

# DEPARTMENT OF SOLID STATE PHYSICS

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*Our research program is focused on studying 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 behavior of these systems, which represent the link between perfectly ordered crystals, on one side, 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 tunneling, 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  $^{17}\text{O}$ -H and  $^{14}\text{N}$ -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

## ***1. Research programme “Magnetic resonance and dielectric spectroscopy of smart new materials”***

The research of the programme group has focused on a study of the 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 attained knowledge provides the key to the understanding of microscopic and macroscopic properties of various types of solids and is an important condition

**The group has investigated important open issues in the electronic properties of quasicrystals and complex metallic alloys, quantum magnetism in low-dimensional spin systems, the physical properties of nanostructures, materials with a giant electrocaloric and thermomechanical effect, and multiferroic and relaxor phases. The research included pharmaceutical and biological substances, where a nuclear quadrupole resonance-based technique for the detection of nitrogen complexes (as found in explosives, drugs and narcotics) was developed.**

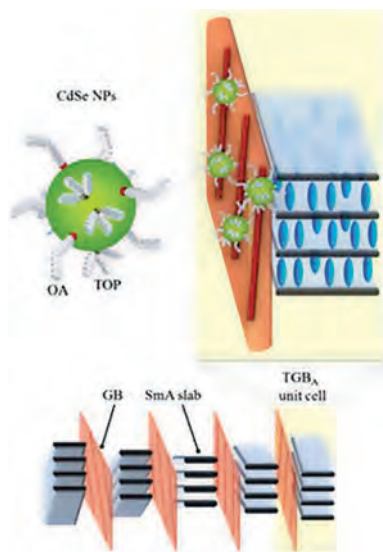


Figure 1: Structure of the TGBA phase and trapping of nanoparticles within the cores of defect lines, thus helping to stabilize the screw dislocations.

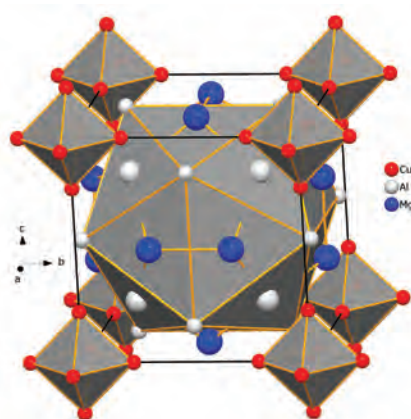


Figure 2: Motif from the crystal structure of the cubic metallic phase  $V-Al_5Cu_6Mg_2$ .

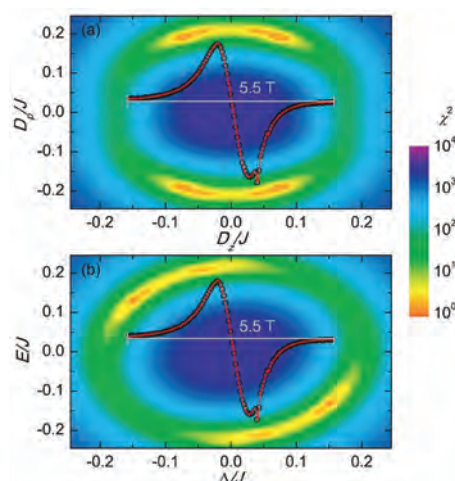


Figure 3: Determination of the magnetic anisotropy parameters of the quantum kagome antiferromagnet  $BaCu_3V_2O_8(OH)_2$  in the case of (a) crystal-field anisotropy and (b) Dzyaloshinsky-Moriya anisotropy.

for the discovery and development of new multifunctional materials and nanomaterials for novel technological applications.

### Study of the critical properties of nanostructured materials and materials with large electrocaloric and thermomechanical effects

Using direct measurements it was shown that the maximum electrocaloric response is achieved at the ferroelectric phase-transition temperature. Field-dependent piezoelectric measurements have demonstrated in  $BaTiO_3$  that the field-induced critical point influences the strength of the electromechanical response and the electrocaloric responsivity, both of which exhibit a maximum in the vicinity of the critical point. Using calorimetric and optical experiments we showed that the anisotropic graphene and  $MoS_2$  nanoparticles stabilize the first blue phase in contrast to spherical nanoparticles, which mainly stabilize the third blue phase. Moreover, CdSe spherical quantum dots stabilize the  $TGB_A$  phase (see Figure 1), which is an analogue of the Shubnikov phase of type-II superconductors. The above results have been published in 14 articles in international scientific journals. Recently published works on electrocalorics and the stabilization of blue phases have been cited more than 100 times in 2013 alone.

### Complex metallic alloys

Combining the measurements of bulk transport properties, specific heat and nuclear magnetic resonance, the group of Janez Dolinšek studied the influence of structural complexity on the physical properties of the cubic intermetallic phase  $V-Al_5Cu_6Mg_2$ . With 39 atoms in a unit cell,  $V-Al_5Cu_6Mg_2$  is an intermetallic phase with an intermediate structural complexity (Figure 2). We found that the free-electron approximation provides a good description of the  $V-Al_5Cu_6Mg_2$  behaviour, despite the presence of the quenched structural disorder at low temperatures, which is very likely intrinsic to the structure of  $V-Al_5Cu_6Mg_2$ . The work was published in M. Klanjšek, S. Jazbec, M. Feuerbacher, J. Dolinšek, "Physical properties of the  $V-Al_5Cu_6Mg_2$  complex intermetallic phase", *Intermetallics* 39, 50 (2013).

### Quantum magnetism

By means of neutron scattering and specific heat measurements, Martin Klanjšek, with French colleagues, studied the magnetic ordering of the quasi-one-dimensional antiferromagnet  $BaCo_2V_2O_8$  at low temperatures in magnetic fields up to 12 T. They confirmed the theoretically predicted incommensurate magnetic ordering in fields above 3.9 T and showed that two types of magnetic domains with equal populations develop in the material. They determined the critical exponents for the transitions into the Néel and incommensurate magnetic ordered state. The work was published in E. Canévet, B. Grenier, M. Klanjšek et al., "Field-induced magnetic behavior in quasi-one-dimensional Ising-like antiferromagnet  $BaCo_2V_2O_8$ : a detailed single-crystal neutron diffraction study", *Phys. Rev. B* 87, 054408 (2013).

By means of  $^{133}Cs$  nuclear magnetic resonance and electron paramagnetic resonance, Denis Arčon, Kristijan Anderle and Martin Klanjšek, with German colleagues, studied the coupling between the electron, lattice, orbital and spin degrees of freedom in the p-electron compound  $Cs_4O_6$ . They realized that the temperature evolution of the measured spectra depends dramatically on the thermal history of the sample. The compound exhibits two competing low-temperature phases, the quenched cubic phase and the low-symmetry phase, where the portion of each phase depends on the cooling protocol. This interesting result is a consequence of the slow reorientation of the p orbitals on cooling. The work was published in D. Arčon, K. Anderle, M. Klanjšek et al., "Influence of  $O_2$  molecular orientations on p-orbital ordering and exchange pathways in  $Cs_4O_6$ ", *Phys. Rev. B* 88, 224409 (2013).

Matej Pregelj, Andrej Zorko and coworkers studied the origin of the magnetic anisotropy in the  $\{Cu_4(tetrenH_5)[W(CN)_8]_4 \cdot 7.2H_2O\}_n$  system. Their results revealed that two-dimensional magnetic correlations start to develop already at 70 K, i.e., well above the magnetic ordering transition. Their modelling of the experimental results shows that the key to the anisotropic response lies within the combination of the dipolar interaction and the axial local anisotropy of the W and Cu ions. Their results were published in O. Zaharko et al., "Source of magnetic anisotropy in quasi-two-dimensional XY  $\{Cu_4(tetrenH_5)[W(CN)_8]_4 \cdot 7.2H_2O\}_n$ ", *Phys. Rev. B* 87, 024406 (2013).

Andrej Zorko, Matej Pregelj, Anton Potočnik, Denis Arčon and collaborators determined the magnetic structure in the ground state of the spin-chain system  $CuSe_2O_5$ . This is characterized by

staggered moments with significantly reduced size, as a consequence of quantum fluctuations. By employing various complementary experimental techniques we also determined the magnetic anisotropy of the system, which is responsible for the staggering of the moment as well as for a relatively small critical field, leading to a spin-flop magnetic transition. Their results were published in M. Herak *et al.*, "Magnetic order and low-energy excitations in the quasi-one-dimensional antiferromagnet  $\text{CuSe}_2\text{O}_5$  with staggered fields", *Phys. Rev. B* 87, 104413 (2013).

Utilizing electron spin resonance, Andrej Zorko and collaborators determined the magnetic anisotropy of the quantum kagome antiferromagnet  $\text{BaCu}_3\text{V}_2\text{O}_8(\text{OH})_2$  and showed that this is of the Dzyaloshinsky-Moriya type (Figure 3). They demonstrated that its dominant component is perpendicular to the kagome planes, which significantly suppressed the quantum fluctuations in this system. Freezing of the fluctuations is responsible for the unexpected long-range magnetic ordering of this system at relatively high temperatures, comparable to the exchange interactions. Their results were published in A. Zorko *et al.*, "Dzyaloshinsky-Moriya interaction in vesignieite: a route to freezing in a quantum kagome antiferromagnet", *Phys. Rev. B* 88, 144419 (2013).

### Multiferroics

Matej Pregelj, Peter Jeglič, Andrej Zorko, Tomaž Apih, Anton Gradišek, Denis Arčon and coworkers studied magnetically ordered states and the accompanying structural changes in the multiferroic  $\text{FeTe}_2\text{O}_5\text{Br}$  (Figure 4). Employing a combination of neutron diffraction and nuclear quadrupolar resonance (NQR) they managed to determine the incommensurate magnetic ordering in the paraelectric state (HT-IC), which exists in a narrow temperature range – just a few Kelvins before the multiferroic state (LT-IC) with finite electric polarization. In addition, they confirmed that electric polarization stems from the magnetostriction of Fe-O-Te-O-Fe exchange pathways, which is related to the phase shifts of the neighbouring magnetic modulation waves. Their results were published in M. Pregelj *et al.*, "Evolution of magnetic and crystal structures in the multiferroic  $\text{FeTe}_2\text{O}_5\text{Br}$ ", *Phys. Rev. B* 87, 144408 (2013).

