the ion-exchange process in the HCl(aq) solution followed by a thermal treatment in air lead to the formation of Mn^{2+} doped TiO_2 nanoribbons. An analysis of the manganese content by X-ray photoelectron spectroscopy of several TiO_2 nanoribbon samples calcinated in the temperature range from 400 to 700 °C, and the analysis performed at the Ti $L_{2,3}$ and Mn $L_{2,3}$ edges with electron-energy-loss spectroscopy showed that calcination at elevated temperatures induced the diffusion of manganese ions towards the nanoribbons' surface. However, the transformation of anatase nanoribbons to rutile nanoparticles was also accompanied by the partial oxidation of Mn^{2+} to Mn^{3+} and Mn^{4+}. Published in Umek et al., J. Phys. Chem C, Nanomaterials and interfaces, 2014.

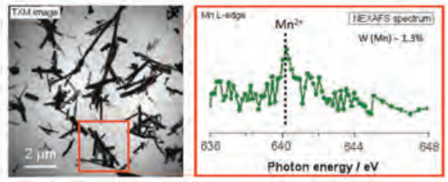

Figure 8: TEM image (left) and Mn L-edge NEXAFS spectrum (right) of Mn^{2+} doped TiO_2 nanoribbons. Spectrum was acquired in the area marked with red square in the TXM image.

Critical properties of nanostructured and electrocaloric materials

Using direct measurements and a simple Kittel model it was shown that the negative electrocaloric effect should be observed in anti-ferroelectric materials. We also calculated the E-T phase diagram for anti-ferroelectrics and corresponding electrocaloric response as a function of temperature and field. By calorimetric and optical experiments we showed that the TGB_A phase (see Figure 9), which is analogous to the Abrikosov lattice vortex state in superconductors, can be stabilized by functionalized nanoparticles added to a highly chiral liquid crystal. The above results have been published in 6 articles in international scientific journals and a chapter published in a book published by Springer. Recently, published works on electrocalorics and the stabilization of TGB and blue phases have been cited more than 100 times in 2014 alone.

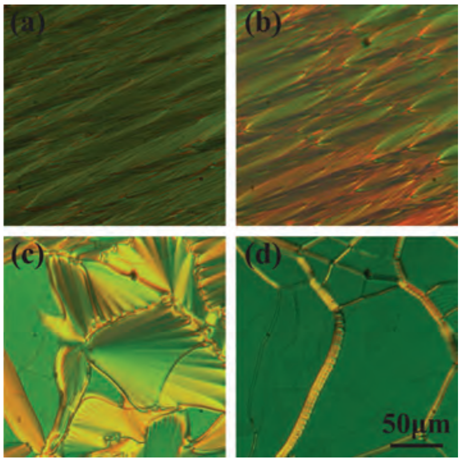

Figure 9: Texture of TGBA phase stabilized by nanoparticles (b). Other phases: smectic A (a), liquid vortex state (c) and the nematic phase (d).

II. Research programme "Physics of Soft Matter, Surfaces, and Nanostructures"

The investigations of the research program "Physics of Soft Matter, Surfaces, and Nanostructures" are focused on novel complex soft-matter systems and surfaces with specific functional properties. We investigated, in particular, liquid-crystalline elastomers and dendrimers as novel multifunctional materials, nematic colloids, molecular motors, soft-matter photonic crystals and novel synthetic or self-assembled micro- and nano-structures. The aim of the program is to understand the structural and dynamical properties of these systems, their interactions, their function at the molecular level, and self-assembly mechanisms in soft matter. The underlying idea is that it is possible to understand complex mechanisms, such as self-assembly, on a macroscopic level, using a simplified physical picture and models. In order to provide a comprehensive approach to the problem, the program combines both experimental and theoretical investigations, supported by modelling and simulations. Special emphasis is given to the possible electro-optic and medical applications.

We have investigated the topology and photonics of liquid-crystal colloids and dispersions, and studied the motion of molecular motors. Tribological properties of nanomaterials and their safety were investigated; the structure of matter has been studied on the atomic level and the infrastructure for cold-atom physics was set up.

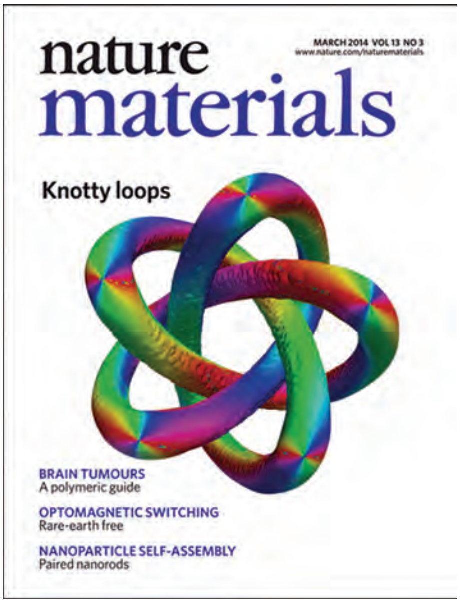

Figure 10: Front cover of a journal Nature Materials, showing a colloidal knot with a surface nematic director field in the case of degenerate planar anchoring. The cover picture was taken from A. Martinez, et al. Nature Mater. 13, 258-263 (2014).

Mutually tangled colloidal knots and induced nematic defect loops

Micron-size particles in nematic liquid crystals induce complex distortions including topological defects, leading to effective inter-particle forces and consequently to self-assembled structures. In collaboration with Smalyukhs's group at UCO Boulder we theoretically and experimentally demonstrated the effect of 'colloidal knots' on the nematic field (Martinez et al., Nature Materials 2014). The micron-scale knotted particles created using two-photon photo-polymerisation induce nematic distortions that were analyzed by three-photon excitation fluorescence polarizing microscopy. Experimental results and computer simulations uncover numerous structures, for example, a knotted particle that induces perpendicular alignment of the director at its surface can lead to a pair of topological defect lines with the same knotted configuration as the particle. We suggest that the interplay between the topologies of the knotted particles and the knotted nematic field may provide the clue to a new types of self-assembled materials.

Quasicrystalline tilings with nematic colloidal platelets

The inclusion of micron-sized facetted particles in liquid crystals opened up a rich new area of research. In collaboration with our former postdoc J. Dontabhaktuni we showed that in such a system the forces mediated by topological defects can form quasicrystalline structures (Dontabhaktuni et al. PNAS 2014). In a thin layer of an aligned nematic with the help of the Landau-de Gennes approach we found that surface defects in the nematic field can cause pentagonal platelets to join with their edges – which is different from stacking in an isotropic liquid, where edges can easily slide. This enables the formation of the Penrose tiling patterns. Interestingly, hierarchical structures can also be made where a given pentagonal platelet is substituted for a number of smaller ones of the same shape. We believe that this may be of interest for photonic metamaterials.

