INSTITUTE OF PHYSICS
POLISH ACADEMY OF SCIENCES

70 Years of Science and Innovation

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Ministry of Education and Science
Republic of Poland

Dear Readers,

I am glad to be able to present the new information booklet about the Institute of Physics of the Polish Academy of Sciences. Apart from updating many pieces of information the new edition also celebrates the 70th anniversary of the Institute foundation.

The mission of the Institute has remained unchanged in these seventy years: to contribute to advancement of our knowledge of physics by extending the frontier between known and unknown, to bring the new science to the society by offering attractive ways of education at many levels, and to create opportunities of making it useful and serving the many needs of people. We think that we have succeeded in achieving progress in all these areas. Naturally, the methods of reaching our goals changed over the seventy years of the Institute's existence. The booklet provides only a brief snapshot of the evolving situation. For a bit broader view, please, pay a visit to our new and refurbished webpage **www.ifpan.edu.pl** which we hope you will find not only informative and interesting but also attractive. In particular, you will find a brief history of the Institute as well as constantly updated info on the newest scientific achievements. You will be able to pay a virtual visit in our laboratories.

As you will be able to note by going through the pages of this booklet, the important novelty that appeared in the Institute within the last ten years is formation of new dynamic research divisions: the theory group ON5, formed on the basis of the International Research Agenda Magtop, Division ON6 that pursues investigation on topological aspects of the physics of condensed matter. Both new divisions are carrying out the investigations at the cutting edge of research and already are assets in the Institute's portfolio.

Other newcomer to the scene is the Doctoral School (**www.warsaw4phd.eu**) which replaces the International Doctoral Studies. The latter has ceased formally to operate at the end of 2022, with the last students to complete their work for their PhD degrees by the end of 2023. The School was formed in collaboration with eight other institutes (most of them from system of institutes of the Polish Academy of Sciences) which introduced a possibility of more interdisciplinary approach to present-day problems that the society faces, but also, at least at the beginning, by adding complexity which made the organization of the School and its running much more complicated and cumbersome. Let us hope that this extra effort will be compensated by many fascinating discoveries made in the course of the doctoral studies. One of the differences the new School brought is the greater number of students from abroad and from relatively far-away countries. This fact resulted in English being spoken commonly and widely in the labs, seminar rooms, and corridors.

As far as new instrumentation is concerned, the spacious cleanroom was finally completed and equipped with basic tools of

semiconductor nanotechnology. New possibilities appeared related to a successful cooperation of several groups in the Institute with large facilities such as Solaris synchrotron in Kraków (**https://synchrotron.uj.edu.pl**) or European x-ray lasers (**www.xfel.eu**). And, in view of rising energy prizes, the Institute had installed on the roofs of its three buildings the photovoltaic panels.

Finally, one has to remember that the past years were also influenced by the COVID-19 pandemic. Changes had to be put up with considering the ways of organization of seminars, lectures, exams, visits and conferences. Let us hope that this disturbance will be more than compensated by our newly acquired prowess to work remotely.

Roman Puźniak

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Scientific Council

The Scientific Council is a collective managing body of the Institute. The Council oversees the Institute's scientific activities, sets the research goals and the yearly research plans, as well as establishes the work program. It also assess the performance of the scientific staff and the quality of research, makes recommendations for improvements and future actions. It also formally confers scientific degrees and oversees the education process of the PhD School.

The Scientific Council consists of 50 eminent scientists and scholars. The members are elected by the scientific staff of the Institute for a four year period. Professor Tomasz Story took office as the Chairman of the Council from January 1st 2023.

Formal Council meetings are held once a month. Between the meetings the Council operates via permanent commissions dealing with staff and program matters and special committees supervising procedures of awarding scientific degrees. There were about 8 PhD degrees and 6 doctor habilitatus degrees awarded each year in the period 2016-2022.

Tomasz Story
Chairman of the
Scientific Council

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Deputy directors for scientific affairs:

Magdalenia Załuska-Kotur

Piotr Deuar

Scientific Divisions and Laboratories:

Research areas and recent achievements

Division ON1: Physics of Semiconductors

The aim of the Division is to advance physics of new semiconductor materials and nanostructures by carrying complementary experimental and theoretical research benefitting from Division's rich semiconductor technological potential. The Division is the leading European center for the growth of crystals as well as experimental and theoretical studies of semiconductor II-VI, IV-VI, V_2-VI_3, and III-V materials. High quality semiconductor bulk monocrystals are grown from the melt (by the Bridgman method) or by the vapor phase growth methods. For manufacturing of the layered II-VI/IV-VI semiconductor heterostructures the molecular beam epitaxy method is used. The experimental and theoretical activities of the Division are mainly devoted to magnetotransport, thermoelectric, magnetic, and optical properties of new semiconductor crystals and nanostructures. The Division is actively engaged in the world-wide research in the field of topological materials as well as semiconductor spintronics with semimagnetic (diluted magnetic) semiconductor alloys and nanostructures. In these fields of research the Division contributed with several seminal discoveries, like exchange interaction induced giant magneto-optical and magnetotransport effects in II-VI semimagnetic semiconductors with Mn, carrier induced ferromagnetism in IV-VI semiconductors with Mn, and the recent experimental discovery of topological crystalline insulator states at the surface of (Pb,Sn)Se monocrystals. The Division also actively participates in applicational research programs aiming at development of new semiconductor materials and nanostructures for X-ray and gamma-ray detectors, thermoelectric energy converters, and infrared detectors.

ATOMIC STEPS AT TOPOLOGICAL CRYSTALLINE INSULATORS

One distinguishes materials that are electrically conducting (metals or semimetals) or nonconducting (insulators or semiconductors). The key physical factor is here the energy gap in the electron structure of valence states, present in insulators and semiconductors but absent in metals and semimetals. Experimentally, at very low temperatures insulators and semiconductors possess zero electrical conductivity whereas metals and semimetals remain conducting. In the world-wide search for new materials this classification was qualitatively extended by the discovery of a new class of materials – topological insulators. Insulating in the bulk, these materials are conducting at their boundaries (i.e. surfaces of bulk crystals or edges of two-dimensional systems). The existence of these states in canonical topological insulators, like $Bi_2(Te,Se)_3$, is guaranteed by the time reversal symmetry. Topological materials possess unique properties, like spin-momentum locking, linear Dirac-like electron energy dispersion, or forbidden back-scattering. It raises hopes for new

applications in nanoelectronics, spintronics, and quantum computing. In the Division we experimentally discovered (Nature Materials 11, 1023 (2012)) a new class of topological materials – topological crystalline insulators (TCI) – in which the crystalline symmetry (mirror plane) warrants the topological protection of the boundary states. The discovery of chemical composition and temperature induced transition between the topologically trivial and the TCI state in $Pb_{1-x}Sn_xSe$ was done with the angle-resolved photoelectron spectroscopy (ARPES) technique that provides direct experimental information on the electron energy dispersion relation E(k) in different energy ranges. Our collaboration with German and Swiss teams on scanning tunneling microscopy and spectroscopy (STM/STS) of TCI materials resulted in 2016 [1] in the discovery of new one-dimensional (1D) topological states residing at the edges of atomic steps at the (001) crystal plane hosting the TCI states (see Figure below). The excellent crystal quality of TCI materials used in the experiments was the key to the successful preparation of atomically clean and flat surfaces [1]. Exploiting the available large pool of TCI crystals and various cleavage regimes permitted the study of electron coupling effects between the 1D electron states at neighboring atomic steps. The experimental observation of the energy splitting in local density of states for close steps resulted in the determination of the upper limit (set by the interstep distance of about 25 nm) for density of surface packing of such 1D states, avoiding hybridization effects and preserving quantum coherent electron character of individual steps [2]. In the very recent experimental and theoretical work, we exploited the method of, so called, surface doping (i.e. low temperature deposition of metal ions on topological surface) to reach a new physical regime corresponding to the energy resonance between the Fermi level (EF) and the Dirac (ED) point of the surface TCI states. In STM/STS experiments the 2-fold or 4-fold splitting of local density of states at the steps was observed when tuned to EF≈ED and explained in a physical model pointing out to the importance of electron correlation effects in the, so called, flat band regime achieved [3].

[1] P. Sessi, D. Di Sante, A. Szczerbakow, F. Glott, S. Wilfert, H. Schmidt, T. Bhaton, P. Dziawa, M. Greitner, T. Neupert, G. Sangiovanni, T. Story, R. Thomale, M. Bode, Science 354, 6317, 1269 (2016).

[2] J. Jung, A. Odobesko, R. Boshuis, A. Szczerbakow, T. Story, M. Bode, Phys. Rev. Lett. 126, 236402 (2021).

[3] G. Wagner, S. Das, J. Jung, A. Odobesko, F. Kustler, F. Keller, J. Korczak, A. Szczerbakow, T. Story, S.P. Parkin, R. Thomale, T. Neupert, M. Bode, P. Sessi, Nano Letters 23, 2476 (2023).

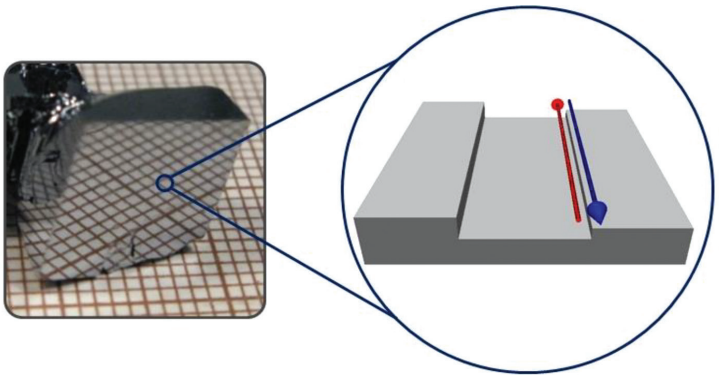

Figure: Single crystal of topological crystalline insulator $Pb_{1-x}Sn_xSe$ (x=0.23) grown by the self-selecting growth method showing natural (001) crystal facets (left). Cleaved under ultra-high vacuum the surface reveals micron-long atomic steps of 1–4 monolayer heights which, for odd monolayer numbers, reveal in STM/STS measurements the unique, one–dimensional topological states (zoomed-in scheme in the right panel).

QUANTUM OSCILLATIONS STUDIES OF TOPOLOGICAL STATES IN SnTe

Experimental studies and theoretical analysis of magnetic quantum oscillations of electrical resistivity (Shubnikov - de Haas effect) and magnetization (de Haas - van Alphen effect) were performed for a cubic single crystal of the topological crystalline insulator SnTe grown from the vapor by the SSVG method. It revealed that the oscillatory electronic contributions to magneto-conductivity and magnetic susceptibility appear simultaneously from two orthogonal {001} crystal facets hosting two-dimensional massless topological Dirac fermions. Measurements were carried out in high magnetic fields and at low temperatures as a function of the angle between the applied magnetic field and the crystal facets of the cubic topological crystal (see Figure). Theoretical model of electronic surface states in quantizing magnetic field (Landau quantization regime of band states) were developed taking into account the exchange of charge carriers between the bulk of SnTe and the surface topological states. The model successfully explained the experimental observations and permitted determination of key electronic parameters of surface Dirac electrons, like Fermi velocity or effective mass of charge carriers.

[1] K. Dybko, M. Szot, A. Szczerbakow, M.U. Gutowska, T. Zajarniuk, J.Z. Domagala, A. Szewczyk, T. Story, W. Zawadzki, Phys. Rev. B 96, 205129 (2017).

SEMICONDUCTOR II-VI CRYSTALS FOR RADIATION DETECTORS AND OPTICAL STUDIES

The Division is the national leader in developing new (Cd,Mn,Mg)(Te,Se) – based II-VI semiconductor materials for applications as high energy radiation detectors. The project covers: (i) growth of large homogeneous crystals of very high electrical resistance and low concentration of defects and dopants (possible carrier traps), (ii) development of ohmic electrical contacts, and (iii) experimental testing of material's performance as a detector. Our

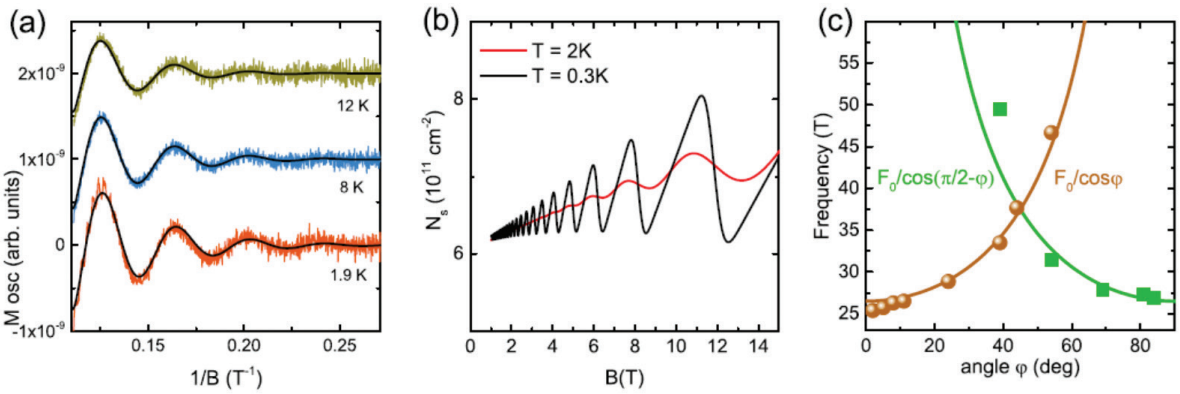

Figure: (a) Quantum oscillations of magnetization vs. magnetic field (de Haas – van Alphen effect) in SnTe cubic single crystal with six {001} facets hosting topological crystalline insulator states; (b) bulk reservoir model calculations of concentration changes of surface topological carriers; (c) angle-dependence of quantum oscillation's frequency showing simultaneous, π/2-phase shifted, contributions from two crystal facets.

research indicates that crystals based on CdTe, when properly doped with manganese, selenium, or magnesium, may serve as X-ray and gamma-ray detectors with state of the art detection parameters. The aim of our technological studies was establishing the conditions for the growth by the low-pressure Bridgman method which enable obtaining large, homogeneous, and high-resistivity single crystals. All the used elements were of the highest purity and the crystals we obtained had diameters of 55 mm (see Figure) which paves the to detector applications [1]. For X-ray and gamma-ray detectors one of the critical parameters determining usability of a system is the product of carrier mobility and life time, μτ. It may be obtained from the analysis of photocurrent-voltage PC-V characteristics. For $Cd_{1-x}Mn_xTe$ samples we showed that the results critically depend on the surface treatment and the space charge distribution. In particular, etching of the sample with 20% HCl leads to appearance of significant concentration of very shallow surface traps, which significantly changes PC-V characteristics. We also proved that the PC-V characteristics for photon energies larger than the energy gap determine the detector plate's surface quality [2].

Excellent quality of our semiconducting materials permits advanced studies of optical properties of, *e.g.*, diluted magnetic (semimagnetic) semiconductors, like $Cd_{1-x}Mn_xTe$ or $Zn_{1-x}Mn_xTe$. In our recent work, we show that in mixed crystal of $Zn_{1-x}Mn_xTe$ manganese ions are in two charge states: Mn^{2+} and Mn^{3+}. The ions in the 2+ charge state strongly interact with zinc vacancies resulting in the formation of Mn-V_{Zn} charge transfer complexes. The presence of manganese in these complexes results in a significant change of the shallow acceptor energy level related to zinc vacancy: from 0.047 eV in ZnTe to 0.138 eV in $Zn_{1-x}Mn_xTe$. This new deep acceptor level induces a new 1.44 eV band in the photoluminescence spectrum. The interaction between Mn^{2+} and Mn^{3+} ions is ferromagnetic while for Mn^{2+}-Mn^{2+} pairs it is antiferromagnetic. The coexistence of two kinds of magnetic interaction leads to paramagnetic – spin glass phase transition at T=3.2 K in $Zn_{1-x}Mn_xTe$ with x=0.06 [3].

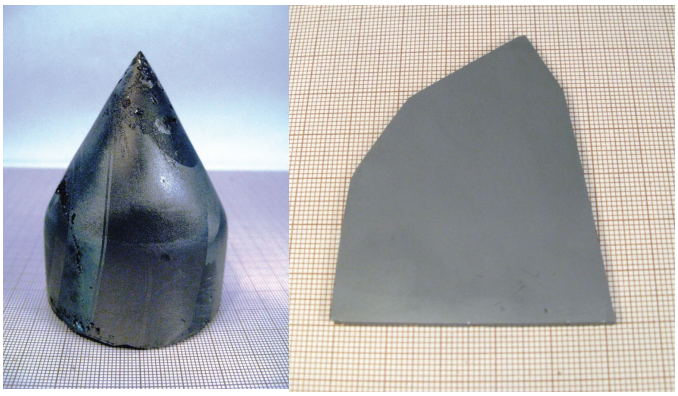

Figure: $Cd_{1-x}Mn_xTe$ (x=0.05) bulk crystal with diameter of 55 mm (left) and monocrystalline plate with dimensions of 40×40×3.5 mm^3 (right) cut off from this ingot along crystal twin boundary for further manufacturing of the crystalline matrix for X-ray detection of 1.5×1.5 mm^2 pixels.

[1] A. Mycielski *et al.*, Prog. Cryst. Growth Charact. Mater. 67, 100543 (2021).
[2] A. Mycielski *et al.*, Sensors, 22, 2941 (2022).
[3] Le Van Khoi *et al.*, Phys. Rev. B 107, 085206 (2023).