As a continuation of the work on the  $\text{FeTe}_2\text{O}_5\text{X}$ ,  $\text{X} = \text{Br}, \text{Cl}$  system, Matej Pregelj, Andrej Zorko, Peter Jeglič, Zdravko Kutnjak, Simon Jazbec and Denis Arčon with coworkers studied the magnetic, structural and dielectric properties of the  $\text{FeTe}_2\text{O}_5\text{Cl}$  compound. They have discovered that its ground state is multiferroic and that the corresponding magnetic ordering is very similar to the one in the isostructural  $\text{FeTe}_2\text{O}_5\text{Br}$  system (Figure 5). They also learned that the main difference between the two isostructural compounds is in the structural effects, accompanying the establishment of the multiferroic phase, which are much more pronounced in  $\text{FeTe}_2\text{O}_5\text{Cl}$ . Moreover, they assigned these structural changes to the shift of the  $\text{O}_1$  ion and correlated them with the polarization of the  $\text{Te}^{4+}$  lone-pair electrons. In this way they confirmed that the lone-pair electrons are indeed the carriers of the electric polarization in these systems. Their results were published in M. Pregelj *et al.*, "Multiferroicity in the geometrically frustrated  $\text{FeTe}_2\text{O}_5\text{Cl}$ ", *Phys. Rev. B* 88, 224421 (2013).

### Clathrates

In collaboration with Prof. Tanigaki from Japan, Denis Arčon, Andrej Zorko and Peter Jeglič studied type-I germanium clathrates – cage structures with promising thermoelectric properties. Their NMR results are in agreement with claims that the conventional picture of purely ionic interactions between the rattling guest atoms and the cage is only approximate and that covalent effects should be taken into account in the clathrates or similar thermoelectric cage materials. Their results were published in A. Arčon *et al.*, "Rattler site selectivity and covalency effects in type-I clathrates", *J. Phys. Soc. Jpn.* 82, 014703 (2013).

### Studies of crystal structures

Matej Pregelj and coworkers studied copper and zinc complexes with the condensation derivative of 2-acetylpyridine and hydrolyzed ethyl hydrazinoacetate. They determined the crystal structure and discovered that the fifth coordination site of the ligand (Zn/Cu) is occupied by a chloride, causing a distortion of the zinc surrounding. In addition, they studied thermal behaviour employing thermogravimetric analysis. Their results were published in N. Filipović *et al.*, "Synthesis, characterization, and thermal behavior of Cu(II) and Zn(II) complexes with (E)-2-[N-(1-pyridin-2-yl-ethylidene)hydrazino]acetic acid (aphaOH), Crystal structure of  $[\text{Zn}_2(\text{aphaO})_2\text{Cl}_2]$ ", *J. Coord. Chem.* 66, 1549 (2013).

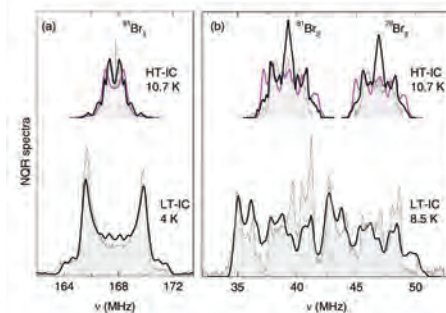


Figure 4: The  $^{81}\text{Br}$  NQR spectra for (a)  $\text{Br}_1$  and (b) for both isotopes of  $\text{Br}_2$  in the high-temperature (HT-IC) and the low-temperature (LT-IC) phases. Thick black lines are simulations considering the magnetic structures determined by neutron diffraction and the derived hyperfine coupling tensors. For a comparison we show simulations of the HT-IC spectra based on the LT-IC structure with an appropriately reduced size of the magnetic moments (thick magenta line).

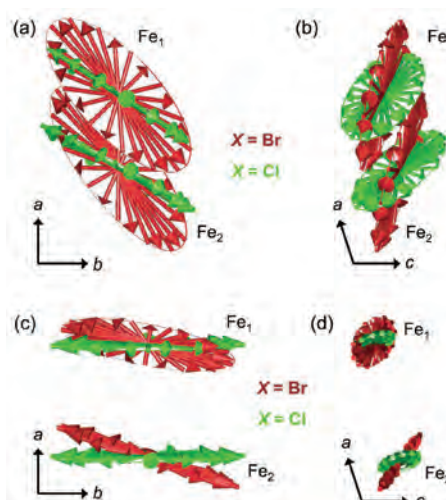


Figure 5: Magnetic structure models for  $\text{FeTe}_2\text{O}_5\text{X}$  ( $\text{X} = \text{Br}, \text{Cl}$ ), compared at  $\text{Fe}_{11}$  and  $\text{Fe}_{21}$  sites for the low-temperature phase in the (a)  $ab$  and (b)  $ac$  projections, and for the high-temperature phase in the (c)  $ab$  and (d)  $ac$  projections. For clarity, the magnetic unit cell along  $b$  is flattened and the sizes of the magnetic moments in (c) and (d) are magnified by a factor of 3.



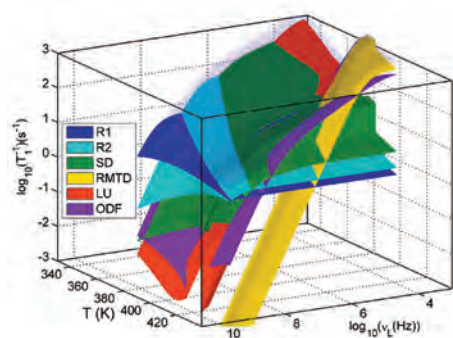


Figure 6: Contributions of various dynamic processes to the total proton relaxation as a function of temperature and magnetic field.

## Zeolites

In collaboration with Prof. Igarashi and Prof. Nakano from Japan, Peter Jeglič and Denis Arčon studied alkali-doped zeolites. Zeolites are nanoporous materials with periodic nanospaces (known as cages), which can accommodate a large amount of alkali atoms. For low-doping levels with sodium atoms the low-silica X zeolites are insulating, whereas they become metallic for high-doping levels. The confined geometry of the alkali-metal nanoclusters imposed by the framework cages make enhanced coupling between the electronic and lattice degrees of freedom leading to the formation of polaron states. The  $^{23}\text{Na}$  and  $^{27}\text{Al}$  nuclear magnetic resonance (NMR) investigation of low-silica X zeolites suggests strong electron-phonon coupling in support of the proposed polaron model. This work is described in the paper M. Igarashi, T. Nakano, P. T. Thi, Y. Nozue, A. Goto, K. Hashi, S. Ohki, T. Shimizu, A. Krajnc, P. Jeglič and D. Arčon, "NMR study of thermally activated paramagnetism in metallic low-silica X zeolite filled with sodium atoms", *Phys. Rev. B* 87, 075138 (2013).

## Molecular dynamics in a blue phase liquid crystal: a 1H fast field-cycling NMR relaxometry study

Liquid crystals exhibiting blue phases are attractive systems to study due to their highly interesting properties in the fields of optics and photonics. We investigated molecular dynamics in a chiral system, called 10BBL, that exhibits blue phase (BP), two twisted grain-boundary phases (TGB), and a smectic C ( $\text{SmC}^*$ ) phase. All these phases are stable over large temperature ranges. By means of fast field-cycling NMR relaxometry, we measured the temperature and field dependencies of proton spin-lattice relaxation times. Using theoretical models for different dynamic processes, we determined correlation times, activation energies, etc. for these processes, which include molecular rotations/reorientations, order director fluctuations, layer undulations, self-diffusion, and rotations mediated by translational diffusion along the helical axis (Figure 6). This is the first relaxometric study of a blue phase liquid crystal, published by Anton Gradišek, Tomaž Apih, Valentina Domenici, Vladimira Novotna, Pedro J. Sebastião, in *Soft Matter*, 2013, 9, 10746-10753.

## NMR study of molecular dynamics in complex metal borohydride $\text{LiZn}_2(\text{BH}_4)_5$

Lithium zinc borohydride  $\text{LiZn}_2(\text{BH}_4)_5$  (LZBH) was investigated as a potentially interesting hydrogen-storage material due to its high hydrogen content and low decomposition temperature. LZBH shows a structure of two identical interpenetrated three-dimensional frameworks with no bonds between them, which is a unique feature in complex metal hydrides. To better understand the relations between the structure and the thermodynamics of the system, we studied molecular dynamics in LZBH by means of  $^1\text{H}$  and  $^7\text{Li}$  NMR spectra and spin-lattice relaxation measurements. Different thermally activated re-orientational processes of  $\text{BH}_4^-$  tetrahedra about their 2-fold and 3-fold symmetry axes were identified from the temperature-dependent proton and lithium spin-lattice relaxation rates and were quantified by their activation energies. Due to the structure, there are two different types of  $\text{BH}_4^-$  tetrahedra; one type is located between two Zn atoms and the other type between one Li and one Zn atom. Our study presents a physical insight into the dynamic properties of LZBH on the microscopic level of atomic groups, providing a link between the microscopic and the bulk properties of this phase. Published by Anton Gradišek, Dorte B. Ravnsbæk, Stanislav Vrtnik, Andraž Kocjan, Janez Lužnik, Tomaž Apih, Torben R. Jensen, Alexander V. Skripov, Janez Dolinšek, in *J. Phys. Chem. C*, 2013, 117, 21139-2147.