Free-standing knots in confined chiral nematic fluids

Knotted fields are an emerging research topic relevant to different areas of physics where topology plays a crucial role. The recent realization of knotted nematic disclinations stabilized by colloidal particles raised the challenge of free-standing knots. We demonstrated the creation of free-standing knotted and linked disclination loops in the cholesteric ordering fields, which are confined as spherical droplets with normal surface anchoring (Seč et al., Nature Comms. 2014). Our approach, using free-energy minimization and topological theory, leads to the stabilization of knots via the interplay of the geometric frustration and intrinsic chirality (Beller et al. Phys. Rev. X 2014). Selected configurations of the lowest complexity are characterized by knot or link types, disclination lengths, and self-linking numbers (Čopar, Phys. Rep. 2014). The droplets with knots could be controlled by optical beams and may be of use for photonic elements.

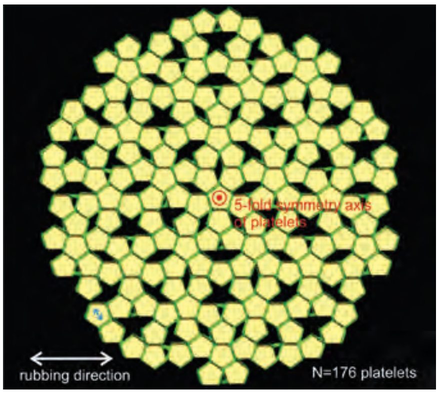

Figure 11: Colloidal quasicrystalline Penrose tiling assembled from 176 pentagonal particles in a nematic liquid crystal layer (J. Dontabhaktuni et al. PNAS 111, 2464 (2014)).

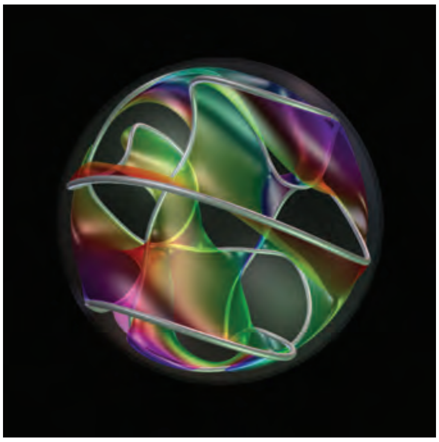

Figure 12: Homeotropic chiral nematic liquid-crystalline droplet with a single disclination loop exhibiting a trefoil knot. The Pontryagin - Thom surface where the directors are in the x-y plane is colored according to the local orientation of the director field (D. Seč, S. Čopar and S. Žumer, Topological zoo of free-standing knots in confined chiral nematic fluids, Nature Comms. 5, 3057 (2014)).

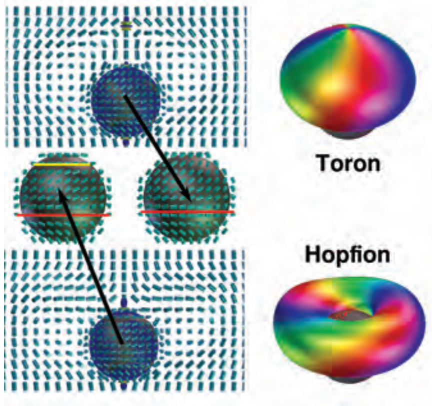

Figure 13: Soliton dressed colloidal particles in an untwisted thin cholesteric liquid crystalline layer. Toron and hopfion director fields appearing in the case of degenerate planar anchoring are visualized using cylindrical glyphs and Pontryagin-Thom surfaces (T. Porenta, S. Čopar, P. J. Ackerman, M. B. Pandey, M. C. M. Varney, I. I. Smalyukh and S. Žumer, Topological switching and orbiting dynamics of colloidal spheres dressed with chiral nematic solitons, Scientific Rep. 4, 7337 (2014)).

Colloidal spheres dressed with chiral nematic solitons

Metastable liquid-crystalline configurations formed by defects, inclusions, and elastic deformations in forms of topological solitons are promising choices for building photonic crystals and metamaterials for new optical applications. Local optical modification of the director or colloidal inclusions into a moderately chiral nematic liquid crystal confined to a homeotropic cell creates localized multi-stable chiral solitons. In collaboration with Smalyukhs's experimental group at UCO in Boulder we induced solitons that "dress" the dispersed spherical particles treated for tangential degenerate boundary conditions, and performed controlled switching of their state using focused optical beams (Porenta et al., Scientific Rep. 2014). Two optically switchable distinct metastable states, toron and hopfion, bound to colloidal spherical micro-particles into nematic superstructures with different topological charges were investigated. Their structures examined using Q-tensor based numerical simulations and topological theory were compared to the profiles reconstructed from the experiments.

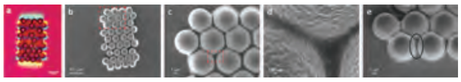

Figure 14: (a) Reflection-mode Optical microscopy images of a colloidal crystal of 5 μm silica particles embedded in a polymerized nematic matrix after the non-polymerized LC was washed out, imaged between crossed polarizers with a retardation plate added; (b-d) SEM images of the same assembly at different magnifications; (e) SEM image of the assembly tilted by 12°. The blue ellipse indicates the region where the topological defect is expected to be observed.

Nematic colloids and photonics

We continued our investigations of nematic colloids for photonic applications by studying the polymerization of colloidal crystals, assembled by laser tweezers in the nematic liquid crystal. After polymerization, the colloidal crystals preserve the structure very well (Figure 14), and they are stable at elevated temperatures as well. After the removal of the polymer, SEM investigations (Figure 14b-e) reveal remnants of a polymer network, attached to the silica colloidal particles. Photo-polymerizable liquid crystals show an excellent potential for assembling the robust photonic superstructures for applications in photonics. Published in Mirri et al., Stabilisation of 2D colloidal assemblies by polymerisation of liquid crystalline matrices for photonic applications, Soft Matter 10, 5797 (2014). Ideas and concept of a new field of soft-matter photonics were presented in an invited article in Liquid Crystals, by I. Muševič (Integrated and topological liquid crystal photonics, Liquid Crystals 41, 418 (2014).

