YOUNG MULTIS 2021

Multiscale Phenomena in Condensed Matter
Online conference for young researchers

Kraków, 5 – 7 July 2021

Institute of Nuclear Physics
Polish Academy of Sciences

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Dear Colleagues, dear Friends,

It is our great pleasure and honour to welcome you to the conference ”Multiscale phenomena in condensed matter — Young Multis 2021”, the online meeting held on 5 – 7 July. The meeting is addressed to students and young researchers. We are happy that you found our idea of a scientific meeting devoted to a wide scope of research into condensed matter materials interesting and worth joining. The rich subject area of the conference, comprising structure, dynamics, relaxation, magnetism and other properties, as well as great diversity of materials, from liquid crystals to molecular nanomagnets, and a variety of experimental techniques, reflects somehow the investigations we have been conducting in the H. Niewodniczański Institute of Nuclear Physics Polish Academy of Sciences for a long time. Our intention is to promote collaborative research among physicists, chemists and natural scientists, which may bring new ideas and important results. For this purpose, a series of biennial Multis conferences dedicated to studies of molecular dynamics and related problems was organized. Staying in a steady contact with the participants of our previous Multis conferences, we decided to arrange a short-time online forthcoming event dedicated to young scientists.

The conference is organized by the Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences. The Institute was established in 1955, the founder and first director was Professor Henryk Niewodniczański. Even though the main research concerns particle and nuclear physics, the condensed matter physics together with other disciplines like nano-materials engineering, dosimetry or medical physics, are being explored as well.

We welcome all of you to the conference and firmly hope that Young Multis 2021 will be an important and valuable scientific event. We expect that lectures and posters will initiate interesting and stimulating discussions. During the Young Multis 2021 conference closing the prizes for the best posters and best oral presentation will be awarded and plans for a follow-up meeting will be announced.

Mirosław Gałązka — Magdalena Fitta

Chairman — Co-chairwoman

The historical panorama of Kraków at the Welcome page is a copy of the copperplate engraving by Meriam Matthaus Elder. In 1619 he wrote „Cracovia Totius Poloniae urbs celeberimma atque amplissima regia atque Academia insignis" (Most celebrated and splendid city in all Poland notable by the royal castle and Academia).

Design of our Logo was inspired by the mosaic from Pompeii (Casa degli Amorini Dorati) as it mimics the multiscale path. The TEX code to draw the mosaic was first published by Daniel Steger http://www.texaple.net/tikz/examples/mosaic-from-pompeii

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Opening lecture — Stephen Blundell

Opening lecture, Mon./10:00

Using muons to study condensed matter physics

S. Blundell

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Muons, radioactive particles produced in accelerators, have emerged as an important tool to study problems in condensed matter physics and chemistry. Beams of muons with all their spins polarized can be used to investigate a variety of static and dynamic effects and hence to deduce properties concerning magnetism, superconductivity, molecular or chemical dynamics and a large number of other phenomena.

I will describe how this technique works and, in particular, how it can be applied to molecular systems. I will give a recent example of how a muon implanted in a fluoride crystal realizes a coherent quantum system, and how the entanglement of muon and nearest-neighbour fluorine nuclear spins gives rise to an oscillatory time dependence of the muon polarization that can be detected and measured.

The decohering effect of more distant nuclear spins can be modelled quantitatively, allowing a very detailed description of the decoherence processes coupling the muon-fluorine ”system” with its ”environment”, and allowing us to track the system entropy as the quantum information degrades. These results show how to precisely quantify the spin relaxation of muons implanted into quantum entangled states in fluoride crystals.

Session I: Conductivity, superconductivity

Contributed talk, Mon./11:00

Stabilization of antiferromagnetic ordered state in π-d system of λ-(BEDT-STF)$_2$Fe$_x$Ga$_{1-x}$Cl$_4$

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Molecular π-d systems, in which π and 3d electrons coexist, show various unique conducting and magnetic properties. For example, λ-(BETS)$_2$FeCl$_4$, where BETS is bis(ethylenedithio)tetraselenafulvalene, shows an antiferromagnetic (AF) transition accompanying a metal-insulator transition at 8.3 K, although λ-(BETS)$_2$GaCl$_4$, which is an isostructural compound with nonmagnetic anions, shows a superconducting transition at 5 K. λ-(BETS)$_2$GaCl$_4$ shows an unconventional magnetic state in the insulating phase that the 3d spins behave as if they stay paramagnetic even below T_{N}. It has been argued that the strong magnetic interaction between π and 3d spins, which is called π-d interaction, plays a crucial role for the unconventional magnetism.

λ-(BEDT-STF)$_2$FeCl$_4$, where BEDT-STF is bis(ethylenedithio)diselenadithiafulvalene, shows an AF transition $T_{\mathrm{N}} = 16$ K. On the other hand, λ-(BEDT-STF)$_2$GaCl$_4$ shows no magnetic transitions down to 0.3 K. The stabilization of the AF ordering in λ-(BEDT-STF)$_2$FeCl$_4$ is expected to be related to π-d interaction. To study the stabilization mechanism of the AF ordering, we performed ^{13}C NMR measurement on λ-(BEDT-STF)$_2$Fe$_x$Ga$_{1-x}$Cl$_4$ ($x = 0.05; 0.1; 0.2; 0.4; 0.6; 0.8$).

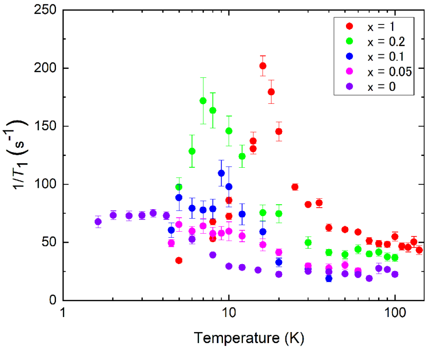

Figure 1. Temperature dependence of nuclear spin-lattice relaxation rate ($1/T_1$).

Figure 1. shows the temperature dependence of nuclear spin-lattice relaxation rate ($1/T_1$). We found that the AF transition temperature decreases with decreasing Fe content x. The transition temperature of λ-(BEDT-STF)$_2$Fe$_{0.2}$Ga$_{0.8}$Cl$_4$ remains at $T_{\mathrm{N}} = 8$ K. Even though a sharp anomaly was observed at $x = 0.2$, the divergence of $1/T_1$ was suppressed and no clear peaks were observed below $x = 0.1$. These results suggest that the introduction of a small amount of 3d spins drastically stabilizes the AF ordering at around $x \approx 0.2$. In this presentation, I will discuss the role of π-d interaction for the stabilization of the AF ordering.

CONTRIBUTED TALK, MON./11:15

Magnetic-field-induced transition of charge-glass former containing a magnetic transition metal

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Geometrical frustration can induce exotic electronic and magnetic states in low temperatures. Charge-glass (CG) state is a novel electronic state caused by the frustration effect of the Coulomb repulsion between itinerant electrons, which is discovered in organic charge-transfer complexes with a triangular lattice.(1) In the CG state, two kinds of short-range domains of charge order patterns coexist randomly. A variety of unique transport properties due to the instability and inhomogeneity of this CG state has been reported.(2,3)

An organic conductor θ-(BEDT-TTF)$_2$CsCo(SCN)$_4$ (CsCo salt) is one of the candidates of the CG former. This compound contains magnetic ions Co^{2+} ($S = 3/2$) in the insulating layers. In organic conductors containing magnetic ions, it is possible that π electrons in conducting layers and localized d-spins in insulating layers can interact with each other, leading to anomalous magnetic responses. In the case of the CsCo salt, a novel magnetic field response of the physical properties is expected due to the interaction between localized d-spins and electrons in the CG state.

In this study, we perform the thermodynamic and transport studies on the CsCo salt under magnetic fields. The heat capacity measurement reveals the presence of a magnetic-field-induced transition showing a sharp thermal anomaly in this compound. In addition, the magnetic heat capacity of Co^{2+} ions shows an anomalous temperature dependence, suggesting that the transition is possibly induced by the π-d interaction in the CsCo salt. In our presentation, we will talk about the transport and thermodynamic properties of this compound under magnetic fields in detail.

(1) F. Kagawa et al., Nature Physics 9, (2013), 419-422
(2) F. Sawano et al., Nature, 437 (2005), 522-524
(3) Y. Takahide et al., Phys. Rev. Lett., 98 (2007), 116602

CONTRIBUTED TALK, MON./11:30

Kohler's rule in cuprates

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In cuprate high-temperature superconductors, the normal state exhibits a plethora of unusual phenomena. A theory which aims at describing the elusive mechanism of high-temperature superconductivity should be based on a comprehensive understanding of these phenomena across the temperature-doping phase diagram. Despite the complexity, we have recently demonstrated that the scattering rate $1/\tau$ behaves remarkably simple. Independent of cuprate compound and doping, it is quadratic in temperature, as in a Fermi-liquid — thus it is universal for cuprates.(1,2) Here, we will demonstrate that Kohler's rule is obeyed throughout the phase diagram of cuprates and provide further evidence of the universal scattering rate. In its essence, Kohler's rule states that, in a Fermi-liquid, the magnetoresistance $\delta\rho/\rho_0$ should be a function of $H\tau$ (H is the magnetic field): $\delta\rho/\rho_0 = F(H\tau)$. By applying this scaling to a variety of magnetoresistance data obtained at different doping levels and cuprate families, we confirm the universality of the scattering rate.(1) As shown in the figure, data for different compounds (Hg1201: this work; LSCO: this work as well as Refs. [3] and [4]; Tl2201: Ref. [5]) fall on a single line. Deviations at low fields are related to paraconductivity contributions close to T_c.

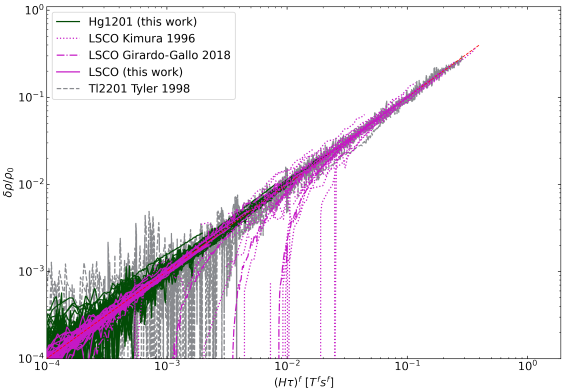

Figure 1. Magnetoresistance $\delta\rho/\rho_0$ versus $F(H\tau) = (H\tau)^f$, where f is a sample dependent parameter, H the magnetic field and τ the lifetime from Ref. [1].

(1) N. Barišić et al., New J. Phys., 21 (2019), 113007
(2) D. Pelc et al., Sci. Adv., 5 (2019), eaau4538
(3) T. Kimura et al., Phys. Rev. B, 53 (1996), 8733
(4) P. Giraldo-Gallo et al., Science, 361 (2018), 479
(5) A. W. Tyler et al., Phys. Rev. B, 57 (1998), R728

Contributed talk, Mon./11:45

Thermodynamic picture of a quantum liquid-liquid transition occurring in the geometrically frustrated organic complexes

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In this presentation, we discuss novel quantum mechanical features of molecule-based compounds studied by thermodynamic measurements using micro single crystals weighing in the microgram order. The compounds we are interested in are alloying charge transfer complexes withchemical formula of κ-$[(\mathrm{BEDT\text{-}TTF})_{1-x}(\mathrm{BEDT\text{-}STF})_x]_2\mathrm{Cu}_2(\mathrm{CN})_3$. The compounds have layered structures of organic donor molecules and counter anions. The charge transport and magnetic properties dominated by electron correlations of π-electrons appear in the organic layers. The donors form a dimer-triangle arrangement typical for the κ-type structure in the layer and the magnetic interactions between dimers show frustrated character.(1) The pristine compound of κ-$(\mathrm{BEDT\text{-}TTF})_2\mathrm{Cu}_2(\mathrm{CN})_3$ are known to show spin liquid ground state.(2) By alloying with BEDT-STF, the overlap of the molecular orbital increases and the system becomes gradually conductive. The electronic ground state changes from the spin liquid state to metallic state around the boundary of X = 10–12%.(3) Therefore, the quantum mechanical change of electronic states occurs across the boundary as a pure Mott transition. Since both sides of the transition have spin itinerancy, this phase boundary can also be considered as a quantum liquid-liquid phase transition.

We performed the systematic heat capacity measurements from the insulating spin-liquid region (SL) to the conductive Fermi liquid (FL) region. The electronic heat capacity gives finite γ values in all concentrations studied. The gapless features for the spin liquid region are consistent with the thermodynamic features of the pristine compound which has $\gamma = 12.6$ mJK^{-1}mol^{-1} and other intermetallic compounds showing spin liquid ground states. The γ values shows slight increase in the SL region and then shows step like increase around X = 10–12% corresponding to the boundary. Those in the metallic region above this concentration has larger γ values in the range of 20–30 mJK^{-2}mol^{-1}. The step like increase around the boundary is interpreted as the closing of the gap due to the charge degrees of freedom. The results can be understood as the formation of Fermi-surface of the spin excitations namely called as spinons. It is interesting to indicate the formation of spinon Fermi-surface in such insulating system where only the spin degrees of freedom shows itinerancy. We also discuss magnetic field effects for the low energy excitations from the analyses of heat capacity data under magnetic fields up to 10 T. Although small change of low temperature heat capacity occurs in the highly doped metallic region, the magnitude of γ values do not show drastic change by applying such high magnetic fields. The results are also consistent of the itineracy of the spins in the dime-based triangle lattice Mott-Hubbard system.

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CONTRIBUTED TALK, MON./12:00

Melting *arctic circles*

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An *arctic circle* is the name given to the phenomenon discovered by Jockush, Propp & Shor(1) when they were looking at dimer coverings of the so-called "Aztec diamond". They found that in the limit of an infinitely large diamond a well-defined curve appeared that demarcated two regions: one in which the dimers were "frozen" — their location was known exactly — and one in which the dimers fluctuated. The shape of this curve was a circle. It gradually became clear that this phenomenon was more widespread, in particular in the context of condensed matter, e.g. six-vertex model, XX chain, when one considers the return probability of electrons.(2) That is, given an initial configuration of electrons, known as a Domain Wall Initial State (DWIS), what is the probability they return to the same configuration at some later time, t (calculations are in fact often done in Wick-rotated imaginary time, $\tau = it$). For the XX chain on a line, with DWIS corresponding to full occupancy for $x < 0$ and emptiness for $x > 0$ and $\tau = 2R$, the density profile of electrons forms a perfect arctic circle(2).

The present work explores what happens when the DWIS for the XX chain is amended so that only an interval $[-L/2, L/2]$ is fully occupied. We find that when $L > 2R$ the electrons' density profile forms two well-separated arctic circles but, once $L \leqslant 2R$, the circles touch, a phase transition occurs and the electrons' density profile quantitatively changes-something which we affectionately refer to as the arctic circles "melting". Remarkably, this transition is third order and of the kind first discussed by Gross-Witten in Ref. [3]. Here we will present the calculations and figures detailing this transition as well as future areas of work.

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(3) D.J. Gross et al., Phys. Rev. D, 21 (1980), 446

Session II: Molecular magnetism

CONTRIBUTED TALK, MON./13:15

Magnetic properties of Ni(*fum*)(*phen*)-ferromagnetic dimer with spin 1

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This work is devoted to the experimental study of magnetocaloric effect in Ni(*fum*)(*phen*) (*fum* = fumarato, *phen* = 1,10-phenanthroline). The compound has been identified as a two-dimensional system of the array of antiferromagnetic $S = 1$ dimers.(1) The monoclinic crystal structure forms layers of Ni dimer connected by bridging fumarato ligands. The measurements established in Ni(*fum*)(*phen*) the single-ion magnetic anisotropy D comparable to the intradimer exchange coupling $J, D/J \approx 1$ and $D/\mathrm{k_B} \approx -6$ K.

Magnetic properties were studied by means of magnetization and heat capacity measurements on polycrystalline sample. A magnetic phase transition has been not observed down to 0.4 K in zero magnetic field. For magnetocaloric effect analysis, isothermal magnetic curves of Ni(*fum*)(*phen*) in the temperature range from 1.8 to 44 K in magnetic field up to 7 T were measured. Sizeable conventional magnetocalorical effect has been found around 5.8 K, where $-\Delta S_{\max} = 8.2$ J/(K·kg) for $\Delta \mathrm{B} = 7$ T. From theoretical analysis of magnetocaloric effect has been found the parameters of singleion anisotropy $D/\mathrm{k_B} \approx -11.5$ K, a rhombic anisotropy $E/\mathrm{k_B} \approx -3.4$ K and the intradimer ferromagnetic exchange coupling $J/\mathrm{k_B} \approx 2.5$ K. Theoretical analysis also shows that the presence of ferromagnetic coupling increases the magnetocaloric effect. Investigation of magnetocaloric properties of Ni(*fum*)(*phen*) suggest that the studied system can be considered as a good material for magnetic cooling at low temperatures.

This work was supported by the Slovak Research and Development Agency Project No.APVV-18-0197

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Contributed talk, Mon./13:30

The synthesis and properties of Prussian blue and its Cr analog nanotubes

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Molecular magnets are compounds assembled out of discrete building blocks, e.g. coordination complexes or organic molecules, that exhibit magnetic properties and can be treated as multifunctional materials. The continuous increase in the interest in molecular magnets can be seen in recent years. Some of them can combine multiple attractive properties, such as low density, the high magnetic moment per unit of volume, or the sensitivity for external stimuli, including temperature and pressure. Prussian blue (PB) and Prussian blue analogs (PBAs) are one of the best-known groups of molecular magnets, especially due to their functional properties (sorption capacity, photomagnetism). It is possible to manufacture these compounds in various forms, e.g. bulk, thin films, or nanoparticles by applying different synthesis methods. The impact of size reduction on magnetic properties is one of the crucial factors to investigate.

In this work, we present the synthesis and physicochemical characterization of the nanotubes composed of Prussian blue ($\mathrm{Fe^{III}Fe^{II}}$) and its Cr analog ($\mathrm{Fe^{II}Cr^{III}}$). The process of manufacturing samples by template-assisted electrochemical deposition is described in detail. The porous polycarbonate (PCTE) membranes covered by a thin film of Au were used as the working electrode in a three-electrode electrochemical cell. The samples were fabricated inside the PCTE membranes of different pore sizes: 50, 80, 100, and 200 nm.

The analysis of scanning electron microscope (SEM) microphotographs confirmed that nanotubes of cylindrical shape with outer diameters from 50 to 200 nm were obtained for both samples. The measurements of magnetic properties showed that synthesized materials are ferromagnets with critical temperatures T_c around 4 K and 20 K for $\mathrm{Fe^{III}Fe^{II}}$ and $\mathrm{Fe^{II}Cr^{III}}$ respectively. These T_c values are comparable to those observed for bulk as well as thin films. This work also covers the core-shell nanotubes composed of both base compounds.

Acknowledgments: W.S. acknowledges the Polish National Science Centre (Grant PRELUDIUM 16: UMO-2018/31/N/ST5/03300) for financial support.

Contributed talk, Mon./13:45

Tuning of magnetic properties of the 3D 2-fold interpenetrating CN-bridged networks

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The formation of interpenetrating networks is relatively rare among CN-bridged assemblies. The known compounds are almost exclusively based on diamagnetic cyanidometallates with low coordination numbers.(1,2) We have recently reported the first three-dimensional interpenetrating network based on diamagnetic $[Mo(CN)_8]^{4-}$ complex which resulted in paramagnetic characteristic of the coordination system.(3) In order to improve the magnetic properties, we have designed a new family of 3D two-fold interpenetrating networks based on paramagnetic $[Ni(\mathit{cyclam})]^{2+}$ and $[Nb(CN)_8]^{4-}$ building blocks of the general formula: $[Ni(\mathit{cyclam})]_5[M(CN)_4][Nb(CN)_8]_2 \cdot nH_2O$ (M = Ni, Pd, Pt). The structures consist of two independent subnetworks, each composed of 2D honeycomb-like layers linked in the third dimension by the linear trimetallic linkages that pass through the center of the hexagonal openings of the another subnetwork. The structures contain discrete cavities filled with crystallisation water molecules that can be reversibly removed or exchanged, what results in structural transformations, often with retention of crystallinity. The type and amount of crystallisation solvent molecules accommodated in the structure strongly influences the magnetic behaviour of the coordination systems. Moreover, the size of the metal in in the diamagnetic $[M(CN)_4]^{2-}$ linker affects the sorption properties of the networks.

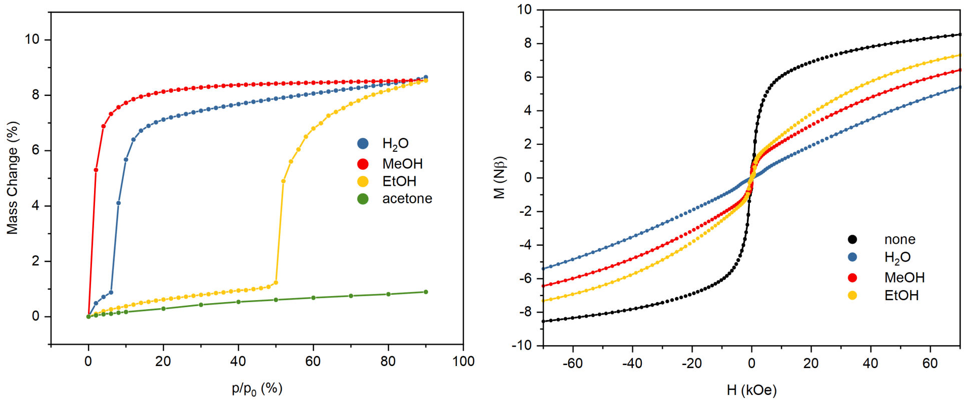

Figure 1. Dynamic vapor sorption studies at 25°C (left) and magnetization vs. magnetic field plot at 1.8 K (right) for $[Ni(\mathit{cyclam})]_5[Pt(CN)_4][Nb(CN)_8]_2 \cdot$ solv.

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Contributed talk, Mon./14:00

High-performance tetrahedral Er^{III} SMMs and their functionalization using radicals and photoswitchable molecules

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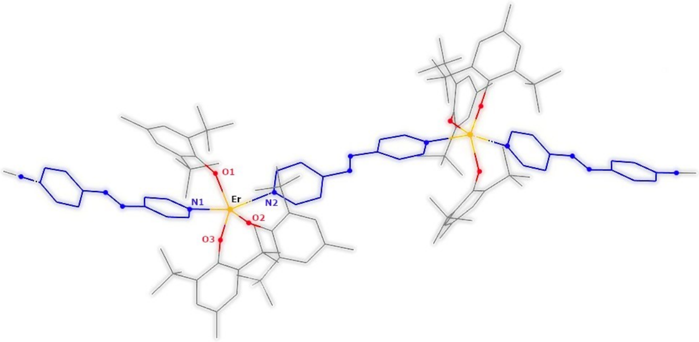
Functional single molecule magnets (SMMs) constitute one of the hottest topics in the field of molecular magnetism. Currently, lanthanide complexes are the most promising candidates for high-performance SMMs and major efforts are being made to improve their SMM characteristics.(1) Herein we present two new high-performance Er^{III} complexes with slow magnetization dynamics:(2) $[Er^{III}(TTBP)_3(THF)]$ (**1**) ($TTBP^-$ = 2,4,6-tri-tert-butyl-phenolate) and $[Er^{III}(BHT)_3(THF)]$ (**2**) (BHT^- = 2,6-di-tert-butyl-4-methylphenolate). We also demonstrate their functionalization using paramagnetic and photoswitchable molecules. Substitution of THF with TEMPO radicals in **1** (TEMPO = 2,2,6,6- tetramethylpiperidine 1-oxyl) leads to the isolation of $[Er^{III}(TTBP)_3(TEMPO)]$ (**3**) while a similar reaction of **2** with azopy (*azopy* = 4,4'-azopyridine; a photoswitchable organic molecule) results in the formation of $[Er^{III}(BHT)_3(\mu\text{-}azopy)]$ chains (**4**) (Figure 1). **1-4** are designed based on the concept of Rinehart and Long taking advantage of the prolate-shaped electron density of Er^{III}.(3)

The slow relaxation of the magnetization of **1** and **2** is controlled mainly by a Raman-like relaxation mechanism and both compounds show waist-restricted magnetic hysteresis loops at 1,8 K. Interestingly, introduction of TEMPO radicals as ligands completely disrupts the slow magnetization dynamics of the parent **1** leading to a typical paramagnetic behavior for the resulting **3**. The reaction of **2** with azopy leads to coordination chains **4**, where each Er^{III} is trigonal bipyramidal. The chains show slow magnetic relaxation typical for isolated Er^{III} SMMs and since the azopy is known to undergo photoisomerization reactions, **4** is tested for the presence of the photoswitching behavior.



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CONTRIBUTED TALK, MON./14:15

Effect of proton irradiation on magnetic properties of two-dimensional Ni(II) molecular magnet

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The broad capability of the molecular magnetic materials emerges from the variety of available systems with unique properties that can be altered by external stimuli such as temperature, pressure, light irradiation, or sorption of guest molecules. Although not popular in the field of molecular magnetism, ion irradiation is the other approach for tailoring the material's parameters. Energetic particles expose solids to the high-density local energy deposition, leading to non-linear and threshold effects that may create new materials with novel properties.

In particular, the irradiation-induced defects may give rise to the magnetism in initially non-magnetic materials and modify the magnetic properties of a system with a non-zero magnetic moment, especially when strong magneto-structural correlations are present. The studies of the response of thin films and bulk samples to ion irradiation show there is a possibility to alternate such parameters as the critical temperature, g-factor, or coercivity by energetic particles deposition. However, no systematic studies can be found regarding the effects of ion irradiation on molecular magnetic materials.

Here we examine the magnetic properties of 2D coordination polymer based on nickel sulfate and a 1,3-phenylenediamine ligand that was irradiated with 1.9 MeV protons using fluences ranging from $5{\cdot}10^{13}$ p·cm^{-2} to $2{\cdot}10^{15}$ p·cm^{-2}. The samples irradiated with the high fluence showed an increase in magnetization saturation up to 200 percent and the reduced coercive field to even 10 percent of the reference level. Simultaneously, the critical temperature remained the same ($T_c = 24.5$ K) regardless of the received radiation dose. The IR spectroscopy showed that the overall structure of the studied compound was preserved after proton irradiation, and only minor changes are present in the local structure.