## Nanomaterials

Tungsten oxide nanostructures functionalized with gold or platinum NPs were synthesized and integrated, using a single-step method via aerosol-assisted chemical vapour deposition, onto micro-electromechanical system (MEMS)-based gas-sensor platforms. This co-deposition method is demonstrated to be an effective route to incorporate metal NPs or combinations of metal NPs into nanostructured materials, resulting in an attractive way of tuning the functionality in metal oxides. The results show variations in the electronic and sensing properties of tungsten oxide according to the metal NPs introduced, which are used to discriminate effectively analytes ( $\text{C}_2\text{H}_5\text{OH}$ ,  $\text{H}_2$ , and  $\text{CO}$ ) that are present in proton-exchange fuel cells. Improved sensing characteristics, in particular to  $\text{H}_2$ , are observed at 250 °C with Pt-functionalized tungsten oxide films, whereas non-functionalized tungsten oxide films show responses to low concentrations of  $\text{CO}$  at

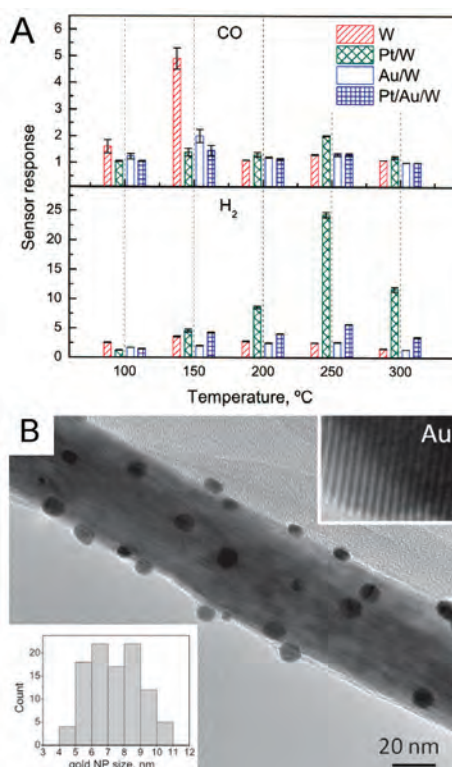


Figure 7: A) Sensor responses and error bars to 100 ppm of  $\text{CO}$  and 100 ppm of  $\text{H}_2$  as a function of the operating temperature; B) TEM image of  $\text{WO}_3$  nanostructure functionalized with Au nanoparticles. Inset on the bottom left side shows the size distribution of the Au nanoparticles. Label L stands for  $\text{WO}_3$  nanostructures, while labels Pt/W, Au/W in Pt/Au/W denote nanostructures decorated with Pt, Au and Pt/Au nanoparticles.

low temperatures. This work was published in several articles by Polona Umek et al., among others in *Advanced Functional Materials* 23, 1313-1322 (2013).

Substituted imidazole and benzimidazole often form polar hydrogen-bonded chains in the solid state. 2-Methylbenzimidazole is known to be a high-temperature organic ferroelectric. We have measured the temperature dependences of  $^{14}\text{N}$  nuclear quadrupole resonance (NQR) frequencies and proton  $T_1$  in 2-methylbenzimidazole and 5,6-dimethylbenzimidazole. The NQR frequencies are assigned to amino and imino nitrogen positions. The NQR data exclude the possibility of proton two-site exchange in an  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bond. The activation energies for the methyl group hindered rotation are determined in both compounds. The present  $^{14}\text{N}$  NQR data are compared to the published  $^{14}\text{N}$  NQR data in solid-substituted and coordinated imidazoles, in substituted benzimidazoles and in imidazole in the gas phase. A linear correlation between the two in-plane principal values of the quadrupole coupling tensor and the out-of-plane principal value of the quadrupole coupling tensor is observed in imidazole, ranging from the amino nitrogen position to the imino nitrogen position. The transition from the amino to the imino nitrogen position is determined on the correlation diagram. The correlation diagram can be used to quantitatively observe the asymmetry of the  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bond. A similar correlation diagram is also proposed for substituted benzimidazoles. The magnitudes of the principal values of the  $^{14}\text{N}$  quadrupole coupling tensor in ferroelectric 2-methylbenzimidazole show that the macroscopic ferroelectric ordering has, in this compound, a minor effect on the asymmetry of the  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds.

### Pharmaceutical and biological substances

$^{14}\text{N}$  nuclear quadrupole resonance frequencies have been measured in solid 2-pyridone, 3-hydroxypyridine, and 4-pyridone by  $^1\text{H}$ - $^{14}\text{N}$  nuclear quadrupole double resonance. Two slightly non-equivalent nitrogen positions are observed in solid 3-hydroxypyridine, whereas only one nitrogen position has been observed in 2-pyridone and 4-pyridone within the experimental resolution. The rather low  $^{14}\text{N}$  quadrupole coupling constants in pyridones are the consequence of the delocalization of the nitrogen lone-pair electrons in the aromatic rings. Two different compounds have been obtained by the crystallization of 4-pyridone from ethanol in a normal and in a dry atmosphere. The compound obtained in the dry atmosphere is identical to the commercial sample. The compound obtained in the normal atmosphere cannot be converted to the commercial polymorph by melting. It is thus not a polymorph of anhydrous 4-pyridone. The temperature coefficient of the  $^{14}\text{N}$  quadrupole coupling constant is negative in 3-hydroxypyridine and positive in 2- and 4-pyridone. Therefore, in 3-hydroxypyridine, molecular librations dominate the temperature variation of the quadrupole coupling constant, whereas in 2- and 4-pyridone, the changes in the hydrogen bonding interactions with temperature seem to give the dominant effect.

### Co-crystals and crystal polymorphs

The  $^{14}\text{N}$  and  $^{17}\text{O}$  nuclear quadrupole resonance frequencies have been measured in 1:1 co-crystals and salts of 2-amino-4,6-dimethylpyrimidine and several carboxylic acids. A systematic decrease in the  $^{17}\text{O}$  quadrupole coupling constant with the increasing strength of the hydrogen bond is observed in co-crystals bound by  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds. The  $\text{O}-\text{H}$  distances deduced from the line widths of the  $^{17}\text{O}$  NQR lines show that the hydrogen atom is in a hydrogen bond formed by a carboxylic groups for about 0.01 nm displaced from the oxygen atom toward the centre of the hydrogen bond. In the  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond formed by the hydroxyl group, which is only slightly longer than the hydrogen bonds formed by the carboxyl group, the hydrogen atom is much less displaced. A linear relation between the  $^{14}\text{N}$  quadrupole coupling constant and the sum of the inverse third powers of the  $\text{H}\cdots\text{A}$  ( $\text{A} = \text{O}$  or  $\text{N}$ ) distances is deduced for the amino group. A linear correlation of the principal values of the  $^{14}\text{N}$  quadrupole coupling tensor in  $\text{NH}_2$ , as observed in the solid phase and in the gas phase, is analysed in a simple model assuming a displacement of the electron charge in the  $\text{N}-\text{H}$   $\sigma$  bond and simultaneous deformation of the nitrogen lone-pair electron orbital. At the ring nitrogen position, hydrogen bonding and proton transfer produce a large decrease in the  $^{14}\text{N}$  quadrupole coupling constant. A linear correlation of the principal values of the  $^{14}\text{N}$  quadrupole coupling tensor is observed in co-crystals and salts of 2-amino-4,6-dimethylpyrimidine. This correlation differs from the correlation observed in substituted pyrimidine, where the hydrogen atoms are replaced by other atoms or functional groups. The difference is analysed in a model, which assumes that the hydrogen bonding and substituents affect the nitrogen lone pair and  $\pi$  electron orbitals. The analysis shows that the two effects are nearly independent. The application of  $^{14}\text{N}$  NQR to the study of co-crystals and crystal polymorphs is reviewed. In ferroelectric and antiferroelectric organic co-crystals  $^{14}\text{N}$  NQR is used to determine the proton position in an  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond and the proton displacement below  $T_c$ . In co-crystal isonicitinamide – oxalic acid (2:1)  $^{14}\text{N}$  NQR is used to distinguish between the two polymorphs and to determine the type of the hydrogen bond ( $\text{N}\cdots\text{H}-\text{O}$ ). The difference in the  $^{14}\text{N}$  NQR spectra of the co-crystal formers and the co-crystal is investigated in the case of carbamazepine, saccharin and carbamazepine-saccharin (1:1). The experimental resolution allows an unambiguous distinction between the  $^{14}\text{N}$  NQR spectrum of the co-crystal and the  $^{14}\text{N}$  NQR spectra of the co-crystal formers. The possibility of the application

of NQR and the double resonance for the determination of the inhomogeneity of the sample and for the study of the lifetime of an unstable polymorph is discussed.

### Amorphous solids

Nuclear quadrupole double resonance (NQDR) is proposed as a method for the quantitative observation of crystallization of amorphous solids. NQDR signals from amorphous and crystalline parts of a sample may be separated. The intensity  $I$  of the NQDR signal from the crystalline part of the sample is proportional to its mass. With increasing time the amorphous phase in the sample transforms to the crystal phase and the intensity  $I$  approaches its limiting value  $I_0$ , corresponding to a complete transformation to the crystal phase. The ratio  $I/I_0$  is equal to the mass fraction of the crystalline part of the sample. The same experimental method can be used to determine the mass fraction of a given crystal polymorph in a mixture of crystal polymorphs. As an example we studied the crystallization of amorphous nifedipine at 100 °C. The results of the NQDR study are compared to the published results of other studies.

### Impact of structure modifications on electrically induced properties of relaxor polymers

In collaboration with researchers from Pennsylvania State University, USA, we have investigated how the dielectric, electromechanical, and electrocaloric properties of ferroelectric and relaxor polymers (systems that exhibit fast response speeds, giant electrostriction, high electric energy density, and large electrocaloric effect) are affected by various processing procedures and/or modifications, such as (i) stretching the relaxor polymer, (ii) irradiating the ferroelectric polymer with high-energy electrons, and (iii) blending a relaxor polymer with the ferroelectric system. We have recently focused on the P(VDF-TrFE) copolymer that is irradiated with low and moderate doses of high-energy electrons - up to now most of investigations have focused either on ferroelectric P(VDF-TrFE) copolymer or P(VDF-TrFE) that is irradiated with high doses and is thus completely transformed into a relaxor system. Using various experimental techniques we found clear evidence that in such a case ferroelectric and relaxor states coexist in the system, which was a key point for the explanation of their enhanced electrocaloric response. Particularly for the nonlinear dielectric spectroscopy (Figure 8) - we have in fact conducted the first measurements of the real and imaginary parts of the nonlinear dielectric response in ferroelectric and relaxor polymers - was found as an extremely powerful tool for investigating the correlation between the structure and the property evolution in relaxor polymer systems. Published in: G. Casar, X. Li, J. Koruza, Q. M. Zhang, V. Bobnar. Electrical and thermal properties of vinylidene fluoride-trifluoroethylene-based polymer system with coexisting ferroelectric and relaxor states. *J. Mater. Sci.* 48, 7920 (2013).