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Head of the division

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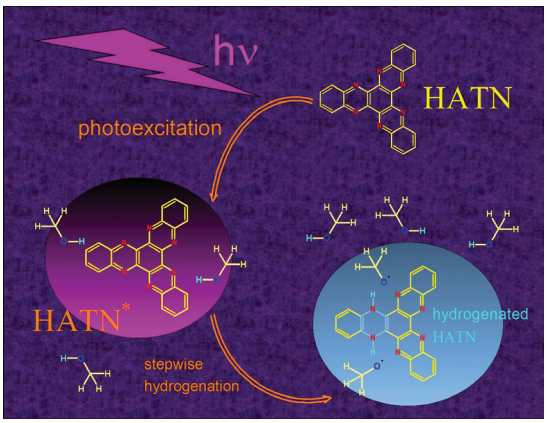
Division ON2: Radiation Physics and Spectroscopy

Research carried out in the Division concerns various aspects of interaction between electromagnetic radiation and matter in the form of atoms, molecules, and their aggregates. Special emphasis is placed on synergy between experiment and computations. The Division has multiple spectrometers enabling measurements in the wavelength range from microwave, through infrared and visible, to ultraviolet. There are also several installations for sample preparation and analysis, including laser ablation and Atomic Layer Deposition, as well as significant activity devoted to applications, documented by multiple patents on novel fluorescing materials, ALD techniques, and active surfaces. The principal research themes are:

MOLECULAR PHOTOPHYSICS:

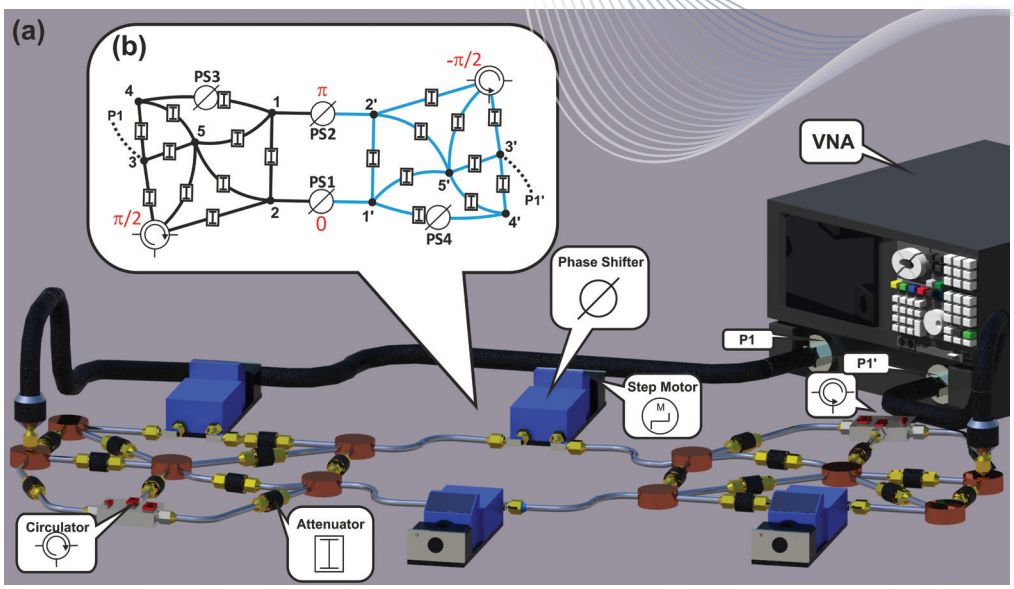
This research focusses on experimental and theoretical investigations of the photophysics and photochemistry of organic molecules. The main research topics are: photoinduced electron, proton, and hydrogen atom transfer, single molecule spectroscopy in a low-temperature matrix, and practical implications of the investigated phenomena.

The figure illustrates photochemical hydrogenation of hexaazatrinaphthylene (HATN) in methanol. The process, induced by violet light, ends up in di-hydrogenated HATN-H_2 and represents an example of the intermolecular Proton-Coupled Electron Transfer as an engine that converts electromagnetic energy of light into chemical energy of the photoproduct (Group ON2.1, A.L. Sobolewski).



QUANTUM CHAOS:

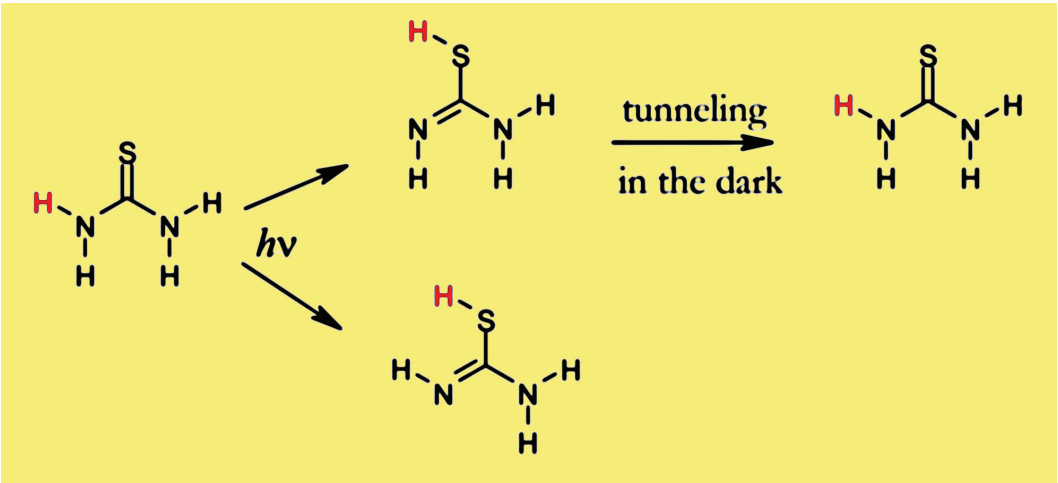
This research concerns manifestations of classical chaos in the properties of the corresponding quantum or, more general, wave-dynamical systems. Such systems include quantum graphs and billiards, atoms in strong electromagnetic fields, and microwave networks. It was shown by this group that quantum graphs can be simulated experimentally using microwave networks. The simulation of quantum graphs by microwave networks is possible because of the formal analogy of the one-dimensional Schrödinger equation describing quantum graphs and the telegrapher's equation for



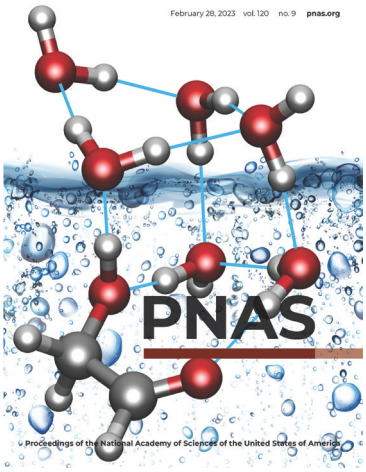
microwave networks. Microwave networks allow experimental studies of chaotic systems with all three types of symmetry within the framework of the random matrix theory. Microwave networks have been applied to demonstrate that the famous question of Mark Kac „Can one hear the shape of a drum?" can be extended to one-dimensional scattering systems. The results of these investigations were highlighted on the cover of Physical Review Letters (Group ON2.2, L. Sirko).

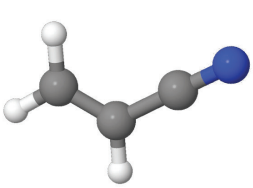
VIBRATIONAL AND ROTATIONAL SPECTROSCOPIES:

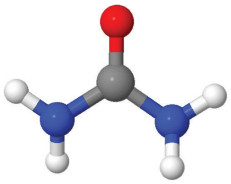
The physical nature of fundamental chemical processes, such as intramolecular transfer of an hydrogen atom, is the main topic of the vibrational spectroscopy research, which is carried out at low temperatures on molecules diluted in inert gas matrices. The main processes studied are phototautomerisations in molecules, tunneling of the hydrogen atom through a relatively high barrier, and photoinduced, long-range hydrogen-atom transfer. Many previous studies have recently been summarized in Int. Rev. Phys. Chem., 2022, 41, 1–47 (Group ON2.3, M.J. Nowak).

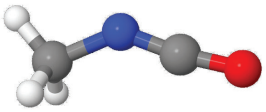


Rotational spectroscopy themes involve studies, in the framework of multipartite international collaborations, of water clusters and multiply hydrated molecules, with publications, *e.g.*, in Science (2012, 2016), Angew. Chem. Int. Ed. 2020, PNAS 2023. Another theme involves laboratory studies of molecules of astrophysical interest, including urea (A&A 2019) and CH_3NCO (A&A 2016, APJ Suppl. Series 2019), and searches for their presence in extraterrestrial environments (Group ON2.3, Z. Kisiel).









PROPERTIES OF OXIDE MATERIALS AND THEIR APPLICATIONS:

These materials are the focus of research targeted at experimental studies of their physical properties and the search for potential applications. The technology of obtaining structures from various oxide materials is being actively developed, with emphasis on possible world wide applications. The materials are fabricated using various methods, including atomic layer deposition, laser ablation or the hydrothermal method, and are most useful in the form of thin films and nanostructures, *e.g.*, nanopowders and nanorods. Ongoing research is directed towards understanding the properties of materials and their various applications in medicine, photovoltaics, electronics, optoelectronics or the civil engineering industry. Potential (already patented) applications include manufacturing silicon photovoltaic cells, hydrothermal preparation of CuO layers, ALD technique, antiallergic layer preparation, and lung cancer cell imaging using oxide nanomarkers (Group ON2.4, B. Witkowski).

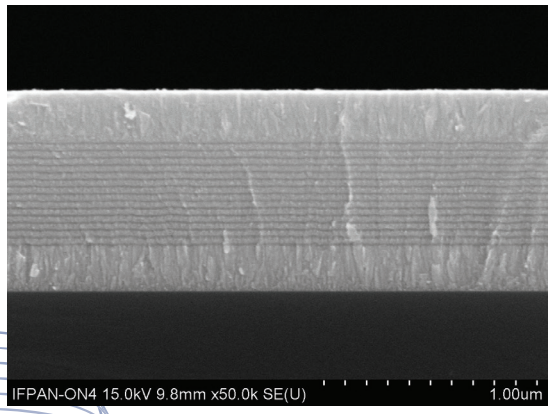
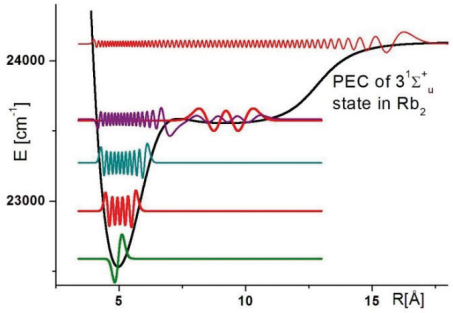


Figure: Multilayer structure grown by ALD.

LASER SPECTROSCOPY OF DIATOMIC MOLECULES:

This involves precise experimental determination of excited electronic state potentials of diatomic molecules. The objects of research are molecules consisting of alkali and/or alkali earth metals which are also used as model diatomic molecules for theoretical calculations and play an important role in physics of ultracold gas media. Two high-resolution spectroscopic techniques are used: laser Polarization Labeling Spectroscopy (PLS) and Laser Induced Fluorescence spectroscopy (LIF) recorded with a Fourier Spectrometer.



The group developed novel numerical methods which allow determination of potential energy curves (PECs) from the obtained spectroscopic data also in cases of exotic PEC shapes, *e.g.*, shelf or double minima, as well as in cases of states which interact so strongly that coupled channel analysis is necessary for interpretation of the experimental data. The raw data have been made available at **www.dimer.ifpan.edu.pl** and in Electronic Supplementary Information of publications (Group ON2.5, W. Jastrzębski).

OPTICAL CHARACTERISATION OF MICRO- AND NANOOBJECTS:

The research concerns characterisation of evaporating nano-liquid microdroplets – the processes of aggregation and formation of (transient) nanostructures on their surface and within them. It is based on elucidating the properties of nanostructured microdroplets from acquired laser speckle images. This opens up the possibility of using machine learning to recognise suspensions in microdroplets, involving characterisation of pathogens in real time! Optical nanodroplet properties can be engineered at low cost, via controlling the composition of the nano-liquid. By depositing such microaggregates on a substrate at different stages of aggregation (drying), the fractal dimension of the created nanostructured films can be controlled. This opens the way to the creation of tailor-made nanomaterials. Particular interesting class of nano-objects are those exhibiting plasmonic properties, created using metal colloids (group ON2.7, D. Jakubczyk).

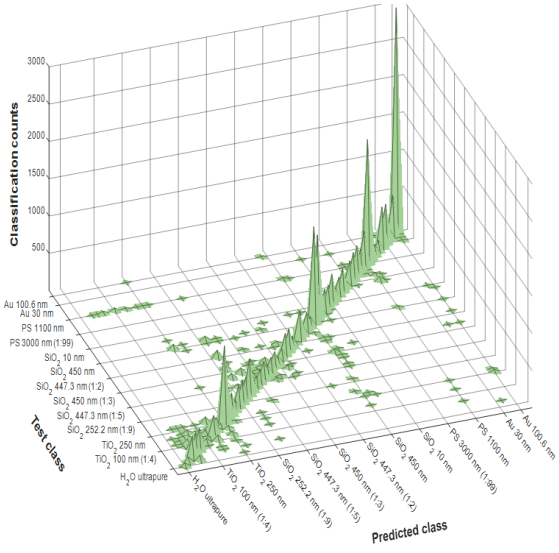


Figure: Graphical representation of the confusion matrix for the neural network trained to classify (recog- nize) ~100 colloidal suspensions (only every 5th class label shown for clarity).

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Division ON3: Physics of Magnetism

RESEARCH ACTIVITY OF THE DIVISION IS FOCUSED ON:

(i) Studies of basic properties of materials suitable for environment friendly energetic applications, among them: materials for hydrogen energetics, *e.g.* cathode materials for solid oxide fuel cells (like layered cobaltites, presented in Fig. 1, which show large oxygen ionic conductivity due to their channel structure), materials for Li-ion batteries (olivines), multifunctional materials, multiferroics, materials showing large magnetocaloric effect (suitable for a new generation of energy efficient magnetic refrigerators). H. Szymczak, A. Szewczyk, and R. Puźniak were the main animators of the magnetocaloric effect studies.

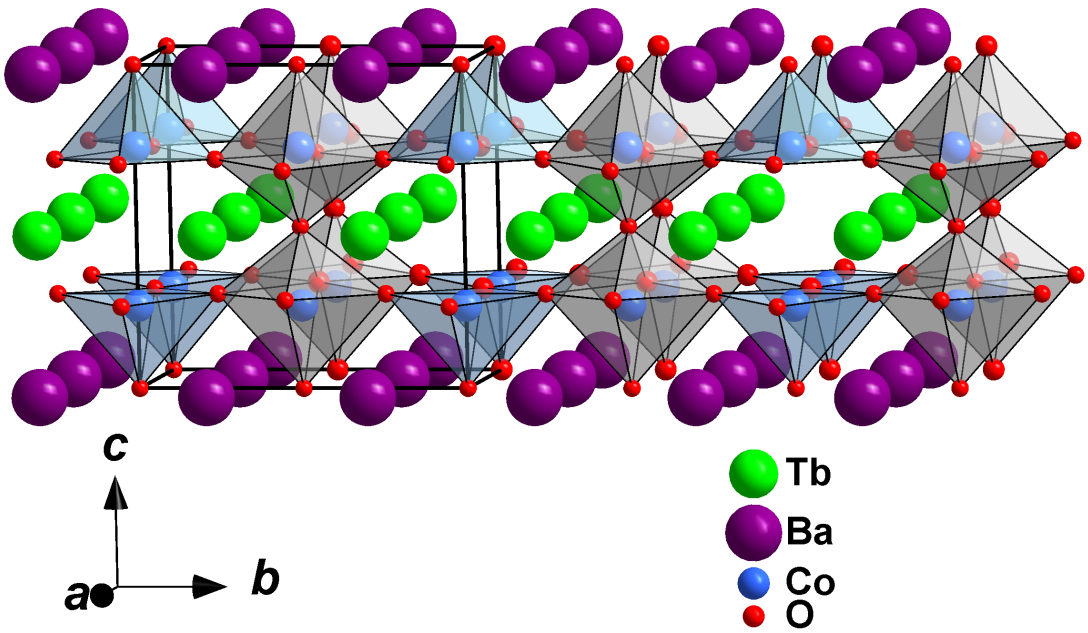

Fig. 1. Layered perovskite $TbBaCo_2O_{5.5}$ considered for cathodes of Solid Oxide Fuel Cells (figure from Phys. Rev. B 86, 054404 (2012), coauthored by Więckowski, Gutowska, Lewińska, and Szewczyk).

(ii) Magnetic and transport properties of high-T_c superconductors (P. Przysłupski, R. Szymczak, H. Szymczak, A. Wiśniewski, and R. Puźniak were leaders of this studies). Recent achievement of critical superconductivity temperature exceeding 200 K, observed under hydrostatic pressure in hydrogen-rich compounds, renewed our interest in high temperature superconductivity. In particular, papers on alleged room temperature superconductivity of lutetium polyhydride synthesized under very high pressure were published. Due to the contradiction in reports concerning superconductivity in this and related compounds, the researchers from the Institute, A. Suchocki, A. Wiśniewski, and A. Wittlin, in collaboration with the Institute of High Pressure Physics PAS, have started synthesis and studies of this family of materials.