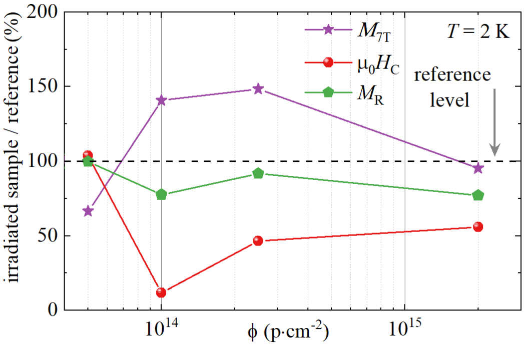

Figure 1. The relative values of magnetic hysteresis loop parameters for studied samples irradiated with various fluencies ϕ normalized to the reference sample's corresponding values. Violet points: magnetization at $\mu_0 H = 7$ T ($M_{7\mathrm{T}}$); red points: coercive field ($\mu_0 H_\mathrm{c}$); green points: remnant magnetization (M_R). The dashed line is placed at 100% and represents the values obtained for the reference sample $\phi = 0$ p·cm^{-2}. The lines between points are only for an eye guide.

CONTRIBUTED TALK, MON./14:30

Modular approach in construction of molecular magnetic materials based on molecular clusters

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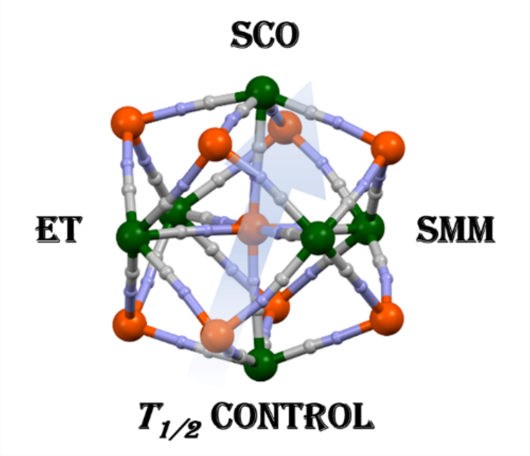
Various synthetic strategies have been developed to control dimensionality and to implement specific magnetic and optical properties into coordination systems during the recent decades, through systematic studies on structure-properties-function correlations.(1) In our study, we are mainly focused on 0-dimensional clusters with molecular bridges, which can be used as independent carriers of properties or used in the construction of more advanced coordination networks, following the Secondary Building Blocks (SBB) concept.(2)

Thanks to various modifications of the cluster core realized by combination of 3d metal ions and 5d policyanidometalates moieties, and/or by the use of organic ligands we obtained recently interesting series of molecular crystals showing essential switchable magnetic properties such as (*i*) spin crossover (SCO), (*ii*) electron transfer (ET) and/or (*iii*) single-molecule magnet (SMM) behaviour.(3,4) In this presentation we disclose the competition between SCO and ET processes and bidirectional control of $T_{1/2}$ thanks to the trimetallic composition within the $\{Fe_9[W(CN)_8]_x[W(CN)_8]_{6-x}(MeOH)_{24}\}$, $x = 1-5$, and $\{Fe_xMn_{9-x}[W(CN)_8]_6(MeOH)_{24}\}$, $x = 1-8$ series. We also disclose the control of the slow relaxation of magnetisation in the bimetallic $\{Mn_9[W(CN)_8]_6(L)_8(MeOH)_8\}$ $L = Bu^t_2bpy$, Ph_2phen series.



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Session III: Soft Matter

Contributed talk, Mon./15:00

Raman spectroscopy, SANS and MD simulation combined study of DPPC lipid bilayer: the competitive effect of cholesterol and melatonin

Y. Arynbek[1,2,3], M. Vorobyeva[1], K. Mamatkulov[1], A. Bekbaev[1,2,3], N. Kucerka[1], J. Genova[4], G. Arzumanyan[1]

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The changes of the structural properties of membrane — most likely underlying its functional modifi-cation, are known to be accompanied by the changes in membrane physico-chemical properties. The role of lipid membrane alternation in Alzheimer's disease has been proposed as a trigger mechanism of amyloid toxicity, thus the membrane-active molecules such as cholesterol and melatonin and their key role in lipid membrane properties is of great importance in understanding molecular mechanisms of membrane functioning.

In the present work, we have studied the impact of cholesterol and/or melatonin on the dynamical and static properties of DPPC phospholipid bilayers using spontaneous Raman spectroscopy, neutron scattering techniques (SANS) and molecular dynamics (MD) simulations. Raman spectroscopy is known to be a sensitive instrument for probing conformational changes manifested in the Raman spectra of biological samples under certain conditions. Primary information regarding the bilayer thickness parameters was obtained from SANS experiments. Molecular dynamics (MD) simulation on the lipid membrane system was performed using the CHARMM-GUI, VMD, PyMOL and GROMACS packages. Figure 1 illustrates some key results of our studies.

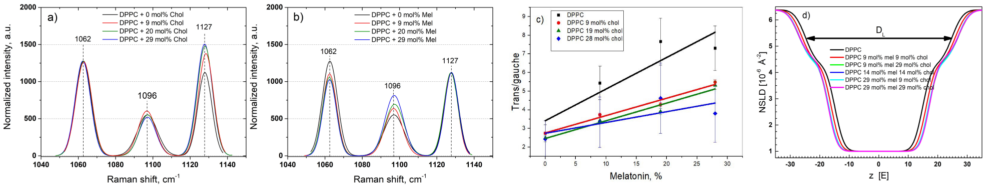

Figure 1. a) Normalized Raman spectra of DPPC/cholesterol and b) DPPC/melatonin complexes at different concentrations; c) values of trans/gauche relation calculated by MD simulation d) Neutron Scattering Length Density profiles (NSLD) for DPPC based unilamellar vesicle samples dispersed in 100% D_2O.

The impact of cholesterol on the increase of the ratio of trans/gauche conformers, accompanied by thickness increase of DPPC bilayers, prompt us to conclude that the region of hydrocarbon chains has been a primary target of cholesterol interactions and its location. These interactions were observed to be modulated by the additional presence of melatonin, though on the studied concentration range it influenced almost solely the dynamics of hydrocarbon chains while has no impact on the bilayer static structure.

The authors acknowledge support from the Joint Institute for Nuclear Research (JINR), and JINR-Bulgaria collaboration program – THEME ♯ 04-4-1133-2018/2023.

CONTRIBUTED TALK, MON./15:15

Vibrational dynamics of chiral smectogenic glassformer

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Infrared spectroscopy has been helpful to elucidate structural variations of molecules accompanying the phase transitions. Such changes become detected by description of the parameters of absorption bands (e.g. wavenumbers, full width at half maxima, areas and heights) observed on infrared spectra measured as a function of temperature. Sometimes, the direct detailed analysis of the IR spectra is difficult due to the overlapping absorption bands.

The two-dimensional correlation analysis (2D-COS) enables new possibilities of interpreting vibrational spectra collected as a function of varying external perturbation, while the perturbation-correlation moving window two-dimensional analysis (PCMW2D) is useful to detect changes in band characteristics and to provide analysis thereof by means of statistical tools. Both correlation analyses are successfully used to interpret the vibrational dynamics of compounds showing glass transition or cold crystallization processes.(1)

Today a study of vibrational dynamics of a novel chiral mesogen (Fig. 1) has been presented.(1–3) The 3F7HPhH7 compound under study is a fluorinated liquid crystal, which gained attention among liquid-crystals researches as a promising compound for the use in new-generation liquid-crystal displays. Hyperspectral FTIR data are examined by means of 2D-COS and PCMW2D analyses. FTIR spectra have been measured for different cooling-heating cycles to detect freezing-in or activation of the stochastic movements during the vitrification and the cold crystallization processes.

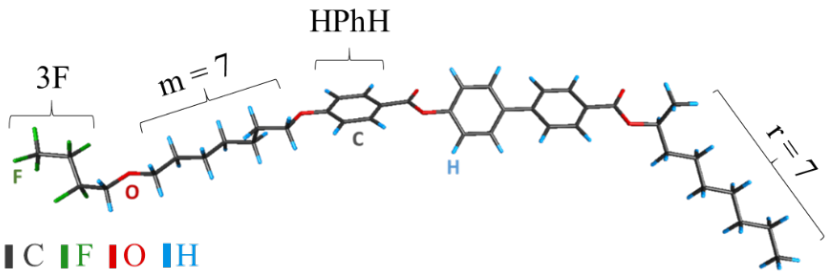

Figure 1. General structure of 3F7HPhH7, optimized with DFT method.

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CONTRIBUTED TALK, MON./15:30

Effect of cross-linking on dynamics of elastomers: insights from ^{1}H field cycling NMR

F. Martini[1], E. Carignani[2], F. Nardelli[1], E. Rossi[1], M. Cettolin[3], A. Susanna[3], S. Borsacchi[2], M. Geppi[1], L. Calucci[2]

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Long polymers experience very complex dynamics covering wide time and spatial scales.(1) ^{1}H field-cycling (FC) NMR relaxometry is an ideal technique to characterize polymer dynamics.(2) Indeed, measurements of ^{1}H longitudinal relaxation rates ($R_1 = 1/T_1$) at different Larmor frequencies allow to study dynamics on a huge range of motion times, especially by combining experiments at different temperatures based on the frequency temperature superposition (FTS) principle. Achieving an in-depth comprehension of dynamics is fundamental in the field of elastomers. In rubber technology, chemical cross-linking and/or the addition of fillers are employed to get elastomers with enhanced elasticity and mechanical properties. The improved mechanical properties arise from the restrictions on chain mobility imposed by the new constrains, and a full understanding of these effects could be of valuable help for the design of materials with optimized performances. In this work, ^{1}H FC NMR was employed to investigate dynamics of elastomers of technological interest for the tire industry. In particular, experiments were carried out over a wide temperature range on polyisoprene, polybutadiene, and poly(styrene-co-butadiene) rubbers, uncured and vulcanized under different conditions.(3) The obtained results pointed out significant differences between uncured and cross-linked elastomers, disclosing insights into the effect of cross-linking on local glassy dynamics as well as on slower and longer-range motions of the polymer chains.

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Contributed talk, Mon./15:45

Characterization and thermoanalytical study of novel valsartan coamorphous systems

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Valsartan, an antagonist of angiotensin II receptor, is a class 2 API according to the Biopharmaceutical Classification System (BCS).(1) The synthesis of coamorphous systems was selected to improve the physicochemical properties of valsartan. Coamorphous are defined as a single phase amorphous solid system composed of low molecular weight binary or multicomponents.(2) Three coformers were selected to synthesize (1:1) coamorphous systems with valsartan: *L*-proline, 4,4'-bipyridyne, and trimethoprim. The systems were synthesized by neat grinding. A halo in the PXR diffractograms showed that the amorphization was efficient. The FTIR of the pure components and the coamorphous systems were compared showing that: *L*-proline interacts weakly with valsartan, a slight shift is observed in the valsartan carboxylic acid stretching band (ν C=O); 4,4'-bipyridyne forms hydrogen bonds with valsartan, giving rise to weak broad bands at 1930 and 2470 cm^{-1};(3) and trimethoprim forms an ionic bond with valsartan, observed as the replacement of the valsartan carboxylic acid stretching band (ν C=O) by the corresponding carboxylate ones. Finally, the glass transition temperatures of pure valsartan and coamorphous systems were determined by DSC. Pure valsartan has a glass transition at 77.9°C. For the binary systems the glass transition was observed at 48.4°C (val:4,4-bipyridine), 73.2°C (val:*L*-proline), and 101.2°C (val:trimethoprim). Therefore, the preliminary study of coamorphous systems showed that the highest glass transition is observed in the salt coamorphous system (val:trimethoprim). Further research is being made to identify how stoichiometry, molecular mobility, and intermolecular interactions affect the glass transition of the coamorphous systems.

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Contributed talk, Mon./16:00

Does the vapor deposited films under confinement follows the bulk behavior?

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The glasses prepared means of physical vapor deposition (PVD) technique got wide attention as they possess properties such as high density, kinetic-stability etc., which can take thousands of years for an ordinary glass counterpart to achieve. Miniaturization being a sought-after criteria in current technological scenario, novel materials in confined geometry is of high significance. We would like to discuss about the properties of vapor deposited glasses under geometric confinement. The segmental dynamics and crystallization behaviour of vapor-deposited organic thin films down to 26 nm which was studied mainly using Broadband dielectric spectroscopic technique will be discussed. Apart from this, the effect of deposition temperature on the thin film properties and a comparison of vapor deposited films with the spin-coated counterparts will also be addressed.

(1) S.F. Swallen et al., Science., 315 (2007), 353-356
(2) M.D. Ediger, J. Chem. Phys., 147 (2017), 210901

CONTRIBUTED TALK, MON./16:15

Fast calorimetric characterization of glass transition and physical ageing of two prototypical glass-forming liquids

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Glycerol and orto-terphenyl (OTP) are well-know glass-forming liquids, very deeply characterized through years with several experimental techniques. Nevertheless, they are of great interest also nowdays because they can be used as a benchmark for the development of experimental protocols or for the development of new experimental techniques: due to the vast amount of results available, novel measurements can be compared with the ones already present in literature to verify the agreement between the two data sets and then to validate the new protocol/measuring machine.

OTP is an hydrocarbon composed by three aromatic rings in a triangular configuration. Through years, it is has been characterized with several experimental techniques, like rheometry, broadband dielectric spectroscopy, conventional calorimetry and so on.

Glycerol is a prototypical glass-formers too and it has lots of practical application as it is often used as a cryoprotectant and as a solvent/eccipient for drugs .

Recently, a study of OTP with fast calorimetry has appeared in literature, while nothing is still present for glycerol. Morover, this study is only devoted to the characterization of the glass transition and crystallization processes; no information are provided about physical ageing.

Fast differential scanning calorimetry (FDSC) is a particular kind of calorimetry, also called *chip calorimetry*, that is based on a thin film of sample deposited on MEMS (*micro-electro-mechanical-systems*) calorimetric devices, instead of the usual sample holded in metallic pans in furnaces 1 as for conventional calorimetry. This switch of paradigm allows the reduc- tion of the involved sample mass and to reach very high heating scan rates, up to 40000 K/s, without loosing precision nor being affected by important thermal lag or gradient.

The consequent improvement (by more than three decades) in the available heating rates compared to conventional calorimetry provides new op- portunities for a more detailed investigation of metastable materials, along with a stronger suppression of diffusive and reorganization processes. It also allows for a better insight in the investigation of kinetic processes down to millisecond timescales.

In this study, these two objects have been used to check for the goodness of fast differential scanning calorimetry (FDSC) and to develop a new data analysis method, different from the ones available in literature. Relaxation times have been estimates with the fast calorimeter by means of two methods: the behavior of the glass transition temperature with scan rate and the physical ageing process. These times have been compared with the ones present in literature belonging to other techniques, namely broadband dielectric spectroscopy and rheometry.

Contributed talk, Mon./16:30

The role of co-formers on the thermal behavior of nateglinide co-amorphous systems

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Bioavailability is an essential property of any drug and plays a significant role in its administration. However, several newly developed drugs have very low aqueous solubility. Consequently, improving the solubility and bioavailability of new formulations is one of the major challenges of the pharmaceutical industry.(1) The main pharmaceutical interest of amorphous solid forms of drugs lies in their improved solubilities and dissolution rates over the respective crystalline forms and amorphization is an increasingly become established as a strategy to enhance the dissolution properties of poorly water-soluble drugs,despite the inherent metastability of the amorphous state that drives it towards recrystallization. Co-amorphous systems of a drug and small-molecule excipient or two complementary drugs often show enhanced stability.(2)

Nateglinide is an effective oral therapy for type II diabetes mellitus with very low aqueous solubility (BCS class II). This study aims to design co-amorphous systems of nateglinide and different small molecule co-formers with better stability. To achieve this purpose, the influence of co-former selection and preparation methods on the thermal behavior of nateglinide co-amorphous systems was investigated. Two amorphization techniques were explored, quench cooling and milling, under different experimental conditions. The thermal behavior of the obtained materials was explored by DSC, and they were characterized by X-ray powder diffraction and FTIR-ATR spectroscopy. Preliminary stability assessment of the obtained co-amorphous phases is also reported.

(1) A. Fahr et al., Expert Opin. Drug Deliv., 4 (2007) 403-416
(2) M. Zhang et al., RSC Adv., 9 (2019) 3946-3955

Contributed talk, Mon./16:45

Influence of molecular weight on the equilibrium phenomena under nanopore-confinement

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Changes in the glass transition dynamics observed under nanoconfinement reveal pronounced out-of-equilibrium features. Therefore, the confinement effects weaken with time. Faster dynamics of the nanopore-confined systems slows down, and ultimately it is possible to regain the bulk-like mobility. The equilibration time increases with reducing the pore size and lowering the annealing temperature much below the glass transition temperature of the interfacial layer. In this talk, we would like to discuss the impact of the molecular weight on the equilibration kinetics of the polymer confined in anodic aluminum oxide (AAO) nanoporous templates. The study polymer is poly(phenylmethyl siloxane) with low and high molecular weight. We have found that the length of the polymer chain has a significant impact on the equilibrium phenomena under nanopore-confinement. Moreover, we also study the influence of the molecular weight on the relationship between the time constant characterizing the equilibration kinetics and the characteristic time of the viscous flow in the cylindrical channels of the nanometer size.

Session IV: Multifunctional Materials, Applied Materials

Contributed talk, Mon./17:15

Investigation of the nature of bifunctional catalysts in rechargeable zinc-air battery with neutron diffraction methods

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A metal-air battery is a type of battery or fuel cell that uses the oxidation of metal with atmospheric oxygen to produce electricity. It is equipped with an anode made of pure metals such as lithium or zinc and an air cathode that is connected to an air source. Catalysts in the air cathode maintain the electrochemical reaction with oxygen gas. Recently, metal-air batteries have attracted the attention of researchers, as the new generation of high-performance batteries are characterized by a simple design, very high energy density and relatively inexpensive production. High-capacity rechargeable batteries are becoming increasingly necessary for mobile devices, and currently the metal-air battery is the most promising for this application. Neutron scattering methods play an important and widely recognized role in structural studies of systems with light atoms, especially hydrogen, and as such neutron diffraction has long made a significant contribution to catalysis, especially in determining the positions of adsorbed hydrogen-containing molecules, such as micropores. catalysts.(1,2) Recently, as a result of significant advances in the intensity of neutron beams and the improvement of neutron detectors, studies with neutron-diffraction apparatus(3) of the catalytic process have become possible. Structure study of series of samples at the following temperatures by the neutron diffraction approach Co_3O_4 IC(23 K, 100 K, 200 K, 290 K), Co_3O_4 MT (25 K, 100 K, 200 K, 300 K), LSCF($La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_3$)(27 K, 100 K, 200 K, 290 K), LSCO($La_{0.6}Sr_{0.4}Ca_{0.8}O_{3-\delta}$) (20 K, 100 K, 200 K, 290 K), LSM($La_{0.8}Sr_{0.2}MnO_{3-\delta}$)(22 K, 100 K, 230 K, 270 K), Ni70_Co_3O_4(290 K), Ni70_$NiCo_2O_4$(21 K, 100 K, 200 K, 290 K), $NiCo_2O_4$ based on fulprofile analysis with program Fullprof.

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(1) A. Fahr et al., Expert Opin. Drug Deliv., 4 (2007) 403-416
(2) N. Q. Minh, J. Am. Ceram. Soc., 76 (1993), 563-88
(3) A.B. Stanbauli et al., Renewable and Sustainable Energy Systems, 6 (2002), 433-455

Contributed talk, Mon./17:30

Magnetic skyrmions in GaM_4X_8 (M = V, Mo; X = S, Se) lacunar spinels

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Lacunar spinels, compounds belonging to the AM_4X_8 family, can display many interesting properties, correlated with the presence of the well-known Jahn-Teller (JT) effect, a geometric distortion associated with lifting of the degeneracy of the ground-state electron configuration. In the case of lacunar spinels, the triply degenerate valence $t2$-symmetry orbitals split due to the JT effect, lowering the energy of the crystal structure when it changes from cubic *F4-3m* to rhombohedral *R3m* space group.(1) At very low temperatures, a ferromagnetic behaviour in some compounds from these family has been reported.(2) Some of them may present magnetic skyrmions below the magnetic ordering temperature T_c. Skyrmions are swirling spin structures carrying a topological quantum number and they occur due to the competition between the ferromagnetic exchange and Dzyaloshinskii–Moriya interactions. Their stability, low required magnetic fields and easy manipulation, turn skyrmions into promising candidates for nanotechnological devices, such as data storage systems.(3)

In this work, we will present and discuss the synthesis, the structural characterisation by XRD and Raman spectroscopy, and the magnetization studies performed by VSM for the GaM_4X_8 (M = V, Mo; X = S, Se) lacunar spinels. Skyrmions can be detected in such compounds by two characteristic anomalies observed in the numeric derivative $\mathrm{d}M/\mathrm{d}H$ curves below T_c. *Ab initio* calculations, performed with the WIEN2k package for both cubic and rhombohedral structures, will be also presented. Such calculations prove the lifting of the degeneracy of electron bands close to the Fermi Energy (EF), related to the JT effect.

Acknowledgements: J.F. Malta PhD grant is supported by FCT- Fundaç ão para a Ciência e a Tecnologia through ChemMat PhD programme. Access to TAIL-UC facility funded under QREN-Mais Centro project ICT_2009_02_012_1890 is gratefully acknowledged. This work was partially supported by funds from FEDER (Programa Operacional Factores de Competitividade COMPETE) and from FCT under the projects UID/FIS/04564/2019 and PTDC/FIS-NAN/6099/2014

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(1) Y. Wang et al., Phys. Rev. B, 100 (2019), 115149
(2) E. Ruff et al., Science Advances, 1 (2015), e1500916
(3) N. Romming et al., Science 341, (2013), 636-639

Contributed talk, Mon./17:45

Exploring the quantum spin liquid candidate 1T-TaS_2 from bulk to atomically thin-layers

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Layered materials are excellent candidates for studying the interplay between the in-plane and out-of-plane entanglement in strongly correlated systems. A relevant example is provided by 1T-TaS_2, which shows a multifaceted electronic and magnetic scenario due to the existence of several charge density waves (CDW) configurations, including quantum hidden phases, superconductivity and even quantum spin liquid (QSL) phases, that are highly dependent on the out-of-plane stacking of the CDW.

Here, we report on bulk and atomically thin-layers of 1T-TaS_2. For bulk, we show experimental evidence for several competing quantum phases, obtained by combining temperature-dependent muon spin relaxation and specific heat measurements, with a switching on the spinon density of states versus energy.(1) Regarding atomically-thin layers of 1T-TaS_2, we fabricate vertical van der Waals heterostructures based on few-layer graphene and we measure their transport properties. Different activation energies in the conductance and a gap at the Fermi level are observed, which may indicate a progressive formation of out-of-plane spin-paired bilayers at low temperatures.(2,3) These features make 1T-TaS_2 a potential candidate for hosting multiple QSL crossovers

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(1) S. Mañas-Valero et al., arXiv:2007.15905 (2020)
(2) C. Boix-Constant et al., arXiv:2009.14550 (2020)
(3) C. Boix-Constant et al., Adv. Electron. Mater., (2021), 2000987

CONTRIBUTED TALK, MON./18:00

Sensing spin transitions on hybrid van der Waals heterostructures

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Spin-crossover (SCO) materials are metal complexes where the spin state of the metallic center changes between high-spin (HS) and low-spin (LS) due to the presence of an external stimulus (light, pressure, temperature . . .), with potential applications as memory devices or in spintronic applications.(1)

In this work, we fabricate hybrid van der Waals heterostructures based on SCO and inorganic two-dimensional (2D) materials. First, we exfoliate mechanically a SCO compound(2) and characterize it by atomic force microscopy, optical microscopy and Raman spectroscopy. Then, these molecular flakes are deterministically combined with inorganic 2D systems like few-layers graphene (FLG) or atomically-thin layers of 2H-$NbSe_2$ and WSe_2, thus creating hybrid van der Waals heterostructures. Interestingly, the hysteretic thermal spin transition is detected by transport measurements in SCO/FLG heterostructures and by photoluminescence in SCO/WSe_2 heterostructures.

Our results illustrate the synergy between the SCO and the inorganic system and opens the door to explore further molecular compounds of interest which properties could not be detected otherwise.

(1) J. Dugay, et al., Nano Letters, 17 (2017), 186-193
(2) V. Martínez, et al., Chem. Eur. J., 15 (2009), 10960-10971

CONTRIBUTED TALK, MON./18:15

Influence of uniaxial pressure on electronic properties of a simple cuprate superconductor

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Since the discovery of high-temperature superconductors in 1986, the ones based on copper oxide (so-called cuprates) are of utmost interest in condensed matter physics. The cuprate superconductors consist of CuO_2 planes separated by material-specific charge reservoir layers. Superconductivity in such compounds appears upon doping with charge carriers (either holes p, or electrons n) and is attributed mainly to the copper-oxide planes. The basic question that remains without a definitive answer concerns the microscopic mechanism of the formation of unconventional superconductivity in these compounds.

It has been demonstrated, that the critical temperature (T_c) depends strongly on the details of the crystal structure, and at doping optimal for superconductivity it varies from about $T_{c,\max} = 30$ K in $La_{2-x}Sr_xCuO_4$ (LSCO), to $T_{c,\max} = 135$ K in $HgBa_2Ca_2Cu_3O_{8+x}$ (Hg1223). Understanding the structural details which are responsible for such a substantial difference in the critical temperature is expected to ultimately help to understand the underlying mechanism of superconductivity in the cuprates.

In my talk, I will present the electrical resistivity and X-ray absorption spectroscopy (XAS) measurements in underdoped LSCO, but with uniaxial pressure applied to the sample. The uniaxial stress applied along one of the crystallographic [100] directions within the CuO_2 planes breaks the lattice symmetry. For example, it can induce an orthorhombic distortion in an initially tetragonal sample (or inverse). It thus allows to explore the impact of the lattice distortion (symmetry) on the physical properties in one sample and does not require comparing different compounds. Such results are naturally free of material-specific details.

After describing the experimental setups I will present the results obtained during the two experiments. First, I will discuss the electrical resistivity measurements along the c axis (perpendicular to CuO_2 planes), which show a substantial increase with increasing the uniaxial pressure. Such change in the electronic transport suggests that the electronic structure is impacted by the applied stress. This motivated us to employ XAS to explore whether the uniaxial pressure induces changes in the distribution of the doped carriers within the copper and oxygen orbitals inside the CuO_2 planes. Although no clear evidence of the charge carriers redistribution was found, the resistivity measurements indicate that not only the CuO_2 planes contribute to superconductivity, but also the reservoir layers may play a role.