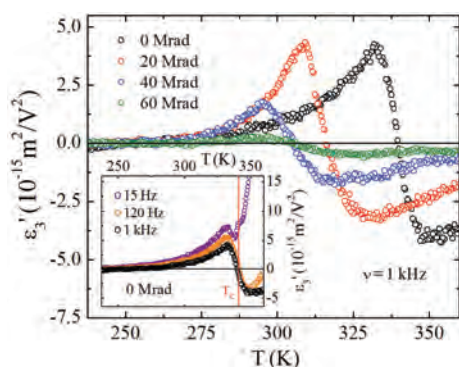


Figure 8: The nonlinear dielectric response revealed the coexistence of ferroelectric and relaxor states in P(VDF-TrFE) copolymer, irradiated with low doses of high-energy electrons, which was a key point for the explanation of their enhanced electrocaloric response.

### High-temperature dielectric investigations of a novel inorganic relaxor system

We have continued high-temperature dielectric investigations of classical inorganic relaxors, which revealed astonishing results - they contradict widely the accepted dogmas on relaxor properties. Also the results obtained in a novel  $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$  ceramic system, prepared from mechanochemically activated powder, clearly reveal that the polar nanoregions do not form at the so-called Burns temperature (approx. 600 K), but are continuously formed over a broad temperature range, starting well above 800 K. We have in fact successfully recognized various distinctive dielectric contributions in a broad temperature range of 150–750 K. Moreover, a detailed analysis of the intrinsic high-temperature dielectric response revealed a critical behaviour associated with universality classes typically found in spin glasses and, particularly, that the low-temperature fingerprint behaviour can be observed at much higher temperatures, well above the dispersive relaxor dielectric maximum.

Published in: V. Bobnar, H. Uršič, G. Casar, S. Drnovšek. Distinctive contributions to dielectric response of relaxor ferroelectric lead scandium niobate ceramic system. *Phys. Status Solidi B* 250, 2232 (2013).

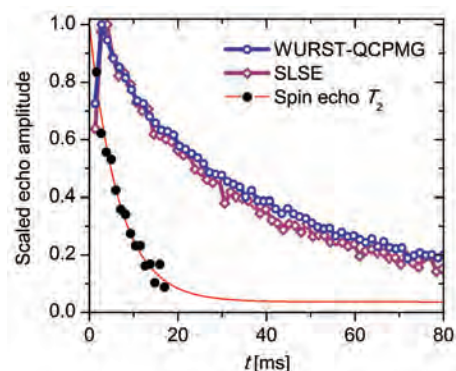


Figure 9: The decay of echo amplitudes during the SLSE experiment with rectangular pulses and QCPMG experiment with WURST pulses. For comparison also the  $T_2$  decay is shown. The sensitivity of each experiment is here roughly proportional to the area below the curves. Published in: A. Gregorovič, T. Apih, *J. Mag. Res.* 233, 96 (2013).

### “WURST-QCPMG sequence and “spin-lock” in 14-N Nuclear Quadrupole Resonance”

The excitation of magnetization in Nuclear Quadrupole Resonance (NQR) is most often accomplished with the use of rectangular RF pulses, where the pulse amplitude and phase are constant during the pulse. These pulses are technically easy to implement. Also, they are easy to include in various theoretical predictions and analysis. However, rectangular pulses also have some disadvantages. When these disadvantages become severe, shaped pulses are often used instead. Here, the amplitude and phase during the pulse follow a prescribed function. WURST pulses are



just one of the many shaped pulses and are in use in NMR for a decade. Their principal advantage is a large excitation bandwidth at low RF powers. In the publication we demonstrate that WURST pulses are suitable for  $^{14}\text{N}$  NQR as well. In particular, we demonstrate, that the “spin-lock” effect is completely preserved compared to rectangular pulses. This is very important, as the spin-lock effect is essential for the  $^{14}\text{N}$  NQR detection. It allows us to increase the otherwise poor sensitivity by 10-100 times (Figure 9). The theoretical prediction/analysis of the spin-lock effect is already challenging for the rectangular pulses. For shaped pulses it would be even more difficult. Thus the existence of the spin-lock effect for WURST pulses is not at all obvious. In the publication we have shown how the WURST pulses combined with the QCPMG sequence can significantly reduce the time required for the acquisition of a very broad  $^{14}\text{N}$  spectrum, usually a very time-consuming task. In addition, WURST pulses require limited RF power, and are as such appropriate for small desktop applications of  $^{14}\text{N}$  NQR.

## 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 nanostructures. The aim of the program is to understand 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. New nanocomposite materials have been developed, the structure of matter has been studied on the atomic level and a new infrastructure for cold atom physics experiments was set up.**

### Highly constrained topological defects in nematics

Topological defects in uniaxial nematics can be compared to the defects in biaxial media. The defects are not equivalent, but similarities can be exploited to better understand the topological rules that govern the disclinations in uniaxial nematics. Disclination lines with variable profiles are systematically described with quaternions, which allow the simple characterization of disclinations by counting geometrically recognizable features (Čopar and Žumer, PRSA 469, 2013). In a similar fashion, the bulk director, away from the defects, can be studied as a biaxial phase by using its derivatives. This formulation finds “quasi-disclinations” that carry additional topological information, potentially useful for a description of the blue phases and general chiral nematics (Čopar et al, PRE 87, 2013).

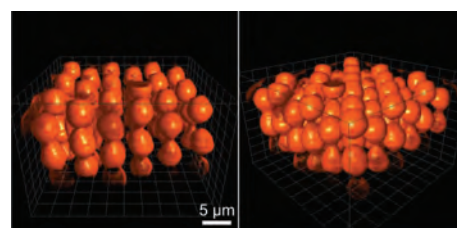


Figure 10: 3D image of a nematic colloidal crystal, reconstructed from fluorescent confocal imaging.

### 3D nematic colloidal crystals

Significant advancements have been made in our understanding of assembling 3D nematic colloidal crystals. We have published in *Nature Communications* (Nych et al, Nature Commun. 4, 2013) an article about the laser-tweezers-assisted assembly of 3D nematic colloidal crystals from dipolar nematic colloids. Using fluorescent confocal microscopy we have found that the unit cell of this 3D crystal is tetragonal with a basis (Figure 10). This crystal shows unusual response to external electric fields; for positive dielectric anisotropy of the nematic liquid crystal, the crystal shrinks up to 30%. If the dielectric anisotropy of the carrier nematic liquid crystal is negative, then the colloidal crystal rotates as a solid unit. The angle of rotation is up to several tens of degrees.

### Nematic colloids

In nematic colloids, advances have been seen in a systematic numerical and theoretical study of disclination networks in the interstitial space of a close-packed lattice of homeotropic particles has revealed a model (Figure 11) that explains the reconfigurable interconnected defects in simplest geometric terms. Local description using tetrahedra and cubes is used to construct all the possible arrangements of defects in this highly frustrated environment (Čopar et al, Soft Matter 9, 2013).

Further pair interactions between colloidal particles in confined cholesteric cells have been measured. The interaction profile contains energy minima and thus allows metastable states, the number of which increases with chirality. A description for this phenomenon has been postulated

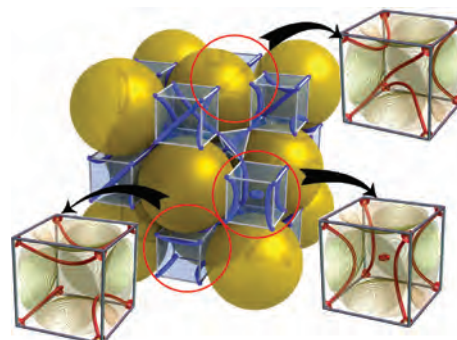


Figure 11: Modelling of the disclination network in nematic permeating opal structure.

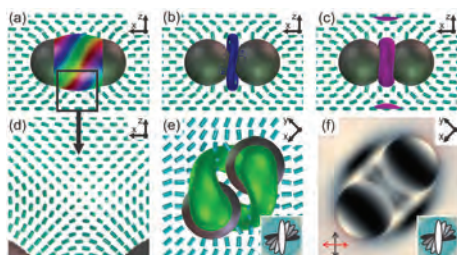


Figure 12: Colloidal pair in an unwound chiral nematic in a bubble-gum structure. a-e visualization of the director fields and ordering tensor derivatives. f simulated polarization microscopy

and probed with computer simulations (Jampani et al, PRL 110, 2013). Related studies of colloidal systems with morphologically and topologically different parameters, performed in collaboration with foreign groups, yielded publications in co-authorship (Gharbi et al, Soft Matter 9, 2013; Geng et al, Soft Matter 9, 2013; Cavallaro et al, Soft Matter 9, 2013; Cavallaro et al, PNAS 110, 2013).

### Visualization of nematic defects

Analysis of the data produced by numerical simulations and advanced experimental methods requires a host of visualization methods to highlight the parameters of interest (Figure 12). An expansive review over the most common methods has been published, together with examples based on well-known models (Čopar, Porenta, Žumer, Liq. Cryst. 2013).

### Nanoparticles dispersed in mesophases

We have demonstrated experimentally and theoretically that the interaction between nanoparticles and topological defects induces a twist-grain boundary phase in a chiral liquid crystal. The occurrence of this phase, the analogue of the Shubnikov phase in type-II superconductors, is driven by the direct interaction between surface-functionalized CdSe quantum dots and screw dislocations. It is shown that, within a universal adaptive-defect-core-targeting mechanism, nanoparticles of the appropriate size and functionalization adapt to qualitatively different cores of topological defects such as disclination lines and screw dislocations. The findings suggest new pathways towards the controlled assembly of superstructures in diverse, symmetry-broken, condensed-matter systems, ranging from nanoparticle-decorated liquid crystals to superconductors (G. Cordoyiannis *et al.*, *Soft matter* 9, 3956 (2013)). Furthermore, we have studied the impact of surface-functionalized graphene nanosheets on the blue-phase range of a chiral liquid crystal. Calorimetric and optical measurements demonstrate that the resulting soft nanocomposite exhibits an increased blue phase temperature stability range for a minute concentration of dispersed graphene. The impact is stronger on the more ordered, cubic structured blue phase I. Experimental results were discussed in the frame of Landau-de Gennes mesoscopic model in terms of the tensor order parameter. These findings suggest that anisotropic nanoparticles may be of great usefulness for stabilizing the blue phases (M. Lavrič *et al.*, *Appl. Phys. Lett.* 103, 143116 (2013)).