(iii) Studies of phase transitions (magnetic, structural, Jahn-Teller, martensitic, quantum, *etc.*). Special emphasis is put on the martensitic transition in materials (*e.g.*, in Ni_2MnGa alloys), in which the transition is accompanied by a huge magnetocaloric effect, which is planned to be the basis of a new generation of energy efficient and environment friendly refrigerators and air-conditioners. The division has a long-standing interest and experience in these investigations (R. Szymczak, H. Szymczak, A. Szewczyk, and R. Puźniak were leading scientists of these studies). They cover studies of critical behaviors of magnetization, susceptibility, and specific heat, as well as optical observations of domain structure near the transitions. For example magnetic transition of quantum character which appears below 1 K in aluminoborates (Fig. 2) was recently studied (Physical Review B 105, 094418 (2022)).

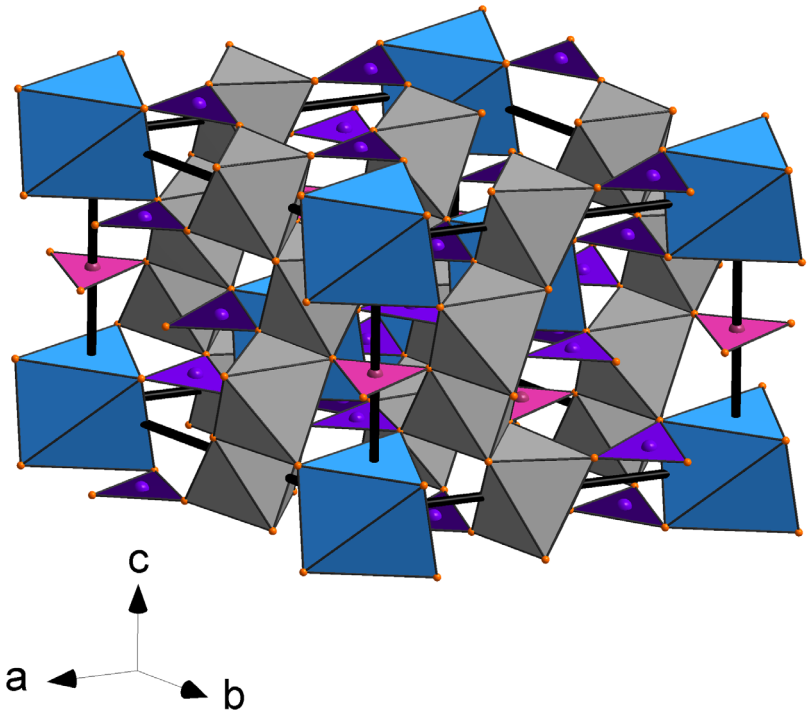

Fig. 2. Crystalline structure of $RAl_3(BO_3)_4$ aluminoborates. Trigonal R-containing oxygen prisms, RO_6, are painted blue, Al-containing oxygen octahedra, AlO_6, are painted grey, and BO_3 triangles appearing in two crystallographic positions are painted pink and violet. The compound with R=Tb shows a magnetic quantum phase transition (figure from Physical Review B 105, 094418 (2022) by T. Zajarniuk *et al.*).

Moreover, the exchange bias (EB) effect, defined as a vertical and horizontal shift of the magnetization hysteresis loops M vs H, as well as temperature-driven spin switching were found in $ErFeO_3$ ferrimagnet near the compensation temperature T_{comp}=45 K (Physical Review B 105, 094424 (2022), coauthored by I. Fita, R. Puzniak, and A. Wisniewski). These phenomena were also analyzed theoretically.

(iv) Studies of thin films, multilayers, half--metallic Heusler alloys (being a source of spin-polarized current and, thus, suitable for dynamically developing spintronics). The main aspect of these studies is understanding the nature of magnetic interactions and their impact on various structural and magnetic properties. In order to realize this goal, the performed experiments are usually supplemented with *ab initio* calculations (performed mainly within the DFT approximation). Recently, in the paper coauthored by L.T. Baczewski (Science 360, 1331(2018)) it was proved that the interaction of chiral molecules (enantiomers) with a perpendicularly magnetized substrate is enantiospecific, i.e. one enantiomer adsorbs preferentially when the magnetic dipole is pointing up, whereas the other adsorbs faster for the opposite alignment of the magnetization (Fig. 3). Thus, it was shown that ferromagnetically magnetized thin films can be used for separation of particles of different chirality. This discovery can have a practical application in pharmaceutical industry as it provides a potentially generic chromatographic method for enantioseparation, which does not require a specific and costly separating columns used up to now. This is a particularly important issue in pharmacology because different enantiomers of the same substance have different toxicity and impact on organisms. It is sufficient to mention the known thalidomide tragedy.

In another paper (Physical Review B 105, 094405 (2022), coauthored by R. Kalvig, E. Jedryka, M. Wojcik), highly ordered carbon penetration into the $Mn_5Ge_3C_x$ epitaxial films (Fig. 4) was investigated by means of the ^{55}Mn NMR method. This material attracts a large attention as a new spintronic material, which can be used as a source of polarized carriers injected directly into Ge. Mn_5Ge_3, a metallic ferromagnet with the Curie temperature of 296 K, shows high spin polarization of the conduction electrons at the Fermi level and a strong magnetocrystalline anisotropy with an easy axis oriented perpendicularly to the film plane, which opens an interesting possibility of combining spintronics with the data storage. Upon doping with carbon, a linear increase of the Curie temperature can be achieved.

In the paper devoted to spintronic Heusler alloys (Physical Review B 106, 054406 (2022)), coauthored by A. Nabiałek, O. Chumak, A.

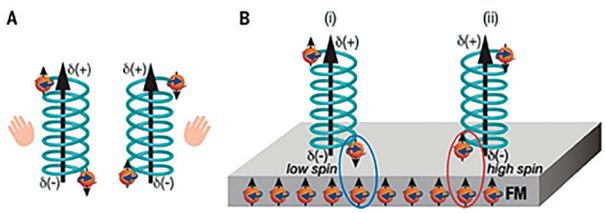

Fig. 3. (A) Schematic cartoon of the polarization. The electrical polarization of the molecule is accompanied by spin polarization. The spin alignment at each electric pole depends on the specific enantiomer. The horizontal arrows indicate the rotation, and the vertical arrows indicate the spin direction. (B) Therefore, for a specific enantiomer, the interaction between the magnetized surface and the molecule (circled in blue and red) follows either a low-spin (i) or a high-spin (ii) potential, depending on the direction of magnetization of the substrate (figure from Science 360, 1331(2018)).

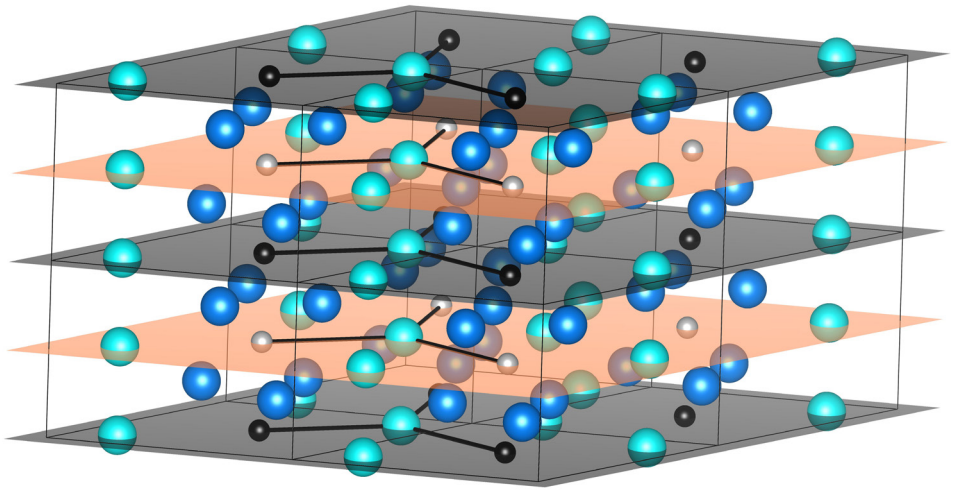

Fig. 4. Schematic representation of a hypothetical carbon superstructure within the $Mn_5Ge_3C_{0.5}$ lattice. Colored spheres denote, respectively, Mn_I (green), Mn_{II} (blue), C (black), and empty 2(b) sites (light gray). Two types of the Mn_{II} planes can be distinguished: gray, all 2(b) voids are filled with carbon, and pink, all 2(b) voids remain empty (figure from Physical Review B 105, 094405 (2022)).

Lynnyk, L. T. Baczewski, and H. Szymczak, the anisotropy of magnetoelastic properties of epitaxial $Co_2Fe_xMn_{1-x}Si$ thin films was studied. The originality of this paper consists in application of a specific strain modulated ferromagnetic resonance technique for determining two cubic magnetoelastic constants of the epitaxially grown 30-nm-thick $Co_2Fe_xMn_{1-x}Si$ magnetic layers.

(v) Physics of topological materials, which is a new branch developing rapidly in recent years. In particular, we are interested in studies of magnetic heterostructures, in which topological skyrmions (considered for memory applications) appear, topological insulators, and Weyl metals.

The paper considering Dzyaloshinskii–Moriya interaction (DMI) in the epitaxial W/Co/Pt multilayers (Nanoscale 13, 7685 (2021)), coauthored by S. K. Jena, E. Milińska, S. Lewińska, A. Lynnyk, A. Pietruczik, P. Aleszkiewicz, and A. Wawro, is an example of such studies. DMI existing in asymmetric layered ferromagnetic films gives rise to non-colinear spin structures stabilizing magnetization configurations with nontrivial topology. A non-collinear spin texture may emerge in the form of skyrmions, spin springs, or chiral domain walls.

(vi) Studies of selected aspects of biomagnetism and nanomaterials suitable for medical applications (among them magnetic nanocapsules in which anticancer medicines could be transported).

MATERIALS STUDIED:

Ceramics, single crystals and thin films of complex oxides (*e.g.*, manganites, layered cobaltites, and high-T_c superconductors); topological insulators and Weyl semimetals; thin films of metals and Heusler alloys; molecular magnets.

TECHNOLOGICAL FACILITIES:

(i) Installations for growing single crystals by means of the Czochralski, chemical vapor transport, floating zone, and Bridgeman methods. (ii) Molecular beam epitaxy systems. (iii) RF sputtering system.

EXPERIMENTAL FACILITIES:

(i) SQUID magnetometers, (ii) Physical Property Measurement Systems, equipped with options for torque, magnetization, transport properties and specific heat measurements from 50 mK to ca 800 K in magnetic field up to 9 T, (iii) Vibrating Sample Magnetometers, (iv) AC- susceptometer, (v) a system of Differential Scanning Calorimetry for high-temperature specific heat measurements (90 K - 1000 K), (vi) broadband spin echo Nuclear Magnetic Resonance spectrometers, (vii) Electron Paramagnetic Resonance and Ferromagnetic Magnetic Resonance (with possibility of using strain modulation) spectrometers, (viii) magneto-optical setup for polar Kerr effect based studies, (ix) optical set-ups for observation of magnetic domain structure, (x) instrumentation for optical absorption, luminescence, and Raman scattering studies, (xi) apparatus for X-ray powder diffraction and single crystal orientation.

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Division ON4: Physics and Technology of Wide-Band-Gap Semiconductor Nanostructures

The mission of the **Division of Physics and Technology of Nanostructures of Wide Gap Semiconductors** is developing the technology of wide band semiconductors, in particular some of the second group metal oxides and third group metal nitrides, with emphasis on structures with reduced dimensionality (1D or 2D) as well as studying physical properties of these systems. The Division consists of four Groups.

The **High-Pressure Spectroscopy Group** (ON4.1) studies optical properties of materials under extreme conditions. For pressure tests, chambers with diamond anvils are used, allowing application of pressures up to about 400 kbar at temperatures down to 4 K. Research is carried out on phosphors for lighting purposes and for applications increasing the efficiency of solar batteries, as well as on modern semiconductor materials and quantum structures based on nitrides and oxides. Recently, research on materials for mechanoluminescent applications has also been initiated.

The **Oxide Nanostructure Technology Group** (ON4.2) deals with fabrication and investigations of new semiconductor and dielectric materials, such as zinc, copper, hafnium, zirconium, and titanium oxides. These materials are produced by atomic and hydrothermal layer deposition, both as thin layers, with thicknesses of several nanometers to about 1 micrometer, and in the form of nanopowders. The conducted research focuses on various types of applications in medicine, photovoltaics, and electronics. The Group has successfully applied for many patents (Polish and European) and won numerous awards at international innovation fairs.

The Group of MBE Growth of Oxide Nanostructures and Electron Microscopy and Spectroscopy (ON4.4) develops epitaxial techniques for the growth of layers and quantum structures from the group II metal oxides: ZnO, CdO, MgO. Its field of activity covers also the growth of rock salt $Mg_{1-x}Zn_xO$ solid solutions or short-period superlattices (digital alloys) of CdO/MgO and ZnO/CdO. The aim of these works is to obtain systems with controlled electronic structures, in particular band gaps, useful in optoelectronic applications in the high-energy ultraviolet range.

The second area of research of the Group is the application of scanning electron microscopy, cathodoluminescence microscopy, and electron beam induced current imaging (EBIC) for the characterization of low-dimensional semiconductor structures (*e.g.*, nanowires made of nitride or oxide semiconductors), as well as the application of photoelectron spectroscopy with use of

synchrotron radiation for studying electronic structure of semiconductors and topological materials.

The **MBE Growth of Nitride Nanostructures Group** (ON4.5) deals with the development of techniques for the preparation of nanostructures of the (Al,Ga,In)N family and studies physical phenomena in such semiconductor systems. In particular, the research is focused on *in-situ* observation and analysis of atomic processes occurring during the crystallization of planar systems and nanostructures of these compounds on unconventional, non-crystalline substrates. The aim of the research is a deeper understanding of the basic mechanisms of nucleation and growth of nanostructures as well as the insight into the impact of these phenomena on the structural, electronic, and optical properties, crucial for applications in modern opto- and microelectronics devices.

Current achievements

EPR AND OPTICAL STUDIES OF THERMOLUMINESCENCE PROCESSES IN Mn DOPED $YAlO_3$ SINGLE CRYSTALS

Yttrium orthoaluminate ($YAlO_3$), also known as yttrium aluminum perovskite (YAP), is widely known as a host material for solid-state lasers and scintillators. Manganese doped YAP became of particular interest after its application potential has been shown as well for holographic recording and optical data storage as for dosimetry of ionizing radiation using thermally (TSL) or optically stimulated (OSL) luminescence.
Manganese ions in YAP:Mn crystals can occur in different sites and charge states: as Mn^{2+} ions in strongly distorted dodecahedral coordination (Y^{3+} sites) or Mn^{4+} ions in octahedral coordination (Al^{3+} sites). The Mn^{4+} ions ($3d^3$ electronic configuration), absorbing in the visible and UV, are sensitive to light exposure. Such exposure, *e.g.*, with blue-green light gives an efficient photochromic effect manifesting itself in blue-grey coloration of the crystal. This coloration is caused by the absorption of Mn^{5+}_{Al} ions created as a result of the Mn^{4+} photoionization (Mn^{4+}_{Al} - Mn^{5+}_{Al} + e) process. The photoinduced absorption of Mn^{5+}_{Al} ions remains stable at room temperature and can be removed completely by subsequent warming of the material at temperatures T=500 K. During warming, the characteristic red emission of Mn^{4+}_{Al} ions near 710 nm is observed in thermal glow peaks at 400, 450 and 570 K, when heated at a rate of 0.4 K/s.

In contrast, Mn^{2+}_{Y} ($3d^5$) ions are not sensitive to visible light exposure because the optical transitions from the ground state to excited ones are spin-forbidden. The presence of Mn^{2+} ions can be revealed in luminescence under excitation above the material band gap, *e.g.*, under X-ray excitation. Under such excitation the emission of Mn^{2+}_{Y} in YAP is observed as a broad band in the green spectral range with maximum near 530 nm. The same green emission from Mn^{2+}_{Y} ions is observed also in thermoluminescence after previous irradiation of the material with ionizing radiation. Exactly this green glow occurring mainly in one TSL peak near 450 K (at 0.4 K/s heating rate) can be used for dosimetry of ionizing radiation.

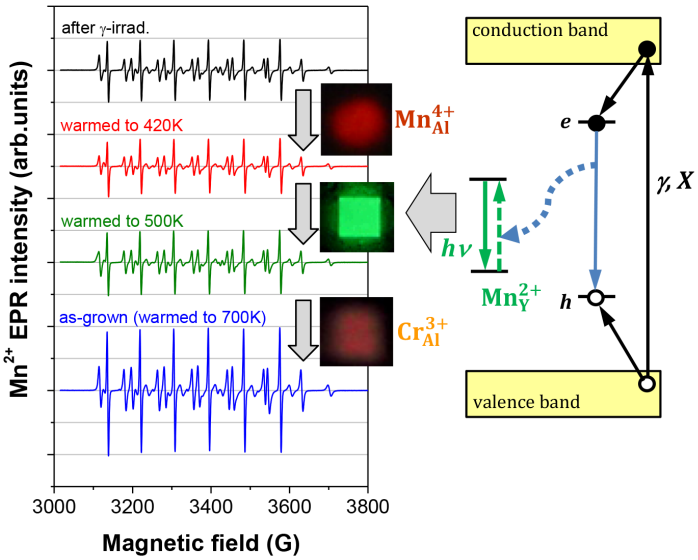
The recharging processes involving Mn^{2+}_{Y} ions under irradiation and subsequent recombination during warming of the irradiated crystals were not unambiguously understood. Therefore, the purpose of the present work was to perform a detailed electron paramagnetic resonance (EPR) study of YAP:Mn^{2+} crystals and to correlate the obtained results with those

of luminescence and optical absorption in order to get an insight into the recharging mechanisms of Mn_Y^{2+} ions under irradiation and subsequent warming in view to application in dosimetry of ionizing radiation. As a result of the conducted experimental studies we confirmed that codoping with Hf instead of Si leads to an increase of the intensity ratio of the green (Mn^{2+} related) to red (Mn^{4+} related) thermoluminescence by over an order of magnitude.