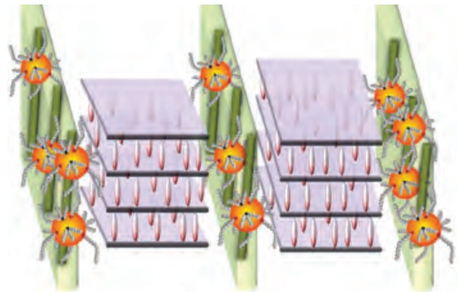

Figure 15: A simple schematic illustration of nanoparticles trapped to screw dislocations.

Interaction between nanoparticles and topological defects

We studied the nanoparticle-driven stabilization of Twist Grain Boundary A phase. By means of high-resolution ac calorimetry and polarizing optical microscopy we have demonstrated that surface-functionalized spherical CdSSe nanoparticles induce a twist-grain boundary phase when dispersed in a chiral liquid crystal (Figure 15). These nanoparticles can effectively stabilize the one-dimensional lattice of the screw dislocations, thus establishing the twist-grain boundary order between the cholesteric and the smectic-A phases. Moreover, a theoretical model that accounts for the trapping of nanoparticles in the defect cores was presented. In particular, we have shown that in addition to the Defect Core Replacement mechanism, also the saddle splay elasticity plays an important role (M. Trček et al., Phys. Rev. E 90, 032501 (2014)).

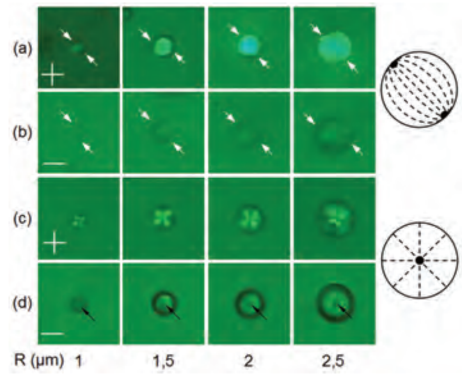

Figure 16: Microscopic images of liquid-crystal droplets in the absence of phospholipids and irradiation (a,b), in the presence of phospholipids (c,d), after 1 minute of irradiation in the absence of phospholipids (e,f).

Combined nanoparticle and UV-irradiation-driven nematic structural transitions

We studied experimentally and theoretically UV-irradiation and phospholipid stimulated bipolar-radial structural transitions of azoxybenzene nematic liquid crystals (NLCs) droplets dispersed in water (Figure 16). It was found that the UV-irradiation that triggered the trans-cis isomerisation of the LC molecules induced a structural transition to a radial configuration at the critical time t_c. In particular, we demonstrated that the critical UV-irradiation time t_c needed for the transition could, under appropriate conditions, sensitively depend on the concentration of phospholipid molecules. This demonstrated a proof-of-principle mechanism could be exploited for the development of sensitive detectors for specific nanoparticles (NPs), where value of t_c fingerprints concentration of NPs (V. Dubtsov et al., Appl. Phys. Lett. 105, 151606 (2014)).

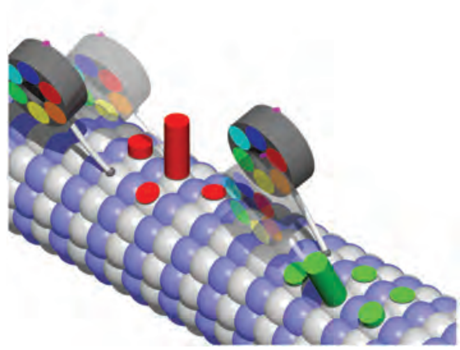

Figure 17: A model molecule of cytoplasmic dynein taking a step with its left or right head.

Molecular motors

We set a mechano-chemical model for the stepping dynamics of cytoplasmic dynein. The results of our elasto-mechanical description of a simplified model object, which mimics the basic properties of this complex molecule, show that such a dimeric molecule can synchronize the ATP hydrolysis cycles of its two heads to produce efficient processive coordinated stepping. The degree of synchronization of the two cycles is tuned by the strength of the coupling between the two heads of the dimer. With weaker coupling the heads lose synchrony and move in an uncoordinated manner with a much broader distribution of steps (Figure 17). In this case the high processivity is retained at the cost of a reduced velocity. These two scenarios seem to be realized in nature: the coordinated stepping for mammalian dyneins and the uncoordinated for dyneins of lower eucaryotes. We showed that the maximum force the loaded motor can withstand is largely limited by motor's processivity (A. Šarlah and A. Vilfan, Biophyisical Journal 2014).

Non-processive molecular motors, such as muscle myosin, can only generate movement when coupled together in larger ensembles. Their ensemble velocity as a function of load has been the subject of many previous studies, but little was known about its dependence on the fuel ATP concentration. We showed that a model with several mechanical states can exhibit non-trivial dependencies that can reveal the sequence of conformational changes in a motor›s cycle. The model also predicts the possibility of velocity reversal depending on the ATP concentration (A. Vilfan, Interface focus 2014). In addition, we contributed to the discussion about the origin of directional motion in myosin-V motors (A. Vilfan, PNAS 2014).

Low-friction nanomaterials

In the paper "The formation of tribofilms of MoS_2 nanotubes on steel and DLC-coated surfaces" (M. Kalin et al. ***Tribology Letters***, 55, 381-391 (2014)) we reported that the addition of the MoS_2 nanotubes to the oil can significantly reduce the coefficient of friction for the steel (up to 65 %) and the DLC-coated (up to 40 %) surfaces, in particular for the boundary-lubrication regime. The major difference between the steel and the DLC contacts is the extent to which the MoS_2-based tribofilm covers the surface, which is 20 % in the case of the DLC/DLC contacts, but almost 40 % in the case of the steel/steel contacts. We found that the chemical and functional properties of the MoS_2-based tribofilm are very similar, or even the same, for both the steel and DLC-coated surfaces.

Nanosafety

In the paper "Sparklers as a nanohazard: size distribution measurements of the nanoparticles released from sparklers" (M. Remškar et al., Air Quality, Atmosphere & Health (2014)), we reported on the high concentrations of nanoparticles released during the indoor combustion of sparklers. Large proportions of the metals making up the sparking material are released into the atmosphere. The sparklers, which consisted of $Ba(NO_3)_2$, elemental Fe, and elemental Al, burned to produce $BaAl_2O_4$, $BaAl_2O_6$, and $BaFe_2O_4$ and emitted nanoparticles that contained Ba, Fe, Al, Na, K, C, and O. The combustion of a single sparkler increased the concentration of nanoparticles in a cubic centimetre of air by at least 150 times, to $350,000/cm^3$. More than 10 % of the metals from the sparklers were released into the local atmosphere. The majority of these released particles were around 100 nm in size, but a substantial amount of them were found to be smaller than 20 nm in diameter (Figure 18). The closest position of the inlet to the sparkler (simulating a child's position) is the most hazardous because of the lowest degree of agglomeration of the nanoparticles. The nanoparticles remained in the atmosphere for several hours. Due to the small size and the chemical composition of the released NPs, and according to the published data on health hazards resulting from their inhalation, the use of sparklers as a children's entertainment should be reconsidered.