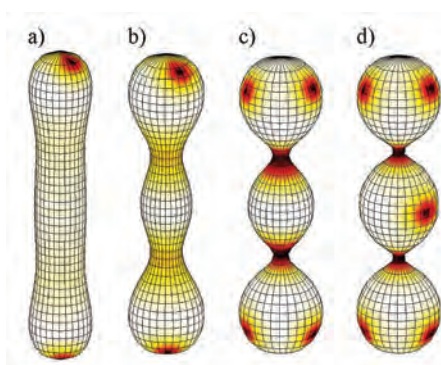


Figure 13: Impact of curvature on the number and position of topological defects.

### Membrane budding and formation and release of microvesicles

The latter might play an important role in long distance cell-cell communication owing to their ability to move with body fluids. Several mechanisms exist that might trigger pinching off of globular buds from the parent membrane (vesiculation). We have considered theoretically the impact of topological defects (TDs) on this process in the membranes exhibiting global in-plane orientational order. Landau-de Gennes type theoretical approach is used in terms of the tensor orientational order parameter. We show on membrane structures exhibiting spherical topology that the coexistence of regions with positive and negative Gaussian curvature might trigger pairs *defect-antidefect* for strong enough local membrane curvatures. Critical conditions for this event are determined for several demonstrative cases (Figure 13). We claim that concentration of TDs at narrow necks might trigger membrane fission neck rupture, enabling a membrane fission process and the release of membrane daughter microvesicles (D. Jesenek *et al.*, *International journal of nanomedicine* 8, 677 (2013)).

### Photonic properties of smectic fibres

In 2013, a lot of attention was paid to our studies of the photonic properties of liquid crystal dispersions. We have studied the resonant transport of light between a planar polymer waveguide and a nematic droplet-optical microresonator in close proximity to the waveguide. White light from a supercontinuum laser that was guided along the planar waveguide, it was seen to be resonantly transferred via photon tunnelling into the Whispering Gallery Modes of the microresonators. A theoretical analysis was also performed within the coupled-mode approach, the article was published in Jampani et al. *Optics Express* 2013. In the same journal we published in December 2013 in cooperation with partners from Max Planck Institute, Goettingen, an article on the lasing and waveguiding in smectic-A optical fibres (Peddireddy et al, *Optics Express* 2013). We observed that in contact with water and CTAB, a smectic liquid crystal spontaneously forms micrometre-diameter fibres. Using confocal microscopy, we reconstructed the layered structure of these fibres. The smectic layers are wrapped-up into a series of closed and concentric molecular layers, forming a +1 topological defect in the core of the fibre. These fibres are excellent waveguides and it is possible to induce laser emission from fibres doped with fluorescent molecules (Figure 14). The article has attracted



Figure 14: Smectic-A liquid crystal spontaneously forms optical fibres that are excellent waveguides and laser emitters.



considerable attention, because it was selected by the editors of all the Optical Society of America journals as the highlight article of December 2013. We have also published a review article on the photonics and topology of nematic colloids and dispersions (I. Muševič, Phil. Trans. Royal Soc. A 2013).

### Molecular motors

We developed a model for the dynamics of cytoplasmic dynein, which is one of the largest and most complex motor proteins. We used an elastomechanical model for each individual dynein head and combined it with a minimal model of the chemical cycle of ATP hydrolysis. We showed that a dimeric molecule, consisting of two heads, can synchronize their cycles and step with regular 8-nm steps if the coupling is sufficiently strong (Figure 15). This is the stepping pattern observed in mammalian dynein. With weaker coupling the heads lose synchrony and move with a much broader distribution of step sizes, but it is still capable of pulling a load. The mode of stepping then corresponds to that observed in yeast dyneins. This shows that the walking mechanism of dynein is robust in itself, but its efficiency and processivity are improved significantly by the coupling between the heads (*A. Šarlah and A. Vilfan, The winch model can explain both coordinated and uncoordinated stepping of cytoplasmic dynein; submitted*).

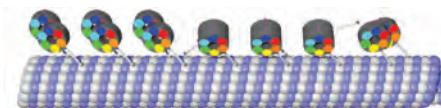


Figure 15: Stepping of a model cytoplasmic dynein molecule.

### LC applications

The Jožef Stefan Institute (JSI) and its spin-off Company, Balder Ltd that was acquired by the multinational Kimberly Clark Corporation (KC) in 2012 were in the past years intensively developing the new concept of LC optical light shutters based on optically compensated birefringence in Super-twisted LCDs. The innovative technical solutions were upgraded (24.9.2013) with a Continuation-in-part Patent US 8,542,334. The new LC light shutter technology is finally protected by 6 granted international patents (USA and EU). The above technology based on the proprietary IP allows Balder (KC) to become the only producer of the LC welding filters in the world that can label its products with the prestigious CE 1/1/1/1 quality certificate. On the grounds of the high performance of Balder's (KC) products, the International Standard Organization invited JSI to participate in the ISO expert group ISO/TC94/SC6/WG2 and WG4 preparing new ISO standard on Eye Protection. The new LC light-shutter technology was recently (2013) upgraded by the emerging spatial light filtering technique (Figure 16). It allows the extension of the application of the LCD optical filters into the field of light hazard (e.g., glare) eye protection against collimated light sources (e.g. car headlights).



Figure 16: Spatial light filtering glass.

### Low-friction nanomaterials

In the paper entitled "Nanoparticles as novel lubricating additives in a green, physically based lubrication technology for DLC coatings", M. Kalin, J. Kogovšek, and M. Remskar, *Wear* 303, 480 (2013), we report on a significant improvement of the friction behaviour of diamond-like carbon (DLC) tribological contacts by addition of MoS<sub>2</sub> nanotubes into PAO oil in 2 wt.%. The friction coefficient measured in the most severe conditions was reduced by up to 50%, compared to using only base PAO oil. In the paper "Influence of surface roughness and running-in on the lubrication of steel surfaces with oil containing MoS<sub>2</sub> nanotubes in all lubrication regimes", by J. Kogovšek, M. Remskar, A. Mrzel, and M. Kalin, *Tribology International* 61, 40 (2013), we reported that the friction at the steel contact drops by 40–65% when 2 wt.% of MoS<sub>2</sub> nanotubes are added to base oil. Furthermore, using MoS<sub>2</sub> nanotubes, the friction is the same for rough and smooth steel surfaces, which indicates a reduced need for fine surface finishing when surfaces are lubricated by MoS<sub>2</sub> nanotubes.

### Nanoelectronics

In the paper "Comparative study of chemically synthesized and exfoliated multilayer MoS<sub>2</sub> field-effect transistors", HS Hwang, M. Remskar, et al., *Applied Physics Letters*, 102, 043116-1 (2013), we report on field-effect transistor (FET) device based on as-synthesized MoS<sub>2</sub> nanoflakes in comparison to thin flakes prepared by exfoliation of bulk MoS<sub>2</sub>. The transistor characteristics were found to be almost identical; the on/off current ratio is 10<sup>5</sup> and transistor behaviour of n-type.

### Polymer nanocomposites

In the paper "A novel structure of polyvinylidene fluoride (PVDF) stabilized by MoS<sub>2</sub> nanotubes", M. Remskar, et al., *Soft Matter* 9, 8647 (2013) we report on the first polyvinylidene fluoride (PVDF)–MoS<sub>2</sub> nanotube based nanocomposites. The results indicate that the polymer–nanotube interaction stabilizes a novel 2b stacking within the  $\gamma$ -phase, which represents a new PVDF crystal structure. Annealing of the PVDF–MoS<sub>2</sub> nanotube films leads to a completely relaxed  $\alpha$ -phase with the nanotubes forming the nucleation centres for crystallization of the dendritic phase. Tribological properties of these films, which evidence that 1 wt.% of MoS<sub>2</sub> nanotubes in PVDF reduces fric-

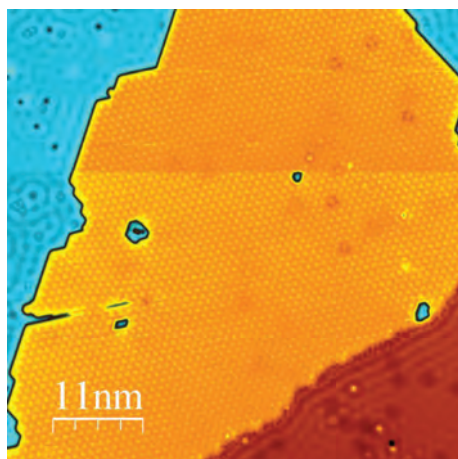


Figure 17: High-resolution STM image of a Pb monolayer on a Cu(111) surface, showing a Moire pattern. (size 50 x 50 nm<sup>2</sup>, It=91 mV, Ut=0.8 nA, T=4.2K).

tion by more than 20% with regard to pure PVDF, while 2 wt.% by more than 70%, were published in the paper "Friction properties of polyvinylidene fluoride with added MoS<sub>2</sub> nanotubes", M. Remškar et al., *Physica Status Solidi. A, Applications and Materials Science*, 210, 2314 (2013). Raman spectroscopy revealed that sliding in the boundary lubrication regime can trigger the phase transformation to polar PVDF phase in similar way as the drawing during crystallization.

### Nanosafety

We prepared a leaflet entitled "Fireworks and other pyrotechnics for entertainment poison air" with the goal to raise awareness of hazardous air pollution by nanoparticles released during fireworks and the combustion of sparklers. The leaflet is available at the public link [http://www.uk.gov.si/fileadmin/uk.gov.si/pageuploads/pdf/Ognjemeti\\_dokoncna.pdf](http://www.uk.gov.si/fileadmin/uk.gov.si/pageuploads/pdf/Ognjemeti_dokoncna.pdf),

### Nanoscale superconductivity

Confined metal nanostructures, such as monolayers or small islands of different thicknesses, are very interesting for probing the ultimate limits of nanoscale superconductivity. We are studying the relationship between bulk and nanostructure superconductive critical temperatures ( $T_c$ ). In particular, we are trying to control  $T_c$  on a nanoscale. High-quality Pb ultra-thin films (from one to few monolayers thick) have been deposited in ultra-high vacuum on an atomically flat Cu (111) surface. For low coverage a monoatomic hexagonal close-packed Pb film is formed, which shows an inverse corrugation (Figure). For higher coverage, a Stranski-Krastanov growth of 3D Pb islands is observed, several monolayers thick. Low-temperature STM and STS measurements were performed down to 1K on such surfaces to study their atomic and electronic structures.