Session V: Advanced Materials, Flash Talks

Contributed talk, Tue./09:00

Neutron diffraction studies of pressure induced phase transitions in Bi_2WO_6

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The Aurivilllius family compounds are one of the most promising and relevant materials for practical applications due to the exhibiting of numerous physical properties like large remanent polarization, relatively low processing temperatures, high Curie temperatures, excellent piezoelectric properties etc. However, from a fundamental point of view, these compounds are extremely interesting to researchers because of the features of their phase transitions and the complex interaction of their structural instabilities. Bismuth tungstate, Bi_2WO_6, is a well-known ferroelectric at ambient conditions, the compound of Aurivilllius family with a high Curie temperature ($T_c \approx 960°C$). However, below the Curie point, the compound undergoes two phase transitions. Nevertheless, the pressure effect on the crystal structure parameters of Bi_2WO_6 haven't been investigated yet. Identification of regularities of structural changes and atomic dynamics near the polymorphic transition from ferroelectric to paraelectric modification at the Curie temperature is necessary to establish its mechanism upon variation of interatomic distance.

In present work the compound of Bi_2WO_6 was chosen at ambient condition, and performed neutron diffraction studies at high pressure. Neutron powder diffraction measurements at ambient and high pressures up to 7 GPa were performed at room temperatures with the DN-12 diffractometer at the IBR-2 high-flux pulsed reactor (FLNP, JINR, Dubna, Russia) using the sapphire anvil high-pressure cell. In order to improve the understanding of the lattice instabilities the Raman spectroscopy studies of the vibration spectra of the Bi_2WO_6 under pressure up to 30 GPa were performed.

The neutron diffraction and Raman spectroscopy investigations show a complex sequence of the pressure-induced phase transitions in the bismuth tungstate Bi_2WO_6. At $P \approx 3.5$ GPa anomalies in pressure behavior of lattice parameters and interatomic distances were observed, which are affected by the phase transition (from *P21ab* to *B2cb* space group). The pressure application leads to mutual rotation of the WO_6 octahedra during the phase transition. Another structural phase transition to the isostructural orthorhombic phase with the *B2cb* space group occurs at pressure $P > 5.9$ GPa. This structural transition is the result of a complex arrangement of WO_6 octahedra, including rotation and changes in the tilting between neighboring octahedra. There are also observed the clear changes of the vibrational modes of Bi_2WO_6 under compression. By increasing the pressure, wave numbers of the majority of modes increase, however, some modes exhibit negative pressure dependence. Changes in the slope of wave number vs pressure at 3.5 and 6 GPa are observed for a lot of modes, which indicates about a second order phase transitions associated with some subtle changes in the crystal structure. Also, at pressures of about 12 and 20 GPa the changes in the Raman spectra indicate the consistent possible transition to new pressure-induced phases of the Bi_2WO_6.

The work was supported by the Russian Foundation for Basic Research, grant RFBR N19-52-45009 IND_a.

CONTRIBUTED TALK, TUE./09:15

Analysis of CNR in molecular MRI using core/shell double contrast NPs

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T_1 and T_2 contrast agents are commonly used in cancer detection using MRI. Recently T_1/T_2 contrast have been developed with an expectation that the contrast to noise ratio (CNR) would increase when compared to T_2 contrast agent. To prove this, we calculated optimal parameters in commonly used Spin Echo and IR TrueFISP pulse sequences that provide optimal CNR for known T_1 and T_2. The results show that the CNR for a T_1/T_2 core shell nanoparticle is greater than that of just a T_2 contrast agent for both pulse sequences. To demonstrate the potential of our core/shell nanoparticles in vivo MRI, we imaged animals with breast tumors after intravenous injection of 0.25 mL of non-targeted core shell contrast agent $NaDyF_4$ (20 nm)/$NaGdF_4$ ($\approx$ 0.5 nm). Post-injection results show that the best CNR comes from the T_1 weighted image subtracted by the T_2 weighted image, and the CNR for the T_1 weighted image is greater than the CNR for the T_2 weighted image.

FLASH TALK, TUE./09:30

Thermoluminescence studies of $Y_3Al_2Ga_3O_{12}$:Cr^{3+} persistent nanophosphors

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From the moment of the first publications to the present day, materials with long-lasting emission, known as persistent luminescence (PersL), have been of interest both from the point of view of fundamental science (trapping and de-trapping mechanisms, traps effect on the decay time etc.) and from the point of view of application in various fields of optics and sensors.(1).

Cr^{3+} doped $Y_3Al_2Ga_3O_{12}$ (YAGG:Cr) nanophosphors are one of the attractive materials in such type of materials. In particular, the YAGG:Cr nanophosphors co-doped with lanthanides have gained attention due to their PersL in the visible, red, and NIR range, where Cr plays an important role for extended the PersL decay time.(2)

In this work, YAGG:Cr nanophosphors synthesized by the Pechini method followed by annealing at temperatures from 800 to 1300°C. The lattice parameters and average grain sizes were calculated from the Rietveld refinement data based on X-Ray powder diffraction data. To investigate the effect of grain size of the materials on its optical properties, absorption, photoluminescence (PL) emission and excitation, as well as luminescence decays and thermoluminescence (TL), were recorded and analysed. It was found that both PL and PersL properties of the YAGG:Cr strongly depend on the grain size. The PL and PersL of the YAGG:Cr have typical Cr spectral features, indicating that both processes originate from the same emitting centres. It is determined that with increasing grain size the electron-phonon coupling decreases, whereas the crystal-field strength increases. The correlation between structural changes and TL behaviour was revealed. In particular, the redistribution of traps and activation energy reach optimal values when the lattice constant reaches the threshold.

Acknowledgements: This work was supported by the OPUS 11 2016/21/B/ST5/02385 project.

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(1) J. Xu et al., Lumin., 205 (2019), 581-620.

(2) V. Boiko et al., Scientific Reports, (2021), 11:141

FLASH TALK, TUE./09:35

Investigation of π-d interaction in λ-$(BEST)_2FeCl_4$

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The quasi-two-dimensional organic conductor λ-$(BETS)_2FeCl_4$, where BETS is bis(ethylenedithio)tetraselenafulvalene [Fig 1(a)], shows a magnetic-field induced superconducting state when a magnetic field is applied precisely parallel to the conducting layers. The mechanism of the FISC is explained by the Jaccarino-Peter compensation mechanism, where the external magnetic field compensates the internal field of aligned d spins through the π-d interaction.(1) However, the details of π-d interaction mechanism is still unknown.

BEST (bis(ethylenediseleno)tetrathiafulvalene) [Fig 1(b)] is an analog of BETS. Comparing BETS and BEST, we can get the information which inner or outer chalcogens are more important in the path of the π-d interaction. λ-$(ET)_2FeCl_4$, where ET is bis(ethylenedithio)tetrathiafulvalene [Fig 1(c)], an alternative candidate, where Se atoms in BETS are substituted with S atoms in ET molecule. However λ-$(ET)_2FeCl_4$ has not been available. Hence BEST is a good candidate for a systematic study of π-d interaction.(2)

In this conference, we will discuss the path of the π-d interaction with the X-ray diffraction and magnetic susceptibility measurements. Moreover, we plan to perform Mössbauer spectroscopy and ^{13}C NMR, and we will discuss the results of microscopic studies.

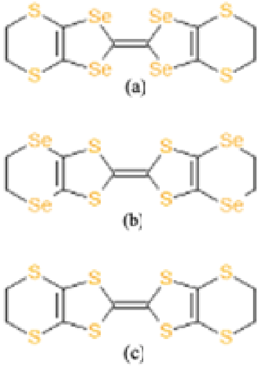

Figure 1. Molecular structure of (a) BETS, (b) BEST, (c) ET.

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(1) S. Uji et al. Nature, 410 (2001), 908
(2) H.B. Cui et al. Chem Lett., 254 (2005)

FLASH TALK, TUE./09:40

Controlling of magnetic properties of iron-based composite particles

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Iron and its oxide nanoparticles have received considerable attention due to their applications in magnetic, electronic, pigmental, catalyst and biomedical purposes.(1,2) The expected magnetic properties for these applications are different, so control of the coercivity is important.

We proposed an unique laser process for preparation of submicron composite magnetic particles. Source magnetite or hematite colloid solutions were irradiated in various organic solvents by Nd:YAG laser with 2nd and 3rd harmonics, various laser fluences and irradiation times. In our work we investigated how size and composition of iron compound particles evolves according to changing irradiation conditions. It was found that during irradiation of magnetite and hematite nanoparticles the dominant phases of the particles are reduced from magnetite and hematite to iron or iron carbide.(3)

The formation of various iron compound particles in controlled laser irradiation process of magnetite and hematite nanoparticles indicates that the magnetic properties of the obtained particles can be tuned.

This work gives us a method for obtaining iron compounds complex particles, which size, composition and magnetic properties can be controlled by the conditions of laser irradiation.

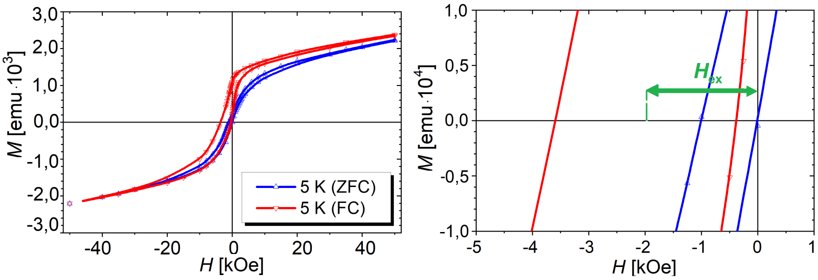

Figure 1. Typical magnetic loop obtained for Fe_3O_4/FeO composite particles.

(1) L.R. Marcelo et al., Environ. Chem. Lett., 19 (2021), 1229-1274

(2) X. Zhao et al., J. Alloys Compd., 513 (2012), 460-465

(3) Z. Swiatkowska-Warkocka et al., Nanoscale Res. Lett., 6 (2011), 226

Flash talk, Tue./09:45

Magnetic and nonlinear optical properties of single-molecule magnets/silica nanocomposite

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The investigation of novel multifunctional nanocomposite materials is the constantly developing topic of numerous modern research. The ability to tailor the nanosized components in order to obtain the material with improved physical properties demands, however precise synthesis methods and proper characterization techniques. Especially noteworthy seems nanocomposite materials showing both significant magnetic and optical properties. Obtaining material with such characteristics in the nanoscale opens up numerous technological applications, for instance in the field of nanophotonics and nanomagnetism.(1)

In the current study, the synthesis of novel silica-based nanocomposite material was carried out. The material was based on the deposition of Mn_{12}-based single-molecule magnets (SMMs) onto the surface of spherical silica nanoparticles of diameter about 300 nm. The SMMs, being separated and regularly organized on the surface, can each act as an individual magnet, due to their unique magnetic properties of the molecular origin.(2) The deposition of SMMs on the silica surface was based on the chemical anchoring using propyl carbonic acid groups. The performed AC and DC magnetic measurements revealed the preservation of basic characteristics of SMMs in the nanocomposite. Another interesting topic of the research was the study of nonlinear optical (NLO) properties of such nanocomposite material. For this goal, the common NLO properties, namely second harmonic generation (SHG) and third harmonic generation (THG) of spherical silica-based nanocomposite material were studied. It was shown that investigated nanocomposite material revealed weak SGH and THG signals. However, structural modifications, such as thermal treatment of initial compound, were resulted in significant enhancement of materials optical nonlinearity.

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FLASH TALK, TUE./09:50

Physico-chemical properties, structure and spectroscopic investigations on iron-containing oxide glasses

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The synthesis of oxide glasses with high concentrations of 3d transition metals is of significant practical interest for environmental monitoring, as catalysts and in biomedicine. Using controlled crystallization procedures enables the preparation of nano-sized glasses-ceramics with narrow size distribution. In order to obtain bulk glass-ceramics with controllable phase composition, size and volume fraction, a thorough knowledge of the structure and the physico-chemical properties of the parent glasses is required.

The present work reports on the synthesis of oxide glasses in the system $Na_2O/CaO/SiO_2/Fe_2O_3$ with high iron oxide concentrations (5–20 mol% Fe_2O_3). The densities of the obtained glasses are determined using a pycnometer; they increase with increasing Fe-concentration. The Becke line method is applied for the evaluation of the refractive indices and it also reveals that increasing Fe-concentrations result in higher refractive indices. IR-spectroscopy is utilized to study the glass structure and shows interconnected SiO_4 tetrahedra but also isolated SiO_4 units in all investigated glasses. The increasing Fe-oxide concentration leads to the depolymerization of the glass-network. Furthermore, absorption bands between 550–590 cm^{-1} occur which are attributed to Fe-O bonds in octahedral FeO_6 groups, typical for ferrites such as Fe_3O_4. X-ray photoelectron spectroscopy is used to gather information on the binding energies and the valence states of the elements constituting the glass. The presence of both Fe^{2+} and Fe^{3+} ions with binding energies at 709 and 711 eV, respectively is observed in all glasses. With increasing Fe_2O_3 concentration, the number of non-bridging oxygens increases at the expense of the number of bridging oxygens.

Acknowledgements: The authors acknowledge the financial support of the Bulgarian National Science Fund under grant КП-06-Н48/4.

Flash talk, Tue./09:55

Role of sublimation in degradation kinetics of carbamazepine

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Carbamazepine (CBZ) is an Active Pharmaceutical Ingredient (API) used in the treatment of epilepsy and different neuralgias, which exhibits high permeability but low solubility and consequently limited bioavailability. Many attempts are made to improve its solubility by e.g. fast cooling of the melt, preparing solid dispersions, milling, compressing, formulating co-crystals. Vitrification of API is usually the easiest way to improve its solubility, as amorphous material has higher internal energy than its crystalline counterpart. However, for APIs thermally unstable in the vicinity of the melting point it is not trivial to obtain liquid phase not contaminated by products of degradation.

CBZ was believed to be stable up to ≈ 225°C, which is about 30°C higher than its melting point.(1) Nevertheless, our studies had shown that iminostilbene (IMB) — main product of CBZ degradation — is present in samples heated just above their melting point.(2–4) Discrepancies in results observed between different groups came out to be the consequence of strong sublimation of CBZ which started to appear dozens of degrees Celsius below melting point. As proved in our latest work,(5) noticed differences are closely related to the choice of the DSC pan. In case of the measurements performed with open pans, sublimating CBZ was able to escape from the system. Therefore, both the pressure of the measurement and the atmosphere did not change. On the other hand, when hermetically sealed pans were used, the appearance of gaseous CBZ led both to the increase of the pressure inside the pan and change of the atmosphere.

Degradation of CBZ placed in hermetically sealed pan was observed both in the vicinity of the melting point and even 20°C below it. The reason of strong degradation was high pressure inside the pan. The role of atmosphere was negligible. On the contrary, for CBZ samples examined in open pans no degradation was observed before and during fusion.

Acknowledgments: AD has been partly supported by the EU Project POWR.03.02.00-00-I004/16

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FLASH TALK, TUE./10:00

Study on the molecular dynamics and structure-related electric properties of poly(dimethylsiloxane) coordinated by metal-ligand complexes

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Nowadays, the new flexible dielectric materials with an elevated value of dielectric permittivity for appliances in fully stretchable electronics are in high demand and polymers cross-linked by metal-ligand coordination are good candidates for serving as fully stretchable dielectrics.

In our research we presented the poly(dimethylsiloxane) dielectrics crosslinked by metal (Me = Ni^{2+}, Mn^{2+}, Zn^{2+})-ligand (bipyridine-bpy) coordination (bpyPDMS-MeX_2). We thoroughly investigated their electrical properties as well as molecular dynamics in order to estimate the effect of various metal-ligand cross-linkers (MeX_2). We found that the chemical incorporation of bipyridine into the PDMS structure and formation of PDMS metal-ligand complexes enhanced the value of dielectric permittivity ε' of obtained materials due to the dipolar nature of the coordination bonds in these systems. The highest value of $\varepsilon' = 4.3$ (at 1 MHz) was observed for the bpyPDMS-$ZnCl_2$ system, which is two times higher than for the neat PDMS.(1) Moreover, we showed that introduction of counter anions results only by slightly higher conductivity values of the materials in comparison to neat PDMS.(2) It was observed that the chemical incorporation of bpy moieties into the polymer matrix suppress PDMS crystallization. Two relaxations α and α_{ac} were found and described as segmental ones. The additional one, i.e. α_{ac} relaxation in studied amorphous materials originates from the lower mobility of PDMS chains, as they are immobilized by metal-bpy coordination centers.

Performed study revealed that double-edged challenge was obtained, i.e. flexible materials with elevated value of dielectric permittivity were synthesized without deterioration of the non-conductive nature of the base polymer.

Acknowledgements: AW gratefully acknowledges the financial support of NATIONAL SCIENCE CENTER (Poland) grant Preludium No. UMO-2019/33/N/ST3/00990.

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Flash talk, Tue./10:05

Kinetics of formation of cobalt (II) complexes in the top layer of thin polymer films

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The presented research focuses on the kinetics of poly(4-vinylpyridine)-Br_2Co complex formation in the top layer of P4VP films. The material obtained in such a process has been proven to successfully combine the advantages of polymers and Single Ion Magnets that exhibit magnetic relaxations.(1) The said material has also found applications in organic field-effect transistor-like geometries, leading to an extraordinary conduction increase by four orders of magnitude.(2) However, the kinetics of the said process was not, until now, investigated, and will be elucidated herein.

To study the kinetics of P4VP-Br_2Co complex formation in the top layer of P4VP films, polymer layers were produced by the spin casting method and subsequently submerged in $CoBr_2$ solution with constant speed. This created a gradient of immersion time. Wrinkled topology was investigated by atomic force microscopy. The samples where then investigated by secondary ion mass spectrometry.

Results indicate a breakthrough model of adsorption, which was confirmed by fitting the Yoon-Nelson model to obtained data using nonlinear regressive method.(3) Parameters such as τ (the time required for 50% adsorbate breakthrough (min)) and k_{YN} (the rate constant) were determined.

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Session VI: Surfaces, New Ideas

Contributed talk, Tue./11:15

Time-resolved measurements from liquid-vapour interfaces using optical pump — X-ray probe technique

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Optical pulses have been routinely used in the last two decades to study the structural and dynamic changes in solids.(1) Currently, there is a growing interest on investigating those phenomena in liquids, such as liquid metals,(2) and aqueous solutions(3), close to their surfaces and interfaces. Critical steps in thermally induced capillary waves and optically induced electron solvation at the liquid-vapour interfaces occur in short time scales. Elucidating the underlying non-equilibrium physics at these interfaces at ultrafast time scales and in atomic spatial resolution associates significant experimental challenges. Short ultrafast optical pulses synchronized with focused synchrotron X-ray pulses are the key to this endeavor, as they can access the structure and dynamics of the liquids at their surfaces and interfaces with atomistic details.

Here, we investigate the thermally induced capillary wave dynamics at liquid mercury and water surfaces and optically induced electron solvation dynamics at water and water-based salt solutions at liquid interfaces scattering apparatus (LISA) at P08 beamline,(4) PETRA III (DESY) in Hamburg. First measurements from a single crystalline Bi (111) reference sample have confirmed a time resolution of 85 ± 2 ps from the setup. Capillary wave dynamics at water-vapour and mercury-vapour interfaces were investigated with X-ray reflectivity (XRR) and time response (TR) pump-probe studies in the time range of ns to s with IR (1030 nm) laser excitation. In addition, UV (258 nm) laser excitation at the vapor interface of salt solutions (NaI, NaCl, RbBr and $K_4[Fe(Cn)_6]$) indicates interesting dynamics close the surface.

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Contributed talk, Tue./11:30

Lubricant-impregnated surfaces and dynamic measurements with drops of liquids

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Slippery liquid-infused porous surfaces (SLIPS) are porous nanostructures impregnated with a low surface tension lubricant. They have recently shown great promise in various applications that require non-wettable superhydrophobic surfaces. These surfaces belong to the class of liquid-repellent and non-adhesive surfaces. Here we show SLIPSs prepared using a carbon-soot superhydrophobic surface. Subsequent infusion of fluorocarbon lubricants (Krytox 100, Krytox 101, Krytox 102 and Fluorinert FC-40) into the porous microtexture results in liquid-repellent slippery surfaces. As these lubricant are immiscible with most liquids, drops deposited on SLIPs slide easily. As drops we use alkanes (hexane, decane, dodecane and hexadecane), alcohols (methanol, ethanol, 2-propanol) and polydimethylsiloxane (PDMS). To image the shape of drops and to calculate the interfacial surface tensions on lubricant-infused surfaces we use an optical tensiometer and a homemade laser scanning confocal microscopy (LSCM).The confocal microscope was used in reflection interference mode. In our project we want to calculate the penetration depth of the different drops on SLIPs. The result of our mesuarements shows that the average penetration depth is about $L \approx 260$ nm. Furthermore, with the assistance of LSCM we managed to calculate the laplace pressure of our liquid-drop system. The results shows a negative sign in the laplace pressure, which indicates that the lubricants are causing the drops to be pulled inwards.

CONTRIBUTED TALK, TUE./11:45

Grafted polymer brush coatings with enhanced temperature response based on poly(di(ethylene glycol)methyl ether methacrylate-co-acrylamide)

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In recent years, considerable attention has been paid to ”intelligent” surfaces with switchable properties, triggered by external factors, such as temperature, pH or light, such as grafted temperature-responsive homopolymer brushes. Copolymer brush coatings exhibit several properties more suitable for different biomedical applications as compared with the „classic” grafted homopolymers. In addition, copolymer composition determines properties that could be adjusted, such as for instance: switching temperature, growth of mammalian oocyte-cumulus cell complexes,(1) or shape of Ag nanoparticles embedded for switchable antibacterial properties.(2) Therefore, copolymer brushes have significant prospects as biocompatible and peptidomimetic materials, temperature as well as pH-sensitive systems, drug delivery devices.

Coatings of statistical copolymer brushes based on acrylamide and di(ethylene glycol)methyl ether methacrylate were fabricated for the first time. The synthesis of grafted p(oegma-co-acrylamide) brushes included three stages using Surface-Initiated Atom Transfer Radical Polymerization. Their composition and properties, such as wettability and surface morphology, were investigated using Time-of-Flight Secondary Ion Mass Spectroscopy, Atomic Force Microscopy and Contact Angle measurements. The obtained grafted copolymer brush coatings are sensitive to two external factors: temperature and pH. Last but not least, they exhibit enhanced temperature-dependent response in wettability, as compared to the ”classic” homopolymer brush-coatings composed of poegma.

The obtained materials can be used for the production of medical equipment, devices for working with blood, tissue engineering, ”smart” carriers of medical drugs.

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Session VII: Soft Matter

Contributed talk, Tue./13:00

Deuterated Liquid Crystals — new materials with higher photochemical stability

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Isotopically labelled compounds are widely used mainly as tracers of chemical and biological processes. High interest of these compounds was induced by two important factors: improvement of highly sensitive and precise analytical methods for isotope identification and development of new synthetic approaches for isotopically labeled compounds. Perdeuterated Liquid Crystals were presented as attractive and prospective new materials with low absorption in the mid-wave infrared region. On the other hand deuterium labelled Liquid Crystals are slightly more studied and play a key role in the study of molecular dynamics, phase behavior and other properties. Liquid Crystals constitute the heart of many optoelectronic devices. Working under harmful conditions causes excitation of delocalized electrons and their transfer to higher energy levels inside organic material, thus initiating photodegradation processes. Until now, Deuterated Liquid Crystals have not been considered as materials with higher photochemical stability.

In this work we present the synthesis of new materials exhibiting higher photochemical stability. Our idea is base on selecting the weakest bond in the molecule and reinforcing it by exchanging the C–H bond to C–D bond systems. The synthetic methodology to a highly birefringent fluorinated 4-alkyl-4"-isothiocyanato-[1,1':4',1"]terphenyls will be presented. The preliminary experimental work carried out on the photochemical stability of synthesized compounds indicates an increased stability of deuterated compounds.

Acknowledgements: This work was co-financed by National Science Centre in Poland project ETIUDA 7 No. UMO-2019/32/T/ST4/00225.

Contributed talk, Tue./13:15

Control crystallization of molecular liquid using AC electric field

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Fully understand the crystallization using electric field is drawing attention from investigators due to a wide application in pharmaceutical science. The outcome in crystallization of a different polymorphism in vinylethylene carbonate, a high polar molecular system, was reported for direct (DC) electric fields. Using dielectric spectroscopy, we study how properties of alternating (AC) electric field affects the crystallization. We discover that crystallization time, and the dimensionality of crystal growth can be manipulated by adjusting the frequency or the amplitude the electric field. Moreover, the crystallization outcome can be controlled to form one or another polymorph. We found that the field effects only are pronounced at below certain frequencies threshold, which orders of magnitude below the characteristic molecular orientation but consistent with the reorientation of polar crystal nuclei. This discovery may serve as new strategies for controlling and tuning crystallization outcomes in the context of materials engineering and pharmaceuticals applications.

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CONTRIBUTED TALK, TUE./13:30

Investigation of the glass transition and comparison of physical properties of the orthoconic liquid crystalline mixture W-1000 and its new modification W-356

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W-1000 is an antiferroelectric orthoconic LC mixture (52.5 w% 3F5HPhF6, 47.5 w% 3F7FPhH6) known of a very wide temperature range of the smectic C$^*_A$ phase.(1) W-356 is a new derivative of W-1000, obtained by addition of a small amount of the C1 and C2 compounds with a terminal -C≡N group.(2) In this study, both mixtures are proved to create the vitrified SmC$^*_\lambda$ phase below ca. 230 K. The dielectric spectroscopy results give the intermediate fragility index $m_f = 79$ and 73 for W-1000 and W-356, respectively. The X-ray diffraction results show that the short-range order in the smectic layers does not evolve in the SmC$^*_\lambda$ glass, while the quasi-long-range smectic layer order is changing even below the glass transition temperature. No cold crystallization is observed on subsequent heating. The experimental results show also that the C1 and C2 dopants lead to decrease of the tilt angle and spontaneous polarization (primary and secondary order parameter, respectively). The X-ray diffraction patterns imply the modulation of the smectic layers in W-356, not observed for W-1000 (Fig. 1). This effect is explained by tendency of the compounds possessing the -C≡N group to create dimers as well as the reversed order of the benzene and biphenyl in the aromatic core of the C2 molecule, which consequently can disturb ordering of molecules in the smectic phases of the W-356 mixture.

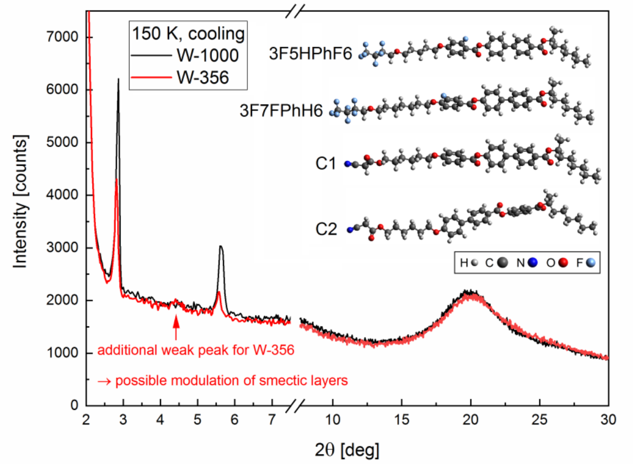

Figure 1. Components of W-1000 and W-356 and X-ray diffraction patterns of the vitrified SmC$^*_\lambda$ phase of both mixtures.