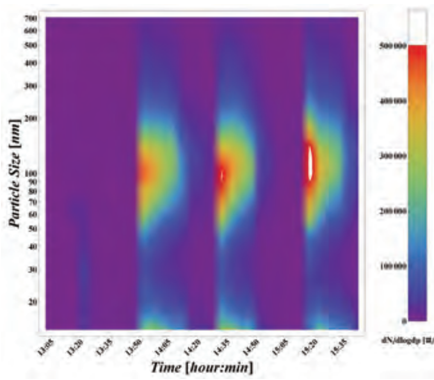

Figure 18: Nanoparticle pollution generated by a sparkler (a toy firework that emits little sparks).

In collaboration with Chemical Office of Republic Slovenia we have built the website Nanoportal (http://www.uk.gov.si/, M. Remškar, U. Lavrenčič Štangar, D. Drobne, M. Pavlin) that represents the contact point for public interesting in nanotechnology and nanosafety. Besides basic information on specific properties of nanomaterials and monitoring tools, a list of researchers specialized on a particular nanomaterial is presented with the aim to strengthen the transfer of knowledge. We performed the monitoring of the pollution of air with nanoparticles in several industrial companies and at public sites using a professional particle sizer that enables a size distribution measurement.

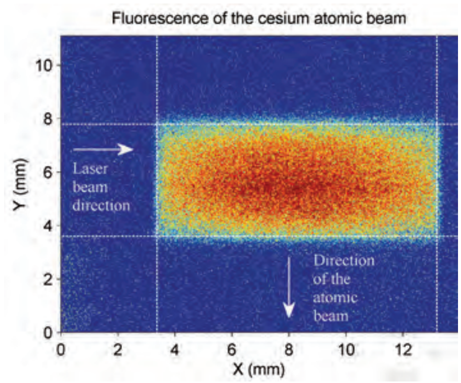

Figure 19: Fluorescence from a beam of Cs atoms in the main chamber of UHV apparatus for cold atoms

Ultra-cold atoms

The first experiments on detecting and characterizing a beam of Cs atoms in ultra-high vacuum apparatus for cold atoms were performed. Using a high-power diode laser locked to selected Cs atomic transition using a modulation transfer spectroscopy we observed fluorescence from the atomic beam in the main experimental chamber (Figure 19). Magnetic fields are being set up, which are needed to slow down and capture a large number of these atoms.

III. Research programme Experimental biophysics of complex systems

In the program "**Experimental biophysics of complex systems**", the processes and structures of various complex biological systems are investigated, ranging from model systems to the structures in living cells, tissues

Our studies have shown that the molecular motional correlation can be estimated directly from the temperature dependence of the local conformational entropy, which can then be used to determine the correct conformational entropy of the entire molecule. We have developed a method of NMR imaging that allows imaging of an electric field during electroporation in vivo. Data about the electric field are crucial for monitoring treatment with electroporation.

and small animals. Investigations also comprise the studies of the impact of numerous bioactive substances such as are toxins and drugs as well as a variety of materials from materials to medical materials on such biological systems. The research is recently focused on the better understanding of the structure of membrane compartments, domains, proteins, glyco-saccharides clusters, molecular structures of polymer gels, etc. and their interaction, accompanying the interaction of cell structures with new materials that enter into their natural environment. New spectroscopic and micro-spectroscopic techniques contribute to the better understanding of the organization of these supramolecular systems, complex cellular and tissue responses and open up new possibilities for the design of medical materials, especially for tissue regeneration, which is one of the main health issues among the aging population of the developed world. In addition, the research field is also directed to the optimization methods for the treatment of tumours, magnetic resonance imaging and the mathematical modelling of thrombolysis, the use of high-resolution magnetic resonance imaging to study materials. This method allows us to study different problems in forestry, wood industry, and food safety. We expect a lot from the development of new methods for measuring diffusion in porous materials, with which we will be able to tell a lot about the microscopic structure of porous materials.

The **cell-material interaction studies**, especially from the viewpoint of bioactivity and biocompatibility, are undoubtedly one of the hottest biophysics research topics. By new micro-spectroscopies we efficiently address the problem of nanoparticles and nanofibres uptake into the cell or the model membrane. Uptake into and through the membrane was proven by the FMS-FRET-experiments acquired on model membranes. We also explored the effect of the properties of nanoparticles such as their size and their surface properties on the interaction of the nanoparticles with biological systems. As a result, some methods to control the size of and surface properties of the nanoparticles have also been undertaken.

Through the studies of the **conformational entropy** of the spin labels incorporated into lipid membranes, significant progress in the development of experimental methods for studying the interaction of nanoparticles with biological systems was shown. Conformational entropy is otherwise a method that has long been used for the theoretical identification of the dynamics of proteins, DNA and other polymers, but its accurate experimental determination has been hampered due to the correlated molecular dynamics. We have shown that the correlated molecular dynamics can be estimated directly from the temperature dependence of local conformational entropy, which can then be used to determine the correct conformational entropy of the entire molecule. The work was published in a journal with the impact factor of 6.7 (J. Phys. Chem. Lett., 2014, 5 (20), pp 3593-3600). This method can be useful in a number of experimental techniques and thus provides an additional insight into the physical properties of various biomolecules.

Fluorescence microspectroscopy is the experimental method by which the fluorescent spectra of each microscopic sample volume element are acquired, revealing the physical properties of the surrounding environment on a molecular scale. Implementation of this method to the nanoparticle uptake problem allows us to analyse the rate and the mechanism of the titanate nanotubes transition into giant liposomes. Special approaches that employ the fluorescence resonance energy transfer concept and the fluorescent labelling of both the nanoparticles and the membranes revealed the accumulation of the nanoparticles onto the model biological membranes. The same method was also used in the study of **interaction between cells and macro-structured polymeric scaffolds** as potential tissue engineering materials, by which morphological properties of the latter and cell ingrowth with its morphology were measured through fluorescent detection. Cell ingrowth was compared and correlated with the molecular and macroscopic properties of the scaffolds, which was done by the analysis of molecular dynamics of polymers by **spin labeling EPR spectroscopy** and rheology. The study was published in a journal with an impact factor 5.9 (ACS Appl. Mater. Interfaces, 2014 6 (18), pp 15980-15990). Further interactions between cell and biomaterials have been studied through the analysis of the dynamics and strength of cell adhesion to these tissue-engineering scaffolds by using a system of **optical tweezers** (sent for publication). Fluorescence microspectroscopy was also applied to **present the effect of antimicrobial technology NANO4AB** developed in our laboratory (Figure 20) to identify bacteria and nanomaterials with an optical set-up that allows us to distinguish them despite the fact that these objects are close to or below the resolution of the microscopy.