### Charge density wave compounds

The real crystal structure of the (NbSe<sub>4</sub>)(10/3)I charge density wave (CDW) compound was studied by simulation of the X-ray diffuse scattering. The average structure of the low-temperature twinned phase was determined and the phase transition was attributed to the formation of a CDW. In addition to the experiments, the electronic properties of the high- and the low-temperature phases were calculated with the extended Hückel tight-binding method. The Fermi surfaces of the average structures above and below the phase transition appear very similar and their shapes support a nesting instability and a CDW formation.

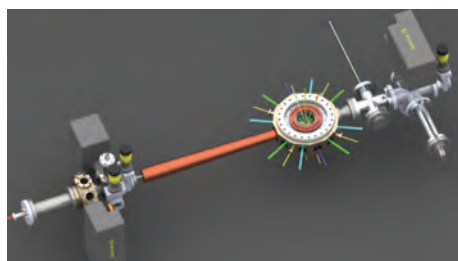


Figure 18: Schematic representation of an UHV system, built and tested for experiments with ultra-cold Cs atoms.

### Ultra-cold atoms

An in-house-built ultra-high vacuum apparatus was constructed and tested for experiments on strongly correlated systems with Cs atoms (Figure). Next, different laser systems are being set up, which will in combination with magnetic fields be used to slow down, capture, compress and cool down atoms to nK temperatures.

## III. Research programme "Experimental Biophysics of Complex Systems"

Within the program "Experimental Biophysics of Complex Systems" we explore processes and structures of various complex systems (from model systems to the structures in living cells, tissues and even small animals) including the effects of various bioactive molecules like toxins, drugs, etc., as well as of various materials like nanomaterials and medical materials on these systems. Our research is focused on the investigation of structural properties of different membrane structures such as membrane domains, membrane proteins and glycosaccharide matrix as well as their interactions with various materials that enter into their native environment. Novel spectroscopic and

**By the analysis of the polarization dependence of fluorescence, we revealed that some widely used membrane probes undertake several lipid phase-dependent conformations at distances below optical spatial resolution. Based on detailed optical microscopy measurements of the dissolution of blood clots model in an artificial perfusion system, we have developed a mathematical model describing the thrombolysis as a corrosion-erosion process.**

microspectroscopic techniques contribute to the understanding of the organization of these supramolecular systems, complex cell and tissue responses as well as opening new possibilities to design new medical materials, like scaffolds for tissue regeneration as one of the most relevant problems in the current aging population of the developed countries. In addition, we focus on medical method optimization, like tumour treatment methods, magnetic resonance imaging and the mathematical modelling of trombolysis, magnetic resonance microscopy in forestry, wood science and food processing as well as to restricted diffusion research.

One of the hottest topics of current biophysics is certainly the study of the interactions between novel materials and cells, especially from the

bioactivity and biocompatibility point of view, which we explore by applying novel microspectroscopies. The basic question is: do nanoparticles and nanofibres enter cell membranes. The partitioning of the nanoparticles was studied via FMS-FRET experiments on model membranes, exposed to the diffusing nanoparticles on a micron scale. The nanoparticles first accumulated on membranes coming into the molecular neighbourhood of the membrane probes, which enhanced the membrane probe signal due to FRET. After approximately 40 min. the liposomes start to degrade and the membrane signal was detected everywhere within the micrometre neighbourhood.

Our system for fluorescence microspectroscopy enables us to acquire fluorescence spectra from microscopic volume elements of the sample and thus to detect physical changes in local molecular environment of fluorescent probes. By stochastic wavelength sampling and efficient computer simulations we improved spectral resolution and bleaching correction reliability, as we reported in the published article "Bleaching-corrected fluorescence microspectroscopy with nanometer peak position resolution. *Opt. Express* vol. 21, no. 21, p. 25291-25306". Upgrading the analysis by polarization dependence of emitted fluorescence, we revealed that some widely used membrane probes undertake several lipid phase-dependent conformations at distances below optical spatial resolution. We published our findings in the article "Coexistence of probe conformations in lipid phases: a polarized fluorescence microspectroscopy study. *Biophys. J.*, vol. 105, no. 4, p. 919-927". As a part of our cell-nanomaterial interaction research, we used resonance energy transfer imaging to investigate rates and mechanisms of titanate nanoparticles' penetration through membranes of giant vesicles. The system for optical micromanipulation was used to study the dynamics and strength of cell attachment to macrostructured biomedical materials that are used as models for potential artificial tissue scaffolds. The results were correlated by molecular (EPR) and macroscopic (morphology, rheology, viscoelasticity) properties of the scaffolds.

In the area of the design and synthesis of probes (nitroxide, fluorophore and combination of both in the same molecule) in 2013 focus was on the synthesis of environment sensitive fluorescent probes (sensitive to polarity and hydration of the environment). A small series of fluorophores was synthesized by linking of 7-(diethylamino) coumarin and different aromatic systems with oxazole. Synthesized dyes display red shift of absorption as well as emission spectra. Fluorescence emission spectra in solvents of increasing polarity exhibit decrease of fluorescence intensity and red shift of emission maxima. Under our experimental conditions synthesized fluorophores display excellent photostability compared to NBD type probes. 7-(diethylamino)coumarin represented also the basis of for a small series of double spin-fluorescent probes. The influence of distance between fluorophore and nitroxide was examined with these probes. Several pH dependant probes of rhodamine type were also evaluated in regard to their photophysical properties.

In collaboration with Biotechnical faculty we have investigated how structural properties of several phenolic substances influence their binding and interaction with liposome membranes. Phenolics are antioxidants with antimicrobial effect and are therefore interesting as bio-additives for food industry. Results obtained using EPR, fluorescence anisotropy and differential scanning calorimetry show that phenolics investigated decrease membrane fluidity and are bounded to a membrane surface predominately via hydrogen bonds (*Food chemistry*, 2013, 139:804-813).

In collaboration with Hacettepe University, from Ankara, Turkey, the influence of tricyclic antidepressant clomipramine (CLO) on model and biological stratum corneum (SC) membrane was investigated by EPR. The fluidizing effect of CLO on pig ear SC throughout the whole membrane indicates that CLO penetrates into the stratum corneum, which is important for its transdermal delivery (*J. Pharm. Sci.* 2013, DOI 10.1002/jps.23687).

In collaboration with Max Delbrück Center for Molecular medicine in Berlin, Germany, we have investigated the role of lysophospholipid, perifosine (OPP) as a constituent of liposome membrane on trans-cell barrier transport of liposome encapsulated drugs. We have shown that liposome membrane fluidity decreases with increasing concentration of perifosine in liposomes. This could be a reason for the increased release of the liposome encapsulated hydrophilic substance measured with the increasing concentration of perifosine. Our results indicate that the efficient transport of liposome-encapsulated hydrophilic drugs across the barrier into a disease-affected tissue is possible with liposomal formulations, which contain sufficient amounts of perifosine to open the channels in the barrier and release the liposome content when the cell barrier is compromised. This opens a new possibility of using lysolipid-containing liposomal formulations as drug delivery systems (submitted for publication).

We have recently shown that the structure of water confined between lipid membranes is perturbed with respect to bulk water. Due to a low light penetration depth the attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy is specifically suited to study interlamellar water structure in multibilayers. Sequential modification of interlamellar water perturbation can be followed with a step-by-step dehydration of samples either by water evaporation or by osmotic pressure. Besides different levels of hydration, the lipid-water interaction can be studied for lipids with different headgroups and for different lipid phases. Modification of interlamellar water properties could explain water-mediated effects on biological processes. This can have implications to membranes adhesion, stacking, and fusion.



Using molecular dynamics (MD) we calculated partition coefficients between the membrane and water phase for several commonly used labels (two spin labels and a fluorescent marker). Coefficients were obtained by first calculating the free energy for the transition from the membrane into water using adaptive biasing force (ABF) MD. The results allow us to perform experiments with greater precision and more economically. Part of the results is summarized in the graduation work of Klare Presecnik with the title "Determination of partitioning coefficients of amphiphilic molecules between membrane and water using molecular dynamics (ABF)". We have created a generally applicable software package for determining position-dependent diffusion coefficients (available at [github.com/lbf-ijs/DiffusiveDynamics](https://github.com/lbf-ijs/DiffusiveDynamics)). The package is capable of obtaining and visualizing diffusion for one- and two-dimensional cases. With the obtained diffusion surface and a known free energy surface, diffusive trajectories can be generated. Thereby the time reach of molecular dynamics, typically a few 100 nanoseconds, can be extended to several 100 microseconds (for the 1D or 2D subspace of interest). The method for determining the diffusion is most efficiently used with ABF MD. With this methodology, the motion of spin labels in the membrane can be studied, thus further improving the empirical approximation used by side-chain conformational space modelling of proteins (CSM). Such estimates allow us to significantly reduce the computational time needed for determining the size of the side-chain conformational space. This also enables us to solve inverse problems – for example, the structural characterization of membrane proteins.

We started experimental work on cysteine mutants of the N-terminal part of the antimicrobial peptide  $\beta$ -defensin. The ultimate purpose of the experiments is to determine the 3D structure of peptides in various environments using CSM. Using circular dichroism (CD) and the EPR we observed two different conformations we have already observed two conformations. We also discovered conditions under which the transition between conformations can be controlled by varying the pH.

The use of one-dimensional nanoparticles, such as  $\text{TiO}_2$  nanotubes, offers a promising low-cost and effective alternative to current disinfection methods used in food processing industry and in hospital environment. In order to improve antibacterial properties of surfaces we developed a stable deposition of  $\text{TiO}_2$  nanotubes on polyethylene terephthalate (PET) surface, a material commonly used in food processing industry and hospital environment. PET surfaces with this kind of antibacterial nanocoating (ABnC) retard growth of bacteria by up to one order of magnitude when illuminated by ordinary fluorescent light bulbs.