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(2) J. Dziaduszek et al., Ferroelectrics, 343 (2006), 3-9

Contributed talk, Tue./13:45

The effect of surface modification on the molecular dynamics of poly(phenyl methyl siloxane) confined in alumina nanopores

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One of very useful strategies allowing for the study of the properties of polymers at the nanoscale level is by constraining them within solid interfaces of nanometer size. From a general perspective the changes in the dynamics and glass transition behavior under nanoscale are controlled by two factors: finite size and surface effect. In this work we will demonstrate if the modification of the surface conditions by the silanization can induce that the effects of confinement on the glass transition dynamics may be partially or even completely lost. The results of the dielectric and calorimetric data for poly(phenyl-methyl siloxane) embedded in nanopores with modification surface will be discussed. Interestingly, our data indicate that the bulk evolution of the segmental relaxation time for nanopore-confined systems can be restored not only by the thermal treatment but also surface modification.

Contributed talk, Tue./14:00

Modelling IR spectra of liquids from MD simulations

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Vibrational spectroscopy is an experimental method commonly used to investigate interactions between molecules in a system of interest or to identify compounds in a sample with unknown composition.

Predictions based on computational methods could be used to support the experiment, e.g. to identify individual bands observed experimentally or to predict possible shape of the spectrum. The most simple approach based on using quantum chemical calculations for isolated molecule in vacuum may provide some useful hints, but usually it is insufficient for condensed phase systems. One could use effective solvent models such as PCM to study the solvent effect on spectra, however, this approach is still not sufficient to deal with more specific interactions like hydrogen bonds.

Our research concentrates on using molecular dynamics (MD) to model IR spectra of liquids, in particular systems that are used as electrolytes for batteries, such as ionic liquids or salt solutions in organic solvents. MD approach does not suffer from limitations of PCM because solvent molecules are explicitly included in the modelled system. However, classical MD based on force fields cannot correctly reproduce the band shifts related to changes in salt concentration and ab initio MD needs to be applied. The IR spectrum can be obtained from the total dipole moment of the system as the Fourier transform of dipole moment autocorrelation function. More detailed information about contribution of different parts of the system to the whole spectrum is available from Fourier transforms of geometrical parameters such as bond lengths or angles.

In the presentation, examples of MD-based investigations of interaction-induced spectral changes will be shown. Discussed systems include Na salt in an ionic liquid and Mg or Na/Li salts in organic solvents. The results show that the approach based on ab initio MD can satisfactorily reproduce the changes induced in IR spectra by solvent interactions with metal ions.

CONTRIBUTED TALK, TUE./14:15

The supramolecular structure of associating alcohols

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Alcohols act as model hydrogen-bonding systems between water and macromolecules due to their exceptional glass formation ability and wealth of chemical structures. It is already known that alcohols in the liquid state may form different kinds of supramolecular structures on a length scale larger than ordinary (non-associating) liquids.(1–3) However, the process of association of alcohols differing in, e.g., the position of the -OH or other functional groups, the type on location of the steric hindrance, which determines the microscopic physical and chemical properties, e.g., solubility, glass transition and boiling temperatures, dielectric constant, is poorly understood. Therefore, the knowledge of the structural models of the supramolecular clustering in alcohols is highly desired.

In this project we perform the molecular dynamics simulations of the structure of alcohols to unveil and to clarify at the molecular level the origin of the diffraction peaks observed at low-scattering vector range. The measured X-ray diffraction data in the form of the structure factor and the pair distribution function provide information on the short- and medium-range intermolecular order in the studied systems. Moreover, they also verify the theoretical models. It is shown that the architecture of the supramolecular clusters in two butanol isomers, n-butanol and t-butanol, differs significantly. The differences are reflected in the dielectric properties of the studied compounds, e.g. Kirkwood factor, which links the macroscopic dielectric constant of polar liquids to their local orientational order.(4,5)

The obtained results also correlates with the outcomes of the infrared spectroscopy. It is demonstrated that the combination of different experimental techniques and computer simulations is an effective tool in solving the complex structure of associating liquids.

Acknowledgments: J. G., K. J., B. H., K. K. and S.P. are thankful for financial support from the National Science Centre, Poland, within OPUS project (Dec. no 2019/35/B/ST3/02670).

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(4) J. Jadżyn et al., J. Mol. Liq., 314 (2020), 113652
(5) V. Durov et al., J. Phys. Chem. B, 112 (2008), 8076-8083

Contributed talk, Tue./14:15

Dielectric spectroscopy measurements of a PEO-based polymer electrolyte using interdigitated electrodes

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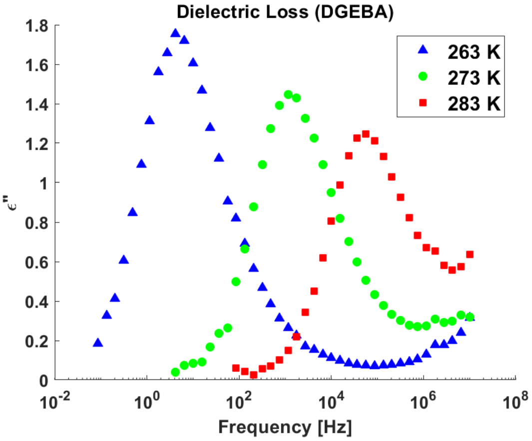
In our work we have targeted the investigation of the ion transport properties of a PEO-based polymer electrolyte (PEO-Na) by means of dielectric spectroscopy (DS). PEO-Na, which has already been used for ionic thermoelectric gating applications, is obtained from the reaction of PEO with metallic sodium and it is composed of mobile sodium cations and fairly immobile anionic polymer chains.(1)

Although DS is usually applied using electrodes with a parallel-plate geometry, we have decided to carry out the measurements using the less conventional geometry of interdigitated electrodes (IDEs),(2) since the use of a carefully designed IDE will enable us to conduct the measurements on a quantity of sample which is comparable to that used for the ionic thermoelectric gating applications (i.e. a drop with a diameter of about 500 μm), thus allowing us to probe ion dynamics on the length scale of actual interest. Using FEM simulations the IDE's geometrical parameters have been determined in such a way that they lead to the optimal value of the IDE's geometrical capacitance and to a sufficiently small area occupied by the conducting combs.

Because of the hygroscopic properties of PEO-Na, the DS measurements will be carried out in a vacuum chamber. In addition, the IDE will be placed inside a copper cell in order to limit thermal losses and gradients due to radiation and conduction. The sample's temperature is measured using a pt100 thermoresistance and regulated by means of a Peltier cell, which is coupled with a thermal circulator and controlled by a PID controller. The effectiveness of the thermal control of our experimental set-up has been checked by DS measurements on a fragile epoxy resin (DGEBA), extensively studied in the past.(3) Specifically, the actual temperature of DGEBA has been inferred by measuring the frequency of maximum dielectric loss and by using its known temperature dependence.



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Session VIII: Computational Physics

CONTRIBUTED TALK, TUE./15:00

New binary copper oxide phases from *ab initio*

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Binary copper oxides (Cu-O) have remarkable technological applications in the field of photovoltaics and all-oxide electronics due to their electronic and optical properties, their sustainability, excellent stability, and non-toxic in nature. They are excellent light absorbers across the visible energy range and furthermore, they give rise to a vast family of semiconductors and superconductors. Though they belong to the most studied transition metal oxides,(1,2), only three binary phases are well known Cu^{I}_2O, $Cu^{II}O$ and $Cu^{I}_2Cu^{II}_2O_3$. There are many indications scattered across the known literature that suggest formation of various other stoichiometries.(3,4) Also, a binary oxide with Cu^{III} is missing even though it is perfectly valid oxidation state of copper. The recognized technological potential of copper oxides as well as our chemical curiosity urges us for their immediate exploration. In this contribution, we provide new theoretical evidence for phase diversity among the binary copper oxides by addressing the „suspected" stoichiometries and oxidation states and their stability with Density Functional Theory methods and Evolutionary Algorithms. We take advantage of the structural diversity observed in the binary and ternary transition metal oxides and evaluate accessibility of their crystal structures to various copper oxidation states, electronic configurations (high-spin, low-spin) and ionic sizes in hypothetical binary copper oxides obtained by M → Cu substitution. Next, we use evolutionary algorithms for prediction of ground state crystal structures. We will present details of calculated crystal, electronic and magnetic structure, and lattice dynamics for the most interesting cases.

Acknowledgement: The European Regional Development Fund, Research and Innovation Operational Programme, for project No. ITMS2014+: 313011W085; Scientific Grant Agency of the Slovak Republic, grant No. VG 1/0223/19; the Slovak Research and Development Agency, grant No. APVV-18-0168; Aurel supercomputing infrastructure in CC of Slovak Academy of Sciences acquired in projects ITMS 26230120002 and 26210120002 funded by ERDF.

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CONTRIBUTED TALK, TUE./15:15

Toward isolated AgF_2 nanowire structure: dynamical and mechanical properties from *ab initio*

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Common known polymorphic form of silver difluoride (AgF_2) at ambient pressure has layered antiferromagnetic structure. The solid phase exhibits numerous structural and electronic similarities with oxocuprate precursors of high-temperature superconductors.(1) X-ray diffraction (XRD) study of phase transitions at high pressure and Density functional theory modeling (DFT)(2) showed that at an elevated pressure of 15 GPa, AgF_2 solid could transform to an unprecedented orthorhombic high-pressure polymorph (HP2) featuring an array of tubular subunits, which are built of corner sharing (AgF_4) squares. This features the first 1D-type of a metal fluoride nanowire, which and also the only one showing rigid square planar rather than common hexagonal or octahedral moieties. The observed tubular structured high-pressure polymorph opens a possibility to paving the way to a new 1D type of silver difluoride based nanomaterials. The fact that the individual AgF_2 nanowire units behave as neutral suggests that they could be in principle isolated from the crystal. In this respect we focused on pure first-principles investigation of the mechanical stability, elasticity and response of electronic structure and lattice dynamics to applied uniaxial strain to an isolated 1D-AgF_2 subunit structure. The mechanical properties, phonon system and vibrational modes in new nanowire were predicted and analyzed by use DFT+U exchange-correlation functionals and quasi-harmonic direct method.(3)

Acknowledgment: We acknowledge the ERDF, Research and Innovation Operational Programme, for project No. ITMS2014+: 313011W085; the Slovak Research and Development Agency, grant No. APVV-18-0168 and Scientific Grant Agency of the Slovak Republic, grant No. VG 1/0223/19. The calculations were performed on Aurel supercomputing facility in CC of Slovak Academy of Sciences acquired in projects ITMS 26230120002 and 26210120002 funded by ERDF and within computational grant GA62-24 at ICM of University of Warsaw.

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CONTRIBUTED TALK, TUE./15:30

Stable magnetic skyrmion without magnetic field

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A spin model for chiral magnets with nearest neighbour exchange interaction and Dzyaloshinskii-Moriya interaction (DMI) describes spin spiral (SS) state and magnetic skyrmion in presence of external magnetic field.(1) In contrary to this paradigm, some experiments show that periodicity of SS state is significantly lower(1) than it is expected from the model, skyrmion at zero magnetic field,(3) and skyrmion in centrosymmetric crystals(4) where DMI is negligibly small. In view of these shortcomings, we propose a new model(5) where we include nearest neighbour biquadratic antiferromagnetic exchange interaction. We find that this model of exchange interaction supports SS structure, even at vanishingly small DMI. Using Monte Carlo simulation with our model Hamiltonian, we find magnetic structures as found in the above mentioned experiments.

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(3) J. C. Gallagher et al., Phys. Rev. Lett. ,118 (2017), 027201
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(5) S. Bera et al., J. Phys. Condens. Matter, 33 (2021), 255801

Contributed talk, Tue./15:45

Local and non-local quantum transport due to Andreev bound states in finite Rashba nanowires with superconducting and normal sections

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We analyze Andreev bound states (ABSs) that form in normal sections of a Rashba nanowire that is only partially covered by a superconducting layer. These ABSs are localized close to the ends of the superconducting section and can be pinned to zero energy over a wide range of magnetic field strengths even if the nanowire is in the non-topological regime. For finite-size nanowires (typically <1 μm in current experiments), the ABS localization length is comparable to the length of the nanowire. The probability density of an ABS is therefore non-zero throughout the nanowire and differential-conductance calculations reveal a correlated zero-bias peak (ZBP) at both ends of the nanowire. When a second normal section hosts an additional ABS at the opposite end of the superconducting section, the combination of the two ABSs can mimic the closing and reopening of the bulk gap in local and non-local conductances accompanied by the appearance of the ZBP. These signatures are reminiscent of those expected for Majorana bound states (MBSs) but occur here in the non-topological regime. Our results demonstrate that conductance measurements of correlated ZBPs at the ends of a typical superconducting nanowire or an apparent closing and reopening of the bulk gap in the local and non-local conductance are not conclusive indicators for the presence of MBSs.

Contributed talk, Tue./16:00

Emergence of Majorana bound states in expansions of Rashba nanowire model

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Typically the Majorana bound states (MBS) can be induced at the ends of a one-dimensional wire, as a phenomenon possible due to the interplay between superconductivity, spin-orbit coupling, and an external magnetic field. Signatures of these states have been observed, e.g. in superconductor-semiconductor hybrid nanostructures or monatomic chains. In the case of the one dimensional chain, condition of the MBS emergence is comfortingly well known to be a dependence on the density of particles, Zeeman energy and proximity induced superconducting gap.

During this talk, I will present few cases when the MBS emerge outside of this topological "comfort zone" by expanding the Rashba nanowire model with the influence of antiferromagnetism, dimerization and extended dimensionality. I will discuss this in context of topological phase diagrams and demonstrate how these topological phases can be confirmed experimentally, e.g. within the non-local transport measurements.

Contributed talk, Tue./16:15

Emergence of Majorana bound states in expansions of Rashba nanowire model

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Recently, the generalization of conventional topological insulators (TIs) and topological superconductors (TSCs) to so-called higher-order TIs and TSCs has raised significant interest. While conventional d-dimensional TIs and TSCs host gapless edge states at their (d-1)-dimensional boundaries, nth-order d-dimensional TIs and TSCs exhibit gapless edge states at their (d-n)-dimensional boundaries. In particular, a two-dimensional second-order TSC hosts Majorana bound states at the corners of a rectangular sample. In this talk, I will consider a system consisting of two layers of tunnel-coupled Rashba nanowires ”sandwiched” between two conventional s-wave superconductors and subjected to an in-plane Zeeman field. I will show that this system exhibits a topologically non-trivial phase with Majorana corner states located at two opposite corners of the sample. Subsequently, I will discuss how the presence of strong electron-electron interactions can ”fractionalize” these Majorana corner states and promote them to even more exotic *parafermion* corner states.(1)

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(1) K. Laubscher et al., Phys. Rev. Research, 1 (2019), 032017(R)

Contributed talk, Tue./16:30

Volkov-Pankratov states in topological superconductors

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We study the in-gap states that appear at the boundaries of both 1D and 2D topological superconductors. While the massless Majorana quasiparticles are guaranteed to arise by the bulk-edge correspondence, we find that they could be accompanied by massive Volkov-Pankratov (VP) states which are present only when the interface is sufficiently smooth. These predictions can be tested in an s-wave superconductor with Rashba spin-orbit coupling placed on top of a magnetic domain wall. We calculate the spin-resolved local density of states of the VP states about the band inversion generated by a magnetic domain wall and find that they are oppositely spin-polarized on either side of the topological phase boundary. We also demonstrate that the spatial position, energy-level spacing, and spin polarization of the VP states can be modified by the introduction of in-plane electric fields.

Session IX: Flash Talsks II

Flash Talk, Tue./17:00

Analysis of information dynamics in chiral spin chain coupled to boson reservoir

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Presentation covers the study of dissipative dynamics of information in chiral spin chain coupled to non-Markovian magnonic reservoir. System of interest is described through the canonical Heisenberg Hamiltonian, including the exchange interactions between nearest and next nearest neighbours. Chirality of the chain is formed due to Dzyaloshinskii-Moriya interaction. The system is coupled to the environment, described in statistical terms (so called ”quantum bath”). The time deririvative of density matrices trace distance was utilzed to determine the direction of information flow and distinguishability of states. Distinct effect of applied electric and magnetic field was found: external electric field can be used to reshuffle the periods of information flow from and to the system, while the magnetic field has the impact on the rate of period transition. This finding reveals a possibility to control the information flow in helical spin rings.

Flash Talk, Tue./17:05

Ferroelectric nanoparticles host Hopfion

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Knot-like structures are very common across many branches of modern physics, like string theory, hydrodynamics, statistical or condensed matter physics. Among different knot-like formations, Hopfions, knotted solitons in three dimensional space, are still explored superficially, with some exceptions for magnetic materials. Present work demonstrates that Hopfion is stable, energetically favorable configuration of polarization field in $PbZrTiO_3$ ferroelectric nanoparticles. We show that Hopfions are responsible for complex electromagnetic properties in ferroelectric nanoparticles. Such properties can form the basis for novel computational devices.

Flash Talk, Tue./17:10

Wenzel to Cassie transition by infusing lubricant

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Liquid drops on lubricant infused surfaces (LIS) show enhanced properties, such as small roll-off angles and small adhesion. In other words, they show great mobility. That is because they are in the Cassie state (air cushions under the drop) or Floating state (no contact between drop and solid). In the case that the drop is in the Wenzel state (fully wet) on a pillared surface, the adhesion forces are big and the drop doesn't move easily. The question we tried to answer is that: could be possible to have a Wenzel to Cassie transition by infusing lubricant on the surface? Images taken by a laser scanning confocal microscope (LSCM) help us to examine the role of surfac's morphology, lubricant's and drop's surface tension and roughness on this transition. The transition occurs at small interpillar distances and big heights.

Flash Talk, Tue./17:15

Ab initio calculations for the α-phase of cooper pyrophosphate

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Amorphous and nanocrystalline pyrophosphates, containing transition metal ions, show unique physical, chemical, mechanical, electrical and thermal characteristics(1). In particular, the study of the magnetic properties of the Cu(II) pyrophosphate shows a rich spectrum of temperature-dependent electronic paramagnetic resonance(2). The electronic band structure obtained within the local density approximation shows an abnormal metallic state, indicating the importance of strong electron interactions in the Cu(3d) states.

Here, we consider copper pyrophosphate in the form of nanocrystals. The materials in the nanometer scale are currently the subject of intensive research due to their unique properties that cannot be obtained in bulk materials. Cooper pyrophosphate crystal structure was optimized starting from the experimental lattice parameters and atomic positions. For such purpose, the generalized gradient approximation (GGA) was applied taking into account the antiferromagnetic (AF) and ferromagnetic arrangements. The lattice parameters show some differences between the two magnetic states, however, they differ significantly from the experimental values. To get a better consistency, the GGA+U method was used. The crystal structure optimization was performed for the ground state AF order and including different van der Waals (vdW) corrections. The calculations show that the local Coulomb interactions and vdW forces influence the crystal structure of $Cu_2P_2O_7$, and they have to be included in the electronic structure and lattice dynamics studies. The calculated phonon dispersion curves and phonon density of states confirmed the dynamical stability of the alpha phase at low temperatures. The calculated frequencies and the assignment of the bands show a good agreement with the experimental non-polarized Raman spectroscopy studies on a single crystal.

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(2) O. Janson et al., Phys. Rev. B, 83 (2011), 094435

FLASH TALK, TUE./17:20

New dioxothiadiazole ligands for organic radical-based magnetic materials

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Organic radicals are a fascinating class of molecules that possess an unpaired electron giving rise to reactivity and physicochemical properties „radically" different than those of their neutral counterparts. In recent years, persistent organic radicals gained much attention in the design of molecular magnetic materials, thanks to their advantageous properties like relative stability over time, intrinsic paramagnetism and high tunability of their physical and chemical characteristics through chemical modifications.(1,2) Among functional motifs capable of displaying radical character the dioxothiadiazole, 1,2,5-thiadiazole 1,1-dioxide to be specific, is strongly underrepresented and the reports on its representatives are scarce, although molecules possessing this functional group are emerging recently as promising candidates for building blocks in molecular magnetism.(3,4) To this day there are no known examples of molecules containing multiple dioxothiadiazole units. Here, the first two members of such family, belonging also to the class of pseudooxocarbons, are presented (Fig. 1) and their remarkable electrochemical properties are discussed based on structural, voltammetric and EPR/magnetic studies. This new and unique class of compounds show four oxidation states providing an unprecedented access to very different electronic and magnetic properties of these molecules.

Acknowledgments: this work was financed by the Polish National Science Centre within the Sonata Bis 6 (2016/22/E/ST5/00055) research project and the Kościuszko Foundation.

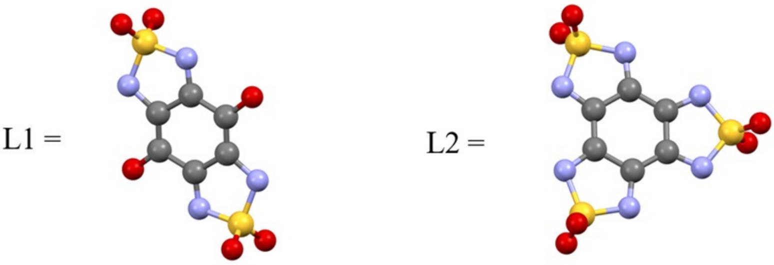

Figure 1. Crystal structures of L1 and L2 dianions.

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(2) P. Pakulski et al., Crystals, 9 (2019), 30
(3) Y. Shuku et al., Inorg. Chem., 50 (2011), 11859-11861
(4) D. Pinkowicz et al., Cryst. Growth Des., 14 (2014), 4878

Flash Talk, Tue./17:25

Dielectric properties of order-disorder phase transition of dimethylammonium zinc formate

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Metal-organic frameworks (MOFs) crystallizing in perovskite-like architecture are extremely interesting for scientists. These compounds are built from metal-oxygen or metal-nitrogen octahedral connected via organic linkers to form three-dimensional frameworks. MOFs have shown various properties or functionalities due to their hybrid inorganic-organic nature but ferroelectric MOFs still remain scare. Most efforts have been devoted to dimethylammonium metal-formate frameworks with general formula $[(CH_3)_2NH_2][M(HCOO)_3]$ (DMAM, where M denotes divalent metal ions). The most studied compound of this family is the dimethylammonium zinc formate. It undergoes an order-disorder phase transition at $T_c \approx 156$ K, surprisingly considered as ferroelectric one without direct proof. Although the nature of the phase transition in this compound has been extensively studied using a number of experimental methods, there are still many questions concerning the mechanism of the phase transition and relaxation processes in these hybrid perovskite structures remaining unanswered. For this compound, the dynamics of the DMA+ cation and framework deformation plays a key role in driving the structural order-disorder phase transition.

Here the analysis of the impact of metal substitution (Cu dopant) and the impact applied of external electric field on the order-disorder phase transition and relaxation processes will be presented. Basing on the dielectric spectroscopy results we will show that doping with Cu ions leads to a decrease of the T_c and change the character of the phase transition and we will look again at the relaxation processes (high- and low-temperatures) that has been enhanced by applying the electric field. These studies served as a window to understanding the origin of the relaxation processes in the DMAZn.

Session X: Positron Annihilation Spectroscopy

Contributed Talk, Wed./09:00

The radiation damage of PIN-diode detectors irradiated with heavy ions studied with the positron annihilation spectroscopy

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Damage of the semiconductor detectors induced by the ionizing radiation is a widely known phenomenon. In particular, the resistance to the radiation of the PIN-diode type of detector used in various measuring systems has been the subject of research in the past. The response of such detectors to the high flux of gamma quanta,(1) neutrons,(2) protons and electrons(3) has been studied. However, the information on the influence of high-flux heavy-ion interaction on the PIN diode-type detectors is still scarce. An example of the PIN-diode charge collection efficiency measurements is reported in paper.(4)

Furthermore, the qualitative deterioration of the acquired energy spectrum of the registered particles could be observed. This effect is of a great importance when designing the particle detection arrays to work in the exposure to high flux of heavy ions conditions.

An attempt was made to document the radiation damage process observed in the 300 μm thick PIN-diode detectors following the set of experiments performed at the Heavy Ion Laboratory in Warsaw, Poland, and at the Joint Institute for Nuclear Research in Dubna, Russia.

Spectroscopic properties of the set of PIN-diodes irradiated with the heavy-ion beam were further evaluated by measuring the α-particle spectrum emitted from the ^{241}Am source. Furthermore, structural defects caused by the heavy ions in the irradiated PIN-diodes were tested using the positron annihilation spectroscopy, which is a sensitive tool for the investigation of the openvolume defects as the vacancies and their clusters.(5–7)

The results of measurements will be presented.

(1) J.S. Miller, Materials Today, 17 (2014), 224-235(R)
(2) P. Pakulski et al., Crystals, 9 (2019), 30
(3) Y. Shuku et al., Inorg. Chem., 50 (2011), 11859-11861
(4) D. Pinkowicz et al., Cryst. Growth Des., 14 (2014), 4878
(5) S. Bera et al., J. Phys. Condens. Matter, 33 (2021), 255801
(6) S. Bera et al., J. Phys. Condens. Matter, 33 (2021), 255801
(7) S. Bera et al., J. Phys. Condens. Matter, 33 (2021), 255801

Contributed Talk, Wed./09:15

Application of nuclear spectroscopies and ion beams in the structural study of nanomaterials

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Due to the rapid scientific and technological development in the last decades, basic research in solid state physics, chemistry and material science has focused on objects and phenomena more and more confined in dimensions and time scale, and well visible for the general publicity by introducing the terms ”nanophysics, nanoscience, nanomaterials, etc.”, often featured in the media. Researchers therefore keep searching for better and better investigative techniques. Various nuclear spectroscopies, such as positron annihilation lifetime (PAL), doppler broadening of positron annihilation energy (DB), electron momentum distribution (EMD), slow positron beam (SPB), neutron diffractions (ND), Rutherford backscattering (RBS), etc., have proved themselves during the last decades as useful tools for microscopic analysis ranging from angstrom (Å) to nanometer (nm) scales. Besides, ion beams generated from accelerators (electron, ^{1}H, ^{2}He, ^{40}Ar, ^{86}Kr, ^{109}Ag, ^{123}Xe, ^{184}W etc.) have also become very effective tools for modifying the micro structures of nanomaterials. These methods have been intensively applied by our group in Ho Chi Minh city in order to study the in-depth structure of different nanomaterials. In this seminar, we will introduce our multidisciplinary research group, our nuclear analytical laboratory and some recent highlighted research results.