Since the properties of **nanoparticles** play an important role in the interaction with biological systems, we started a collaboration with the laboratory of Nobel Prize winner Oliver Smithies from the University of North Carolina and developed two methods for the synthesis of gold nanoparticles with the controlled size from 3 nm to 30 nm and with an optionally functionalized surface. This work was published in the journal Langmuir with an impact factor of 4.4 (Langmuir 11;30(44):13394-404). Based on this work, we were invited to prepare a paper for the journal, Journal of Visualized Experiments (JoVE).

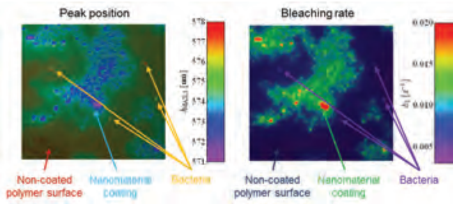

Figure 20: Fluorescent microspectroscopy was used to demonstrate the anti-microbial properties of our technology NANO4AB and the identification of bacteria and nanomaterials using an optical set-up. The image on the left is coding the peak of the emission spectra; the image on the right is coding the speed of the bleaching of fluorophore. One can clearly resolve the nanomaterial and bacteria.

Our results indicate that the formation of lipid corona is possible, where the nanoparticle is wrapped by a lipid membrane. We hypothesize that such lipid-wrapped nanoparticles may resemble lipid vesicles derived from platelets, usually known as "microparticles". An important characteristic of microparticles is that a key reaction of **blood coagulation** takes place on them, the **activation of factor Xa**. Microparticles are membranous vesicles in blood derived from activated platelets or other cells containing the phospholipids of the parent membranes. Microparticles are detectable in normal human blood and are increased in patients with coagulation abnormalities. We therefore studied the activity of an enzyme factor Xa and found that the regulation of the activity of Factor Xa depends critically on the concentration of calcium in the plasma and that this process is likely to be physiologically important in the initial stage of blood clotting. This work was published in the Biochemical Journal with impact factor of 4.7 (Biochem. J. (2014) 462, 591-601) in collaboration with another group of researchers from the University of North Carolina. We also showed that a similar process occurs on activated platelets, which further confirms the physiological role of factor Xa activity on lipid membranes (accepted for publication in the Biochemical Journal).

We also focused on the problem of **diffusion in one- and two-dimensional cases** efficiently tackled by Adaptive Bias Force Molecular dynamics and created a generally applicable software package for determining multidimensional position-dependent diffusion coefficients (J. Chem Phys 140, no. 8, 084109; github.com/lbf-ijs/DiffusiveDynamics). With the obtained diffusion surface and a known free-energy surface, diffusive trajectories can be generated. Using this approach the time scale of molecular dynamics, typically a few 100 nanoseconds, can be extended to several 100 microseconds (for the 1D or 2D subspace of interest). By this approach, we studied the side-chain motion of spin labelled a-helices in the membrane and improved the description of the lipid effect within the side-chain conformational space modelling of proteins (CSM) which drastically reduces the computational time needed for determining the size of the side-chain conformational space. This allowed us to apply the improved CSM method on the **structure characterization of the anti-microbial peptide β-defensin** in water and in SDS-micelles. By comparing experimental side-chain conformational spaces, obtained from EPR spectra and calculated side-chain conformational spaces using the improved CSM method, we were able to determine the insertion of the peptide into the membrane and estimate the local diffusion of the spin-labelled side chain at each mutant position.

In the field of the design and the **synthesis of labels** (nitroxide, fluorophore and combined nitroxide-fluorophore), the research was focused on the environmentally sensitive fluorophores, especially on the surrounding polarity and hydration. We were able to synthesize a small series of fluorophores based on 7-(diethylamino)coumarin, where the batochrome shift in both the excitation and emission spectrum was achieved due to rational planning of the synthesized fluorophores. Fluorescent spectra measured in different solvents showed very large to moderate sensitivity of different fluorophores to the surrounding polarity, while all showed high photostability. These finding were published in Tetrahedron Letters journal (Tetrahedron Letters (2014), 55 (44), 6044-47). To investigate the differences in polarity within the membrane associated with different membrane processes, new membrane probes are designed based on the synthesized environmentally sensitive fluorophores. We furthermore continued the synthesis and evaluation of rhodamine-type pH-sensitive fluorescent labels for the identification of pH-change in the environment, more specifically for the study of cell organelles with lower pH values.

We developed **a MR imaging method** enabling the imaging of an electric field during electroporation ***in vivo***. The information on the electric field is essential **for monitoring of electroporation treatment** (Figure 21). Plasmin is a direct-acting thrombolytic agent with a favourable safety profile upon intra-arterial delivery in pre-clinical and phase I studies. However, the **thrombolytic efficacy of plasmin**, relative to that of rt-PA, remains to be established. We conducted a study in which the differences in thrombolysis between clots exposed to equimolar concentrations of plasmin and rt-PA after partial vessel recanalization were tested in a model system. Model blood clots were prepared in glass chambers enabling direct observation by dynamic optical microscopy. The incubation of clots with plasmin or rt-PA, allowing for the initial biochemical clot degradation, was followed by "flushing" the clots with a tangentially directed plasma flow devoid of a thrombolytic agent, mimicking blood flow after partial vessel recanalization. The acquired images were analysed for non-dissolved blood clot area as a function of time. With both thrombolytic agents, the relative clot area decreased rapidly in the first 30 s after the initiation of perfusion due to "flushing" the degraded clot fragments. In the following minutes the clot size showed a linear time dependence: after incubation with plasmin the clot size did not change substantially any more, while after incubation with rt-PA the clot size continually decreased. The slopes of the regression lines differed significantly. The thrombolytic action of the plasmin was terminated rapidly by contact with flowing blood plasma, while the thrombolytic action of rt-PA was prolonged. The findings of this study were published in the journal Thrombosis Research.