Thrombolysis is the process in which the addition of specific agents (thrombolytic agents) in the bloodstream can dissolve the blood clots. The usual way that a thrombolytic agent functions is that it initially activates a molecule of plasminogen to its active form plasmin and this in turn degrades the fibrin network of which the clot is made. In a large study, which was started two years ago, we studied the possibility of using a direct thrombolytic agent in which the conversion of plasminogen to plasmin would no longer be needed. Namely, in the bloodstream was directly added plasmin. Its effect on thrombolysis was then followed by an optical microscope, by which we monitored the progress of degradation of artificial blood clots in contact with plasmin molecules. The process of blood clot dissolving was also recorded with a digital camera and images were then analysed so that we could analyse the dynamics of blood clot dissolution. The obtained results were then analysed by an appropriate mathematical model of blood clot dissolution. The findings of this study were published in the journal *Blood coagulation and fibrinolysis*, another article with similar content is in the publishing process in the *Thrombosis Research*.

The magnetic resonance imaging (MRI) can also enable monitoring of the development of caries of the teeth and dental tissue impairment caused by caries. However, MRI has of course a number of limitations. The first is that MRI of teeth is currently too demanding that it could be performed *in vivo* successfully. Therefore, our study had to be performed on extracted teeth. Another limitation is that MRI is not capable of imaging of hard dental tissues such as enamel and dentin, at least not in its standard way. However, we still come up with interesting findings with regard to caries. Namely, one of the effects of caries is also dentin demineralization. Due to the demineralization carious dentin produces much more signal than intact dentin, so that regions of demineralized dentin can be easily detected with T1-weighted imaging. Another interesting finding is that caries also affects dental pulp tissue. The changes can be clearly seen in maps of relaxation time T2, as well as in maps of apparent diffusion constants (ADC). The findings of the study were recently published in the *Caries 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 cell membrane is a tissue are made temporary permeable and therefore absorb more drugs than normally, as for example anti-cancer drugs. In this area in the past year, 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 last year. Until last year these experiments were successfully done only on model samples, but not on experimental animals. Experiments on animals have greater importance because

they can be used for determination of the presence and extent of the region of reversible electroporation. In this region, the tissue cells open for a short time and in this time an anticancer drug can enter the cells, after that 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 electric field strength on the basis of the measured current density distribution. The findings of this study were sent to the journal Radiology.

Controlled drug-delivery systems are widely used in pharmaceutical industry because of their numerous advantages. For hydrophilic polymers, it is generally accepted that, once in contact with body fluids, they hydrate and swell, forming a gel layer that regulates the penetration of body fluids into the tablet and the dissolution of the incorporated drug. Therefore the knowledge of the gel layer characteristics is of a crucial importance for the use of controlled drug delivery systems. Combination of different MRI methods enables accurate determination of medium penetration into the tablet as well as hydrogel formation *in situ*. MR imaging was used to study the impact of a soluble active substance in the dynamics of the penetration of the medium into the tablet and the formation of the gel layer. Acquired knowledge in this area was found interesting for our pharmaceutical company Krka, for which numerous studies were conducted within the last year.

The method of application of the gradient pulses in combination with the spin-echo (PGSE method) enables measurement of the translational motion. In this method there several free parameters of the PGSE sequence, which may affect how sensitive this method is for detection of the diffusion spectrum. The same method can be adjusted for measurement of the fast motion on a short time scale as well as of the slow motion on the longer time scale, depending on the parameters of the method. These features of the PGSE method were confirmed by measurements on molten polyethylene. The results confirm a model of constraint release in a system of entangled polymer chains as a sort of tube Rouse motion. The results of this research were published in the Journal of Magnetic Resonance.

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 2013, the Department had cooperations with 108 partners from Slovenia and abroad. Among them:

- The high magnetic field centers in Grenoble, France, and Nijmegen, The Netherlands
- The high magnetic field center 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 Saarbrücken 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 Delbrück Center for Molecular medicine in Berlin
- The Dartmouth Medical School, Hanover, NH, USA
- The Mayo Clinic, Rochester, USA

made the above studies possible.

### Some outstanding publications in the past year

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., Bomholdtravnbsbaek, 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  $\text{LiZn}_2\text{BH}_4$ . *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  $\text{FeTe}_2\text{O}_5$ . *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/ncomms 2486.2013
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 ( $\text{WO}_x$ ) 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)

### Some outstanding publications in 2012

1. Guttmann, P., Rembein, S., Bittencourt, C., Umek, P., Ke, Xi., van Tandeloo, G., Ewels, C. P., Schneider, G.: Nanoscale spectroscopy with polarized X-rays by NEXAFS-TXM. *Nature Photonics* **6**, 25–29 (2012)
2. Dolinšek, J.: Electrical and thermal transport properties of icosahedral and decagonal quasicrystals. *Chem. Soc. Rev.* **41**, 6730–6744 (2012)
3. Pregelj, M., Zorko, A., Zaharko, O., Arčon, D., Komelj, M., Hillier, A. D., Berger, H.: Persistent spin dynamics Intrinsic to amplitude-modulated long-range magnetic order. *Phys. Rev. Lett.* **109**, 227202-1-5 (2012)
4. Novak, N., Pirc, R., Wencka, M., Kunjak, Z.: High-resolution calorimetric study of  $\text{Pb Mg}_{1/3} \text{Nb}_{2/3} \text{O}_3$  single crystal. *Phys. Rev. Lett.* **109**, 037601-1-5 (2012)
5. Zupančič, B., Diez-Berart, S., Finotello, D., Lavrentovich, O. D., Zalar, B.: Photoisomerization-controlled phase segregation in a submicron confined azonematic liquid crystal. *Phys. Rev. Lett.* **108**, 257801-1-5 (2012)
6. Vilfan, A.: Optimal shapes of surface slip driven self-propelled microswimmers. *Phys. Rev. Lett.* **109**, 128105-1-5 (2012)
7. Hwang, W. S., Remškar, M.: Transistors with chemically synthesized layered semiconductor  $\text{WS}_2$  exhibiting  $10^5$  room temperature modulation and ambipolar behavior. *Appl. Phys. Lett.* **101**, 013107-1-4 (2012)
8. Essone Mezeme, M., Kranjc, M., Bajd, F., Serša, I., Brosseau, C., Miklavčič, D.: Assessing how electroporation affects the effective conductivity tensor of biological tissues. *Appl. Phys. Lett.* **101**, 1–4 (2012)
9. Bajd, F., Vidmar, J., Fabjan, A., Blinc, A., Kralj, E., Bizjak, N., Serša, I.: Impact of altered venous hemodynamic conditions on the formation of platelet layers in thromboemboli. *Thromb. Res.* **129**, 158–163 (2012)

### Awards and appointments

1. Matjaž Gomilšek: Prešeren Award of the Faculty of Mathematics and Physics for Diploma thesis, University of Ljubljana, Ljubljana, Time irreversible billiards
2. Primož Koželj: Best paper award, Ljubljana, The European Integrated Center for the Development of New Metallic Alloys and Compounds, C-MAC days 2013, Ljubljana
3. Zdravko Kutnjak: Mentor awards in 2013, the Society of Young Researchers Slovenia

### Organization of conferences, congresses and meetings

1. "C-MAC days 2013", Ljubljana, Slovenia, 9.–12. 12. 2013

### Patent granted

1. Janez Pirš, Matej Bažec, Silvija Pirš, Bojan Marin, Bernarda Urankar, Dušan Ponikvar, Variable contrast, wide viewing angle LCD light-switching filter, US8542334 (B2), US Patent Office, 24.9.2013.
2. S. G. Psakhie, Volia Isaevich Itin, D. A. Magajeva, O. G. Terehova, E. P. Najden, Olga Vasiljeva, Georgij Mihajlov Andrejevič, Urška Mikac, Boris Turk, Contrast agent for T1 and/or T2 magnetic resonant scanning and method for preparing it, RU2471502 (C1), Federal'naja služba po intelektual'n'noj so'stvennosti, 10.1.2013.
3. Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih, Procedure for synthesis of threadlike tungsten oxide  $\text{W}_5\text{O}_{14}$ , US8496907 (B2), US Patent Office, 30.7.2013.



## INTERNATIONAL PROJECTS

- MERCK - AFM Investigations  
Merck KGaA  
Asst. Prof. Miha Škarabot
- 7FP - DIAGNO-RAIL; Combining Innovative Portable Visual, Acoustic, Magnetic and NMR Methods with In-situ Chemical Diagnostic Tools for Effective Failure Assessment and Maintenance Strategy of Rail and Subway Systems  
European Commission  
Prof. Janez Dolinšek
- 7FP - LEMSUPER; Light Element Molecular Superconductivity: An Interdisciplinary Approach  
European Commission  
Prof. Denis Arčon
- 7FP - ESNSTM; Electron Spin Noise Scanning Tunneling Microscopy  
European Commission  
Prof. Janez Dolinšek
- 7FP - NanoMag; Magnetic Nanoparticles and Thin Films for Spintronic Applications and High Performance Permanent Magnets  
European Commission  
Prof. Janez Dolinšek
- 7FP - NEMCODE; Controlled Assembly and Stabilisation of Functionalised Colloids in Nematic Liquid Crystals  
European Commission  
Prof. Igor Muševič
- COST MP1003; ESNAM - European Scientific Network for Artificial Muscles  
COST Office  
Prof. Boštjan Zalar
- COST; IMC-SRM; Network for Intermetallic Compounds as Catalysts for Steam Reforming of Methanol  
COST Office  
Prof. Janez Dolinšek
- NATO ARW 984375; Magnetic Resonance Detection of Explosives and Illicit Materials, 2.-7.9.12, Turkey  
NATO - North Atlantic Treaty Organisation  
Asst. Prof. Tomaž Apih
- COST MP1201; Rational Design of Hybrid Organic-Inorganic Interfaces: The Next Step Towards Advanced Functional Materials  
COST Office  
Dr. Polona Umek
- Factor Xa Dimerization and Its Role in Prothrombinase Complex Formation and Activity on Membrane Surfaces  
Slovenian Research Agency  
Dr. Marjeta Šentjurc
- Synthesis, Microscopy Characterization and Magneto Resonance Study of New Functional Nanomaterials  
Slovenian Research Agency  
Dr. Polona Umek
- Unconventional Ground States of Quantum Matter  
Slovenian Research Agency  
Dr. Martin Klanjšek
- Exotic Electronic Properties arising from Geometrical Symmetry  
Slovenian Research Agency  
Prof. Denis Arčon
- Physiological Role of Factor Xa and Protein S in Coagulation and Inflammation  
Slovenian Research Agency  
Dr. Tilen Koklič
- Novel Polymeric and Ionomeric Materials with Giant Dielectric and Electrocaloric Response  
Slovenian Research Agency  
Asst. Prof. Vid Bobnar
- Liquid Crystals Blue Phases in Confined Geometries: Structure, Optical Properties and Photonic Applications  
Slovenian Research Agency  
Prof. Igor Muševič
- Elastically Tuned Soft Nanocomposites  
Slovenian Research Agency  
Prof. Samo Kralj
- Promotion of Science and Cooperation of International Scientific Associations  
European Commission  
Prof. Igor Muševič