The Mn^{2+} centers occurring in Mn doped YAP single crystals were unambiguously identified by EPR as stemming from isolated Mn^{2+} ions occupying Y^{3+} sites. The same single Mn_Y^{2+} centers were observed both in yttrium-rich YAP:Mn,Si and YAP:Mn,Hf crystals as well as in stoichiometric YAP:Mn,Hf. Investigations of Mn^{2+} EPR signal intensity under UV illumination allowed us, moreover, to place the Mn^{3+}/Mn^{2+} energy level more than 5.4 eV below the YAP conduction band minimum. We found that only in yttrium-rich crystals Mn_Y^{2+} ions can be metastably ionized to Mn_Y^{3+} under γ- or X-ray irradiation at room temperature and the recharging process is limited by the availability of deep electron traps. The lack of such traps in stoichiometric YAP:Mn,Hf shows unambiguously that they must be related to defects introduced by yttrium excess.

The presented results demonstrate, moreover, that Mn_Y^{3+} + e - Mn_Y^{2+} recombination is not the most efficient excitation channel of the green $^4T_1 \rightarrow {}^6A_1$ emission of Mn_Y^{2+}, possibly because of the huge energy difference between the recombination (>5.39 eV) and excitation (3 eV) energies. In contrast, energy transfer to Mn_Y^{2+} proves to be dominant. Thus, ionization of Mn_Y^{2+} is not a necessary condition for Mn_Y^{2+} thermoluminescence, provided that other impurities or defects are present.

Comparative analysis of the EPR results together with those of luminescence, thermoluminescence, and optical absorption studies of the crystals allowed us to propose a general model of trapping and recombination mechanisms responsible for thermoluminescence of YAP:Mn crystals above room temperature that is consistent with all findings. Beside Mn_Y^{2+} ions acting as deep hole traps (with trap depth - 2.1 eV) and some defect-related electron and hole traps intrinsic to the YAP lattice (with depths between 1.2 and 1.7 eV), the model includes also the influence of unintentional impurities, such as Fe_{Al}^{2+} and Cr_{Al}^{3+} ions detected in all investigated crystals, as well as Mn_{Al}^{4+} ions, present despite Si or Hf co-doping. Fe_{Al}^{2+} was found to act as a deep hole trap, while Cr_{Al}^{3+} and Mn_{Al}^{4+} act both as deep hole and electron traps.



Hanka Przybylińska, Yaroslav Zhydachevskyy, Aneta Grochot, *et al.*, J. Phys. Chem. C 2022, 126, 1, 743–753.

Fig. 1. A scheme of thermoluminescence effects related to Mn^{2+}, Mn^{4+} and Cr^{3+} emission in $YAlO_3$:Mn crystals.

VALENCE-BAND ELECTRONIC STRUCTURE OF ZnO AND ZnO:N

EXPERIMENTAL AND THEORETICAL EVIDENCE OF DEFECT COMPLEXES

Today's electronic devices are mainly based on silicon, which is associated with its common occurrence in nature and relatively easy p-type and n-type doping, however, due to the narrow and indirect band gap silicon is not a suitable material for optoelectronic applications. For this purpose, materials with wide and direct band gaps, such as GaN and ZnO, are investigated. ZnO would be an ideal material for optoelectronic devices if stable p-type conductivity is achieved. Despite extensive research in this field, this problem has not been solved and p-type conductivity of ZnO remains difficult to obtain in a predictable way. Photoemission studies carried out at the ELETTRA synchrotron in Trieste and supported by DFT calculations shed light on this problem.

Thin ZnO films, undoped and nitrogen doped, were cleaved under ultra-high-vacuum conditions and the cross-sections were investigated by scanning photoelectron microscopy (Fig. 1a). A state-of--the-art resolution of 130 nm allowed the study of the electronic structure of individual crystallites shown in Fig. 1 (b, c) and a series of photoemission spectra from different crystallites were taken. As found, only two types of electronic band structure in the valence band region were recorded, both for N-doped (Fig. 1d) and undoped (Fig. 1e) ZnO. This finding, confirmed by cathodoluminescence images showing clustering of the acceptor- and donor-related emission (Ref. 1), unveiled that acceptors and donors occupy separate crystallites. Density Functional Theoretical (DFT) calculations revealed that complexes involving zinc vacancy, hydrogen, and nitrogen (in case of ZnO:N) modify the density of states in the valence band region, so the experimentally observed differences in photoelectron spectra between crystallites evidence the accumulation of acceptor complexes in some crystallites (Ref. 2). DFT calculations also point at the dual role of nitrogen as an acceptor dopant in ZnO, which can both passivate shallow donors and facilitate creation of n-V_{Zn} complexes providing shallow acceptor states. The reason for separate acceptor and donor domains is not clear and requires further studies. Earlier photoemission investigations performed on Zn- and O-polar surfaces of single ZnO crystals and the SPEM measurements of ZnO nanostructures showed a similar modification of the valence band shape, indicating that formation of acceptor complexes is associated with distortion of the crystal lattice, so microstrain might play a role in this phenomenon. On the one hand, the separation of donors and acceptors explains the uniqueness of electrical results obtained on polycrystalline ZnO and ZnO:N films. On the other hand, it is of great importance for future applications. It paves the way to obtain homogeneous ZnO acceptor conductivity without incorporation of donors, at least on the nanometer scale if necessary strain conditions are ensured. It also indicates that eventual devices should be rather constructed in a vertical architecture, enabling transport of carriers along the grown columns.

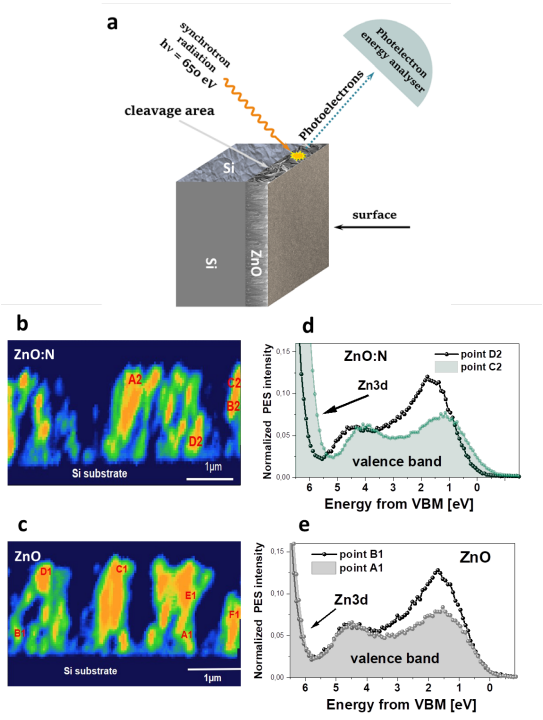


Fig. 1. (a) Experimental scheme used in the SPEM measurements; SPEM images of the films' cross-sections measured for ZnO:N (b) and ZnO (c) films; PES spectra of ZnO:N (d) and ZnO (e) in the valence band region measured at different points.

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SHORT PERIOD ZnO-BASED NANOSTRUCTURES TOWARD EFFICIENT LIGHT SOURCES

Wide gap II–VI semiconductors such as ZnO-based heterostructures have reached their technological importance for the development of optoelectronic devices, in particular near-UV emitters and sensors, active material in light emitting diodes and lasers. This is due to the wide band gap and large 60 meV exciton binding energy permitting excitonic recombination well above room temperature. Additionally, ZnO is a binary compound which can form ternary $Zn_{1-x}Mg_xO$ alloys with Mg moving optical emission towards deeper UV. On the other hand, alloying ZnO with CdO in form of $Zn_{1-x}Cd_xO$ lowers the band gap down to 1.73 eV and offers possibility of green light emission. While ZnO crystallizes in the thermodynamically stable wurtzite structure, the high ionicity of the Mg-O bond makes the octahedral coordination of Mg atoms more favorable than the tetrahedral one. Therefore, the stable wurtzite structure in $Zn_{1-x}Mg_xO$ alloys is limited to about 33% of Mg content, above which metastable material occurs. At 45% it tends to segregate into a mixture of cubic and hexagonal phases due to phase instability, which leads to reduced conductivity and mobility of charge carriers and lower luminescence efficiency.

An alternative method for fabricating ZnMgO alloys with high Mg contents that would be stable without a tendency to phase separation during growth or thermal annealing is highlighted here. It seems that one of the possible approaches is to grow artificial (ordered) alloys in form of short period superlattices (SLs). This approach allows covering a wide spectral range by manipulation of the average composition of ZnMgO structures without phase separation, a drawback present in random alloys. The ordered alloys, also called quasi-ternary alloys (QTA), are composed of a sequence of MgO and ZnO layers, thin enough to avoid strain relaxation via generation of misfit dislocations. The change of layer thicknesses allows obtaining ZnMgO alloys potentially with any average composition.

In the proposed ZnO/MgO superlattices, grown with the molecular beam epitaxy technique, the barrier heights (conduction band offset) exceed 2 eV therefore excitons are being easily localized in ZnO quantum wells and such a ZnO/MgO superlattice may become a system of independent quantum wells for MgO barrier thicknesses of a few nanometers only. Another issue comes from the fact that retaining WZ crystalline structure at high mean Mg concentrations in ZnO/MgO SL structures may have a direct influence on intrinsic and extrinsic effects through an accumulation of strains.

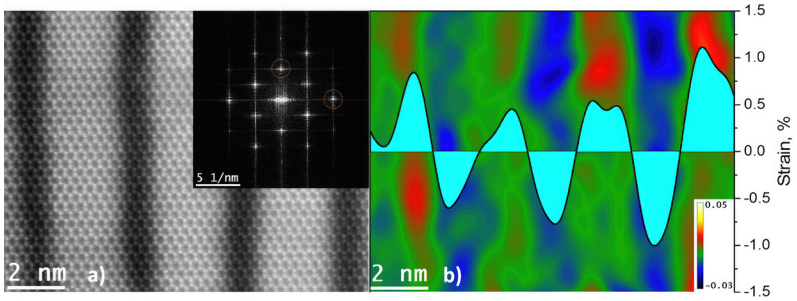

Figure: STEM-HAADF images, inset shows reflections selected for GPA analysis, b) strain distribution and stain line plot along [11-20] growth direction of structure A 2.5/1.

To accurately design a photoelectronic device, it is crucial to understand the influence of SL design on QW emission. The obtained SLs contain from 27% up to 72% of mean Mg concentration. The results allow drawing following conclusions:

- SLs with MgO layers below 2 nm represent excellent crystallographic quality retaining the wanted wurtzite structure.
- For MgO layers thickness above 3 nm, the crystalline quality detoriates forming a mixture of cubic and wurtzite crystallites.
- The thicker are the MgO layers, the more severe is the generation of the biaxial strains, which influence emission energy, and beyond a critical value, lead to poor crystallinity.
- All the results evidenced that bandgap engineering through deposition of wurtzite quasi-ternary alloys in the form of superlattices is feasible and potentially allows overcoming phase separation for above 40-50% of Mg content.

Authors: M. Stachowicz, A. Wierzbicka, J.M. Sajkowski, M.A. Pietrzyk, P. Dłużewski, E. Dynowska, J. Dyczewski, K. Morawiec, S. Kryvyi, S. Magalhães, E. Alves, A. Kozanecki

GaN NANOWIRES FOR NEW DESIGNS OF OPTOELECTRONIC DEVICES AND SENSORS

Group-III nitride nanowires (NWs) are a promising alternative to planar heterostructures from this material system and have significant potential to drive new applications, especially when integrated on low-cost substrates. In general, due to the advantage of efficient elastic strain relaxation at the sidewalls, NWs are almost strain-free objects without lattice misfit defects even if grown on highly lattice-mismatched substrates. Therefore, complicated heterostructures can be ideally grown in the form of NWs with a crystallographic quality not achievable in similar planar heterostructures. As example, Figs. (a-b) show SEM images of NW-based LED device structure grown by plasma-assisted molecular beam epitaxy (PAMBE) on nitridated Si(111) substrate. The NW structure consisted of an initial GaN:Si segment, followed by Si doped AlGaN with increasing Al content up to 15%, three 3.5 nm thick GaN quantum wells with 10 nm thick $Al_{0.15}Ga_{0.85}N$ barriers and the top p-type $Al_{0.15}Ga_{0.85}N$ part doped with Mg. In

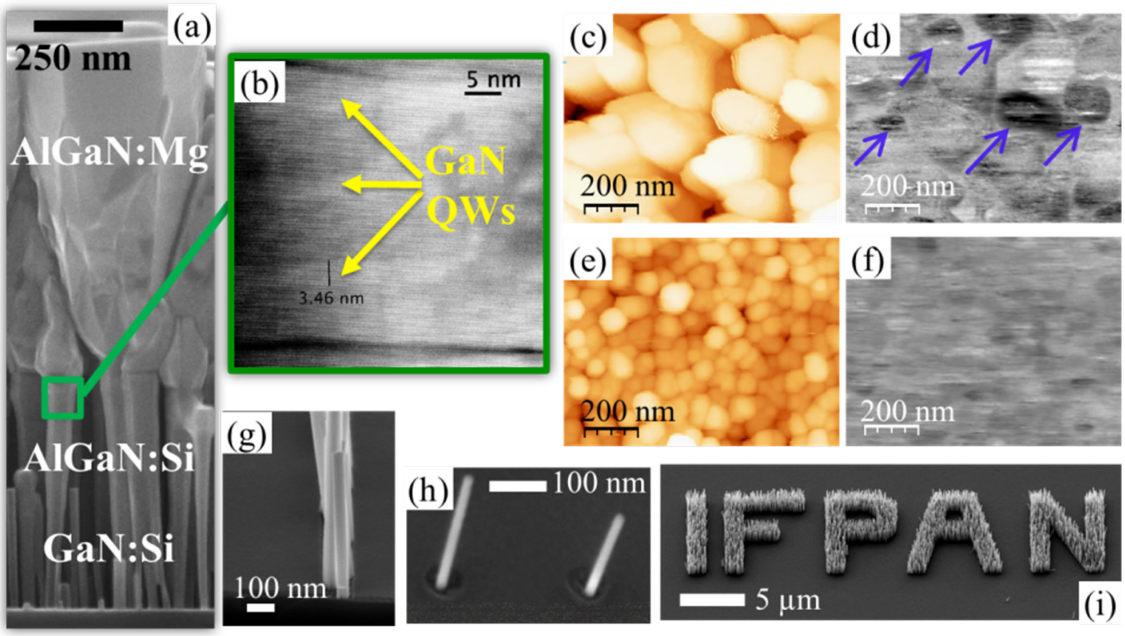

Figure: (a-b) structure of GaN/AlGaN nanowire LED device [1]; KPFM topographic (c, e) and contact potential difference (d, f) maps of GaN NWs with (c, d) and w/o (e, f) mixed polarity. The arrows in (d) mark the NWs with reversed polarity [2]; (g-i) SAG of GaN NWs on SiN_x-masked AlO_y nucleation layer [3].

Ref. [1] we provided the nano-scale correlation of the morphological, electrical, and optical properties of such GaN/AlGaN NW LEDs. Two types of nanowire LEDs, having opposite growth polarities were analyzed. We showed that switching the polarity of the nanowires from the N- to Ga-face had a significant impact on their optical and electrical properties. In particular, our studies revealed quantum wells emissions at ~3.5 eV, which were significantly brighter in Ga-polar NWs than in N-polar ones. Moreover, the electron beam induced current mapping proved that the p–n junctions were less active in N-polar NWs.

The example above shows that control of NWs' polarity is crucial for the development of efficient NW-based LED structures. However, coexistence of nanowires with different polarities inside one NW ensemble is commonly observed. Therefore, in Ref. [2] we used Kelvin probe force microscopy (KPFM) to assess the polarity of GaN NWs grown on Si(111). We showed that uniformity of the polarity of GaN NWs critically depends on substrate processing prior to the growth. For example, nearly 18% of NWs with reversed polarity were found if the most common way of Si deoxidation (HF etch) was used (Figs. c-d). Alternative treatments of Si substrates were tested. The best results, i.e., purely N-polar ensemble of NWs, were obtained on Si wafers thermally deoxidized under UHV in the growth chamber at ~1000°C (Fig. e-f). Interestingly, no mixed polarity was found for GaN NWs grown under similar conditions on Si(111) with a thin AlO_y buffer. Our results show that reversal of NWs' polarity can be fully prevented by growing them on a perfectly uniform substrate surface, in our case on clean, *in situ* formed SiN_x or *ex situ* deposited AlO_y buffers.

The main drawback of NWs formed by self-assembly is that they nucleate spontaneously and are distributed randomly on the substrate. Thus, control of NW number density is an issue and the growth of core-shell radial heterostructures becomes difficult due to a shadowing effect in a dense NW ensemble. Selective area growth (SAG) offers a spatial ordering of NWs on the substrate. This can be achieved when a part of the substrate is covered by a mask material and the growth conditions are adjusted so that GaN nucleates exclusively on the mask-free areas. Figs. (g-i) show the results of our experiments on SAG of GaN NWs with AlO_y nucleation layer and SiN_x film as the mask [3]. As seen, perfect growth selectivity is obtained. We continue this work developing SAG of GaN NW on metallic nucleation layers that will act in LED devices as a low resistive ohmic contact to the bottom parts of NWs as well as efficient buried mirror preventing light losses by absorption in the substrate.