Magnetic resonance imaging allows monitoring of the distribution of electric current density in the conductive samples. By using current images in several different arrangements of electrodes, it is possible to determine the **electrical conductivity of the sample** and consequently also the electric field for a given electrode arrangement. This is of paramount importance **in electroporation**, which is a method in which by the use of high voltage the cell membrane is a tissue that is made temporary permeable and therefore absorbs more drugs than normally, as for example anti-cancer drugs. In this area, we worked with a group of prof. Damian Miklavčič from the Faculty of Electrical Engineering. Within this collaboration, we conducted a number of important ***in vivo*** MRI experiments of current distribution during electroporation and were able to determine the presence and extent of the region of reversible electroporation ***in vivo***. In the electroporated region, the tissue cells open for a short time and the anticancer drug can enter the cells and stays there since the cells close again. Cancer cells in this process die, while most of healthy cells should survive. In our experiments, instead of the anticancer drug a MRI contrast agent was injected into experimental animals. In the region of reversible electroporation the contrast agent remained in the tissue also after several days, while it was not present at that time in other tissues that were not reversibly electroporated. Thus, we were able to detect the region of reversible electroporation and also to compare its extent with predations for the region that were done based on calculations of the electric field strength on the basis of the measured current density distribution. We published the findings of this study in the distinguished journal Radiology.

Our collaboration with the group of Prof. Eung Je Woo from Kyung Hee University in Korea led to some interesting results in the field of advanced methods for **MR imaging of electrical conductivity**. Among other results we also developed a new imaging method that allows simultaneous tissue conductivity mapping at the radiofrequency (RF) range and at near zero frequency (DC) range. The method was tested on test samples as well as on experimental dogs. The result of the study are published in IEEE transactions on medical imaging.

In the journal Angewandte Chemie International Edition an article entitled "Selective Targeting of Tumor and Stromal Cells By a Nanocarrier System Displaying Lipidated cathepsin B inhibitor" was published in collaboration with department B1. A novel system for targeted drug delivery to tumours (LNC-NS-629) was developed. The system consists of nanoliposoms with incorporated lipidated CtsB specific inhibitor allowing targeting of cathepsin B (CtsB), a cysteine proteinase that is specifically up-regulated in cancers and translocated from its intracellular lysosomal locations to the cell surface and/or secreted into the extracellular milieu by tumour and tumour-associated stromal cells. The basis of the system are nanoliposoms, inside which there is enough space for small and large molecules, i.e., for the encapsulation of a drug or a diagnostic agent, such as a contrast agent for magnetic resonance imaging (MRI). In the paper T1-weighted MRI imaging ***in vivo*** was used to demonstrate the efficiency of the LNC-NS-629 system containing Magnetvist (T1 MRI contrast agent) targeting to the tumour microenvironment. The MRI images showed significant enhancement of contrast at the tumour site only 1 hour post-administration of the system. After 24 hours, the increased signal in the area of the tumour was still observed, reflecting the slower elimination of the LNC-NS-629 system with Magnevist than in the case of Magnevist alone. The system has been tested on healthy animals, where no accumulation of LNC-NS-629 was observed on the MRI images, indicating the rapid elimination of the LNC-NS-629 system from a healthy organism. It was shown that the new system has the potential to increase the efficacy of cancer diagnosis and treatment.

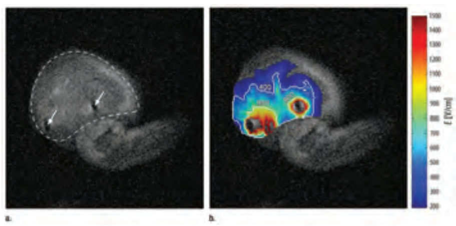

Figure 21: MR EIT images demonstrate electric field distribution in a mouse tumour during electroporation. (a) The tumour t1 (marked with a dashed white line) is situated on an animal leg in this T1-weighted image, acquired in the section perpendicular to the electrodes. Locations of the two inserted electrodes are marked with arrows. (b) The electric field distribution in the tumour, obtained with MR EIT, was superimposed onto the T1-weighted image acquired before the application of electric pulses. A white contour line encloses an area exposed to an electric field strength between reversible (400 V/cm) and irreversible (900 V/cm) electroporation threshold values. Tumour cells located outside the area are either irreversibly electroporated (the area close to the electrodes) or remain unelectroporated (the area toward the tumour boundary).

Our research has been supported by a number of international projects financed by the European Union within the 6th and 7th Frameworks. It was also supported within the bilateral Slovenian–USA, Slovenian–German and Slovenian–Greek and other scientific cooperations. In 2014, the department had cooperations with 108 partners from Slovenia and abroad. Among them:

- The high magnetic field centres in Grenoble, France, and Nijmegen, The Netherlands
- The high magnetic field centre at the University Florida, Tallahassee, Florida, USA
- The ETH, Zürich, Switzerland
- The Ioffe Institute in St. Petersburg, Russia
- The University of Duisburg, the University of Mainz and the University of Saarbrucken in Germany
- The University of California, the University of Utah and the Liquid Crystal Institute, Kent, Ohio, USA,
- National Institute for Research in Inorganic Materials, Tsukuba, Japan
- NCSR Demokritos, Greece
- Institut für Biophysik und Nanosystemforschung OAW, Graz, Austria
- Bioénergétique et Ingénierie des Protéines, CNRS Marseille, France
- Architecture et Fonction des Macromolécules Biologiques, CNRS Marseille, France
- The Max Delbruck Center for Molecular medicine in Berlin
- The Dartmouth Medical School, Hanover, NH, USA

- The Mayo Clinic, Rochester, USA
- Kyung Hee University, Suwon, Korea
- Technische Universität Ilmenau, Ilmenau, Germany
- Elettra Sincrotrone Trieste, Trieste, Italy
- University if North Carolina at Chapel Hill
- Max-Delbrück-Centrum für Molekulare Medizin (MDC)

made the above studies possible.