## RESEARCH PROGRAMS

- Magnetic Resonance and Dielectric Spectroscopy of „Smart“ New Materials  
Prof. Janez Dolinšek

- Physics of Soft Matter, Surfaces and Nanostructures  
Prof. Slobodan Žumer
- Experimental Biophysics of Complex Systems  
Prof. Igor Serša

## R&D GRANTS AND CONTRACTS

- New Metallic Materials for Thermal Storage of Digital Information  
Prof. Janez Dolinšek
- Design, Formulation and Characterization of Biomimetic Nanocomposite Systems for Effective Tissue Regeneration  
Dr. Mojca Urška Mikac
- Theory of the Nematic Nanodroplet and Ordering of DNA, Encapsidated in Simple viruses  
Asst. Prof. Andrej Vilfan
- Collective and Molecular Dynamics of Photosensitive Liquid Crystal Elastomers  
Prof. Boštjan Zalar
- Use of Green Energy Sources: New Functional Nanomaterials on the Base of Polyoxometalates and TiO<sub>2</sub> Nanostructures for Production of Hydrogen by Catalytic Oxidation of Water -NANOleaf  
Dr. Polona Umek
- Oligomers of Amyloidogenic Proteins from A to Z: Biophysical Properties, Structure, Function and Mutual Interactions  
Asst. Prof. Miha Škarabot
- Optimization Strategies in Biological and Artificial Microfluidic Systems  
Asst. Prof. Andrej Vilfan
- Selective and Hipsensitive Microcapacitive Sensor System for Targeted Molecular Detection in the Atmosphere  
Prof. Igor Muševič
- Textured Ceramic Layers for Sensors and Actuators  
prof. dr. Zdravko Kutnjak
- Optical Microresonators Based on Liquid Crystals  
Prof. Igor Muševič
- Biotechnological Processes of Treatment of Lignocellulosic Materials  
Prof. Janez Štrancar
- Behaviour of Dissipative Systems Under Extreme Thermo-Mechanical Loading  
Dr. Andrej Zorko
- Water Exclusion Efficacy, Measure for Prediction of Wood Performance against Wood Decay Fungi  
Prof. Igor Serša
- New Materials for Power Conversion: Oxide Semiconductor Thermoelectrics  
Prof. Boštjan Zalar
- A Spectrometer for Automatic <sup>14</sup>N Nuclear Quadrupole Resonance Characterization of New Substances  
Dr. Alan Gregorovič
- Exchange Interactions in Selenides and Tellurides – Key for New Functional Low-Dimensional Magnetic Systems  
Dr. Matej Pregelj
- TABANA: Targeting Antimicrobial Activity via micro/Nano-structured surfaces for civil Applications  
Prof. Janez Štrancar
- Nanomaterials and Scaffolds Preparation and Characterization  
Prof. Janez Štrancar
- New Polymer and Ceramic Materials for Potential Use in Capacitors  
Dr. Andreja Eršte
- Influence of Mechanical Field on Electrical Properties of Oxide Semiconductor Materials  
Dr. Nikola Novak
- Irradiation and Analysis of Si Samples  
Prof. Igor Muševič

## NEW CONTRACTS

- Protocol for Validation of the Analytical Method  
Lek d. d.  
Asst. Prof. Miha Škarabot
- A Spectrometer for Automatic <sup>14</sup>N Nuclear Quadrupole Resonance Characterization of New Substances  
Gorenje Gospodinski Aparati d.d.  
Dr. Alan Gregorovič
- Balder - Technology Development  
BALDER d.o.o.  
Prof. Igor Muševič
- Behaviour of Dissipative Systems under Extreme Thermo-Mechanical Loading  
BALDER d.o.o.  
Prof. Igor Muševič

## VISITORS FROM ABROAD

1. Dr. Hae Jin Kim, Nano-Energy Materials Team, Korea Basic Science Institute, Daejeon, South Korea, 1. 3. 2012–28. 2. 2013
2. Dr. Adam Ostrowski, Poland, EUPF7 project "ESR-STM", 1. 11. 2012–31. 10. 2013
3. Mag. Venkata Subba Rao Jampani, India, EU Marie-Curie, 1. 11. 2009–15. 7. 2013
4. Maryam Nikkhou, Iran, EU Marie-Curie, 1. 6. 2012–31. 12. 2013
5. Dr. Anna Ryzhkova, Russia, EU project Marie-Curie, 1. 6. 2012–31. 1. 2013
6. Dr. Mirta Herak, Institute of Physics, Zagreb, Croatia, 4.–5. 1. 2013
7. Silvio Preda, Ilie Murguescu Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania, 14.–25. 1. 2013
8. Prof. Yishay Manassen, Ben Gurion University, Beer Sheva, Israel, 5.–12. 2., 17. 9. 2013
9. Prof. David Sherrington, University of Oxford, Oxford, Great Britain, 13.–14. 2. 2013
10. Dr. Sanjiv Sonkaria, Dr. Varsha Khare, Seoul National University, Kwanak, Seoul, South Korea, 15.–30. 3. 2013
11. Prof. Horst Beige, Martin-Luther Universitaet, Halle, Germany, 18. 3. 2013–21. 3. 2013
12. Dr. Magdalena Wencka, Polish Academy of Sciences, Institute of Molecular Physics, Poznan, Poland, 3. 4.–30. 4., 23. 11.–15. 12. 2013
13. Prof. Luigi Colombo, Texas Instruments Incorporated, Texas, USA, 9. 4. 2013
14. Dr. Shehab Mansour Hassan, University of Menofia, Menofia, Egypt, 14. 4.–27. 4. 2013
15. Dr. Giorgio Mirri, Italy, EU Marie-Curie project, 6. 5. 2013–6. 5. 2015
16. Nerea Sebastian Ugarteche, Universidad del Pais Vasco UPV/EHU, Leioa, Spain, 16. 4.–3. 6. 2013
17. Prof. Wilfried Schranz, University of Vienna, Faculty of Physics, Vienna, Austria, 27. 5.–30. 5. 2013
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20. Dr. Valentina Domenici, Università di Pisa, Pisa, Italy, 15. 7.–15. 8. 2013
21. Donatella Ancora, Università di Pisa, Pisa, Italy, 15. 6.–15. 10. 2013
22. Mutsuo Igarashi, Gunma National College of Technology, Maebashi, Japan, 5. 8.–22. 9., 12. 10.–12. 11., 28. 11.–27. 12. 2013
23. Dr. Rama Rao Partibho, Raman Research Institute, Bangalore, India, 7. 9.–21. 9. 2013
24. Dr. Takehito Nakano, University of Osaka, Toyonaka, Osaka, Japan, 8. 9.–13. 9. 2013
25. Prof. Qiming Zhang, University of Pennsylvania State, Pennsylvania, USA, 18.–21. 9. 2013
26. Džiugas Jablonskas, University of Vilnius, Faculty of Physics, Vilnius, Lithuania, 23. 9.–31. 12. 2013
27. Dr. Toni Shiroka, ETH Zuerich, Hoenggerberg, Laboratorium fuer Festkoerperphysik, Zurich, Switzerland, 6. 11.–8. 11. 2013
28. Dr. Katarina Čirić, dr. Jana Radaković, Vinča Institute of Nuclear Sciences, University of Belgrade, Serbia, 12. 11.–17. 11. 2013
29. Dr. David Wilkes, Merck, Darmstadt, Germany, 14. 11.–15. 11. 2013
30. Dr. Andriy Nych, National Academy of Science of Ukraine, Kiev, Ukraine, 19. 11. 2013–31. 1. 2014
31. Dr. Uliana Ognysta, National Academy of Science of Ukraine, Kiev, Ukraine, 19. 11. 2013–15. 12. 2013
32. Dr. Ticijana Ban, Institute of Physics, Zagreb, Croatia, 20. 11. 2013
33. Dr. Valentin Laguta, Ukrainian Academy of Sciences, Kiev, Ukraine, 24. 11.–15. 12. 2013
34. Dr. Emmanuella Lacaze, Institut des Nano-Sciences de Paris, Paris, France, 10.–13. 12. 2013
35. Dr. Anna Ryzhkova, ASML, Eindhoven, The Netherlands, 11. 12.–16. 12. 2013
36. Dr. Jun-ichi Fukuda, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, 18. 12. 2013–11. 2. 2014

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## ORIGINAL ARTICLE

- Andreja Abina, Uroš Puc, Anton Jeglič, Aleksander Zidanšek, "Structural analysis of insulating polymer foams with terahertz spectroscopy and imaging", *Polym. test.*, vol. 32, issue 4, pp. 739-747, 2013.
- Denis Arčon, Kristjan Anderle, Martin Klanjšek, A. Sans, C. Mühle, P. Adler, W. Schnelle, M. Jansen, C. Felser, "Influence of O<sub>2</sub> molecular orientation on p-orbital ordering and exchange pathways in Cs<sub>4</sub>O<sub>6</sub>", *Phys. rev., B, Condens. matter mater. phys.*, vol. 88, no. 22, pp. 224409-1-224409-7, 2013.
- Denis Arčon, Andrej Zorko, Peter Jeglič, Jingtao Xu, Jun Tang, Yoichi Tanabe, Satoshi Heguri, Katsumi Tanigaki, "Rattler site selectivity and covalency effects in type-I clathrates", *J. Phys. Soc. Jpn.*, vol. 82, no. 1, pp. 014703-1-014703-6, 2013.
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- Vid Bobnar, Hana Uršič, Goran Casar, Silvo Drnovšek, "Distinctive contributions to dielectric response of relaxor ferroelectric lead scandium niobate ceramic system", *Phys. status solidi, b Basic res.*, vol. 250, no. 10, pp. 2232-2236, 2013.
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