CONTRIBUTED TALK, WED./09:30

Structure of $BaTiO_3$ nanopowders modified by annealing treatment

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An important direction of many studies is focused on seeking an effective route to fabricate a rare room-temperature material that possesses ferroelectric and ferromagnetic properties and magneto-electric coupling.(1) The origin of these properties is different and can be observed simultaneously only in nanoscale. It was found that many diamagnetic materials in the form of nanoparticles become ferromagnetic.(2,3) It is believed that the reason for the appearance of magnetic properties is the presence of surface vacancy defects. Technologically essential is developing an effective way for modification of $BaTiO_3$ nanopowders properties and practical tools for controlling their surface defect structure. In current studies, we investigated a structure of $BaTIO_3$ nanoparticles modified by annealing treatment using positron annihilation, XPS, Raman, IR spectroscopies, and XRD, SEM methods. The obtained results were confronted with magnetic measurements to find interrelations between structural defects in nanoparticles with their magnetism. It reveals that low-temperature annealing causes the appearance of additional oxygen vacancies, and high-temperature annealing favors the reduction of Ti. These changes affect nanoparticle magnetism.

(1) The-Long Phan et al., J. Appl. Phys., 113, (2013), 17E305
(2) R. V. K. Mangalam et al., J. Phys.: Condens. Matter, 21 (2009), 445902
(3) A. Sundaresan et al., Nano Today, 4 (2009), 96-106

CONTRIBUTED TALK, WED./09:45

Research on biopolymer matrices synthesized on the basis of soybean oil in the construction of biosensors of trace water pollutants and analysis of the impact of the matrix composition on its nanostructure

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The biopolymer matrices were synthesized from epoxidized soybean oil (AESO), vanillin dimethacrylate (VDM) and vanillin diacrylate (VDA) and triarylsulfonium hexafluorophosphate salts (PI). The samples were examined using Positron Annihilation Lifetime Spectroscopy (PALS). The showed results are based on the ortho-positronium (o-Ps) lifetime τ_3 and intensity I_3 as a function of temperature (120–320 K). The tested samples contained the substance VDM or VDA, which differ from each other by the presence of two more methyl groups in the case of VDM substances. In addition, the matrices contained AESO + VDM/VDA substances in various molar ratios. Some of the tested samples also contained PI. The PALS technique investigated the influence of the molar ratio of the tested substances, the presence of PI and the type of admixture (VDA or VDM) on the nanostructure. The temperatures of phase transitions were also determined. Sample results for 3 selected samples are shown in Figure 1.

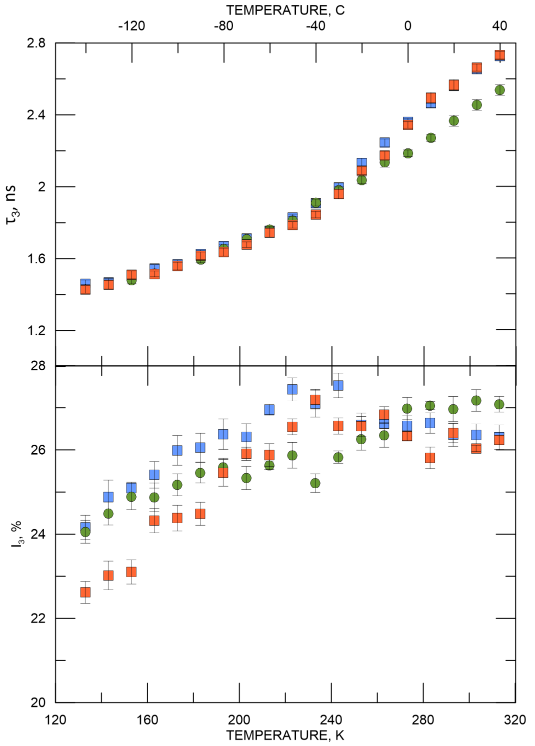

Figure 1. Sample results for 3 selected samples.

CONTRIBUTED TALK, WED./10:00

Gradient microstructure induced by Surface Mechanical Attrition Treatment (SMAT) in magnesium studied by positron annihilation spectroscopy

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[2] Faculty of Metals Engineering and Industrial Computer Science, AGH University of Science and Technology, Kraków, Poland
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Surface mechanical attrition treatment (SMAT) was used to generate a gradient microstructure in commercial-grade magnesium. The SMAT process is based on surface plastic deformation induced by repeated impacts on the treated surface with high-velocity spherical shots of a few millimeters in diameter. Multidirectional impacts induce grain refinement to the nanometer scale at the target surface. SMAT was performed in the stainless-steel chamber at room temperature in air using 2 mm diameter stainless steel balls and a vibration frequency of 20 kHz, for 60 s and 120 s with twice the vibration amplitude. The normal speed of shots depends on the vibration amplitude, i.e. increase in the amplitude leads to a higher impact velocity. Doubling the vibration amplitude leads to doubling the velocity of shots and hence their kinetic energy rises approximately fourfold.

Polarized light microscopy, EBSD, and XRD revealed a gradient microstructure within the deformed surface layer of the SMATed magnesium. It was found that SMAT causes an increase in dislocation density and grain refinement, which was indicated by the X-ray diffraction measurements and high values of the mean positron lifetime.

The mean positron lifetime indicates trapping of positrons in vacancies associated with dislocations and dislocation jogs. Its value decreases with the distance from the treated surface to the values measured for the reference sample indicating the end of SMAT induced region at the depth of about 800–900 μm. It is in good agreement with the thickness of the hardened layer and is confirmed by the images obtained by optical microscopy and electron backscatter diffraction.

The variable energy positron beam measurements showed a thicker oxide layer formation on the surface of the sample SMATed for 120 s in comparison to the one SMATed for 60 s. Electrochemical corrosion tests revealed that the structural changes induced by SMAT increased the susceptibility of magnesium to anodic oxidation, leading to the enhanced formation of hydroxide coverage at the surface and, as a consequence, leading to apparent better corrosion resistance.

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Session XI: Magnetism, Multifunctional Materials

Contributed Talk, Wed./10:30

Dynamics and magnetic properties of NO molecules encapsulated in open-cage fullerene derivatives evidenced by low temperature heat capacity

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A better understanding of the dynamics of caged atoms/molecules can lead to several new applications in nanoscale science and technology. Especially, open-cage fullerene derivative is an ideal molecular cage for encaging small gas molecules as an isolated form. In this work, we conducted the heat capacity analyses for nitric oxide (NO) molecules confined in the open-cage fullerene for the purpose of capturing the dynamics and the magnetic properties. We have captured the thermal anomaly below 10 K, which associates with the motion of the NO molecule. We also have revealed that NO accommodated in the cage molecule shows strong magnetic anisotropy, which originates from unquenched orbital angular momentum. Complete-active-space self-consistent field (CASSCF) calculations revealed that magnetic properties of NO molecule are sensitive to the conformation of the molecular cage.

CONTRIBUTED TALK, WED./10:45

Magnetic investigations of single crystals of spin chains

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The slow relaxation of magnetization in spin chains based on Co(II) ion is a very complex issue. For that reason, we started investigations of single crystals of spin chains from family $[Co(NCS)_2(ligand)_2]_n$ in hope of getting new information, not possible to extract from powder samples. The first single crystal we obtained was $[Co(NCS)_2$(4-(3-phenylpropyl)pyridine$)_2]_n$ **(1)**, which orders ferromagnetically at 3.39 K.(1) For the first time, for the compound from the investigated family, we observed two different relaxation processes (Fig. 1., left), one of which is single chain relaxations. The second relaxation process we assign to spin waves. None of these processes were observed for a powder sample. To check whether the presence of the second process is a unique property of **(1)**, we prepared another single crystal proper for magnetic investigations — $[Co(NCS)_2$(4-methoxypyridine$)_2]_n$ **(2)**. This compound orders antiferromagnetically at 3.93 K. The single crystal sample shows, similarly to the powder sample,(2) single chain relaxation process, and another process, dominant above T_c (Fig. 1., right). Contrary to **(1)**, the relaxation time of the second process is temperature-independent. Apart from the observation of new relaxation processes, the single crystal samples provide us with information about the location of the magnetic easy axes, which confirms the theoretical predictions of ab initio calculations.

This project is supported by National Science Centre, Poland (Project Preludium 19 No. UMO2020/37/N/ST3/02526).

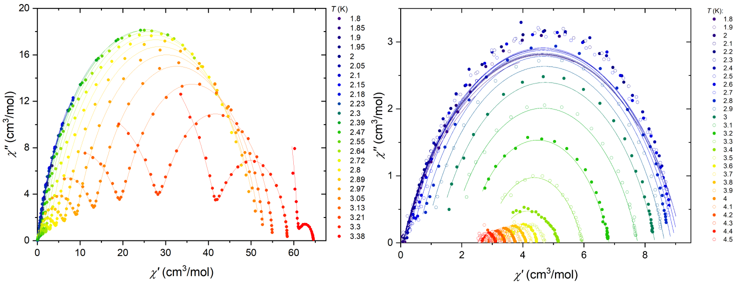

Figure 1. The Argand plot of ac magnetic susceptibility measured for **(1)** at $H_{dc} = 0$ Oe (left) and **(2)** at $H_{dc} = 1100$ Oe (right).

(1) M. Ceglarska, et al., Phys. Chem. Chem. Phys., 23 (2021), 10281-10289
(2) M. Rams, et al., Chem. Eur. J., 26 (2020), 2837-2851.

Contributed Talk, Wed./11:00

Nanopatterned MOM junctions

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The MOM junction is a system composed of a trilayer structure where M is a transition metal and O is a metal oxide. This type of structure can be designed as a magnetic tunnel junction when the metal layers are ferromagnets and the interlayer is an insulator. Magnetic junctions are the first spintronic elements used commercially in the electronic industry. Another type of junction is a system in which the spacer layer is a semiconductor. The connection between metal and the semiconductor lead to the creation of the Schottky diode.

To produce a semiconducting oxide we use the anodization method, which allows to obtain the nanopatterned layer with spatially ordered structures with sizes typically tens of nanometers. The anodization method makes possible easy control of the nanostructures' size by the change of the anodization voltage. Introducing structurization leads to formation of defects influencing the electric and magnetic properties of junctions.

In this study, we focus on the characterization of the nanostructured titanium/titanium oxide/iron junctions with various size of nanostructures. The crystal structure of the junctions was observed with X-Ray Diffraction (XRD) and the images of the surface were obtained by SEM measurements. The magnetic properties were investigated with SQUID magnetometry and the transport measurements were performed with a standard four-probe technique. The results showed that the hysteresis curves are a combination of two magnetic phases including iron and its oxides formed at interfaces. The magnetoresistance characteristics showed the transition from positive to negative values with decreasing temperature. The positive MR comes from the titanium/titanium oxide interface and the negative MR has a source at the titanium oxide/iron interface. Introducing the structurization increased the values of magnetoresistance and also caused the appearance of the glass-like behavior.

The support from the NCN grant 2015/19/D/ST3/01843 is acknowledged.

Contributed Talk, Wed./11:15

Spin relaxation in molecular nanomagnets: first-principles modeling and case studies

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Molecular nanomagnets is an emerging field within molecular magnetism that has been recently reinvigorated by record hysteresis temperatures above the nitrogen boiling point. In the path to prevent nanomagnets from magnetization reversal and harness them as tiny classical memories, crystal field engineering via synthetic chemistry has displayed an undoubted key role. The current step to clear in the pursuit of new nanomagnets able to operate at higher temperatures is the control and suppression of the spin-phonon coupling.

In this contribution, we will firstly overview the recent experimental advances with special focus on lanthanide- and actinide- based molecular nanomagnets. On top of that, we will provide an inexpensive first-principles methodology devoted to simulate spin relaxation in f-block nanomagnets, which will be illustrated with two case studies. The theoretical results allow identifying those molecular vibrations that mostly promote spin relaxation and proposing a molecular structure re-design to suppress them.

CONTRIBUTED TALK, WED./11:30

^{13}C-NMR study of λ-(BETS)$_2$GaBr$_x$Cl$_{4-x}$($x = 0.9$)

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The organic conductor λ-(BETS)$_2$GaCl$_4$ undergoes a superconducting (SC) transition at 5 K. In the investigation of the mechanism of superconductivity, the nature of the adjacent insulating phase is important, and a systematic understanding of the physical properties using phase diagrams is necessary. H. Mori et al. attempted to understand the P-T phase diagram of λ-D$_2$GaCl$_4$ by donor substitution.(1) On the other hand, H. Tanaka et al. investigated the adjacent insulating phase in the alloy system λ-(BETS)$_2$GaBr$_x$Cl$_{4-x}$, and reported that the non-magnetic insulating (NMI) phase is adjacent to the SC phase in λ-(BETS)$_2$GaCl$_4$. However, the details of the magnetic state are not clear.(2) Recently, T. Kobayashi et al. carried out ^{13}C-NMR in λ-(BETS)$_2$GaBr$_{0.75}$Cl$_{3.25}$ and concluded that the insulating phase adjacent to the SC phase is the spin density wave (SDW) phase.(3) To further investigate ground state of the phase with increasing Br concentration, we focused on λ-(BETS)$_2$GaBr$_{0.9}$Cl$_{3.1}$ which locates in a more negative pressure position.

The sample was a single crystal of BETS with one side of the central C=C bond substituted with ^{13}C. Resistivity, spectra, and spin-lattice relaxation time (T_1) were performed on the same batch of samples and confirmed that the behavior was consistent with the results of Tanaka et al.

Figure 1. shows the temperature dependence of $1/T_1$ and $1/T_1T$. Different from λ-(BETS)$_2$GaBr$_{0.75}$Cl$_{3.25}$, the $1/T_1$ increases monotonically and diverse at 11 K, suggesting an antiferromagnetic (AF) transition at 11 K and the existence of a different AF phase adjacent to the SDW phase. In the presentation, we will discuss the insulating phase of λ-type salt.

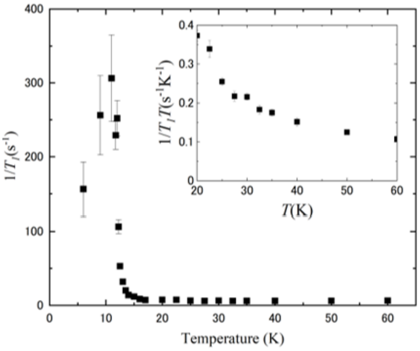

Figure 1. Temperature dependence of $1/T_1$ and $1/T_1T$.

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(1) H. Mori et al., Phys. C Supercond., 103 (2001), 357-360
(2) H. Tanaka et al., J. Am. Chem. Soc., 121 (1999), 760
(3) T. Kobayashi et al., Phys. Rev. Research, 2 (2020), 02307

CONTRIBUTED TALK, WED./11:45

Dielectric and thermodynamic properties of mixed valence coordination polymer $[\mathrm{Cu^{I}_{7}Cu^{II}Br_{7}}\ (n\text{-}\mathrm{Bu_{2}dtc})_{2}]_{n}$

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Coordination polymers are potential candidates of functional materials with high electrical conductivity in which metal ions and cross-linked organic ligands self-assemble to form coordination networks. (1)

In this study, we investigated the dielectric and thermodynamic properties of mixed valence coordination polymer $[\mathrm{Cu^{I}_{7}Cu^{II}Br_{7}}\ (n\text{-}\mathrm{Bu_{2}dtc})_{2}]_{n}$, in which complexes of Cu(II) with di-n-butyl dithiocarbamate $[\mathrm{Cu^{II}}(n\text{-}\mathrm{Bu_{2}dtc})_{2}]$ and Cu(II)Br$_2$ are coordinated.

The impedance measurements revealed that $[\mathrm{Cu^{I}_{7}Cu^{II}Br_{7}}\ (n\text{-}\mathrm{Bu_{2}dtc})_{2}]_{n}$ showed an anomaly in dielectric constant at around 350 K (Fig. 1●). However no thermal anomaly was detected at this temperature by the differential scanning calorimetry (DSC), expect that two phase transitions were observed at 239 and 389 K. We carefully investigated the exothermic and endothermic behaviours by using an adiabatic calorimeter, and finally found an exothermic behaviour at above 360 K, which was attributed to a spontaneous stabilization from a metastable to a stable phase (Fig. 2●). When the sample was annealed at 387 K for 24 h, the exotherm disappeared (Fig. 2△). The annealed sample did not show the anomaly in the dielectric constant at 350 K, while a step-like increase was found at 400 K (Fig. 1△), which was possibly associated with the structural transition at 389 K. These results indicated that the dielectric anomaly observed at 350 K were characteristic to the metastable phase.

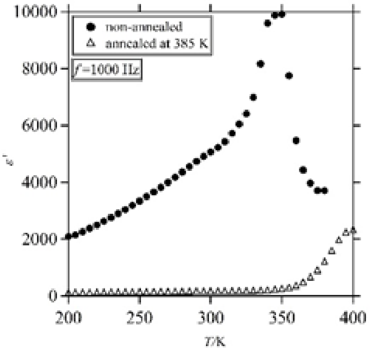

Fig. 1 Temperature dependence of dielectric constant of $[\mathrm{Cu^{I}_{7}Cu^{II}Br_{7}}\ (n\text{-}\mathrm{Bu_{2}dtc})_{2}]_{n}$ between 200 K and 385 K

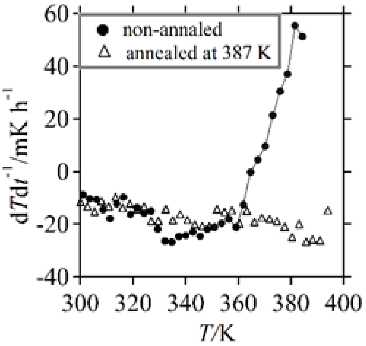

Fig. 2 Temperature dependence of the rate of temperature change of $[\mathrm{Cu^{I}_{7}Cu^{II}Br_{7}}\ (n\text{-}\mathrm{Bu_{2}dtc})_{2}]$ in adiabatic condition

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(1) T. Okubo et al., Dalton Trans, 40 (2011), 2218-2224

Session XII: Multifunctional Materials, Miscellany, New Ideas

Contributed Talk, Wed./13:00

Spin-resolved thermoelectric properties of correlated magnetic molecules

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Thermoelectric transport studies through nanostructures such as molecular junctions, quantum dots and nanowires, owing to their discrete density of states exhibit striking thermoelectric efficiency compared to their bulk counterparts. Besides, (spin) thermoelectric coefficients of these nanostructures were shown to provide insights into the signatures of quantum correlations present in the system, the Kondo effect in particular. With the advent of the spin Seebeck effect, fascinating interplay of charge, heat and spin gives rise to a broad range of behavior in the spin-dependent thermoelectric coefficients. Although studied extensively in the presence of weak correlations, the behaviour of such systems in the strongly correlated case remains to be deeply investigated.

Thus, in this work, we investigate the spin-resolved thermoelectric properties through a molecular junction modelled as an orbital level exchange coupled to a large spin magnetic core in the linear response regime using the numerical renormalization group method. In particular, we study the molecule in the presence of both nonmagnetic and ferromagnetic electrodes having fast and slow spin relaxation times. We analyze the signatures of the Kondo effect in the transport and the (spin) thermoelectric properties of the system and show how the ferromagnetism in the leads and parameters of the molecule, such as the exchange interaction and magnetic anisotropy, affect the Kondo resonance in the system. In addition, we observe a new sign change in the Seebeck coefficient for antiferromagnetic exchange interaction in the molecule at low temperatures. Our work provides a comprehensive analysis of (spin) thermopower in the case of large-spin molecules dependent on the exchange interaction and finite magnetic anisotropy of the molecule.

This work was supported by the Polish National Science Centre grant No. 2017/27/B/ST3/00621.

Contributed Talk, Wed./13:15

Local structure studies of multifunctional $CuMoO_4$ and $CuWO_4$ solid solutions

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Copper molybdate ($CuMoO_4$) and related solid solutions are multifunctional materials exhibiting several chromic-related properties, including thermochromism, tribochromism, piezochromism, halochromism. $CuMoO_4$ also has thermosalient, photoelectrochemical, catalytic and antibacterial features. To control the functionality of the material, its structure-property relationship must be understood.

In this study, $CuMo_{1-x}W_xO_4$ thermochromic compounds were investigated to elucidate the structural origin of their optical properties. The results of temperature and composition-dependent X-ray absorption and resonant X-ray emission spectroscopy (XAS and RXES) studies are presented. XAS provides information on the local environment around absorbing atoms. Reverse Monte-Carlo calculations allowed us to create a 3D structural model consistent with the experimental data and to follow a change of the local structure of $CuMoO_4$ upon temperature variation. The RXES method was used to understand the role of W^{6+} ions in $CuMo_{1-x}W_xO_4$ solid solutions and determine changes in the crystal field-induced splitting of the 5d(W) states across the phase transitions.

The ability to adjust the thermochromic properties in a controllable manner to more desired temperature ranges may make the material interesting for applications as an indicator for monitoring storage/processing conditions of temperature-sensitive products (drugs, vaccines, chemicals, biological materials, etc.).

The work has been supported by the Latvian Council of Science project No. lzp-2019/1-0071. I.P. acknowledges the L'ORÉAL Baltic „For Women In Science" Program with the support of the Latvian National Commission for UNESCO and the Latvian Academy of Sciences.

CONTRIBUTED TALK, WED./13:30

The "core-shell" type magnetic nanoparticles in biomedicine: preparation, physical properties and applications

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One of the promising areas of nanotechnology development is the medical field of application of nanostructures. Nanomedicine is a rapidly developing area in the last decade, including methods for the prevention, diagnosis and treatment of a wide range of diseases using various types of nanostructures. The control of the shape, size, and chemical composition of nanostructures allows to set their physical properties at the synthesis stage and opens up new possibilities for bioprocessing. A rather interesting possibility of using nanostructures is the targeted delivery of useful goods (drugs or proteins) using a magnetic field. In this method, a drug or protein is attached by functional groups to a magnetic nanostructure and introduced into the circulatory system, after which it is transported to a problem area through a magnetic field. One of the most promising materials for creating magnetic nanostructures is iron oxide or an alloy of iron with nickel due to its greater saturation magnetization compared to this value for pure ferromagnetic metals Co, Ni, and Fe.

The use of magnetic nanostructures in medicine can not only efficiently deliver biologically active molecules through various body barriers that they are not able to overcome on their own (skin, blood-brain), but also significantly change the nature of the drug. Nanostructures of magnetic metals (iron, cobalt and nickel) are rarely used in pure form for therapeutic purposes. Usually they are encapsulated or placed in bioinert matrices (various organic compounds or polymers, including those of natural origin) in order to reduce the possible toxic effects of the magnetic phase, increase its physico-chemical stability and create the possibility of immobilization of the surface of such capsules or matrices of drugs. Coating magnetic metals with a carbon shell or noble metals such as gold and silver increases their effectiveness in medical applications.

CONTRIBUTED TALK, WED./13:45

Design and microfluidic flow of a vesicle prototissue

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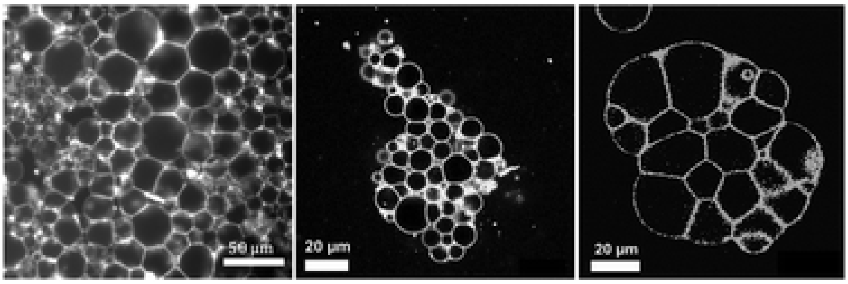
Bottom-up synthetic biology and biomimetic approaches are promising tools that allow reconstitution of biological systems with reduced degrees of complexity. The aim of this work is to build an artificial biomimetic tissue with tunable properties through the controlled assembly of Giant Unilamellar Vesicles by using the Streptavidin-Biotin pair or DNA complementary strands. By combining the ligand-to-receptor ratio and the vesicle volume fraction we are able to obtain vesicle aggregates of known size and degree of internal adhesion. The latter can also be controlled by changing the type of ligand. The morphology of such systems can be changed by applying different incubation techniques: we can obtain sheet-like structures (2D) or spheroidal (3D) aggregates (Fig. 1). We believe that frequency of vesicle-vesicle collisions, diffusion of free ligands in solution and lateral diffusion of bound ligands are the main mechanisms that govern the kinetics of vesicle assembly. The rheological behavior of this vesicle aggregates will be studied in microfluidic confinement, and the ability to tune its physical features will allow us to selectively probe specific mechanisms involved in their microfluidic flow. The study of this model system will help deepen the knowledge in tissue flow, which takes place in relevant biological processes like embryogenesis, metastasis, and would healing.



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(1) L. Casas-Ferrer et al., Soft Matter., 17 (2021), 5061-5072

CONTRIBUTED TALK, WED./14:00

Influence high hydrostatic pressure on electrical properties of ferroelectric $(Ba_{0.83}Ca_{0.17})TiO_3$ ceramics

A. Szeremeta[1], A. Molak[1], A. Winiarski[1], D. Mahato[2], J. Macutkevic[3], I. Gruszka[1], S. Miga[4], J. Koperski[1], E. Palaimiene[3], S. Pawlus[1]

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Ferroelectric materials are characterized by wide application possibilities in microelectronics, microwave, and memory devices. The Pb-based ferroelectric materials have been the subjects of a large class of materials showing the perovskite ABO_3 structure. However, there is an urgent need to study Pb-free materials to overcome environmental concerns and toxicity restrictions.

In our studies, we have sintered the Pb-free barium calcium titanate, $(BaCa)TiO_3$, ceramic compound, with a Ca content of 17%, by the solid-state reaction procedure, which was modified in comparison to literature data. The electric impedance was measured by using broadband dielectric spectroscopy (BDS). At ambient pressure, the ferroelectric to paraelectric phase transition was diffused and markedly shifted to the lower temperature, $T_c = 339$ K, in relation to barium titanate. After the sample is pressurized up to 1.4 GPa, the phase transition temperature decreased by ≈ 52 K. The scanning electron microscope measurement showed fluctuation in chemical composition.

The authors are grateful for the financial support provided by the National Science Centre within the framework of the Opus 13 project (Grant No. DEC-2017/25/B/ST3/02321).