Some outstanding publications in 2014

1. Zorko, A., Adamopoulos, O., Komelj, M., Arčon, D., Lappas, A.. Frustration-induced nanometre-scale inhomogeneity in a triangular antiferromagnet. Nature Comms 5, 3222 (2014).
2. Koželj, P., Vrtnik, S., Jelen, A., Jazbec, S., Jagličić, Z., Maiti, S., Feuerbacher, M., Steurer, W., Dolinšek, J.: Phys. Rev. Lett. 113, 107001 (2014).
3. Pirc, R., Rožič, B., Koruza, J., Malič, B., Kutnjak, Z.: Negative electrocaloric effect in antiferroelectric $PbZrO_3$. Europhysics Letters 107, 17002-1-5(2014).
4. Martinez, A., Ravnik, M., Lucero, B., Visvanathan, R., Žumer, S., Smalyukh, I. I.: Mutually tangled colloidal knots and induced defect loops in nematic fields, Nature Mater. 13, 258-263 (2014).
5. Seč, D., Čopar, S., Žumer, S.: Topological zoo of free-standing knots in confined chiral nematic fluids, Nature Comms. 5, 3057 (2014).
6. Dontabhaktuni, J., Ravnik, M., Žumer, S.: Quasicrystalline tilings with nematic colloidal platelets, Proceedings of the National Academy of Sciences of the United States of America 111, 2464 (2014).
7. Čopar, S.: Topology and geometry of nematic braids, Phys. Rep. 538, 1-37 (2014).
8. Vilfan, A.: Myosin directionality results from coupling between ATP hydrolysis, lever motion, and actin binding. Proceedings of the National Academy of Sciences of the United States of America 111, E2076 (2014).
9. Urbančič, I., Ljubetič, A., Štrancar, J.: Resolving Internal Motional Correlations to Complete the Conformational Entropy Meter. J. Phys. Chem. Lett. 5, 3593–3600 (2014).
10. Podlipec, R. et al.: Molecular Mobility of Scaffolds' Biopolymers Influences Cell Growth. ACS Appl. Mater. Interfaces 6, 15980–15990 (2014).
11. Mikhaylov, G. et al.: Selective targeting of tumor and stromal cells by a nanocarrier system displaying lipidated cathepsin B inhibitor. Angew. Chem. Int. Ed Engl. 53, 10077–10081 (2014).

Some outstanding publications in 2013

1. Vallejos, S., Umek, P., Stoycheva, T., Annanouch, F., Llobert, E., Correig, X., de Marco, P., Bittencourt, C., Blackman, C.: Single-step deposition of Au- and Pt-nanoparticle-functionalized tungsten oxide nanoneedles synthesized via aerosol-assisted CVD, and used for fabrication of selective gas microsensor arrays. Advanced Functional Materials 23, 1313-1322(2013).
2. Gradišek, A., Bomholdtravnsbaek, D., Vrtnik, S., Kocjan, A., Lužnik, J., Apih, T., Jensen, T., Skripov, A. V., Dolinšek, J.: NMR study of molecular dynamics in complex metal borohydride $LiZn_2 BH_{45}$. Journal Phys. Chem. C 117, 21139-21147(2013).
3. Pregelj, M., Zorko, A., Zaharko, O., Jeglič, P., Kutnjak, Z., Jagličič, Z., Jazbec, S., Luetkens, H., Hillier, A. D., Berger, H., Arčon, D.: Multiferroicity in the geometrically frustrated $FeTe_2 O_5Cl$. Phys. Rev. B 88, 224421-1- 10(2013).
4. Nych, A., Ognysta, U., Škarabot, M., Ravnik, M., Žumer, S., Muševič, I.: Assembly and control of 3D nematic dipolar colloidal crystals. Nature Communications 4, 1489-1-8 (2013) doi: 10.1038/ncomms2486. 2013,
5. Jampani, V. S. R., Škarabot, M., Čopar, S., Žumer, S., Muševič, I.: Chirality screening and metastable states in chiral nematic colloids. Phys. Rev. Lett.110, 177801-1-5(2013).
6. Novak, S., Drobne, D., Vaccari, L., Kiskinova, M. P., Ferraris, P., Birarda, G., Remškar, M., Hočevar, M.: Effect of ingested tungsten oxide (WO_X) nanofibers on digestive gland tissue of Porcellio scaber (Isopoda, Crustacea) : fourier transform infrared (FTIR) imaging. Env. Sci. & Tech. 47, 11284-11292(2013).
7. Bajd, F., Serša, I.: Mathematical modeling of blood clot fragmentation during flow-mediated thrombolysis. Bioph. Journal 104, 1181-1190(2013).
8. Urbančič, I., Ljubetič, A., Arsov, Z., Štrancar, J.: Coexistence of probe conformations in lipid phases : a polarized fluorescence microspectroscopy study. Bioph. Journal 105 919-927(2013).

Awards and appointments

1. Simon Čopar: Jožef Stefan Golden Emblem Prize
2. Simon Čopar: Glenn Brown Prize, International Liquid Crystal Society
3. Slobodan Žumer: Honoured member of the International Liquid Crystal Society, International Liquid Crystal Society

Organization of conferences, congresses and meetings

1. Alpine NMW Workshop, Bled Slovenia, 18-21 September 2014
2. Midterm Review Meeting, JSI, Ljubljana, Slovenia,10-11 April 2014

INTERNATIONAL PROJECTS

1. MERCK - AFM Investigations
   Asst. Prof. Miha Škarabot
   Merck KGaA
2. Development of Curved LCD Shutter
   Prof. Igor Muševič
   Kimberly-Clark
3. 7FP - LEMSUPER; Light Element Molecular Superconductivity: An Interdisciplinary Approach
   Prof. Denis Arčon
   European Commission
4. 7FP - ESNSTM; Electron Spin Noise Scanning Tunneling Microscopy
   Prof. Janez Dolinšek
   European Commission
5. 7FP - NanoMag; Magnetic Nanoparticles and Thin Films for Spintronic Applications and High Performance Permanent Magnets
   Prof. Janez Dolinšek
   European Commission
6. 7FP - NEMCODE; Controlled Assembly and Stabilisation of Functionalised Colloids in Nematic Liquid Crystals
   Prof. Igor Muševič
   European Commission
7. 7FP - LIVINGLASER; A Laser Made Entirely of Living Cells and Materials Derived from Living Organisms
   Prof. Igor Muševič
   European Commission
8. 7 FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability
   Prof. Maja Remškar
   European Commission
9. 7FP - SIMDALEE2; Sources, Interaction with Matter Detection and Analysis of Low Energy Electrons 2
   Prof. Maja Remškar
   European Commission
10. COST MP1003; ESNAM - European Scientific Network for Artificial Muscles
    Prof. Boštjan Zalar
    COST Office
11. COST MP1201; Rational Design of Hybrid Organic-Inorganic Interfaces: The Next Step Towards Advanced Functional Materials
    Dr. Polona Umek
    COST Office
12. Exotic Electronic Properties arising from Geometrical Symmetry
    Prof. Denis Arčon
    Slovenian Research Agency
13. Elastically Tuned Soft Nanocomposites
    Prof. Samo Kralj
    Slovenian Research Agency
14. Liquid Crystals Blue Phases in Confined Geometries: Structure, Optical Properties and Photonic Applications
    Prof. Igor Muševič
    Slovenian Research Agency
15. Novel Polymeric and Ionomeric Materials with Giant Dielectric and Electrocaloric Response
    Asst. Prof. Vid Bobnar
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16. Physiological Role of Factor Xa and Protein S in Coagulation and Inflammation
    Dr. Tilen Koklič
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17. Key Role of Magnetic Anisotropy in Low-dimensional Spin Systems
    Dr. Andrej Zorko
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18. Hybrid Solar Cell Based on Conducting Polymers and 1D Nanostructured TiO2
    Dr. Polona Umek
    Slovenian Research Agency
19. Solar Cell Application of Rf Rotating Plasma Modified Inorganic Nanotubes
    Prof. Maja Remškar
    Slovenian Research Agency
20. Low Dimensional Structures of Metal Sulfides and Selenides for Use in Transistor Electronics
    Prof. Maja Remškar
    Slovenian Research Agency
21. Local Studies of Frustrated Quantum Antiferromagnets
    Dr. Andrej Zorko
    Slovenian Research Agency
22. Crystal and Electronic Structure of Quasi One-dimensional Transition-metal Chalcogenides
    Dr. Erik Zupanič
    Slovenian Research Agency