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Division ON5: Theoretical Physics

The research in the division encompasses a broad range of topics – including hard and soft condensed matter, ultra-cold atomic gases, and biophysics – which can be gathered under the umbrella of “investigations of complex quantum and classical systems”. There are currently 10 research groups within the Division, and below we give examples or recent results obtained by some of them.

SOFT MATTER AND FLUID PHYSICS

Substrates that gradually change their properties along a particular direction can be used to provoke, steer, and sustain the motion of fluids, which is relevant for a range of applications, such as microfluidics, microfabrication, coatings, nanoscale actuation and energy conversion. Our group has proposed a new substrate design based on polymer brushes with a stiffness gradient along a specific direction, which can cause spontaneous and unidirectional fluid motion, a phenomenon known as durotaxis [1]. The results have indicated that the grafting density of the brush chains and the droplet adhesion to the substrate are two key parameters for this substrate design and moderate values of these parameters can with certainty lead to the fastest fluid motion. In contrast, the droplet motion is not affected by the droplet viscosity or the length of the substrate brush polymers. This research has also unraveled the underlying mechanism of the durotaxis motion of the droplet for the brush substrate design, which suggests that the substrate roughness is the ultimate factor that determines the droplet motion, that is the droplet will move from rougher regions to those with less roughness as a result of the stiffness gradient, thus minimizing its energy.

[1] R. Kajouri, P.E. Theodorakis, P. Deuar, R. Bennacer, J. Židek, S.A. Egorov, A. Milchev, Langmuir 39, 2818 (2023).

BIOMEMBRANES

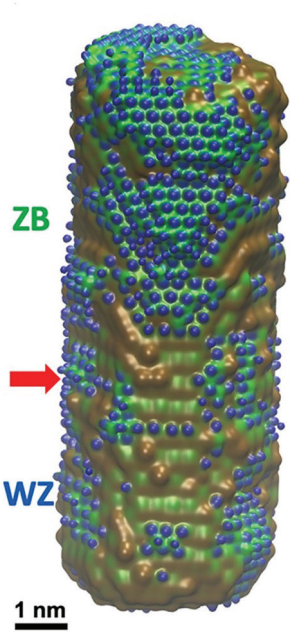
The research is focused on membranes that separate biological cells from the surrounding environment as well as different organelles inside cells. They are composed primarily of lipids and proteins that govern diverse biological processes, such as tissue formation and repair, nutrient uptake, neuronal communication, and immune responses. They are central players in numerous diseases and host-pathogen interactions, while membrane proteins (such as transporters, channels, and receptors) are the targets of almost 70% of FDA-approved drugs. We have recently focused on nanoscale lipid clusters in cell membranes that can serve as platforms to recruit membrane proteins for various biological functions. A central question is how these nanoclusters respond to physical contacts between cells. Using methods of classical statistical mechanics we explored how adhesion of cell membranes affects the distribution of lipid clusters associated with membrane adhesion receptors. Our results show that intercellular receptor-ligand binding can induce coalescence of these clusters and simultaneous condensation of the receptor-ligand complexes within the adhered membranes [1]. We also found that formation of these membrane biomolecular condensates leads to significant cooperativity of the receptor-ligand binding [2]. The interplay between the receptor-ligand binding cooperativity and the receptor condensation manifests acute sensitivity of the membrane system to changes in control parameters. This sensitivity can be relevant in cell signaling and immune responses.

[1] L. Li, J. Hu, B. Różycki, F. Song, Nano Lett. 20, 722-728 (2020).
[2] L. Li, J. Hu, X. Shi, B. Różycki, F. Song, Soft Matter 17, 1912-1920 (2021).

STRUCTURAL, ELECTRONIC, SPIN, AND TOPOLOGICAL PROPERTIES OF SEMICONDUCTOR NANO-STRUCTURES

A theoretical analysis of the growth of nanostructures, in particular nanowires, concentrates on processes which take place mostly on the surface and which determine the crystal structure, shape and composition of the structure. The studies of such processes

are carried out using in parallel an analytical approach, solving differential equations, using Monte Carlo or molecular dynamics simulations. They allowed us to explain the shape, growth direction, and crystal structure of various structures observed in experiments, *e.g.*, formation of craters and inclined nanowires [1], the growth of so called nanoflags [2], or the crystal structure of magnetic (EuIn)As nanowire shells [3]. The effects of such studies are projected and compared with mesoscopic models based on cellular automata approach [4, 5]. With this type of models, surface stability diagrams and scaling properties of pattern formation for given crystal symmetry, type, and orientation are studied [5, 6].



Theoretical studies were also devoted to the topological properties of IV–VI materials, their nanostructures and defects. The tight binding approach was employed to model the electronic properties of topological crystalline insulator $Pb_{1-x}Sn_xSe$ quantum wells confined by $Pb_{1-y}Eu_ySe$ barriers on one side and by vacuum on the other and to study the structure inversion asymmetry and Rashba effects in heterostructures with non-equivalent interfaces [7]. Recently, we have shown that in the range of parameters such as pressure, temperature, and chemical composition of crystalline alloys for which the bulk crystals belong to the phase of topological crystalline insulators, also the atomic steps on their surfaces are characterized by a non-trivial topology [8]. We have also demonstrated that twinning defects are two-dimensional topological crystalline insulators, and have spin-polarized chiral states on their edges [9].

[1] J.H. Kang *et al.*, Nano Lett. 18, 4115 (2018).
[2] M.S. Song *et al.*, Nano Lett. 21, 10215 (2021).
[3] H. Shtrikman *et al.*, Nano Lett. 22, 8925 (2022).
[4] H. Popova *et al.*, Crystal Growth & Design 20, 7246 (2020).
[5] F. Krzyżewski *et al.*, Crystal Growth & Design 19, 821 (2018).
[6] O. Toktarbaiuly *et al.*, Phys. Rev. B 97, 035436 (2019).
[7] R. Rechciński *et al.*, Advanced Functional Materials 31, 2008885 (2021).
[8] R. Rechciński, R. Buczko, Phys. Rev. B 98, 245302 (2018).
[9] S. Samadi, R. Rechciński, and R. Buczko, Phys. Rev. B 107, 205401 (2023).

POLARITONS

We have demonstrated hardware neural network systems where strong optical nonlinearity results solely from interactions of exciton-polaritons, i.e., quantum superpositions of light and matter [1]. Such superpositions, in the form of mixed quasiparticles of photons and excitons, are characterized by excellent photon--mediated transport properties and strong exciton-mediated interactions. These semiconductor microcavity systems can be used to construct fully all-optical neural networks characterized by extremely high energy efficiency. We show why using polaritonics in place of standard nonlinear optical phenomena is the key to achieving

such a high performance and discuss the scalability of polariton neural networks.

[1] M. Matuszewski *et al.*, Phys. Rev. Appl. 16, 024045 (2021).

SPIN QUBITS AND OPEN QUANTUM SYSTEMS

We have been providing theoretical support for experimentalists working with quantum-dot based spin qubits, mostly focusing on decoherence caused by nuclear spins and sources of charge noise [1, 2]. In the last few years, a lot of work has been done on the problem of spin-coherent shuttling of single electrons in silicon based nanostructures [3], as mastering of such shuttling is currently considered to be necessary for building scalable quantum computers with silicon quantum dots. Our research on the description of decoherence of solid-state based qubits provides a valuable ”reality check” for our more fundamental investigations into the emergence of classical stochastic behavior from the dynamics of a complex quantum system.

[1] F.K. Malinowski *et al.*, Phys. Rev. Lett. 118, 177702 (2017).
[2] T. Struck *et al.*, npj Quantum Information 6, 40 (2020).
[3] J.A. Krzywda, Ł. Cywiński, Phys. Rev. B 101, 035303 (2020); Phys. Rev. B 104, 075439 (2021); V. Langrock, J.A. Krzywda *et al.*, PRX Quantum 4, 020305 (2023).
[4] P. Szańkowski, Ł. Cywiński, Sci. Rep. 10, 22189 (2020); P. Szańkowski, SciPost Phys. Lect. Notes 68 (2023).

ULTRA-COLD ATOMS AND MOLECULES

We are working on the theoretical aspects of the applications of these systems in modern metrology, *e.g.*, atomic clocks, quantum computing, or simulators are considered. The common feature of these applications is the preparation of appropriate quantum states, the so-called spin-squeezed or entangled states. The group of E. Witkowska is developing methods to obtain such states in systems of ultra-cold atoms loaded in a periodic optical lattice. Recently, together with colleagues from Vilnius University and Institute of Photonic Sciences in Castell-defels, a dynamic method for generating spin-squeezed states in fermionic systems used in optical atomic clocks has been developed, see Phys. Rev. Lett. 129, 090403 (2022). In addition, the level of Bell correlation in the states created in this way was calculated. In collaboration with researchers from University of Warsaw and Institute of Photonic Sciences in Castell-defels, the critical time of occurrence of Bell correlations was determined and their levels were classified, which was summarized in Phys. Rev. Lett. 129, 250402 (2022).

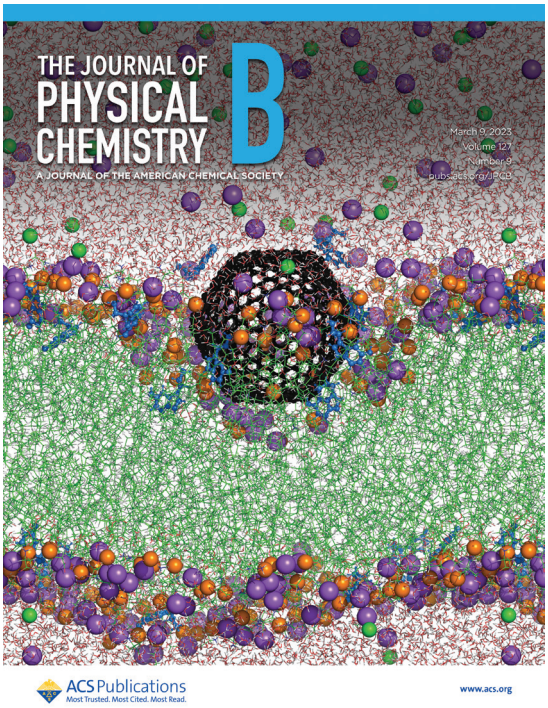
The Quantum Noise group led by P. Deuar focuses on the study of quantum fluctuations, pairing, and thermally induced phenomena in ultra-cold many-body quantum systems, such as Bose-Einstein condensates, quantum droplets, optical cavity arrays, and wave dark matter. To be able to simulate these macroscopic quantum systems without (hopefully) running afoul of the exponential growth of Hilbert space, members of the group also develop new theoretical and numerical approaches. These include: implementation of the positive-P and gauge-P representations with stochastic evolution to new systems, Fock state sampling algorithms for study of condensate fluctuations (*e.g.*, Phys. Rev. Lett. 126, 153601 (2021)), study of higher-order correlations in the Lieb-Liniger one-dimensional gas, modifications of the classical wave field and stochastic Schrödinger equation in order to avoid the ultraviolet catastrophe, and extensions of the stochastic Gross-Pitaevskii model and truncated Wigner representation to new

systems, such as quantum droplets and driven dissipative cavities (*e.g.*, Quantum 5 455 (2021), PRX Quantum 2, 010319 (2021)).

COMPUTATIONAL BIOPHYSICS

The stability of neurotransmitter vesicles in the presence of high serotonin concentrations strongly depends on their lipid composition. To investigate this, we analyzed the mechanical properties of lipid bilayer membranes composed of phosphatidylcholine (PC), phosphatidylethanolamine (PE), phosphatidylserine (PS), and cholesterol (Chol) using AFM, molecular dynamics simulations, and solid-state NMR measurements. We show that the specific lipid mixture in vesicular membranes allows for an appropriate response to serotonin by maintaining stability and facilitating exocytosis. Molecular dynamics simulations revealed the localization and interactions of serotonin with the lipid bilayer, showing that the mechanical response varies among lipids due to differences in serotonin interaction and lipid ordering. The formation of a layer comprising charged PS head-groups, ions, and serotonin contributes to increased mechanical stability of the lipid bilayer under mechanical stress. This effect was not observed with other investigated lipid heads, as they are uncharged and do not exhibit strong electrostatic interactions with other molecules. These insights shed light on the role of lipid composition in achieving optimal mechanical stability of neurotransmitter vesicles in the presence of serotonin (J. Phys. Chem. B 127, 1947 (2023)).

In another study, we demonstrated that the driving force for co-translational protein folding is weaker in the ribosome exit tunnel due to enhanced water ordering (Chem. Sci. 2021, 12, 11851-11857). Electrostatic interactions were found to govern extreme nascent protein ejection times from ribosomes, potentially delaying ribosome recycling (J. Am. Chem. Soc. 2020, 142, 13, 6103-6110). A significant finding in Covid-19 research is the increased binding strength of SARS-CoV-2 to human cells compared to the older SARS-CoV-1, potentially explaining its high contagious- ness (J. Phys. Chem. B 2020, 124, 34, 7336–7347).



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DIVISION ON6: International Centre for Interfacing Magnetism and Superconductivity with Topological Matter – MagTop

The core MagTop's activity is directed to solve grand challenges of topological matter interfaced with magnetism and superconductivity, and to discover experimentally and theoretically new materials and unanticipated topology-related phenomena, which enlarge research horizons and, possibly, lead to new applications. MagTop's motto is: "Experimental and application results inspire theory; theory inspires materials development and applications".

MagTop operates within the International Research Agendas Programme of the Foundation for Polish Science, supported by the European Regional Development Fund under Smart Growth Operational Programme (SG OP), Priority Axis 4: Increasing the research potential, Measure 4.3: International Research Agendas (IRAs).

The IRAs programme provides support for specialised, independent research units in Poland which pursue international research agendas in strategic cooperation with renowned scientific institutions from other countries. The scope of the proposed research, as well as the international standing of the project leaders, are key for the research centre's success and its international scientific visibility. The IRAs programme is aimed at enabling the creation of research organizations (scientific units) led by scientists with considerable experience in science management as well as their own area of expertise, which have international teams of renowned scientists from different fields who conduct research in order to solve a specific global scientific challenge and apply the best international practices with regards to:

- HR policy
- R&D management
- Commercialisation of R&D results.

Research centres implementing the IRAs programme conduct their R&D work in line with a pre-approved research agenda. According to the programme documentation the agenda has to highlight a specific scientific issue – a challenge and a means of addressing it. The challenge itself as well as the proposed means of solving it must be important enough so that the results of the research will likely be published in top scientific journals and presented at prestigious scientific meetings. The intellectual property developed over the course of the research should have the potential for legal protection and the developed solutions should be applicable. The suggested challenge must be contained within the National Smart Specialization framework.

The grant, awarded to MagTop's Leaders

Tomasz Dietl and Tomasz Wojtowicz in 2017, provided funding of forty million PLN (about 9 M€) for initial 5 years. Later, MagTop received additional financing in the amount of 8.5 million PLN (about 1.8 M€), which allows extending its operation until December 31, 2023. Furthermore, two MagTop groups obtained additional funding of about 1 M€ and 0.8 M€ for upgrading GENxplor MBE system and purchasing Variable Temperature and Magnetic Field Characterization equipment package and a microscope-base set-up for local Brillouin Light Spectroscopy (BLS). A call for proposals that could provide MagTop financial support for the next five years within the EU supported FENG Programme (European Funds for Modern Economy) was posted by the Foundation for Polish Science in May 2023.

Julius-Maximilians-Universität Würzburg is MagTop's strategic partner unit. MagTop's employment processes and R&D activities are supervised by the International Scientific Committee (ISC) chaired by Laurens Molenkamp. As detailed in the home page www.MagTop.ifpan.edu.pl, MagTop's forty employees have originated from thirteen countries, which constituted a game changer in the IFPAN internationalization. As shown in Graph 1, MagTop's six groups (Theory, MBE, Characterization, Dirac, Majorana, and Weyl) are headed by leaders with extensive international experience and acclaimed accomplishments [T. Dietl (since 2017), T. Wojtowicz (since 2017), V. Bhat (since 2019), M. Trif (since 2019), T. Hyart (since 2018), C. Autieri (since 2022), M. Matusiak (since 2020)]. The hiring procedures of team leaders, young and senior postdocs, PhD and MSc students have obeyed high standards of openness, equal opportunity, and broadly understood diversity and inclusiveness. In addition to PIs' international experience, good practices in HR, R&D management, commercialization, and outreach have been gathered by study visits of all group leaders in the strategic partner unit University of Würzburg and, in particular, in its Institute for Topological Insulators, and by acquiring good practices from visiting other relevant centres such as Advanced Institute for Materials Research at Tohoku University, which was funded within World Premier International Research Center Initiative (WPI), and together with a parallel initiative of the Japanese Government, Top Global University, aims in modernizing and internationalizing Japanese's academia landscape.

The presence of MagTop was instrumental in acquiring by IFPAN a Welcome to Poland grant from the Polish National Agency for International Exchange (NAWA). The Welcome Centre at IFPAN, in addition to day by day help in arranging foreigners' life in Warsaw, organized, also together with MagTop, various cultural and mixer activities for IFPAN's researchers from abroad as well as seminars concerning mobbing and related challenges. Garden parties for all MagTop employees and their families have routinely been organized by MagTop's Management Board.