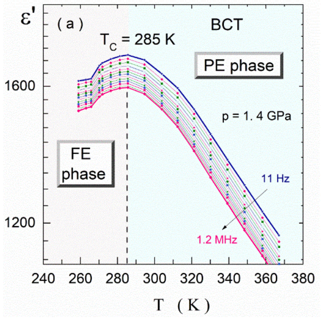

Figure 1. Real part of the permittivity temperature dependence, $\varepsilon'(T)$, obtained at 1.4 GPa.(1)

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(1) A. Molak et al., J. All. Comp., 856 (2021), 158216-1-13

Contributed Talk, Wed./14:15

Applying Density Functional Tight Binding approach to study X-ray-induced phase transitions in solid materials

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[2] Center for Free-Electron Laser Science, DESY, Hamburg, Germany
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Modern X-ray free-electron lasers generate intense XUV and X-ray pulses able to trigger ultrafast electronic and structural transitions in solids. This opens unique opportunities for material processing as well as new challenges in the related computer simulations. Here we present a dedicated computational approach developed to study X-ray and XUV-induced phase transitions in a broad range of solid materials. This is possible due to the utilization of the well-known density functional tight binding code, DFTB+ to follow band structure evolution of the irradiated targets. The outstanding performance of the implementation is demonstrated with a comparative study of the XUV induced graphitization in diamond.

Contributed Talk, Wed./14:30

Effect of tacticity of PtBMA thin films on interactions with proteins, peptides and bacteria

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Tacticity of polymers has a major role in adsorption of biomacromolecules to polymer thin films. In our work, we investigated three forms of tacticity of poly(tert-butyl methacrylate) (PtBMA): atactic (at), isotactic (iso) and syndiotactic (syn). Our studies by Secondary Ion Mass Spectrometry, Fluorescence Microscopy and X-ray Photoelectron Spectroscopy revealed that the orientation of side groups in the polymer main chain modifies the interactions with biomacromolecules. For iso-PtBMA the side groups are exposed to the external environment which results in differences in adsorption of proteins and peptides in comparison to at-PtBMA and syn-PtBMA. In the case of peptides, this is caused by interactions between the polar ester group of iso-PtBMA and positively charged peptides. The tacticity of the polymeric thin film does not affect the amount of adsorbed protein, but it does affect the orientation and conformation of the protein. Additionally we noticed, that tacticity of the polymers also affects the interactions with bacteria. In case of Gram-positive bacteria (in this case S. aureus) the higher adhesion is observed for iso-PtBMA compared to the other two tacticities.

This work was financially supported by the National Science Centre of Poland under Grants No. UMO-2016/21/D/ST5/01633.

Poster Session I: 10:10-11:10

POSTER NO. 1

Development of a tabletop femtosecond electron diffraction system

S. Banu[1], M. Hada[2], Y. Hayashi[2], T. Ishikawa[1], S. Jin[1], M. Kaneko[1], S. Koshihara[1], K. Takubo[1], Y. Okimoto[1]

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[2] University of Tsukuba, Tsukuba, Japan
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Ultrafast electron diffraction (UED) is a developing technique which provides new insights of molecular/atomic movements in solid materials with high time resolution. This technique has been utilized for the study of photoinduced structural changes in realistic systems such as conformational changes in crystal symmetry, the mechanism of phase transition and structural dynamics after the photo-excitation.(1–3) In order to directly observe the changes in crystal structure followed by photo-excitation, we are developing an electron diffractometer with a time resolution of several tens of fs based on a new synchronization method between laser light and electron bunch compressor. By capturing the structures on the ultrafast timescale, we are able to develop concepts that correlate structure with photoinduced changes in various properties of solid materials. As an instrumentation, an optical pulse from Ti: sapphire regenerative amplifier (1 kHz, 30 fs, 800 nm) synchronized with an oscillator with a frequency of 3 GHz is splits into two arms by an upstream beam splitter. The third-harmonic light (THG) (266 nm) is generated from one of the arms and focused on a gold thin film to generate an fs electron pulse for the probe of UED. The other light is used as excitation light by wavelength conversion. This realizes pump-probe measurements based on the transmission electron diffraction method. The acceleration voltage of the electron beam is set to 100 kV to minimize the damage to the target sample.

In order to get ultrashort electron pulses, it is necessary to compress the electron bunch with a radio frequency (RF) cavity which works at 3 GHz synchronized with the master oscillator.(4) Here we demonstrate fs-UED system with a new synchronization method to reduce the timing jitter between the laser and the RF cavity. We use the laser oscillator (30 fs pulse, FemtoLock) equipped with phase lock loop, to synchronize the laser pulse with the frequency of 3 GHz RF master oscillator. To check the time resolution (pulse width of electron bunch) of our developed UED, we measured photoinduced structural dynamics of 50-nm-thick silicon film (Fig. 1A). As shown in Fig. 1B, very fast decay of the diffraction intensities from the (220) and (400) planes were observed within 100 fs. The results in detail will be discussed in the presentation.

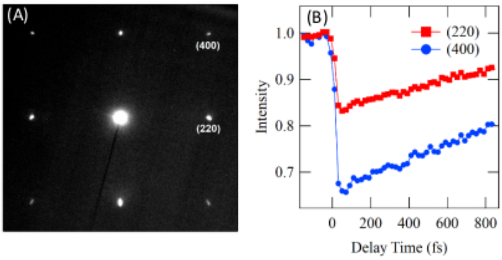

Figure 1. (A) The diffraction pattern of 50-nm-thick silicon film. (B) The time-evolution of the diffraction intensities at the (220) and (400) peaks after the photo-excitation, fast decay of the intensity was observed within 100 fs after photo-excitation.

(1) J. Edbert et al., Nature, 565 (2019), 61-66
(2) M. Eichberger et al., Nature, 468 (2010), 799-802
(3) A. Kogar et al., Nat. Phys., 16 (2020), 159
(4) M. Gao et al., Opt. Express, 20 (2012), 12048

Poster No. 2

Electronic properties of quasi-one-dimensional organic conductor $(\text{DMET-TTF})_2\text{AuBr}_2$

T. Kato, Y. Iida, Y. Sasaki, M. Sawada, N. Matsunaga, A. Kawamoto, K. Nomura

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DMET-TTF is an asymmetric donor molecule that combines one side of a TMTTF molecule and one side of a BEDT-TTF molecule. DMET-TTF molecules are alternately stacked, and the normal to the molecular plane is tilted largely from the stacking axis, which is expected to have a stronger dimerization effect than TMTCF family. $(\text{DMET-TTF})_2\text{AuBr}_2$ is a quasi-one-dimensional organic conductor with a Fermi surface similar to $(\text{TMTCF})_2\text{X}$. In our previous study, we found that $(\text{DMET-TTF})_2\text{AuBr}_2$ transitions to the antiferromagnetic (AF) phase at ambient pressure and to the spin-density-wave (SDW) phase under pressure.(1) In order to clarify the magnetic structures of these phases, we performed ^{13}C-NMR measurements under 6 T. The NMR spectrum in the paramagnetic phase is a single peak because two ^{13}C in a unit cell are crystallographically equivalent (interpolated figure of Fig.1).

At ambient pressure, the spectrum splits at 22 K (Fig.1), and T_1^{-1} also shows a peak structure at 22 K. The magnetic moment is estimated to be 0.06 μB/molecule, which suggests nesting type AF, i.e., commensurate SDW (C-SDW). In $(\text{TMTTF})_2\text{Br}$, $(\uparrow - \text{o} - \downarrow - \text{o})$ type C-SDW has been reported from the $2k_F$ instability.(2) On the other hand, in $(\text{DMET-TTF})_2\text{AuBr}_2$, the NMR spectrum suggests $(\uparrow - \uparrow - \downarrow - \downarrow)$ type C-SDW, which can be explained by the strong dimerization.(3)

Under 0.5 GPa, a SDW transition with multiple peaks in the NMR spectrum was observed at 14 K. On the other hand, T_1^{-1} is constant below 10 K. In our transport measurements, we observed threshold electric fields that can be explained by impurity pinning in the incommensurate SDW. In a high electric field region, negative differential resistance was observed.

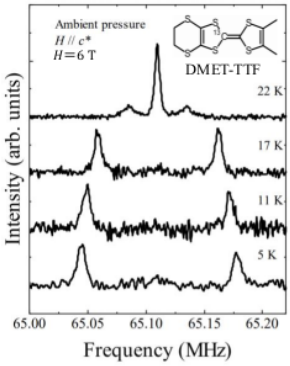

Figure 1. Temperature dependence of NMR spectrum of $(\text{DMET-TTF})_2\text{AuBr}_2$ at ambient pressure.

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(1) Y. Sasaki et. al., J. Phys. Soc., 13ak23-6 (Autumn 2019)

(2) S. Hirose et. al., Phys. Rev. B, 88 (2013), 125121

(3) H. Seo et. al., J. Phys. Soc. Jpn., 66 (1997), 1249

Poster No. 3

Observation of CN stretching mode below magnetic phase transition temperature on a MnW octacyanide molecule-based magnet

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Introduction: Molecule-based magnets are attractive from the viewpoints of rational molecular design and various functionalities.(1) In the molecule-based magnets, influence of long-range magnetic ordering such as ferromagnetic (or ferrimagnetic) ordering on the phonon mode is of high interest. In this work, we synthesized an octacyanide-bridged manganese tungstate bimetal assembly and observed an shift of the CN-stretching frequency below magnetic phase transition temperature.

Experiment: $Mn_3[W(CN)_8]_2(\textit{pyrimidine})_4 \cdot 6H_2O$ (MnW) was prepared using the reported method,(2) i.e., adding a 5.0 mL aqueous solution of $MnCl_2 \cdot 4H_2O$ to an aqueous solution of $Cs_3[W(CN)_8] \cdot 2H_2O$ and an aqueous solution of pyrimidine, yielding a dark brown microcrystal. The crystal structure was determined by Single-crystal X-ray structural analysis. The magnetic properties were measured using SQUID magnetometer. The IR spectrum was measured by using a SHIMADZU IRAffinity-1S spectrometer.

Result: Single-crystal X-ray structural analysis revealed that MnW has a 3D crystal structure (monoclinic; space group *P21/n*).(Fig.1) Magnetic measurements showed that MnW exhibited spontaneous magnetization below the magnetic phase transition temperature (T_c) of 47 K. In the temperature dependence of the IR spectrum, eight peaks due to the CN stretching frequency were observed around 2150–2200 cm^{-1}, and they showed frequency-shifts below 50 K. From the first-principles calculation, the origin of the frequency-shifts of the peaks were assigned to the contraction of the Mn^{II}-CN-W^{V} bonds. The mechanism of this phenomenon can be explained by the competition of the magnetic energy and the elastic energy.

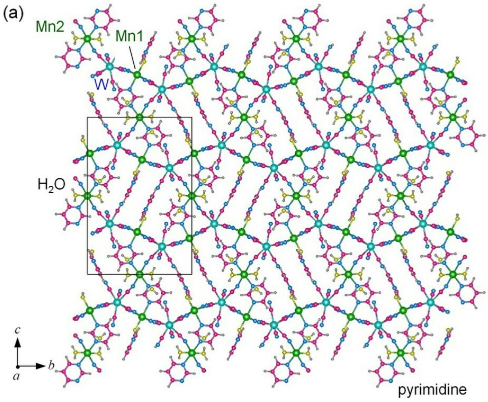

Figure 1. Crystal Structure of MnW.

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(1) S. Ohkoshi et. al., Nature Chem., 12 (2020), 338
(2) T. Kashiwagi et. al., J. Am. Chem. Soc., 126 (2004), 5024

Poster No. 4

Thermodynamic properties of metastable gel phase for cationic surfactant cetyltrimethylammonium bromide (CTAB)/water system

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Surfactant/water systems form various types of self-aggregates such as micellar, lyotropic liquid crystal (LC), and gel phases. The gel phase is less popular than the other phases, which consists of bilayer membranes and water molecules occupying the space between the membranes. The alkyl chains in the membranes adopt all-trans conformations and the rotational motions around the long axis are limited. Although gel phase has been observed for many surfactant/water systems, its location has rarely been determined in precise phase diagrams, which provoked a discussion from the view point of thermodynamics whether gel phase can be treated as an equilibrium phase or not.(1)

Cetyltrimethylammonium bromide ($[(C_{16}H_{33})N(CH_3)_3]Br$; CTAB) is a popular cationic surfactant, which has been used in the synthesis of gold nanoparticles and mesoporous materials. In this study, we have investigated thermodynamic properties of CTAB/water binary system by differential scanning calorimetry (235–320 K) and adiabatic calorimetry (78–320 K), and revealed that the gel (L_β) phase appears as metastable state.(2) L_β phase was obtained by rapidly cooling the micellar phase or LC phases, and the metastable phase diagram was successfully established (Fig. 1). Details of the thermodynamic quantities associated with the transition between L_β and micellar or LC phases will be discussed in the presentation.

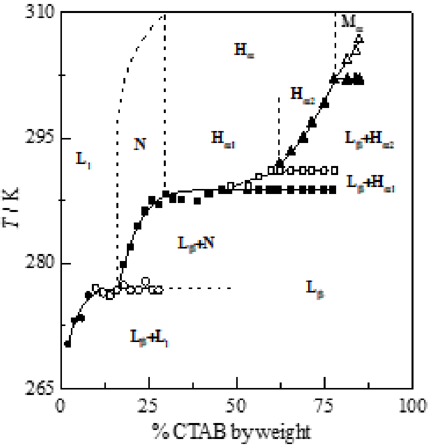

Figure 1. Metastable phase diagram of the CTAB/water.

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(1) K. Holmberg, Handbook of Applied Surface and Colloid Chemistry, Wiley, New Jersey, 2002

(2) T. Yamamoto et. al., Colloids and Surf. A Physicochem. Eng. Asp., 625 (2021), 126859 (1-9)

Poster No. 5

Pressure effect on the magnetic properties of MnW cyanide-bridged bimetal assemblies

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Cyano-bridged bimetallic assemblies are promising for molecular magnets that exhibit magnetic functionalities, such as external-stimulus responsive magnetisms, etc.(1,2) Especially, octacyanide-bridged bimetallic assemblies are expected to exhibit magnetic functionalities due to their diverse coordination geometries. In this work, octacyanide-based bimetal assemblies $\{Mn^{II}(\mathit{pyrimidine})(H_2O)\}_2\{Mn(H_2O)_2\}\{W^V(CN)_8\}_2 \cdot zH_2O$ are synthesized and their pressure effect on the magnetic properties are reported.

Target compounds were prepared by reacting an aqueous solution of $Cs_3[W(CN)_8]$ to an aqueous solution of $MnCl_2{\cdot}4H_2O$ (or $NiCl_2{\cdot}6H_2O$) and pyrimidine under stirring.(2) Analysis of the composition by ICP-MS and CHN elemental analysis indicated that the synthesized compounds consist of the chemical formula of $\{Mn^{II}(\mathit{pyrimidine})(H_2O)\}_2\{Mn(H_2O)_2\}\{W^V(CN)_8\}_2 \cdot zH_2O$ (**1**) ; Calculated values : Mn, 11.91; W, 26.30; C, 27.97; N, 24.41; H, 2.10%; Found: Mn, 12.17; W, 26.21; C, 28.04; N, 24.34; and H, 2.21%. Single-crystal X-ray structural analysis indicates that (**1**) had a monoclinic crystal structure in the *P21/n* space group with a lattice constant of a = 7.2319(4) Å, b = 14.9477(8) Å, c = 22.4483(13) Å. Magnetic measurements showed that MnW exhibited spontaneous magnetization below the magnetic phase transition temperature (T_c) of 47 K. Next, magnetic measurements under applying pressure (P) were performed. The T_c value linearly shifts toward a higher temperature from $T_c = 47$ K to $T_c = 58$ K as P increases up to 1.0 GPa, indicating that the slope of (dT_c/dP) is 11 K GPa^{-1}.

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(1) S. Ohkoshi et al., Nature Photonics, 8 (2014), 65-71
(2) T. Kashiwagi et. al., J. Am. Chem. Soc., 126 (2004), 5024-5025

POSTER NO. 6

Effects of stretching on the melting behaviors of silicone rubbers

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Rubber is liquid as a thermodynamic state, which can be crystallized with decreasing temperature. On heating the crystallized rubbers, melting and recrystallization occur successively, which is characteristic to crystalline macromolecules. Rubbers can also be crystallized by stretching even above the melting temperature because polymer chains are forced to be aligned. In this study, we investigated the melting behavior of stretched silicone rubbers in the temperature range from 78 to 380 K using adiabatic calorimetry. The stretching ratios of the rubbers to the free length L_0 were 1.00, 1.78, and 2.56 (i.e., $\lambda = L/L_0 = 1.00; 1.78$, and 2.56).

Fig.1 shows the specific heat capacities in the vicinity of the melting point. It was found that the melting peak became broader and slightly shifted to higher temperature with increasing stretching ratio. Exothermic behaviors due to the recrystallization were also observed at around 200–260 K for all the samples. The fusion enthalpies, including the heat generated during the recrystallization, were estimated to be 18.92; 19.72 and 20.94 J/g for the sample of $\lambda = 1.00; 1.78$, and 2.56, respectively, which indicated that the higher the stretching ratio, the greater the amount of crystals at low tem-perature.

The annealing effects on the recrystallization and melting behaviors will be discussed in the presentation.

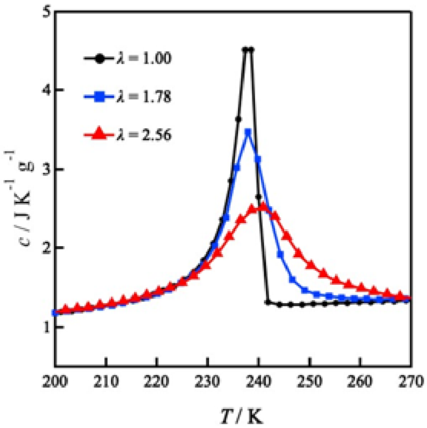

Figure 1. Specific heat capacities of silicone rubbers with the stretching ratios of 1.00; 1.78; 2.56.

POSTER NO. 7

Investigation of π-d interaction in λ-(BEST)$_2$FeCl$_4$

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The quasi-two-dimensional organic conductor λ-(BETS)$_2$FeCl$_4$, where BETS is bis(ethylenedithio)tetraselenafulvalene [Fig 1(a)], shows a magnetic-field induced superconducting state when a magnetic field is applied precisely parallel to the conducting layers. The mechanism of the FISC is explained by the Jaccarino-Peter compensation mechanism, where the external magnetic field compensates the internal field of aligned d spins through the π-d interaction.(1) However, the details of π-d interaction mechanism is still unknown.

BEST (bis(ethylenediseleno)tetrathiafulvalene) [Fig 1(b)] is an analog of BETS. Comparing BETS and BEST, we can get the information which inner or outer chalcogens are more important in the path of the π-d interaction. λ-(ET)$_2$FeCl$_4$, where ET is bis(ethylenedithio)tetrathiafulvalene [Fig 1(c)], an alternative candidate, where Se atoms in BETS are substituted with S atoms in ET molecule. However λ-(ET)$_2$FeCl$_4$ has not been available. Hence BEST is a good candidate for a systematic study of π-d interaction.(2)

In this conference, we will discuss the path of the π-d interaction with the X-ray diffraction and magnetic susceptibility measurements. Moreover, we plan to perform Mössbauer spectroscopy and ^{13}C NMR, and we will discuss the results of microscopic studies.

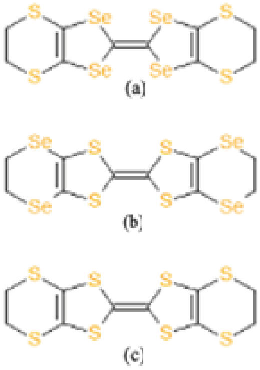

Figure 1. Molecular structure of (a) BETS, (b) BEST, (c) ET.

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(1) S. Uji et al. Nature, 410 (2001), 908
(2) H.B. Cui et al. Chem Lett., 254 (2005)

Poster No. 8

Kramers-like problem for underdamped Levy flights

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The noise driven motion in a bistable potential acts as the archetypal model of various physical phenomena. In the weak noise limit, for the overdamped particle driven by a non-equilibrium, α-stable noise the ratio of forward and backward transition rates depends only on the width of the potential barrier separating both minima. The poster presents analytical and numerical results showing that in the regime of full dynamics the ratio of transition rates depends both on widths and heights of the potential barrier separating minima of the double-well potential.

Poster No. 9

Thermoluminescence studies of $Y_3Al_2Ga_3O_{12}$:Cr^{3+} persistent nanophosphors

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From the moment of the first publications to the present day, materials with long-lasting emission, known as persistent luminescence (PersL), have been of interest both from the point of view of fundamental science (trapping and de-trapping mechanisms, traps effect on the decay time etc.) and from the point of view of application in various fields of optics and sensors. (1)

Cr^{3+} doped $Y_3Al_2Ga_3O_{12}$ (YAGG:Cr) nanophosphors are one of the attractive materials in such type of materials. In particular, the YAGG:Cr nanophosphors co-doped with lanthanides have gained attention due to their PersL in the visible, red, and NIR range, where Cr plays an important role for extended the PersL decay time. (2)

In this work, YAGG:Cr nanophosphors synthesized by the Pechini method followed by annealing at temperatures from 800 to 1300°C. The lattice parameters and average grain sizes were calculated from the Rietveld refinement data based on X-Ray powder diffraction data. To investigate the effect of grain size of the materials on its optical properties, absorption, photoluminescence (PL) emission and excitation, as well as luminescence decays and thermoluminescence (TL), were recorded and analysed. It was found that both PL and PersL properties of the YAGG:Cr strongly depend on the grain size. The PL and PersL of the YAGG:Cr have typical Cr spectral features, indicating that both processes originate from the same emitting centres. It is determined that with increasing grain size the electron-phonon coupling decreases, whereas the crystal-field strength increases. The correlation between structural changes and TL behaviour was revealed. In particular, the redistribution of traps and activation energy reach optimal values when the lattice constant reaches the threshold.

Acknowledgements: This work was supported by the OPUS 11 2016/21/B/ST5/02385 project.

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(1) J. Xu et al., Lumin., 205 (2019), 581-620.

(2) V. Boiko et al., Scientific Reports, (2021) 11:141

POSTER NO. 10

Retardation of quantum correlation decay of two spin qubits by quantum measurements

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We study a system of two electron spins each interacting with its small nuclear spin environment (NSE), which is a prototype system of two quantum dot (QD) spin qubits. In such a system it is possible to initialise, to coherently manipulate, to entangle and to read out electron spins only, the NSEs of QDs are beyond of direct experimentalists' control. (1,2)

The two electron spins subsystem (TESSS) initially being in an entangled state in course of time evolution loses its coherences and quantum correlations due to the Fermi contact hyperfine coupling with NSEs. Quantum correlations (coherences) initially present solely in TESSS changes into the quantum correlations between TESSS and its NSEs. With connection to that one may propose a way to counteract decay of entanglement in TESSS by performing some manipulations with TESSS, e.g. repeatable quantum projective measurements (PMs) of TESSS. Performing a few cycles of free evolution of the system for a some time τ followed by a quantum measurement of TESSS with subsequent postselection of TESSS state (the same as the initial one) produces quantum correlations in NSEs and also restores the quantum correlations in TESSS. By numerical calculation of the system evolution (full density matrix $\widehat{\rho}(t)$) we show that in contrast to a fast decay of TESSS entanglement on timescale $\sim T_2^*$ (shown in Fig. 1 of [3] or [4]), performing a few cycles of evolution of initially entangled two electron spins interacting with their NSEs followed by quantum measurement performed on TESSS gradually build up coherences in the entire system and the rest decay of quantum correlations of TESSS may be significantly slowed down for specific cycle durations τ and numbers of the performed cycles (see Fig. 1).

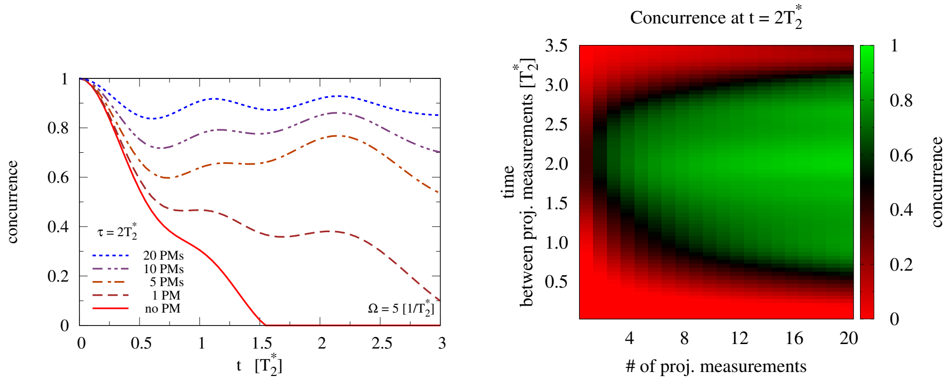

Figure 1. Plot: time evolution of entanglement (concurrence) of TESSS initially being in the Bell state $\widehat{\rho}(0) = |\Psi_- >< \Psi_-|$. Map: concurrence of TESSS calculated for $\widehat{\rho}(t = 2T_2^*)$. Electron Zeeman splitting $\Omega = 5[1/T_2^*]$. NSEs consist of 5 spins 1/2 each.

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(1) D. Kim et al., Nature Phys., 7 (2011), 223-229

(2) K. De Greve et al., Rep. Prog. Phys., 76 (2013), 092501

(3) P. Mazurek et al., Phys. Rev. A, 89 (2014), 062318

(4) I. Bragar et al., Phys. Rev. B, 91 (2015), 155310

Poster No. 11

Phase composition and microstructure of iron-containing glasses and glass-ceramics

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The synthesis of oxide glasses and glass-crystalline materials with advanced electrical and magnetic properties is of great potential to apply them in electronics, medicine and for environmental monitoring.

The present work reports on the synthesis of oxide glass-crystalline materials in the system $Na_2O/CaO/SiO_2/Fe_2O_3$ by the melt-quenching technique. The prepared materials crystallize during cooling of the melt due to their high iron oxide concentrations. The phase composition of the obtained materials studied by X-ray diffraction shows the spontaneous crystallization mainly of magnetite, Fe_3O_4 and besides of some hematite, Fe_2O_3. The electron microscopy studies, combined with energy-dispersive spectroscopy analyses allow to evaluate the chemical composition of the obtained Fe-containing crystals. Results were in agreement with the predictions of the X-ray diffraction. As a last step of the microstructural characterization of the prepared materials, micro-computed tomography investigation is performed on selected samples. It shows the occurrence of a relatively high-volume fraction of platelet-like crystals, which are supposed to correspond to the Fe-containing crystalline phase.

Acknowledgements: The authors acknowledge the financial support of the Bulgarian National Science Fund under grant КП-06-Н48/4.