RESEARCH PROGRAMS

1. Experimental Biophysics of Complex Systems
   Prof. Igor Serša
2. Physics of Soft Matter, Surfaces, and Nanostructures
   Prof. Slobodan Žumer
3. Magnetic Resonance and Dielectric Spectroscopy of "Smart" New Materials
   Prof. Janez Dolinšek

R & D GRANTS AND CONTRACTS

1. Optical Microresonators based on Liquid Crystals
   Prof. Igor Muševič
2. New Metallic Materials for Thermal Storage of Digital Information
   Prof. Janez Dolinšek
3. Design, Formulation and Characterization of Biomimetic Nanocomposite Systems for Effective Tissue Regeneration
   Dr. Mojca Urška Mikac
4. Theory of the Nematic Nanodroplet and Ordering of DNA, Encapsidated in Simple Viruses
   Asst. Prof. Andrej Vilfan
5. Collective and Molecular Dynamics of Photosensitive Liquid Crystal Elastomers
   Prof. Boštjan Zalar
6. Optimization Strategies in Biological and Artificial Microfluidic Systems
   Asst. Prof. Andrej Vilfan
7. Thermophoretic Guidance, Accumulation and Sorting of Biomolecules in Microfluidic Devices
   Prof. Igor Muševič
8. Thermophoretic Guidance, Accumulation and Sorting of Biomolecules in Microfluidic Devices
   Asst. Prof. Andrej Vilfan
9. Intra-pocket-targeted Nanomedicines for Treatment of Periodontal Disease
   Prof. Maja Remškar
10. Use of Green Energy Sources: New Functional Nanomaterials on the Base of Polyoxometalates and TiO2 Nanostrucutres for Production of Hydrogen by Catalytic Oxidation of Water –NANOleaf
    Dr. Polona Umek
11. New Advanced Electrocaloric Materials for Novel Environmentally Friendly Dielectric Refrigeration Technology
    Prof. Zdravko Kutnjak
12. The Textural Analysis of Spatiotemporal Changes for Breast Lesions Diagnosis on Ultrafast Breast MRIs
    Prof. Igor Serša

13. Role of Calcium and Lipid Membranes in Survival of Critically Ill Patients
Dr. Tilen Koklič
14. Oligomers of Amyloidogenic Proteins from A to Z: Biophysical Properties, Structure, Function and Mutual Interactions
Asst. Prof. Miha Škarabot
15. Selective and Hipersensitive Microcapacitive Sensor System for Targetted Molecular Detection in the Atmosphere
Prof. Igor Muševič
16. Behaviour of Disipative Systems under Extreme Termo-Mechanical Loading
Dr. Andrej Zorko
17. New Materials for Power Conversion: Oxide Semiconductor Thermoelectrics
Prof. Boštjan Zalar
18. Micro-electromechanical and Electrocaloric Layer Elements
Prof. Zdravko Kutnjak
19. Water Exclusion Efficacy, Measure for Prediction of Wood Performance against Wood Decay Fungi
Prof. Igor Serša
20. A spectrometer for Automatic 14N Nuclear Quadrupole Resonance Characterization of New Substances
Dr. Alan Gregorovič
21. Light-controlled Layer-by-layer Formation of Scaffolds for Faster Tissue Regeneration
Dr. Iztok Urbančič
22. New Polymer and Ceramic Materials for Potential Use in Capacitors
Dr. Andreja Eršte
23. Implementation Services MRI Recording Samples
Prof. Igor Serša
24. TABANA: Targeting AntimicroBial Activity via Micro/Nano-structured Sufaces for Civil Applications
Prof. Janez Štrancar
25. NQR Measurements of Active Pharmaceutical Ingredients
Dr. Alan Gregorovič
26. Nanomaterials and Scaffolds Preparation and Characterization
Prof. Janez Štrancar
27. Analysis with NQR (Nuclear Quadrupolar Resonance) Method
Prof. Igor Muševič
28. Irradiation and Analysis of Si Samples
Prof. Igor Muševič
29. SCOPES; Spin-liquid and Spin-ice States in Frustrated Rare-earth and Transition Metal Spinels
Dr. Matej Pregelj
30. Irradiation and Analysis of Nano Si Samples
Asst. Prof. Vid Bobnar

NEW CONTRACTS

1. CONPHIRMER: Counterfeit Pharmaceuticals Interception using Radiofreqency Methods in Realtime
Asst. Prof. Tomaž Apih
Jožef Stefan International Postgraduate School
2. Cooperation within the R&D Program of the Company Akripol
Prof. Maja Remškar
Akripol, d. o. o.
3. Research and Development Agreement
Prof. Igor Muševič
Balder, d. o. o.

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BIBLIOGRAPHY

Original Article

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2. Nina Bizjak, Franci Bajd, Jernej Vidmar, Aleš Blinc, Maja Pohar Perme, Victor J. Marder, Valery Novokhatny, Igor Serša, "Direct microscopic monitoring of initial and dynamic clot lysis using plasmin or rt-PA in an in vitro flow system", *Thromb. res.*, vol. 133, issue 5, pp. 908-913, 2014.
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6. Simon Čopar, Miha Ravnik, Slobodan Žumer, "Janus nematic colloids with designable valence", *Materials (Basel)*, vol. 7, iss. 6, pp. 4272-4281, 2014.
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October 4, 2013, Honolulu, Hawaii, USA, *Mol. cryst. liq. cryst.*, Vol. 594, iss. 1, pp. 70-77, 2014.

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