In accord with the implemented agenda, one of MagTop's strengths is the **molecular beam epitaxy of 2D and 1D quantum structures** of topological IV-VI and II-VI com pounds that can be interfaced with magnetic and superconducting materials. Another is **bulk growth** of top-quality single crystals of topological crystalline insulators and Weyl semimetals. The developed materials and their hybrid structures with normal, superconducting, or magnetic metals, as well as with amorphous insulators, after **extensive structural and chemical characterization**, are processed into experimental devices and studied in-house by a broad range of experimental methods, comprising **charge and heat magnetotransport, magnetooptics including Brillouin scattering, magnetization, and magnetic resonances** down to millikelvin temperatures and in magnetic fields up to 16 T. Theory research, oriented to propose new R&D directions and to elucidate the in-house and external experimental discoveries,

is a prominent part of MagTop activities. In addition to broad national and **international research collaborations** that involved 43 scientific institutions on three continents, the MagTop researchers are systematic users of European **large facilities**, including synchrotron radiation sources (SOLARIS synchrotron in Kraków, in particular), high magnetic fields' laboratories, and supercomputer centres, available via competitive calls.

Joint research, workshops, papers, and patent applications have been completed with **industrial partners** in the frame of agreements that MagTop/IFPAN signed with six companies: VIGO Photonics S.A., PUREMAT Technologies Sp. z o.o., KrioSystem Sp. z o.o., MeasLine S.A., PREVAC Sp. z o.o., and Robert Bosch GmbH.

Until May 2023, MagTop's researchers have co-authored **240 articles**, delivered **87 invited talks**, presented **94 conference contributions**, submitted **four European patents**, and organized **four international focussed meetings**. The updated lists are in MagTop's home page and in the Web of Science. Two publications and three patents have been jointly submitted with collaborating companies, two other are in a pipeline. All publications are posted in arXiv, *i.e.*, are available via green open access. MagTop's community is also active in **outreach activities**, including teaching in the Doctoral School and many actions for public at large with a special focus on talented and curiosity-driven high-school students.

As conspicuous examples of MagTop's R&D achievements, we present here 25 highlights: 22 are more on the R&D side, the other four involve direct collaboration with industrial partners. They are group into six major topics: **(1) Quantum spin Hall and quantum anomalous Hall materials; (2) Topological crystalline insulators; (3) Weyl semimetals; (4) Towards Majorana zero modes and beyond; (5) Beyond electronic topological matter; (6) Collaboration with industrial partners.** More detailed descriptions of highlights are given in the MagTop home pages and, of course, in relevant MagTop's publications and patents.

QUANTUM SPIN HALL AND QUANTUM ANOMALOUS HALL MATERIALS

Understanding the quantum spin Hall effect

Unlike in the quantum Hall effect [1,2] and quantum anomalous Hall effect, the quantization precision in the quantum spin Hall effect depends on unavoidable background impurities and defects [3,4]. However, doping with magnetic ions restores the quantization accuracy [3,4]. In specific systems, topologically trivial edge states [5] and spontaneous formation of excitonic liquid can play a role [6].

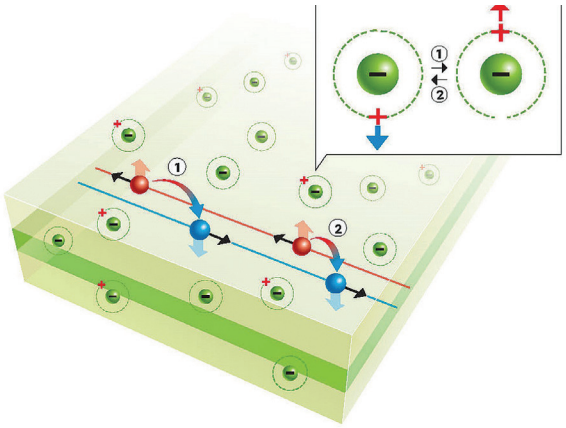

Figure: Destructive role of acceptors occupied by holes in the quantum spin Hall effect regime, e.g., in HgTe quantum wells. Two backscattering processes between helical states are allowed in the presence of electron-hole exchange and spin-orbit interaction: (1) spin-conserving and (2) spin non-conserving leading to backscattering for spin-momentum locking case. As the Kondo limit is reached, the scattering rate is large provided that no bound magnetic polarons are formed around occupied acceptors (after [3,4]).

[1] I. Yahniuk *et al.*, npj Quantum Materials 4, 13 (2019); [2]] I. Yahniuk *et al.*, arXiv:2111.07581 (2021); [3] T. Dietl, Phys. Rev. Lett. 130, 086202 (2023); [4] T. Dietl, Phys. Rev. B 107, 085421 (2023); [5] N. M. Nguyen *et al.*, Phys. Rev. B 107, 045138 (2023); [6] T. Paul *et al.*, Phys. Rev. B 106, 235420 (2022).

New topological phases in mercury compounds

Since the beginning of the era of topological materials, HgTe has been one of the most attractive compounds due to a large band inversion that makes it a robust topological system [B. A. Bernevig *et al.,* Science, 1757 (2006); M. Koenig, Science 318, 766 (2007)]. MagTop's computational team engineered new topological phases of two kinds of HgTe-based superlattices, one preserving time-reversal symmetry and another violating it by magnetic ions.

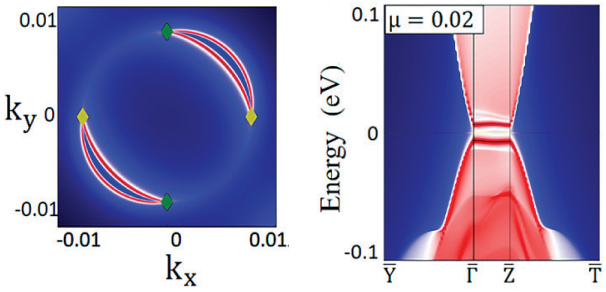

Figure: Fermi arcs (red) in a HgTe/HgSe superlattice around the Γ point and projected onto (001) surfaces (left panel). Diamond markers indicate Weyl points with chirality −2 (yellow) and +2 (green) (after [1]). Surface states (red) on the (100) surfaces in HgTe/MnTe superlattices (right panel). A small gap is visible but the system represents the axion insulator phase protected by C_2T symmetry (after [2]).

[1] R. Islam *et al.*, Phys. Rev. Research 4, 023114 (2022); [2] R. Islam *et al.*, Phys. Rev. B 107, 125102 (2023).

Developing quantum spin Hall materials: grey tin and mercury compounds

Experimental and theoretical studies carried out at Wuerzburg University, MagTop, and elsewhere call for extensive progress in developing 3D, 2D, and 1D systems of non-magnetic and magnetic mercury-based chalcogenides, and related topological materials, such as grey tin, in order to find new topological phases (such as axion insulator) and explore the interplay between Kondo, Luttinger, and magnetic polaron effects in a topological setting. MagTop's MBE Group has launched an extensive programme on the growth and characterization of grey tin and, in collaboration with the University of Rzeszów, is striving to develop its own MBE growth technology for mercury compounds that so far were taken from abroad [1].

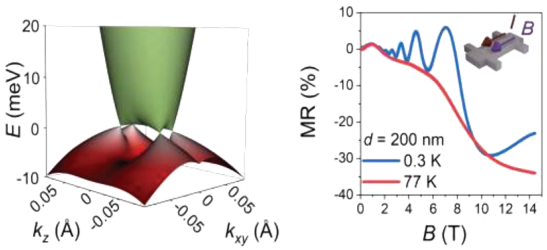

Figure: Band structure of compressively strained α-Sn in in-plane magnetic field B = 10 T showing Weyl semimetal band structure and an example of α-Sn magnetoresistance in a magnetic field parallel to the current, measured at two temperatures, and assigned to chiral anomaly (after [2]).

[1] I. Yahniuk *et al.*, arXiv:2111.07581 (2021); [2] J. Polaczyński *et al.*, to be published.

Predicting new quantum spin Hall systems in atomically-thick 2D materials

In quantum spin Hall (QSH) materials studied so far the longest topological protection length is of the order of a few micrometers and the operation temperature is too low for potential applications. MagTop's researchers have theoretically demonstrated a large topological gap and

a strong sensitivity to an electric field of $MoSi_2N_4$ and related 2D systems [1-6].

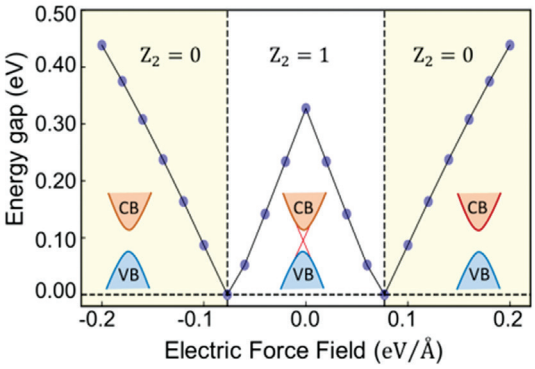

Figure: Topological invariant Z_2 and band gap of 1T′-$MoGe_2P_4$ as a function of the applied out--of-plane electric field. The critical electric force fields qE_C = ±0.077 eV/Å, within which the quantum spin Hall phase exists, are marked with vertical dashed lines (after [6]).

[1] R. Islam *et al.*, Phys. Rev. B 104, L201112 (2021); [2] G. Hussain *et al.*, Appl. Surf. Sci. 590, 153131 (2022); [3] G. Hussain *et al.*, Physica E 144, 115471 (2022); [4] G. Hussain *et al.*, J. Magn. Magn. Mat. 563, 169897 (2022); [5] R. Islam *et al.*, Phys. Rev. B 106, 245149 (2022); [6] R. Islam *et al.*, Adv. Electron. Mater. (2023); arXiv:2211.06443 (2022).

Magnetic impurities in topological semiconductors: superexchange vs. Van Vleck

A consensus appeared [He Ke *et al.*, Annu. Rev. Cond. Mat. Phys. 9, 329 (2018); Y. Tokura *et al.*, Nat. Rev. Phys. 1, 126 (2019)] that the enhanced interband magnetic susceptibility leads to a strong and foremost ferromagnetic coupling between transition-metal spins in quantum anomalous Hall effect materials. A series of works [1-3] carried out by MagTop/IFPAN collaboration shows why superexchange, rather than the interband Van Vleck/Bloembergen-Rowland mechanism, dominates exchange coupling between localized spins in topological materials and why there is no ferromagnetism in Fe-doped topological systems [4].

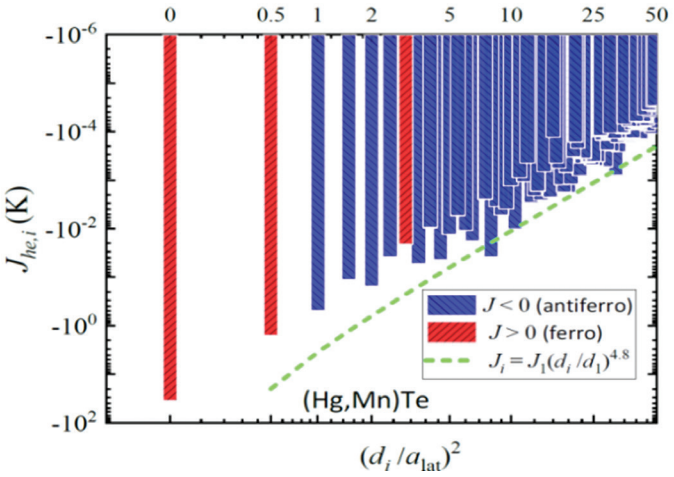

Figure: Contribution of the interband (he) Van Vleck-Bloembergen-Rowland mechanism to the exchange energies J_i in topological (Hg,Mn)Te vs. the pair distance d_i. The interband term contains a dominating ferromagnetic self-interaction component ($J_{he,i}$ at d_i = 0). The total interaction including super-exchange is sketched by the green line (after [3]).

[1] C. Śliwa, T. Dietl, Phys. Rev. B 98, 035105 (2018); [2] C. Autieri *et al.*, Phys. Rev. B 103, 115209 (2021); [3] C. Śliwa *et al.*, Phys. Rev. B 104, L220404 (2021); [4] Y. Satake *et al.*, Phys. Rev. Materials 4, 044202 (2020).

Quantum and topological phase transitions

One of the central questions in the field of condensed matter physics is understanding the microscopic mechanisms governing phase transformations. MagTop's theoretical teams addressed conditions for the appearance of quantum or topological phases in selected systems, including (i) a subtle interplay between

itinerant ferromagnetic and antiferromagnetic correlations in various strongly correlated metals under pressure [1-3]; (ii) the formation of the quantum anomalous Hall phase for electrons experiencing the Rashba interaction, Zeeman splitting, and ionic potential, and (iii) the effect of many-body interactions on the Chern insulator clarifying a misleading notion of the first-order topological transition (see Figure) [4].

[1] M. M. Wysokiński, Sci. Rep. 9, 19461 (2019); [2] M. M. Wysokiński, Phys. Rev. B 97, 041107(R) (2018); [3] G. Cuono *et al.*, Phys. Rev. B 104, 024428 (2021); [4] M. M. Wysokiński, W. Brzezicki, arXiv:2303.04454.

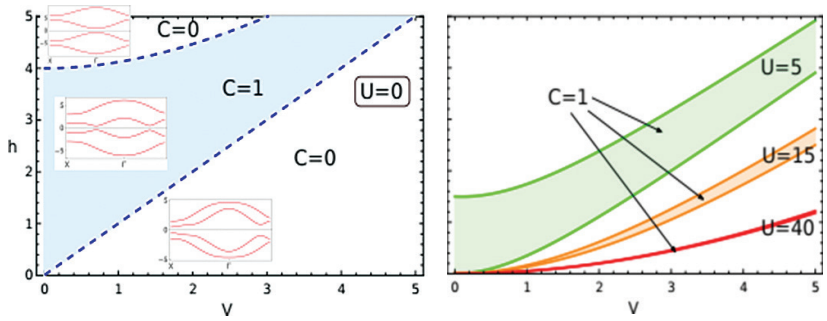

Figure: Topological phase diagrams (Chern number C) vs. ionic potential V and Zeeman field h for an uncorrelated system U = 0 (left panel) and correlated case for selected values of U. Solid lines denote transitions at which spectral gaps do not close [4].

TOPOLOGICAL CRYSTALLINE INSULATORS (TCI)

Interfacing topological materials with magnetic metals

Whether magnetism really opens a gap in topological surface states has become one of most intriguing question in topological physics [see, *e.g.*, Y. L. Chen *et al.*, Science 329, 659 (2010); E. D. L. Rienks *et al.*, Nature 576, 423 (2019)]. MagTop's researchers demonstrated that the effect may come from chemical substitution of heavy cations by lighter ones, rather than from the effect of time-reversal symmetry breaking. At the same time, spin-momentum locking, relevant for spin current generation, remains present on the both sides of the topological phase transition [1].

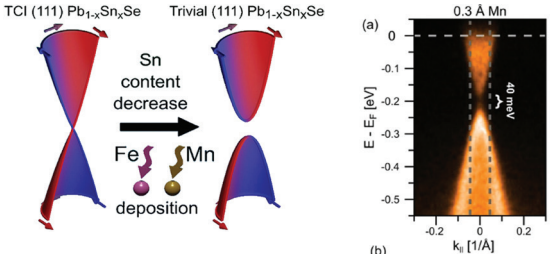

Figure: Deposition of a transition metal on the surface of a topological crystalline insulator (TCI) n-type $Pb_{1-x}Sn_xSe$ opens a gap in the surface Dirac cones (ARPES, right panel), but helical spin texture is preserved (after ([1]).

[1] B. Turowski et al., Appl. Surf. Sci. 610, 155434 (2023)].

One-dimensional topological states along surface atomic steps

High-quality TCI crystals grown at IFPAN/MagTop allowed to demonstrate by scanning tunneling spectroscopy (STS) the presence of 1D higher-order topological states residing at the edges of odd-atom-high steps at (001) $Pb_{1-x}Sn_xSe$ hosting TCI states [P. Sessi *et al.*, Science 354, 1269 (2016)]. These states undergo hybridization splitting by coupling to neighbouring steps [1]. Experimental [2] and theoretical [3] arguments were presented that step states account for Andreev-like point-contact spectra observed in a number of topological systems, including TCI, the insight corroborated by STS data showing a gap when metal overlayers shifted the Fermi energy to these states [4].

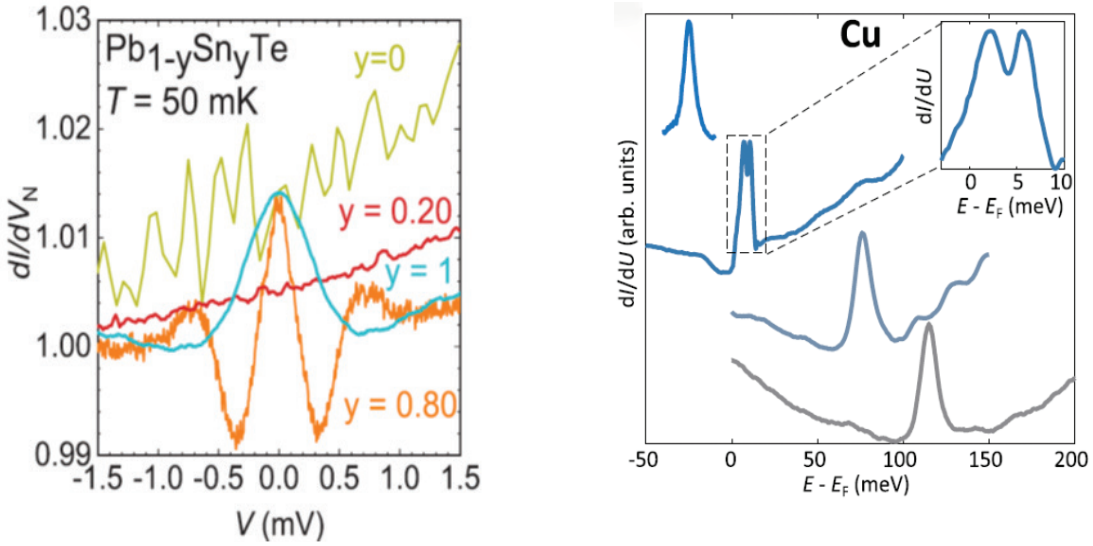

Figure: Scanning tunnelling spectroscopy [2] (left panel) and point contact spectroscopy [3] (right panel) showing features for Sn concentrations corresponding to the topological phase. Deposition of Cu shifts the Fermi energy towards 1D states leading to the appearance of a gap in the energy spectrum [2], as predicted in Ref. 4 to explain the origin of the point contact spectra [3].