POSTER NO. 12

Vibration spectroscopy and neutron diffraction studies on glasses and glass-ceramics in the system $Na_2O/BaO/TiO_2/B_2O_3/SiO_2/Al_2O_3$

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Glasses were synthesized in the system $Na_2O/BaO/TiO_2/B_2O_3/SiO_2/Al_2O_3$ using a conventional high-temperature glass melting technique and thereon based glass-ceramics were prepared by applying different time-temperature crystallization schedules to the glasses.

The structures of the obtained glasses and selected glass-ceramics were investigated using Fourier-transformed infrared and Raman spectroscopy and the existence of SiO_3, SiO_4, Si_2O_7, BO_3 and BO_4 structural units was proposed. Also, the occurrence of multiple prenucleation clusters inhomogenously distributed in the amorphous matrix with compositions close to that of the barium titanate, $BaTiO_3$ phase could be suggested from subsequent IR-data processing.

The phase composition of the obtained glass-ceramics was initially proposed by conventional X-ray diffraction and further investigated by Raman spectroscopy and as main crystallizing phases $BaTiO_3$ and barium fresnoite, $Ba_2TiSi_2O_8$ were identified.

Additional information on the crystallization behaviour, phase formation and occurrence of phase transitions for the glasses was gathered by using in situ crystallization combined with neutron diffraction analysis. The neutron diffraction data reveals crystallization of $BaTiO_3$ in all compositions. The kinetics of crystallization was also studied and revealed the phase transition of tetragonal to cubic $BaTiO_3$ taking place in some of the compositions.

Acknowledgements: The authors express their gratitude to the Bulgarian National Science Fund, contract КП-06-Н28/1 for the financial support.

Poster No. 13

Influence of the parallelepiped form localized defects on ellipsometry data: scale modeling

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This paper is devoted to the problem of the analysis of ellipsometric data of the surface with localized defects (different phases, blistering, grains etc.). In these cases, often is not even a clear understanding of how certain types of defects affect the values measured in an ellipsometric experiment. Earlier, in the works devoted to the study of the radiation stability of the precipitation-hardened CuCrZr alloy, anomalous (non-classical) angular dependences of the ellipsometric parameters were found. It was assumed that this is due to the scattering of radiation by the secondary phases protruding above the surface of the copper matrix. Accordingly, when the angle of incidence is changed, the detector receives the radiation that is reflected from different parts of the sample.

This experiment was carried out using a terahertz ellipsometer with an operating wavelength of 2.14 mm. The ellipsometric parameters of ferrite samples with a defect in the form of a parallelepiped are measured. The size of the defect was varied, which made it possible to determine the minimum size of the defect distinguishable by the ellipsometric technique. The trend of the dependences of the ellipsometric parameters was determined as a function of the incidence angle in the presence of a defect several times larger than the wavelength. A qualitative change in the dependences of the ellipsometric parameters on the angle of incidence of radiation with a decrease in the size of the defect has been determined. The size of the defect at which the ellipsometric parameters practically coincide with the data for a clean surface is determined. The comparison of the results of the ellipsometric and the reflectometric techniques are carried out. The model was confirmed, according to which localized defects, the dimensions of which are slightly smaller than the probe radiation wavelength, become "invisible" for ellipsometry, although they strongly affect the specular reflection coefficient.

POSTER NO. 14

Electrical conductivity of lithium-sodium tetragernabate glass

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Lithium-sodium tetragermanate $LiNaGe_4O_9$ (LNG) is one of the representatives of germano-germanates complex oxides family. Earlier it was shown that charge transfer in LNG single crystal was strongly anisotropic and determined by Li ions motion.(1,2) In this work we study electrical conductivity of LNG glass devitrified on heating. The LNG glass was prepared by fast quenching the melts between two massive copper plates. The samples were then polished to the shape of rectangular parallelepipeds 0,5 mm thick with the main faces being 5×5 mm^2. These main faces were covered by Pt electrodes.

Electrical conductivity σ of lithium-sodium tetragermanate (LNG) glass was measured in an alternating current field. The experiment was conducted with the sample being heated from 300 K to 900 K at a rate of 8 K/min and then cooled. The results of the measurements are presented in the Arrhenius scale in Fig.1. One can see that on heating σ of LNG glass increases exponentially and abruptly decreased above $T_{\max} = 820$ K as a result of the glass crystallization. Subsequent cooling of the crystallized sample showed nearly linear behavior of $\sigma(1/T)$ dependence. Conductivity of LNG glass is three orders of magnitude higher as compared with σ values for LNG polycrystal. One can assume that thermal treating of LNG glass between glass transition temperature T_g and $T_{\max}$ can be used for preparation of nanocrystallized glass-ceramic compounds with increased ionic conductivity in analogy with lithium heptagermanate glass-ceramics.(3)

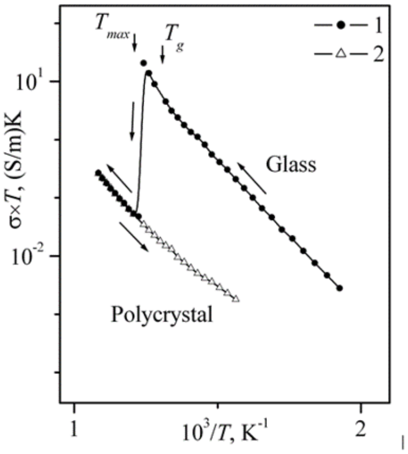

Figure 1. Arrhenius plot for the conductivity of LNG on heating (1) and following cooling (2).

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(1) M. Volnianskii et al., Ferroelectrics, 443 (2013), 16-19

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(3) M. Volnianskii et al., Phys. Sol. St., 54 (2012), 945-946

Poster No. 15

Positron Annihilation Spectroscopy study of defects in doped diamonds

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Positron annihilation spectroscopy (PAS) study of defects in doped diamonds is important for solving different applied problems in X-ray optics and quantum sensorics.

Generation of the diamond plates was conducted by HTHP method with addition of nitrogen in different concentrations (12.5 ppm, 75 ppm, 88 ppm). At the first stage diamond plates were investigated by methods of IR-spectroscopy, UV-spectroscopy, Raman-spectroscopy and XRS-spectroscopy. At the second stage crystalline structure of the diamond plates was studied with Positron Annihilation Spectroscopy (PAS). PAS is nowadays well recognized as a powerful tool of microstructure investigations of crystalline materials. It can be used in cases where other popular methods such as scanning electron microscopy (SEM) or /mboxX-ray diffraction are not applicable. PAS is non-destructive method of detecting open-volume defects such as vacancies, vacancy clusters, dislocations and microvoids.

Positron spectroscopy of doped diamond defects can be performed by Doppler broadening spectroscopy of annihilation radiation and positron lifetime spectroscopy (PALS). Each method used a radioactive isotope of sodium (^{22}Na). PALS method is based on determination of the positron lifetime in the doped diamond plate. This method shows average lifetime of the positron, what in turn reveals defects in their type in the material. The positron lifetime gives information about the electron density inside the defect. Doped diamond plates in this study show typical vacancy-type defects from monovacancies up to large clusters. Second method investigates doppler broadening on ^{22}Na source. Third method is Doppler Broadening on positron beam with energy of positrons from 0 to 20 keV.

This study reveals dependence between nitrogen concentration and appearance of the defects in the diamond plates. All the defects are of the vacancy-type. Dependence of the amount of such defects is also in accordance with the depth of the layer in diamond plate.

POSTER NO. 16

Towards thin films of multi-responsive molecular switches

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In the field of molecular materials, there has been a constant development of novel tuneable materials, for which different properties such as magnetic behaviour can be controlled by external conditions. Preparation of stimuli-responsive molecule-based materials in the form of thin films is an important step towards the exploration of their application potential as molecular switches or sensors. Compounds in the form of thin films react more efficiently to external stimuli and are more suitable for the construction of molecular devices. Various methods, including Langmuir-Blodgett, vapour deposition, spin- and dip-coating as well as electrochemical techniques, were employed in the studies on the formation of thin films for several classes of molecular magnetic materials.(1) However, in the group of CN-bridged coordination polymers, the surface deposition was studied almost exclusively for Prussian blue analogues (PBAs). While PBAs, thanks to high connectivity, usually show higher temperatures of magnetic ordering, hybrid organic-inorganic CN-bridged coordination polymers are exceptionally efficient in the development of switching characteristics, implemented at the molecular level, while at the same time they can accommodate different functionalities.

In our recent study, we have focused on the thin film preparation of multi-responsive chain-like coordination compound $NH_4[Ni(cyclam)][Fe(CN)_6] \cdot 5H_2O_n$ ($cyclam$ = 1,4,7,11-tetraazacyclotetradecane), which display drastic magnetic and optical changes under ambient conditions in response to various stimuli such as temperature, pressure, humidity or light.(2) Herein we present preliminary results of thin film deposition using the drop-casting technique containing mentioned CN-bridged coordination compound with switching abilities.

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POSTER NO. 17

Controlling of magnetic properties of iron-based composite particles

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Iron and its oxide nanoparticles have received considerable attention due to their applications in magnetic, electronic, pigmental, catalyst and biomedical purposes.(1,2) The expected magnetic properties for these applications are different, so control of the coercivity is important.

We proposed an unique laser process for preparation of submicron composite magnetic particles. Source magnetite or hematite colloid solutions were irradiated in various organic solvents by Nd:YAG laser with 2nd and 3rd harmonics, various laser fluences and irradiation times. In our work we investigated how size and composition of iron compound particles evolves according to changing irradiation conditions. It was found that during irradiation of magnetite and hematite nanoparticles the dominant phases of the particles are reduced from magnetite and hematite to iron or iron carbide.(3)

The formation of various iron compound particles in controlled laser irradiation process of magnetite and hematite nanoparticles indicates that the magnetic properties of the obtained particles can be tuned.

This work gives us a method for obtaining iron compounds complex particles, which size, composition and magnetic properties can be controlled by the conditions of laser irradiation.

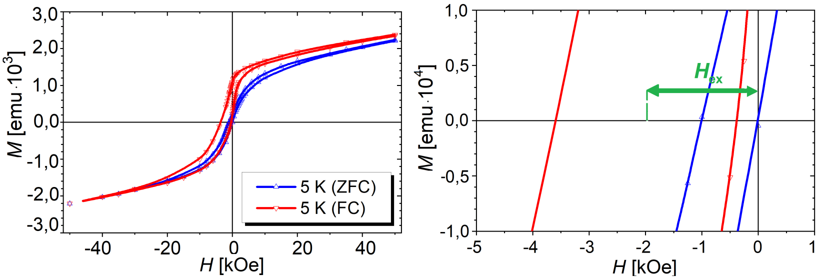

Figure 1. Typical magnetic loop obtained for Fe_3O_4/FeO composite particles.

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(3) Z. Swiatkowska-Warkocka et al., Nanoscale Res. Lett., 6 (2011), 226

POSTER NO. 18

Crystal structure and luminescence of $Gd_{1-x}Yb_xAlO_3$:Mn^{4+}

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In the last decade, high-performance phosphors capable to convert visible blue and UV light into red light are attracting considerable attention of researchers as perspective materials for warm white light sources, luminescence thermometry, biological applications, etc.

Polycrystalline samples of $Gd_{1-x}Yb_xAlO_3$:Mn^{4+} ($x = 0.2; 0.4; 0.6$) were obtained by common solid-state synthesis from initial oxides of Gd_2O_3, Yb_2O_3, Al_2O_3 and MnO_2. High-temperature annealing in air was performed at 1500°C in three stages each of 10 h with two intermediate grindings. According to X-ray phase analysis main orthorhombic perovskite phase along with traces of monoclinic $Gd_4Al_2O_9$ and garnet $(Gd_{1-x}Yb_x)_3Al_5O_{12}$ phases were revealed. The additional annealing at 1650°C during 10 h led to a decrease in content of undesirable phases.

Photoluminescence (PL) properties of the studied $Gd_{1-x}Yb_xAlO_3$:Mn^{4+} samples were measured in the temperature range from 4.5 to 300 K. It was revealed that intensity of Mn^{4+} photoluminescence observed near 715 nm decreases significantly with increasing of ytterbium content, which is associated with an interaction and excitation energy transfer between Mn^{4+} and Yb^{3+} ions. This interaction is also responsible for reduction of the PL decay time (τ) of Mn^{4+} ions. The highest specific sensitivity $|(\Delta\tau/\Delta T)\tau - 1|$, which determines performance of a material for the luminescence thermometry based on temperature dependence of the decay time, was obtained for the sample $Gd_{0.4}Yb_{0.6}AlO_3$:Mn^{4+} in the temperature range 57–175 K that correlates with the lowest absolute values of decay time for this particular sample (about 70 μs at $T \leq 50$ K).

The work was partially supported by the National Research Foundation of Ukraine under Grant no. 2020.02/0373.

Poster No. 19

Decomposition of water molecules on titanium dioxide nano powder under neutron irritation

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It is known that TiO_2 has been extensively used in various areas, such as medicine, food industry, and nuclear applications. The paper aims in understanding the behavior of titanium dioxide nano powders subjected to fast neutron irradiation with different fluences. Neutron irradiation was conducted at 1 atm, 293.15 K, with fluencies of 4.0×10^{12} n/cm^2, 8.0×10^{12} n/cm^2, 1.3×10^{13} n/cm^2, 4.0×10^{14} n/cm^2 and 10^{15} n/cm^2 (neutron energy $E > 0.1$ MeV). X-ray Ray Diffraction, Raman spectroscopy, Neutron Diffraction, and FTIR spectroscopic complementary techniques were used to characterize the crystal structure of the samples before and after the irradiation. The lattice parameters of TiO_2 nanopowders samples were obtained using XRD and ND. X-ray diffraction study has been performed using Panalytical EMPYREAN diffractometer with Cu Kα radiation ($\lambda = 1.5406$ Å) and the neutron diffraction was conducted on RTD instrument at IBR-2 research reactor using Time-of-flight diffraction technique. All five irradiated and one original nano powder sample were successfully fitted by Rietveld refinement in anatase phase, SG $I41/amd$ with unit cell parameters ($a = 3.791$ Å and $c = 9.52$ Å), values differing slightly from values for bulk samples. Analysis of Raman spectroscopy revealed that the peak intensities increased with increasing fluences which can be interpreted as thermal annealing effect of the neutron irradiation. On the other hand, the formation mechanism of OH radicals was studied by using FTIR spectroscopic techniques. The major changes before and after irradiations were presented in detail. In conclusion, the obtained experimental results were evaluated comparatively with each other.

Poster No. 20

Study of pressure-induced polymorphic phase transitions in pharmaceutical compounds

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Due to the wide variety of phenomena realized in organic crystals at high pressure: polymorphic phase transitions, amorphization, etc.,(1–3) studies of pressure-induced changes in the crystal structure and atomic dynamics of complex molecular crystals is an urgent task in condensed matter physics.(2,4) In addition, structural studies of molecular crystals are important for optimization the of pharmsaceutical production process, where, under additional mechanical influences (grinding or tabletting), irreversible polymorphic phase transitions or its amorphization can develop in the initial material,(5) which entails significant changes in the physicochemical and pharmaceutical properties of materials.(3)

The use of Raman spectroscopy under high pressure to study pharmacological components makes possible investigation of their vibrational properties in the most complete way, which is necessary to understanding the nature and mechanisms of physical phenomena observed in them.

Therefore, the main objective of this study was detail investigation of vibrational properties of the group of pharmaceutical compounds by means of Raman spectroscopy in wide pressure range.

Investigation of internal structure and atomic dynamics of pharmacological components: anti-inflammatory drug meloxicam $C_{14}H_{13}N_3O_4S_2$ and antiulcerous component ranitidine hydrochloride $C_{13}H_{22}N_4O_3S \cdot HCl$ were carried out.

At pressure $P > 4$ GPa, several changes in the Raman spectra of meloxicam were observed, which can indicate a pressure-induced phase transformation. Near the polymorphic transition pressure, the changes in the part of Raman spectra were obtained. In additional, the new Raman lines were detected at pressure $P > 10$ GPa. These changes can indicate another polymorphic phase transition in the meloxicam. Around this phase transformation, the noticeable anomalies in the pressure behaviour of different vibration frequencies of the meloxicam were found.

The pressure dependence of vibrational modes of ranitidine hydrochloride measured at high pressures up to 9.8 GPa and room temperature were shown. The changes in a pressure behavior of the Raman lines were observed at pressures 2.2 and 6 GPa. Those changes can indicate the polymorphic phase transitions ranitidine hydrochloride under pressure.

The structural mechanisms of the phase transition in presented pharmaceutical compounds were discussed.

This work was supported by the JINR youth grant No. 21-402-01.

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Poster No. 21

Vibrational spectroscopy study of $SrTiO_3$-based quantum paraelectrics

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Study of ferroelectric materials is of exceptional interest due to the combination of dielectric, piezoelectric and optical properties appearing at phase transitions. Quantum paraelectrics also attract the great attention because structural transformations are observed in a wide temperature range due to the presence of random quantum motion of ions. One of the most interesting quantum paraelectric materials is strontium titanate $SrTiO_3$, which dielectric permittivity on cooling follows the Curie-Weiss law, but the macroscopic ferroelectric phase transition doesn't occur even at low temperatures. Also $SrTiO_3$ is characterized by the antiphase rotations of the oxygen octahedra at $T_a \approx 105$ K. It is worth noting, that structural changes in $SrTiO_3$ may be influenced drastically by external and internal deformations, such as epitaxial strains or chemical doping.

The aim of the research is to understand the role of polar and nonpolar instabilities in the formation of ferroelectric transition in $SrTiO_3$. We studied the barium-doped strontium titanate ceramics, $Ba_xSr_{1-x}TiO_3$ ($x = 0; 0.01; 0.02$), using X-ray diffraction and optical vibrational spectroscopy methods. X-ray diffraction revealed that on cooling lattice parameters of $Ba_xSr_{1-x}TiO_3$ decrease and around 100 K additional parameter appears indicating tetragonal distortion in studied systems. It is also confirmed by Raman spectroscopy. On cooling additional lines $B_{1g} + E_g$ from R-point are observed at $\approx$140 cm^{-1} and $\approx$450 cm^{-1} in Raman spectra of $Ba_xSr_{1-x}TiO_3$ on the background of two-phonon scattering bands. They appearing points out the unit cell's doubling, namely the structural phase transition. According to Raman spectroscopy data, non-polar structural phase transition in pure ceramics $SrTiO_3$ occurs at $\approx$110 K, in solid solutions $Ba_{0.01}Sr_{0.99}TiO_3$ and $Ba_{0.02}Sr_{0.98}TiO_3$ at $\approx$120 K and $\approx$140 K, respectively. Apart from that, Raman spectra of studied samples consist of polar modes TO_2 ($\approx$170 cm^{-1}) and TO_4 ($\approx$540 cm^{-1}), prohibited in a paraelectric phase according to the symmetry selection rules. Their appearing indicates the local polar clusters in a host lattice. The temperature analysis of the parameters of TO_2 and TO_4 modes reveals a critical temperature, at which the polar clusters begin to expand. For pure $SrTiO_3$ a critical temperature is $\approx$110 K, for $Ba_{0.01}Sr_{0.99}TiO_3$ is $\approx$120 K, and for $Ba_{0.02}Sr_{0.98}TiO_3$ is $\approx$140 K. Temperature dependences of the transmission THz-IR spectra of the $Ba_xSr_{1-x}TiO_3$ solid solutions demonstrate soft mode behaviour of ferroelectric mode TO_1. Temperature dependence of TO_1 soft mode squared frequency follows Cochran's law for ferroelectrics, but does not vanish on approaching the extrapolated Curie temperature $T_0 \approx 30$ K and forms the saturation plateau. Moreover, the dielectric strength also saturates on approaching T_0 and is well described by Barret's equation for quantum paraelectrics. Thus, despite the dynamic growth of polar clusters at higher temperatures, the phonon impact to dielectric permittivity points out that the macroscopic ferroelectric phase transition at low temperatures is suppressed by the quantum fluctuations.

Acknowledgments: This work was supported by the RFBR, project No. 20-32-90222/20.

Poster Session II: 17:30-18:30

Poster No. 22

Mechanical and bioactive properties of nanopatterned TiO_2/HAp coatings

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Nanostructured interfaces are promising for orthopedic applications, as they could not only improve the osseointegration between the implant and the living bone but also be used as drug delivery systems. Nanoporous structure, could also be used as drug carrier to the surrounding tissue, with the intention to accelerate the tissue-implant integration, as well as to reduce and treat bacterial infections occurring after implantation of an orthopedic device. Titanium oxide nanotubes are promising for such applications, however, their brittle nature could be a significantly limiting factor. In this work, the topography of titanium foil was modified by two-method approach: anodization process and hydrothermal treatment. In the first step, a crystalline nanoporous u-shaped structure (US) of anodized titanium oxide with improved resistance to scratch compared to TiO_2 nanotubes was obtained. Next, the US titanium substrate was successfully modified with hydroxyapatite coating and investigated for bioactivity. Biological studies showed high bioactivity in SBF after 2 weeks of incubation. The mechanical and bioactive results indicate that the nanopatterned US structure covered with HAp could be an alternative surface modification for titanium-based stem endoprosthesis.

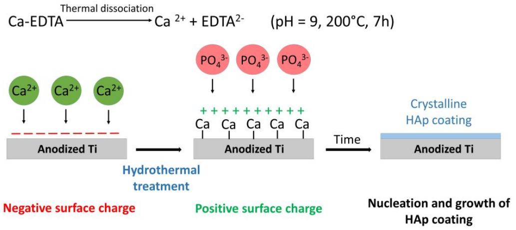

Figure 1. shows schematic presentation of chemical reactions occurring during the hydrothermal synthesis of HAp coatings on anodized and annealed Ti substrates in the form of US and NT.(1)

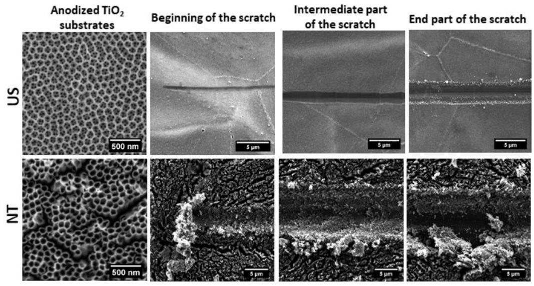

Figure 2. presents SEM images with evolution of grooves after a scratch test on samples with crystalline TiO_2 layers in the form of US and NT.

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POSTER NO. 23

Field induced magnetic ordering in the singlet-ground state magnet Cu(en)$_2$SO$_4$

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Metal-organic compound Cu(en)SO$_4$(H$_2$O)$_2$ (en = C$_2$H$_8$N$_2$) is a realization of the $S = 1/2$ Heisenberg antiferromagnet on the zig-zag square lattice with intralayer interactions $J/k_\mathrm{B} = 3.5$ K, $J' = 0.35\ J$. The interlayer coupling ≈0.01 K leads to the onset of magnetic long range order at 0.93 K.(1) The substitution of water by en leads to the formation of Cu(en)$_2$SO$_4$ with the absence of magnetic order down to 0.3 K. Considering the structure of this material, the formation of magnetic dimers can be expected. Within mean-field approximation, very good description of the magnetic susceptibility in the field applied along the b axis was achieved using the Heisenberg antiferromagnetic dimer model with intradimer coupling $J/k_\mathrm{B} = -5.52$ K, interdimer coupling $z'J'/k_\mathrm{B} = -2.7$ K and $g = 2.12$. The energy gap in the spin excitation spectrum was estimated $\Delta/k_\mathrm{B} \approx 11$ K and corresponding critical field $B_c^b \approx 7.8$ T required for closing the gap. This simple model was also applied in the analysis of specific heat. While in fields from 0 to 3 T, only a round maximum was observed with the exponential decrease down to 0.4 K, suggesting any absence of a phase transition to the magnetic ordered state, in the fields ranging between 4 and 7 T a small additional bump appears at the low-temperature side of the main round maximum. Finally, for fields above 7 T, a sharp λ-like anomaly is formed which grows with increasing magnetic field. The mapping of the anomalies enabled construction of magnetic phase diagram which shows the persistence of the singlet-ground state in the fields up to 7 T, then some kind of magnetic ordered state is established in the fields above 7 T. Further measurements in higher magnetic fields are desirable to achieve saturation field.

The financial support of APVV-18-0197 is acknowledged.

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POSTER NO. 24

Experimental study of low-temperature properties of As_xS_{100-x} glassy systems

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Disordered systems are characterized by universal remarkable behaviour, such as the presence of the boson peak in the reduced specific heat C_p/T^3, or by a presence of a plateau region in thermal conductivity in the low-temperature area between 1 and 20 K. (1,2) This behaviour can be related to the resonant scattering of sound waves by low-frequency localized vibrations observed in the non-crystalline solids.

Our work is focused on the experimental study of As_xS_{100-x} glassy systems with various compositions: As_6S_{94}, $As_{20}S_{80}$, $As_{28.6}S_{71.4}$ (As_2S_5), $As_{40}S_{60}$ (As_2S_3), $As_{45}S_{55}$, $As_{50}S_{50}$. The localized vibrations in such materials can be described with 12 membered ring nanocluster approximation. (3) The topology of such network-forming nanoclusters could be associated with the medium-range order structures of selected systems (3).

The specific heat and thermal conductivity data were measured in the temperature range between 1.8 K and 300 K on a set of As_xS_{100-x} glassy systems in order to identify the exact position of anomalies. The boson peaks in specific heat data were observed at about ≈ 5 K with small changes in temperature depending on composition. The plateaus in thermal conductivity are located in the temperature range from 5 to 20 K. The data were analysed within the Soft Potential Model (SPM). (4)

The quantitative analysis of the obtained experimental data will be presented as the main result of this work.

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(2) M.A. Ramos, Low Temp. Phys., 46 (2020), 104
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Poster No. 25

Solid-State NMR study of a multiple-cation lead mixed-halide perovskite with high efficiency

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Hybrid metal-halide perovskites have emerged as highly interesting materials for various applications, such as thin-film photovoltaics or light-emitting devices, due to their outstanding optoelectronics properties. A main advantage of these materials is the fact that their macroscopic properties are intrinsically related to their microscopic features (i.e. atomic and molecular organization and dynamics), so mixtures of different cations and anions can be used to tune the optoelectronic properties and to enhance efficiencies and stabilities.

Several variations to the perovskite structure have been tested. In particular, the use of mixed-ion structures, in which the compositional complexity is increased by introducing dopants into the perovskite structure, has resulted in a remarkable improvement in perovskite solar cell performance. Some of the latest top efficiencies have been reached by multiple-cation lead mixed-halide perovskites $(Cs,FA,MA)Pb(I,Br)_3$.

However, the role of the dopants and additives in the high performance of the perovskite solar cells has not been fully understood yet, and its transferability to other perovskites is not straightforward.