[1] J. Jung *et al.*, Phys. Rev. Lett. 126, 236402 (2021); [2] G. Wagner *et al.*, Nano Lett. 23, 2476 (2023); [3] G.P. Mazur *et al.*, Phys. Rev. B 100, 041408(R) (2019); [4] W. Brzezicki *et al.*, Phys. Rev. B 100, 121107(R) (2019).

Interfacing topological crystalline insulators with amorphous semiconductors: breaking of reflection symmetry

Topological crystalline insulators (TCIs) have revealed that topologically protected gapless surface states can be brought about by crystal symmetries. MagTop's researchers demonstrated experimentally and theoretically that breaking of reflection symmetry by an overlayer of an amorphous semiconductor leads to a temperature independent phase coherence length controlling quantum localization in magnetoresistance [1]. Furthermore, in agreement with MagTop's ARPES data

[2], spin-momentum locking and, thus quantization of the Berry phase - exist on both sides of the topological phase transitions [1].

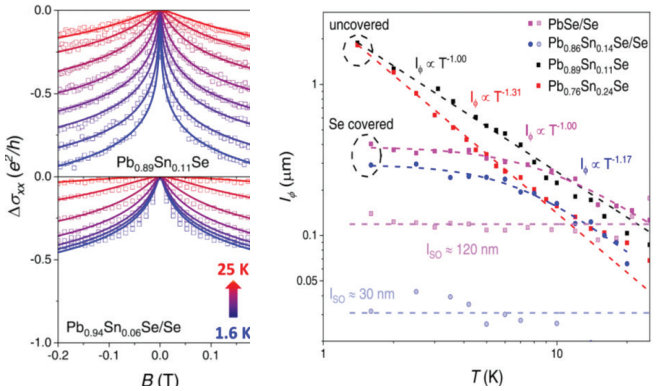

Figure: Evolution of the WAL magnetoresistance with increasing temperature in uncovered (left, upper panel) and Se covered (left, lower panel) epilayers. Experimental points (empty squares) are fitted using one-channel Hikami--Larkin-Nagaoka expression for a strong spin-orbit interaction (solid lines). Right panel shows, that l_φ(T) in uncovered epilayers do not saturate down to 1.5 K (black and red), while in Se covered epilayers l_φ saturates below 5-7 K (blue and magenta) (after [1]).

[1] A. Kazakov *et al.*, Phys. Rev. B 103, 245307 (2021); [2] B. Turowski *et al.*, Appl. Surf. Sci. 610, 155434 (2023)].

WEYL SEMIMETALS

Interfacing Weyl semimetals with heavy metals: Lifshitz transition in surface bands

Revealing and functionalizing interfacing effects is in the heart of MagTop's activities, and brought a number of surprising developments in the case of topological crystalline insulators with gapless 2D and 1D Dirac states at the surface, as described in other highlights. MagTop's studies demonstrated that deposition of heavy metals Pb and Nb on the surface of the Weyl semimetal NbP strongly affects non-topological surface states and displaces arches connecting Weyl points, substantiating theory of the topological Lifshitz transition [G. E. Volovik, Low Temp. Phys. 43, 47 (2017)] .

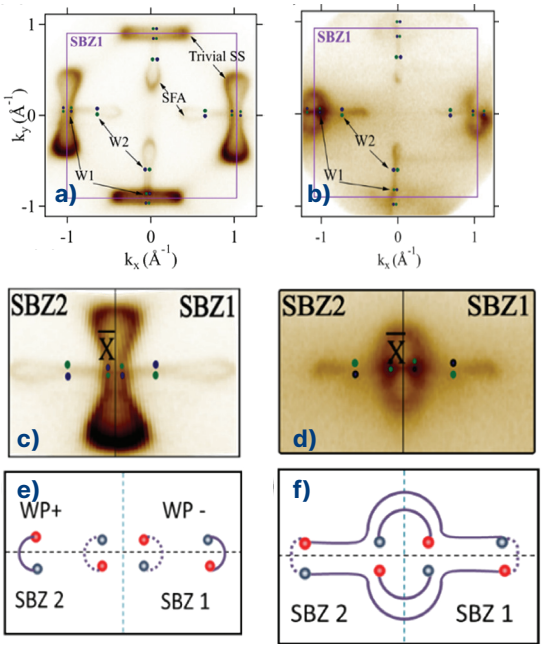

Figure: ARPES visualization of P-terminated surface of NbP before (a,c) and after deposition of 1 ML of Pb (b,d) (after [1]). Possible reconstruction of topological arches is also shown (e, f).

[1] A.S. Wadge *et al.*, Phys. Rev. B 105, 235304 (2022).

Interfacing Weyl metals to polar insulators: topological reconstruction of bands

Charge transfer that appears at the interface of ultrathin itinerant ferromagnet $SrRuO_3$ and polar insulator $LaAlO_3$ exceeds capacities of ordinary electrostatic gates. MagTop's theoreticians, after determining the Chern numbers for a $SrRuO_3$ monolayer [1], showed that such interfacial doping

affects the Berry curvature, and in an extreme case leads to a change of the sign of the Hall conductivity below Curie temperature [2]. This effect is due to a conversion of the Chern numbers of partially occupied bands, *i.e.*, due to topological reconstruction in the momentum space, occurring in the presence of both strong or weak charge pinning (redistribution) in the Weyl metal layer.

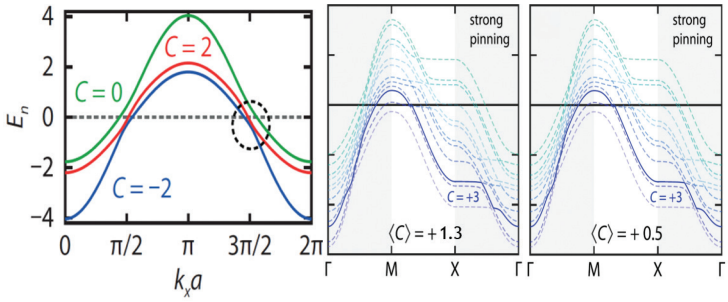

Figure: Chern number C for Ru t_{2g} bands for a single monolayer (left panel) [1] and bilayer of $SrRuO_3$ (right panels). Different magnitudes of the charge transfer between the two monolayers leads to a sign change of the average C value and of the anomalous Hall conductivity (after [2]).

[1] D. J. Groenendijk *et al.*, Phys. Rev. Research 2, 023404 (2020); [2] T.C. van Thiel *et al.*, Phys. Rev. Lett. 127, 127202 (2021).

Heat vs. charge transport in Weyl semimetals

Topologically non-trivial materials exhibit a variety of extraordinary transport phenomena affecting both charge and heat flow. The latter is considered to be more robust to experimental artefacts than may appear in electrical measurements [D. Vu *et al.*, Nat. Mat. 20, 1525 (2021)]. MagTop's Weyl group found novel effects in thermal conductivity, the chiral zero sound, leading to the breaking of the Wiedemann-Franz law, and the gravitational anomaly, in two different Weyl semimetals: NbP [1] and NdAlSi [2].

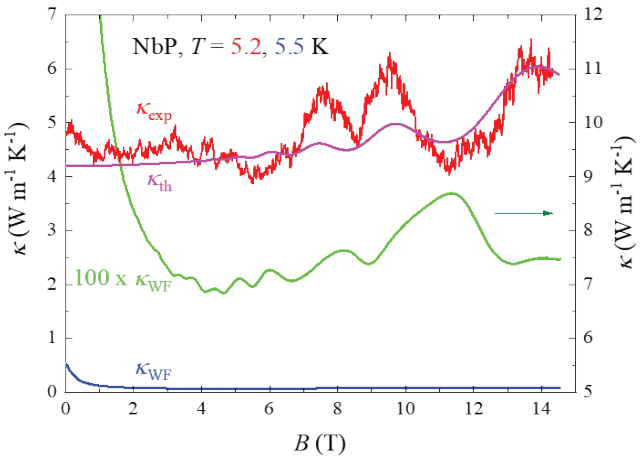

Figure: Magnetic field dependence of the thermal conductivity (κ_{exp}) of NbP at T = 5.2 K (uppermost red line) compared to the electronic thermal conductivity (κ_{WF}) calculated from the Wiedemann-Franz law at T = 5.5 K (lowermost blue line). The middle (green) line shows κ_{WF}(B) multiplied by 100 (right axis). The pink line is the total thermal conductivity including the calculated CZS contribution (κ_{th}) (after [1]).

[1] P.K. Tanwar *et al.*, Phys. Rev. B 106, L041106 (2022); [2] P.K. Tanwar *et al.*, arXiv:2305.04650.

Fixing the topological phase diagram for Eu-based antiferromagnets and related compounds

Surprising physics of magnetic topological materials and possible applications in sensors, metrology, computing, and catalysis [B. A. Bernevig *et al.* Nature 603, 41 (2022)] have triggered experimental and computational search for compounds with robust topological functionalities coexisting with or brought about by a magnetic order. In particular, high-throughput first-principles calculations, implementing the

density functional theory (DFT) within the generalized gradient approximation (GGA)+Hubbard U, indicated that 130 compounds out of 430 magnetic materials studied have topological phases when scanning U, primarily having Weyl points [Y. Xu *et al.*, Nature 586, 702 (2020)]. MagTop's researchers called those results into question demonstrating that more computationally demanding approaches are necessary to properly identify topological classes and, in particular, explain the experimentally observed band gap in $EuCd_2As_2$ and its red shift in a magnetic field.

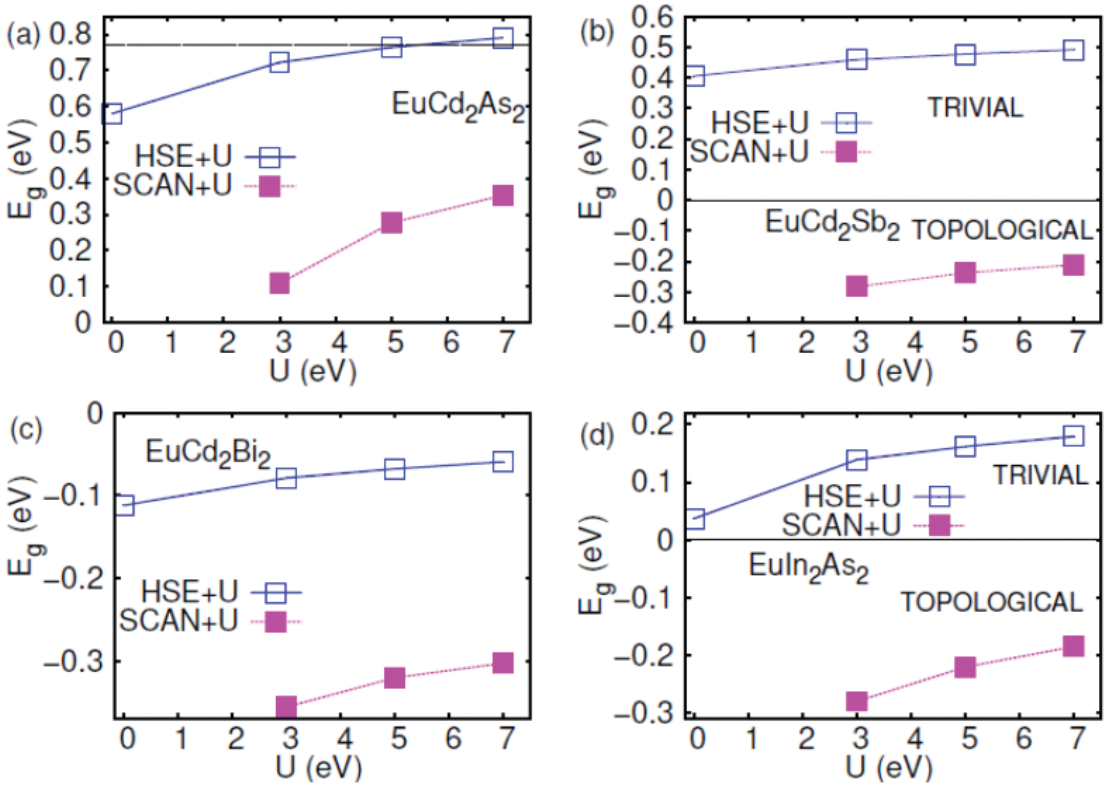

Figure: Band gaps for (a) $EuCd_2As_2$, (b) $EuCd_2Sb_2$, (c) $EuCd_2Bi_2$ and (d) $EuIn_2As_2$ as a function of Coulomb repulsion U in the AFM configuration with spins along the a-axis by considering HSE+U hybrid functional method (blue solid line). SCAN+U approach results are shown for comparison by the purple dashed line. The horizontal dashed line for $EuCd_2As_2$ represents the experimental value [1]. Negative band gaps point to the topological phase (after [2]).

[1] D. Santos-Cottin *et al.*, submitted to Phys. Rev. Lett. (2023); arXiv:2301.08014; [2] G. Cuono *et al.*, submitted to Phys. Rev. B Letters (2023); arXiv:2305.10804.

Three-dimensional flat bands

After explaining how the flat band in twisted graphene can carry a non-zero supercurrent [1], MagTop's theoreticians demonstrated that strain engineering can be used to generate quasi-flat three-dimensional energy bands in materials known as topological nodal-line semimetals, thereby paving the way to tunable correlated phases in three-dimensional materials [2]. HgTe/CdTe superlattices, as core-shell nanowires, can constitute a practical realization of that concept [3].

1] Xiang Hu *et al.*, Phys. Rev. Lett. 123, 237002 (2019); [2] A. Lau *et al.*, Phys. Rev. X 11, 031017 (2021); [3] R. Islam *et al.*, Phys. Rev. Research 4, 023114 (2022).

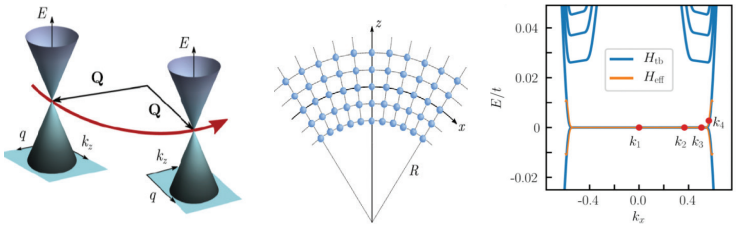

Figure: In a nodal-line semimetal, Dirac cones are formed with respect to the perpendicular momentum components q and k_z (left). Strain profile (middle) leads to a flat band (right) (after [2]).

TOWARDS MAJORANA ZERO MODES AND BEYOND

Search for topological superconductivity

As, so far, the experimental signatures that identify a topological superconductor (TSC) are elusive [see, *e.g.*, M. Mandal *et al.*, arXiv:2303.15581] and there has been no conclusive experimental observation of Majorana bound states in proximitized topologically trivial semiconductors [see, *e.g.*, R. Hess *et al.*, Phys. Rev. Lett. 130, 207001 (2023)], particularly timely is the search for intrinsic or proximitized superconductivity in topological materials. In addition to comprehensive MagTop's theoretical effort [1], MagTop/IFPAN's growers and experimentalists have been exploring four paths: (i) Weyl semimetals with superconductors' overlayers [2]; topological crystalline insulators in the form of (ii) bulk crystals [3]; (iii) superlattices [4], and (iv) nanowires. Surprising and not yet understood results, calling for further work, have been gathered.

[1] N. M. Nguyen *et al.*, Phys. Rev. B 105, 075310 (2022); [2] G. Grabecki *et al.*, Phys. Rev. B 101, 085113 (2020); [3] G. P. Mazur *et al.*, Phys. Rev. B 100, 041408(R) (2019); [4] P. Sidorczak *et al.* (unpublished).

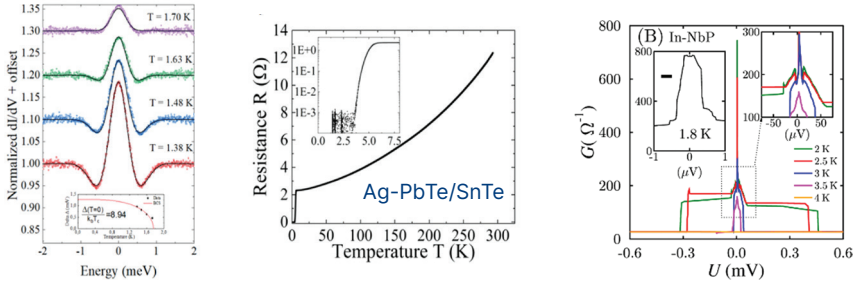

Figure: Differential conductance and four contact conductivity in In-NbP [2] and Ag-PbTe/SnTe super-lattices [4]showing signatures of superconductivity in topological materials.