For this reason, it is important to be able to gain atomic-level understanding of these materials.

Solid-State NMR (SSNMR) spectroscopy is strongly sensitive to the local chemical environment, and as such, it proved to be a perfectly suited technique to investigate mixed perovskites.

In this study, we focused on the perovskite with formula $Cs_{0.05}FA_{0.81}MA_{0.14}PbI_{2.55}Br_{0.45}$ because of its high performance. We investigated it by means of SSNMR for the first time, with $MAPbI_3$ being used a reference compound. ^{207}Pb, ^{13}C and ^{1}H high-resolution SSNMR experiments allowed us to characterize the structure and composition of the samples, highlighting phase homogeneity and/or segregation, and to investigate ion dynamics by exploiting both spectral and relaxation properties.

Poster No. 26

2D Ruddlesden-Popper perovskites $BA_2MA_{n-1}Pb_nI_{3n+1}$ as studied by Solid-State NMR Spectroscopy

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Lead Halide Perovskites are interesting semiconductors used in different optoelectronic devices (e.g. sensitizers for solar cells, photodetectors, LEDs). Recently, 2D analogues of Hybrid Lead Halide Perovskites (HLHP) have attracted considerable attention because they offer the possibility of tunable band gap and enhanced environmental stability with respect to the corresponding 3D systems. 2D Ruddlesden–Popper (RP) perovskites can be prepared by adding a large organic mono ammonium cation L^+ in the precursor solution. In this way the 3D structure of corner-sharing octahedra (ABX_3) is disrupted and a structure with a bilayer of spacer cations between metal halide sheets is formed ($L_2A_{n-1}B_nX_{3n+1}$). For example, butylammonium (BA) is a suitable organic cation to force the archetypical perovskite $MAPbI_3$ into 2D RP perovskites $BA_2MA_{n-1}Pb_nI_{3n+1}$ (Figure 1), which are the object of the present study. The layer thickness of metal halide sheets is specified by n and can be adjusted by tuning precursor stoichiometry.

Solid-State NMR stands out as characterization technique for HLHP for its ability to study ion dynamics, compositional variations and ion incorporation, chemical interactions and degradation mechanisms. In this work, the 2D RP perovskites $BA_2MA_{n-1}Pb_nI_{3n+1}$ with $n = 1, 2, 3$ have been characterized by Solid-State NMR and compared with 3D $MAPbI_3$ as a reference compound. The structural features of these systems have been investigated by ^{207}Pb, ^1H, and ^{13}C spectra recorded under Magic Angle Spinning and static conditions; the obtained results have been discussed also by comparison with very recent literature.(1) In addition, the variable temperature measurement of ^{13}C and ^1H spin-lattice relaxation times (T_1) allowed dynamic properties of the organic cations in the series of samples to be investigated.

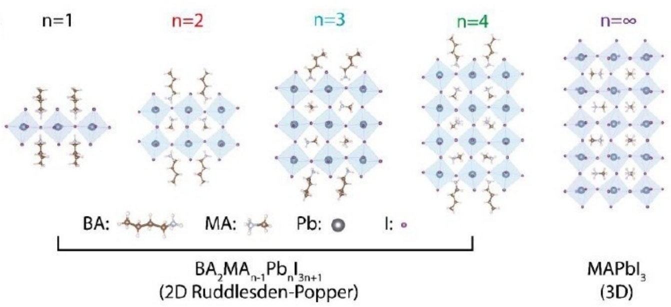

Figure 1. Schematic structure of 2D RP perovskites $BA_2MA_{n-1}Pb_nI_{3n+1}$ for $n = 1, 2, 3, 4$, and of the corresponding 3D perovskites $MAPbI_3$.

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Poster No. 27

Analysis of information dynamics in chiral spin chain coupled to boson reservoir

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Presentation covers the study of dissipative dynamics of information in chiral spin chain coupled to non-Markovian magnonic reservoir. System of interest is described through the canonical Heisenberg Hamiltonian, including the exchange interactions between nearest and next nearest neighbours. Chirality of the chain is formed due to Dzyaloshinskii-Moriya interaction. The system is coupled to the environment, described in statistical terms (so called "quantum bath"). The time deririvative of density matrices trace distance was utilzed to determine the direction of information flow and distinguishability of states. Distinct effect of applied electric and magnetic field was found: external electric field can be used to reshuffle the periods of information flow from and to the system, while the magnetic field has the impact on the rate of period transition. This finding reveals a possibility to control the information flow in helical spin rings.

Poster No. 28

Ferroelectric nanoparticles host Hopfion

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Knot-like structures are very common across many branches of modern physics, like string theory, hydrodynamics, statistical or condensed matter physics. Among different knot-like formations, Hopfions, knotted solitons in three dimensional space, are still explored superficially, with some exceptions for magnetic materials. Present work demonstrates that Hopfion is stable, energetically favorable configuration of polarization field in $PbZrTiO_3$ ferroelectric nanoparticles. We show that Hopfions are responsible for complex electromagnetic properties in ferroelectric nanoparticles. Such properties can form the basis for novel computational devices.

Poster No. 29

The effective mass of fluxon for the process of its interaction with inhomogeneity in the Josephson junction

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A particular role for the modern description of nonlinear phenomena is taken by structures such as solitons. In mathematical physics, the concept of soliton appeared due to the work of N. Zabusky and M. Kruskal. At present, the concept of soliton is used to describe many phenomena appearing in the field of physics. In particular, in 1962 the British physicist B. Josephson presented a model describing the tunneling of Cooper pairs between two superconductors through a thin insulator layer. Currently, a system composed of two superconductors separated by a thin insulator layer is called a Josephson junction. The junctions have found a wide variety of science and technical applications, and research into their possible further development is continuing. In the description of the Josephson junction the equation (sine-Gordon) appears which also has soliton solutions including the so-called fluxon defined as soliton carrying the magnetic flux quantum.

The research concentrates on the dynamics of the fluxon in the Josephson junction. We consider the sine-Gordon model with translational invariance braking by the position dependent function $F(x)$. The function $F(x)$ represents the inhomogeneity, which is a kind of potential barrier for the fluxon propagating in the junction. The analysis of the interaction of the fluxons with the curved regions of the Josephson junctions in the framework of the collective variables approach is compared with exact results derived from the field equation. Three methods are considered. In the first one, the energy carried by the kink is analyzed. The second approach is motivated by the perturbation scheme and the last one relies on the method of projection onto the zero mode of the system. Investigations have revealed that in considered system, only a part of the kink is involved in the interaction with the inhomogeneity. To verify this hypothesis, the mass correction depending on the curvature of the junction is proposed.

Poster No. 30

Phase transitions in systems with anisotropic order parameter modulations

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A model that allows one to describe phase transitions in systems with anisotropic scaling and higher-order parameter nonlinearities is considered. The systems under consideration have critical points with joint multicritical and Lifshitz-point-like properties. Physical space is considered separated into an arbitrary number of subspaces with different types of critical behavior. Dependence of critical dimensions on model parameters is found. It allows one to define mean-field theory applicability for study critical phenomena in systems with anisotropic modulations. Possible types of critical behavior in such systems were discussed.

POSTER NO. 31

Magnetocaloric properties of V6 and Cu5 molecular magnets

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The purpose of calculations was a theoretical study of magnetocaloric properties of molecular nanomagnets: V6 and Cu5 (both containing spins $S = 1/2$).(1,2) The thermodynamic properties of systems in question was described using the quantum Heisenberg model solved within the field (canonical) ensemble using exact numerical diagonalization. The dependence of the magnetic entropy and magnetic specific heat on the temperature and external magnetic field was calculated and extensively discussed. The isothermal entropy change for a wide range of initial and final magnetic fields was also investigated. A high degree of tunability of magnetocaloric effect was demonstrated what is an interesting behaviour of isothermal entropy change.

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POSTER NO. 32

Topological polarization textures in a ferroelectric nanodot

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Ferroelectric nanostructures host a variety of chiral topological excitations, including domain walls, vortices, skyrmions, vortex or skyrmion arrays. In this work, we discuss the possibility of switching between different polar configurations in a cylindrical ferroelectric nanodot. We build the Ginzburg-Landau free energy functional for the model system and analyze the stability of various non-uniform textures depending on temperature, anisotropy, and electric field.

We show that a stable skyrmionic state can occur in a ferroelectric nanodot and propose the algorithm for tuning the skyrmion chirality by applied electric field.(1) Employing the phase-field approach, we construct the hysteresis diagram of the chirality switching. A set of four controlled chiral states $L_-/R_-/L_+/R_+$ (Fig. 1) may serve as a platform for a ferroelectric-based multivalued (namely, 4-level) logic element.(2,3)

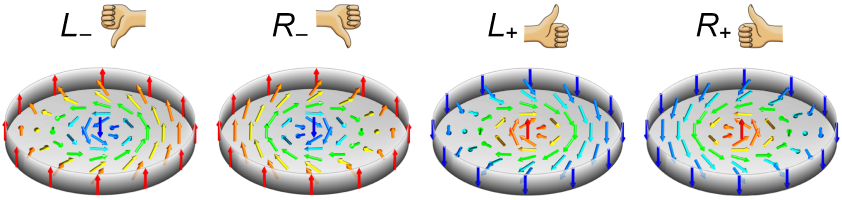

Figure 1. Four skyrmionic states with different chirality and polarity. The hand pictograms are used to classify the skyrmions.

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(3) I. Lukyanchuk et al., Ferroelectrics, 543 (2019), 213-221

Poster No. 33

Magneto-transport in the planar Hall setup for a periodically driven multi-Weyl semimetal

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The transport properties of a time driven system has been studied extensively in literature. In our work we will compute the magneto-transport in the planar Hall setup for a periodically driven multi-Weyl semimetal. We will subject our system to a circularly polarised light and investigate the changes in the transport properties by computing the Hall coefficients. We assume a non-adiabatic limit, where the Floquet theorem is applicable. In this limit the driven part of the hamiltonian appears as a perturbation on the static part and the problem becomes analytically solvable. We ignore expansion in inverse of high frequencies.

Poster No. 34

Fabrication of Self-Assembled Monolayers SAMs based on dithiocarbamate head group

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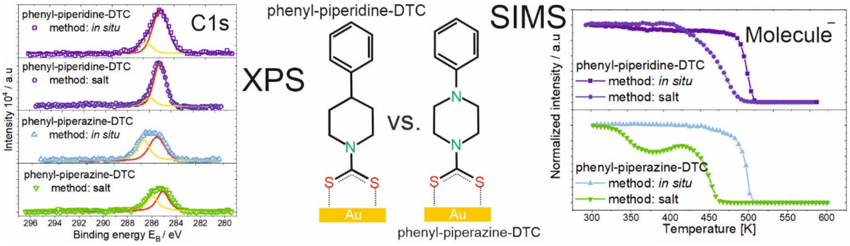
Further development of new technologies relies on combination of different types of materials. In many cases such a new combination involves merging inorganic and organic materials which leads to the formation of an inorganic-organic interface. From this perspective self-assembled monolayers (SAMs), which form well-defined monomolecular films on desired solid substrate, are considered one of the most prototypical systems for investigating physicochemical properties of an inorganic-organic interface. The most broadly examined class of SAMs is derived from the adsorption of alkanethiols on different metals. (1) Nevertheless, the thiolate-metal interface shows a lack of sufficient thermal stability and relatively inefficient charge transport which are required mainly for applications in molecular electronic.

In the view of the above limitations, the dithiocarbamate DTC anchoring group has been proposed. In the current research we have analyzed SAMs of dithiocarbamate monolayers based on phenylpiperidine and phenylpiperazine linked to the Au (111) substrate by two methods of synthesis *in situ* or *from salt solutions*. Structural properties as well as thermal and chemical stability of these SAMs were examined by a combination of infrared reflection absorption spectroscopy (IRRAS), X-ray photoelectron spectroscopy (XPS), secondary ion mass spectroscopy (SIMS) and water contact angle (WCA) measurements. The obtained spectroscopic analysis using IRRAS and XPS revealed that structures based on DTC group and piperidine or piperazine linkers show a desirable high density structures with upright orientation of molecules in the monolayer. Thermal stability analysis based on SIMS indicates that for both types of monolayers the *in situ* synthesis provides more stable structures which show higher thermal stability compared to the conventional thiolate SAMs. The exchange experiments, monitored by the WCA measurements, exhibit that increased thermal stability of DTC based SAMs is not connected with a higher chemical stability of this system which is comparable to thiolate SAMs.



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POSTER NO. 35

Structural and magnetic properties of FePc chains and hybrid superlattices

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The discovery of new materials classes with low dimensionality has driven much of basic research and the development of novel theoretical concepts. Also, low dimensional magnetic materials have led to new technologies in diverse areas. However, when the magnetic ordering energy in nanometric systems becomes comparable to thermal fluctuations, long-range correlations are destroyed. In one-dimensional (1D) magnetic systems long-range ferromagnetic (FM) order can be achieved by the interaction between the magnetic atoms and their supporting frames, such as substrates or inert (non-magnetic) crystal lattices, in which the system is embedded.

Metal-Phthalocyanines (MPc) are planar molecules that can host different transition metals M (M = Fe, Co, Cr, Cu, Mn) in their center and also two H (H_2Pc). They can be deposited on a substrate due to self-assembly phenom that ends in the formation of arrays of MPcs and their metal center M produce macroscopic arrays of 1D metallic chains widely separated from their neighbors.

Here, we present density functional theory (DFT) results of the magnetic and structural properties of FePc and H_2Pc chains, and also mixed FePc-H_2Pc superlattices (SLs). The structural properties, like planar distances and growing angles of both MPcs chains and SLs were calculated with results in concordance with experimental results. We found that a few molecules closer to the interface FePc-H_2Pc show a PDOS distorted with respect to the one for the infinite chain (FePc). The magnetic J exchange and anisotropy parameters D and E for chain FePc molecules were calculated. In particular, it was obtained that there's a nonzero value of transverse anisotropy E in the FePc infinite chains not reported before. We also present experimental results of hysteresis cicles in FePc chains and SL that are in line our theoretical calculations.

Acknowledgments: This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562 under project TG-DMR200083.

Poster No. 36

Synthesis and crystal engineering of d^{10} complexes based on multifunctional pyridinic blocks

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Nowadays, there is much more concern about the planet's future sustainability due to the increasing rate of pollution, and mainly the contamination of groundwater and oceans by heavy metal ions from industrial waste. That's why their removal is necessary or even primordial in order to preserve our environment.(1)

The use of nanoparticles synthesized from organically modified silica is an interesting alternative to deal with this problem. The accumulated knowledge on this subject indicates that the adsorption properties of these hybrid materials depend mainly on the choice of ligands. The molecules carrying donor sites such as sulfur (S), oxygen (O) or nitrogen (N) promote the formation of an active sites able to chelate the metal ion specially transition metal ions.

In this work,(2) we have prepared a novel pyridinic ligand bearing in position 2 and 6 flexible heterocyclic pyrazole molecules variously functionalized: diethyl 2,2'-(pyridine-2,6-diylbis(5-methyl-1H-pyrazole-3,1diyl)) diacetate (L) to react with $MnCl_2\cdot 4H_2O$ and $CdCl_2 \cdot 2.5\ H_2O$ salts.

The quality of the obtained crystals was verified by FT-IR spectroscopic analysis and mass spectroscopy, which confirms the coordination of central metal ions by the heterocyclic ligand. Structural analysis by X-ray diffraction revealed the formation of two different supramolecular structures where the ligand L acts as a tridentate clamp with metal: ligand ratio 1:1 leading to formula $[MnLCl_2]$ (**1**) and $[CdLCl_2]$ (**2**). The single crystal structures of **1** and **2** are discussed in the context of the effect of hydrogen bonding functionalities and counter anions on the supramolecular structural diversities observed in these new coordination complexes.

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Poster No. 37

The role of structural defects in optical absorption of $Bi_{12}SiO_{20}$ crystals

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Crystals of sillenites with the general formula $Bi_{12}MO_{20}$ (M = Ge, Ti, Si, etc.) are photorefractive and photosensitive materials used in dynamic holography.(1) The optical and photoelectric properties of these crystals are determined by defective centers, the levels of which are located in the band gap. Such centers are associated with structural abnormalities or stoichiometry. According to X-ray diffraction analysis, $Bi_{12}GeO_{20}$ (BGO) germanosilenite crystals (BGO) have a perfect crystal structure, and $Bi_{12}TiO_{20}$ (BTO) titanosilenite crystals have the largest number of intrinsic defects. At the same time, in terms of application, they are the most promising. This led to our choice of BSO crystals for research.

It is known that within the range of homogeneity in the system Bi_2O_3:SiO_2 stoichiometric composition contains 14.3 mol.% SiO_2 and 85.7 mol.% Bi_2O_3. Deviation of the crystal composition from stoichiometric leads to a change in the charge state of bismuth ions ($Bi^{3+} \leftrightarrow Bi^{5+}$), their displacement of structure-forming cations Si^{4+} from oxygen tetrahedra, the appearance of charge compensation defects in oxygen sublattices and the formation of high concentrations of their own points. They are the most characteristic defects for BSO.

The paper presents the results of an experimental study of the effect of nonstoichiometry defects (excess-Bi deficiency) on the spectral dependences of the photochromic effect (PHE) of BSO crystals. We grew crystals with a deficiency (BSO - Bi) and an excess (BSO + Bi) of bismuth at the $x = 10.5$ and 12.5, respectively (within the range of homogeneity of BSO) from the $Bi_xSiO_{1.5x+2}$ melt by the Czochralski method.

It is established that the spectra of PHE $\Delta\alpha^{\mathrm{PCE}} = \alpha^{\mathrm{f}} - \alpha^{\mathrm{st}}$ (α^{f} – photoinduced absorption (after light irradiation), α^{st} – stationary absorption) of nonstoichiometric crystals in the range $\lambda = 450 - 700$ nm are similar to the spectra of stoichiometric BSO. The latter are consistent with the data in the literature.(2) However, in the BSO - Bi crystals there is an absorption band with a maximum at $\lambda_{\max} = 420$ nm. In BSO + Bi crystals, in contrast to BSO, in the IR range (at $\lambda = 700 - 900$ nm) the quenching of the photochromic effect is observed. PHE spectra have common bands with spectra of additional absorption caused by excess (deficiency) of Bi. In General, the excess or deficiency of bismuth causes, respectively, an increase or decrease in PHE in BSO crystals.

The $\Delta\alpha^{\mathrm{PCE}}(\lambda)$ spectra of the investigated crystals were decomposed into individual Gaussian components. Estimation of the oscillator power of these components gives $f \approx 10^{-2}$. This value of f is characteristic of electronic transitions due to charge transfer of the ligand-metal type and electric-dipole transitions between the ground and excited states of defects. The nature of such defects is discussed.

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Poster No. 38

Thermal conductivity of the glass-like molecular solids

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It is known the temperature dependence of thermal conductivity for orientational-ordered molecular crystals has the bell-shaped form with pronounced maximum. To the left of the maximum, thermal conductivity is determined by the scattering of phonons on various defects of the crystal lattice such us boundaries, dislocations, impurities. To the right of the maximum of thermal conductivity, the main mechanism of phonon scattering is three-phonon scattering processes, which are described as the sum $\kappa(T) = \kappa_{\mathrm{ph}} + \kappa_{\mathrm{diff}}$, where first term $\kappa_{\mathrm{ph}} = A/T$ ascribes three-phonon scattering processes, and second term κ_{diff} is the contribution from short-wave excitations or diffusons.(1)

From a lot of experimental data it is known that thermal conductivity of disordered solids is more lower than in their analogous crystal in the wide temperature range. Below 1 K thermal conductivity is proportional to $\propto T^2$ and often at 2–10 K it demonstrates "plateu" and next increasing of $\kappa(T)$. The absence of a unified theoretical model for explaining the glass-like behavior of $\kappa(T)$ stimulated the development of various phenomenological models,(2) the most famous are the tunneling model (TM) and soft potential model (SPM).

In the theoretical work,(3) the authors proposed the concept of quantum-mechanical heat transport, so phonons can propagate not only as quasiparticles, but also it can tunnel as waves between phonon branches. This concept is called the "unified theory of heat transport" and it allows to describe heat transfer in both ordered/disordered cases of solids.

From the general theory of dissipative quantum systems, the authors obtained a general transport equation which is the sum of two contributions and it takes the form either as Peierls limit (first term is dominated, for ordered substance) or Allen-Feldman limit (second term is dominated) in the case of disordered solids. For complex crystals these two contributions can be comparable.

As an example we have considered crystals with glass-like behavior mainly which have a clathrate structure, and also we have shown that the unified theory of heat transport is universal to describe the thermal conductivity $\kappa(T)$ of any solid regardless of order/disorder in the system. We have been proposed the tunneling contribution to thermal conductivity κ_{diff} written as the exponential dependence: $\kappa(t) = \kappa_0 \cdot \exp(-E/T)$.(4)

The work has received funding from the National Research Foundation of Ukraine (NRFU project No. 2020.02/0094).

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Poster No. 39

Wenzel to Cassie transition by infusing lubricant

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Liquid drops on lubricant infused surfaces (LIS) show enhanced properties, such as small roll-off angles and small adhesion. In other words, they show great mobility. That is because they are in the Cassie state (air cushions under the drop) or Floating state (no contact between drop and solid). In the case that the drop is in the Wenzel state (fully wet) on a pillared surface, the adhesion forces are big and the drop doesn't move easily. The question we tried to answer is that: could be possible to have a Wenzel to Cassie transition by infusing lubricant on the surface? Images taken by a laser scanning confocal microscope (LSCM) help us to examine the role of surfac's morphology, lubricant's and drop's surface tension and roughness on this transition. The transition occurs at small interpillar distances and big heights.

Poster No. 40

Dipole-induced extraordinary conduction increase in R-P3HT/P4VP metal complex cross-linked

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The increase of the conductivity of the conjugated material, in contact with an organic insulator, is an effect well documented in the literature. However, to this day there is no consistent explanation for this phenomenon. Recently, we developed a new polymer material, poly(4-vinylpyridine) (P4VP) cross-linked with cobalt (II) bromine complexes, and such material can be prepared in the thin film form. In such a system, $\text{pyridine}_2\text{CoBr}_2$ complexes are formed only on the very surface of the film.(1) In the presented work, we use P4VP cross-linked with two d-block metal salts: cobalt (II) and zinc (II) bromides to form, with regioregular poly(3-heksylthiophene) used as a model organic semiconductor, bilayer, and blended laterally arranged systems. In the bilayer system, after the said modification, the overall device in-plane conductivity increased from (for pure R-P3HT thin film) to. The observed increase in the system's conductivity is attributed to the electric field induced in the semiconductor area by the dipole moments directed by surface-oriented metal complexes. We proposed a model based on the introduction of an electric field into the semiconductor area from the ordered dipole moments of both pyridine and/or $\text{Br}_2\text{X}(py)_2$ complexes. The proposed model properly described the behavior of the system where the P4VP film thickness was gradually changed, simultaneously reducing the distance between the semiconductor and cross-linked surface. Conducting the experiment, we excluded the conductivity of the cross-linked thin film surface as well as the influence of each sample preparation step.(2)

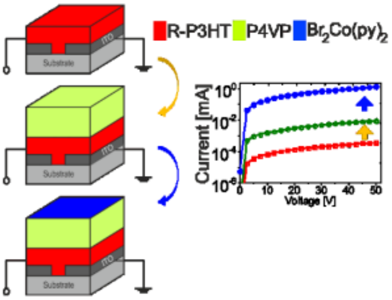

Figure 1. Schematic diagram of the system with the current voltage characteristic.(2)

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POSTER NO. 41

Characterisation of the positron annihilation in Zr/Nb nanoscale multilayer coatings

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Hexagonal-cubic systems (HCP/BCC and HCP/FCC) have the most significant structural mismatch of crystal lattices. In addition, HCP/BCC systems have the potential to produce radiation-resistant composites. Samples were studied by Doppler broadening spectrometry (DBS) using variable energy positrons at the JINR LNP in Dubna. A monoenergetic positron beam with a diameter of 5 mm and an intensity of 10^6 e$^+$/s was used. The positron energy varied from 0.1 keV to 30 keV. Figure 1. shows the dependence of the S, W parameter on the positron energy for Zr/Nb nanoscale metallic layers (NMCs) with an average layer thickness of 100 ± 10 nm, 50 ± 5 nm, and Zr and Nb monolayer coatings.

Figure 1. The graph of dependence of S parameter (a) and W parameter (b) on the positron energy of Zr/Nb NMCs with individual layer thicknesses of 100 ± 10 nm and 50 ± 5 nm, as well as of monolayer Zr and Nb coatings.

Figure 2. shows the dependence of the S, W parameter on the positron energy for Zr/Nb NMCs with an average layer thickness of 25 ± 2 nm, 10 ± 1 nm, and Zr and Nb monolayer coatings.

Figure 2. Plots of the dependence of the S parameter (a) and W parameter (b) on the positron energy for Zr/Nb NMCs with individual layer thicknesses of 25 ± 2 nm and 10 ± 1 nm, as well as monolayer Zr and Nb coatings.

A layer-by-layer positron analysis in Zr/Nb NMCs showed that increasing the thickness of the individual layers leads to a change in the annihilation parameters. If the layer thickness in Zr/Nb NMCs is less than or equal to the positron diffusion length, positrons predominantly annihilate near Zr at the interface. Increasing the monolayer thickness to 100 nm leads to increased positron annihilation in the Nb region.

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Poster No. 42

Ultrafast non-thermal phase transitions of carbon and silicon

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Radiation of modern high-intensive free-electron lasers allows to transform solid materials into their other solid states or to the new states, such as liquids, amorphized systems or warm dense matter. Such transitions may also occur exclusively or partially via non-thermal channels, thus, on ultrafast time scales. Here we analyze particularly two non-thermal phenomena: graphitization of diamond and melting of silicon. The first process is an example of a pure nonthermal event, as diamond can be graphitized on a time scale of 200-300 fs due to significant creation of conductive free electrons and subsequent interatomic potential change. This was confirmed by experiment at FERMI@Elettra FEL facility and predicted by our hybrid code XTANT which combines tight-binding approximation, classical molecular dynamics, Monte-Carlo scheme and Boltzmann collision integrals to properly keep track of all relevant microscopic processes on electronic and atomistic levels. The silicon melting at high pump fluences typically goes through both non-thermal and thermal channels. To describe results obtained in experiments on LCLS and SACLA, in addition to XTANT we also use our XSINC code which calculates diffraction intensities on crystallic structures with respect to the spatial FEL pulse profile and non-uniform sample transformation. By seeing fairly good agreement with the experiment in both cases, we can establish our models as useful tools to investigate ultrafast non-equilibrium dynamics including various nonthermal transitions.

List of presenters and authors