Interfacing ferromagnets and superconductors: Majorana physics

One of the most challenging aims in the current condensed matter physics research is the demonstration of non-Abelian Majorana statistics — the underlying fundamental property that would enable the realization of a topological quantum computer. Though not experimentally proven, it is theoretically well established that Majorana zero modes (MZMs) can be realized in semiconducting nanowires with strong Rashba spin-orbit coupling in the presence of induced superconductivity and external magnetic field. MagTop's team studied theoretically ferromagnetic-semiconducting-superconducting hybrids with MZMs, and demonstrated that this system; (i) constitutes a novel topological charge, spin, and heat transistor [1,3]; (ii) shows quantization of spin under spin pumping conditions [2].

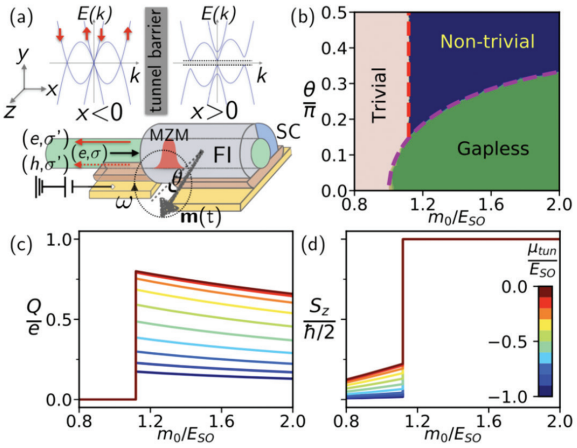

Figure: (a) Rashba nanowire (green) with proximity induced superconductivity (blue) and magnetization (gray) supports MZM (red). The precessing magnetization m(t) pumps spin and charge into the lead due to the normal and Andreev reflection processes. (b) Topological phase diagram of the nanowire as a function of the exchange coupling m_0 and the precession angle Θ (c), (d) The pumped charge Q and spin S as a function of m_0 for different tunnel barriers μ_{tun}. The pump spin is quantized to $S_z = \hbar/2$ in the topologically nontrivial regime (after [2]).

[1] V. Fernández Becerra *et al.*, Phys. Rev. B 103, 205410 (2021); [2] V. Fernández Becerra *et al.*, Phys. Rev. Lett. 130, 237002 (2023); [3] V. Fernández Becerra *et al.*, European patent nr EP3975275A1, submitted.

Quantum computing with magnetic adatoms in superconductors

Magnetic impurities in s-wave superconductors provide a viable platform for realizing a topological quantum computer based on Majorana zero modes (MZMs). However, MZMs alone do not provide a universal set of quantum gates and manipulating coherently quantum degrees of freedom in these systems remains an open challenge. MagTop's team introduced a new type of quantum bit, a Yu-Shiba-Rusinov qubit [1], stemming from two nearby magnetic impurities on a superconductor and demonstrated how to determine relevant quantum gates and topological characteristics, including interactions with MZMs, by scanning tunneling microscopy-electron spin resonance techniques [1,2], couplings to microcavity modes [3], and dynamic magnetic susceptibility [4].

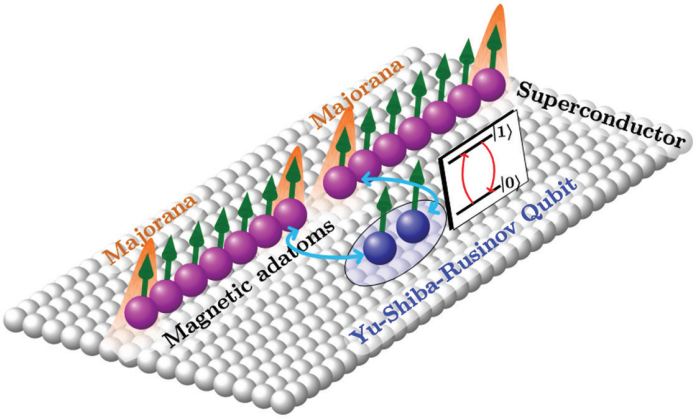

Figure: Two magnetic adatoms (blue balls) deposited on an s-wave superconductor generate an electronic Shiba that encodes a YSR qubit {<0|, <1|}. Coupling this molecular qubit to Majorana zero modes hosted by topological Shiba chains (pink balls) and controlling the orientation of the adatom spins in STM-ESR setups (green arrows) allows implementation of a universal set of quantum gates (after [1)].

[1] A. Mishra *et al.*, Phys. Rev. X Quantum 2, 040347 (2021); [2] A. Mishra *et al.*, Phys. Rev. B 103, L121401 (2021); [3] Pei-Xin Shen *et al.*, Phys. Rev. Research 3, 013003 (2021); [4] Peixin Shen *et al.*, arXiv:2303.13513 (under review in Phys. Rev. Lett.).

Topological systems with dissipation: the discovery of long-range entanglement

Making coupling to the reservoir a resource rather than an obstacle emerges as one of the most promising roads in topological quantum computing. MagTop's researchers proposed a 1D non-Hermitian model, in which they revealed the presence of a hidden Chern number [1]. They used that model to describe lasing in a polariton system [2] and, most recently, to examine a chain of transmon devices [3], the qubits of the most mature quantum computers. The dynamics of this system with dissipation, examined employing the third quantization methods, revealed the presence of controllable long-range quantum entanglement between distant end states of the chain.

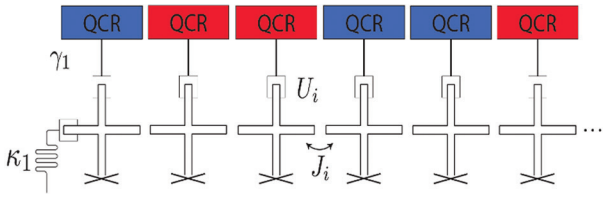

Figure: Non-Hermitian Bose-Hubbard transmon ABBA chain (A – blue, B – red) with the on-site and inter-site energies U_i and J_i, respectively. The dissipation strength is tuned by the coupling to the measurement circuit κ_1 and loss caused by the quantum circuit refrigerator γ_1 (QCR) (after [3]).

[1] W. Brzezicki *et al.*, Phys. Rev. B 100, 161105(R) (2019); [2] P. Comaron *et al.*, Phys. Rev. Research 2, 022051(R) (2020); [3] W. Brzezicki *et al.*, Phys. Rev. B 107, 115146 (2023).

BEYOND TOPOLOGICAL ELECTRONIC MATTER

Interfacing ferromagnets and semiconductors: phonon-mediated exchange

How to control a long-range phonon-mediated exchange interaction discovered by photoluminescence of CdTe quantum well (QW) in a hybrid Co/(Mg,Cd)Te/CdTe/(Mg,Cd)Te heterostructure grown by MBE at IFPAN [V. L. Korenev *et al.*, Nat. Phys. 12, 85 (2016)]? Figure presents two structures fabricated by MagTop/IFPAN MBE teams, which made it possible to affect that exchange by low voltage U [1] and by the distance between the ferromagnetic layer and CdTe QW [2].

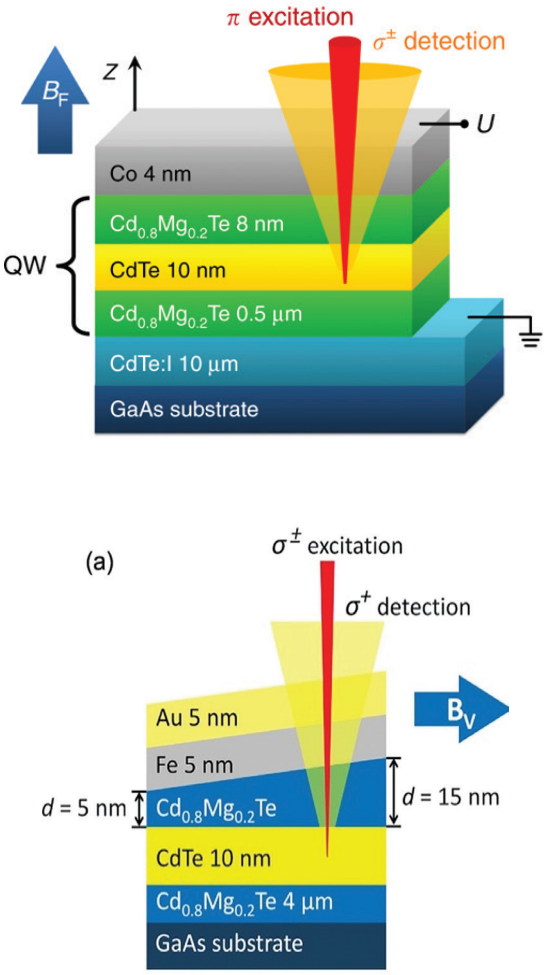

Figure: Hybrid structures grown in a two-chamber MBE set-up allowing for magnetooptical probing of exchange coupling between ferromagnetic layers (Co or Fe) and carriers in CdTe QW vs. voltage U (upper panel) (after [1]) and distance d (lower panel) (after [2]).

[1] L. Korenev *et al.*, Nat. Commun. 10, 2899 (2019); [2] I. V. Kalitukha *et al.*, Nano Lett. 21, 2370 (2021).

A new class of transverse magneto-optical phenomena with potentials for applications in nanophotonic circuits

High-quality quantum structures produced by MagTop/IFPAN MBE groups became building blocks of hybrid plasmonic-semiconductor nanostructures, which were used by MagTop's collaborators to demonstrate [1] and study in details [2] new phenomena of transverse magnetic routing of light emission (TMRLE), as well as to demonstrate optical control of transverse electron spin components normal to the direction of light propagation [3]. In these hybrids, the plasmonic metal grating of Au was fabricated by electron beam lithography and lift-off on the surface of structure containing a diluted magnetic semiconductor $Cd_{1-x}Mn_xTe$ quantum well (QW) (see Figure).

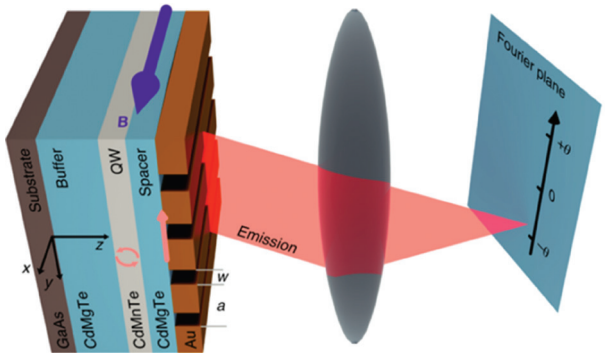

Figure: Schematic representation of experimental setup to demonstrate the TMRLE effect. An external in-plane magnetic field B is applied to the plasmonic structure (left part). The angular distribution of light emitted by the structure is converted by a lens into a spatial distribution in the Fourier plane (right) and recorded by a two dimensional CCD matrix (after [1]).

[1] F. Spitzer *et al.*, Nature Phys. 14, 1043 (2018), corrections; [2] L. Klompmake *et al.*, Phys. Rev. Research 4, 013058 (2022); [3] I. A. Akimov *et al.*, Phys. Rev. B 103, 085425 (2021).

Nematicity in solids: role of anisotropic spinodal decomposition and orbital polarization

The origin of nematicity, *i.e.*, breaking of in-plane rotational symmetry, and in particular the relative role played by spontaneous unidirectional ordering of spin, orbital, or charge degrees of freedom, is a challenging issue of magnetism, unconventional superconductivity, and quantum Hall systems. While MagTop's and collaborators' results indicated uneven d_{xz} and d_{yz} orbital occupation in the superconducting iron pnictide pointed to the important role of orbital polarization [1], experimental and theoretical results for $In_{1-x}Fe_xAs$ demonstrated that anisotropic distribution of Fe cations at the growth surface (that has a lower symmetry than the bulk) can lead to a quenched nematic order of alloy components, which then governs low-temperature magnetic and magnetotransport properties [2].

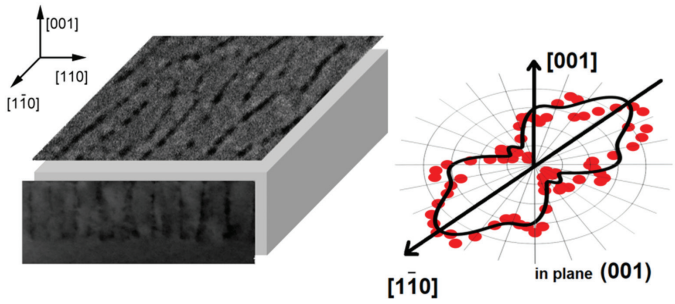

Figure: Non-uniform and anisotropic distribution of Fe cations in a 200 nm-wide slab of (In,Fe)As (black lines along the [1-10] crystallographic direction) according to HR-TEM (left panel) and the corresponding low-temperature anisotropic magnetoresistance (right panel) (after [2]).

[1] D. Rybicki *et al.*, Phys. Rev. B 102, 195126 (2020); [2] Ye Yuan *et al.*, Phys. Rev. Materials 2, 114601 (2018).

COLLABORATION WITH INDUSTRIAL PARTNERS

III-V and IV-VI/II-VI infrared detectors – collaboration with VIGO Photonics

MagTop's and VIGO Photonics's R&D teams examined theoretically optical characteristics of semiconductor quantum superlattices (SL) of III-V compounds [1]. Extensive collaboration concerned also contact and etching properties of detector structures. Furthermore, a new class of highly perspective detectors, combining advantages of II-VI and IV-VI compounds was developed at MagTop (see Figure).

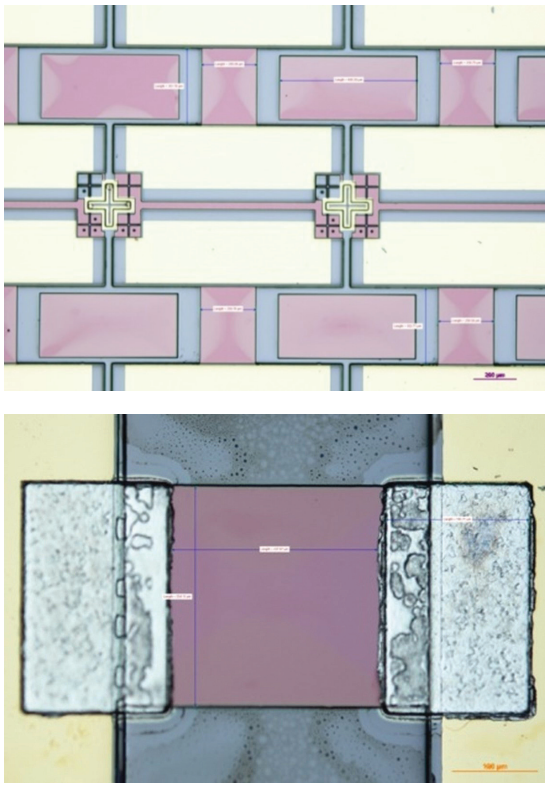

Figure: Optically active PbTe/CdTe structure after photolithographic preparation of detector fields and a single detector structure with electrical contact pads (lower panel). [After Szot et al., unpublished].

[1] G. Hussain *et al.*, J. Phys. D: Appl. Phys. 55, 495301 (2022).

PbTe-CdTe crystalline nanocomposites for thermoelectric energy conversion – collaboration with PUREMAT Technologies

Thermoelectric generators and coolers are semiconductor devices that directly convert heat into electricity (thermoelectric generators - TEGs) or vice versa (thermoelectric coolers - TECs) using the ability of electrons to simultaneously transfer heat and electric charge. Thermoelectric devices with sufficiently high energy conversion efficiency could become a technological solution in the worldwide search for electron systems that efficiently harvest waste industrial heat. MagTop's and PUREMAT Technologies's researchers developed nanocomposite PbTe-CdTe in which enhanced thermal resistance is not compromised by the deterioration of electrical conductivity [1-3].

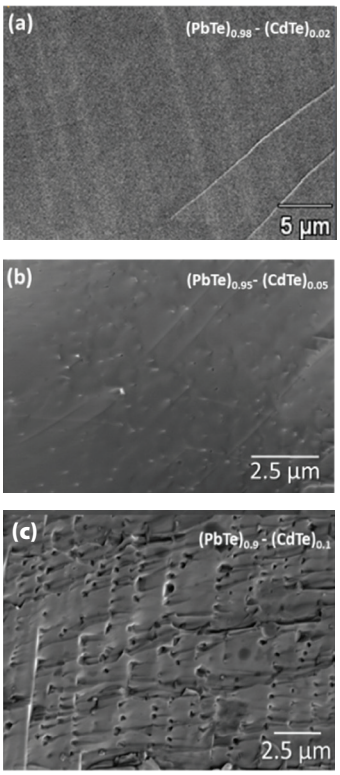

Figure: SEM images of $(PbTe)_{1-x}$-$(CdTe)_x$ nanocomposites with x = 0.02, 0.05, and 0.1 [2].

[1] M. Szot *et al.*, Phys. Rev. Materials 4, 044605 (2020); [2] M. Szot *et al.*, arXiv.2212.14616; [3] European Patent nr EP4036057A1.

Magnetosputtering of ferromagnetic metals – collaboration with PREVAC

Magnetron sputtering is an industry- and research-relevant high-rate vacuum coating technique that allows the deposition of many types of materials, including metals and ceramics, onto as many types of substrate materials by the use of a specially formed magnetic field applied to a diode sputtering target.

Figure: 2” target with a visible narrow and uneven erosion track, indicating that the flux was not constant during deposition (upper). After source modification (lower panel), the surface was flat after several sputtering processes, meaning that the material was consumed evenly (after [1]).

This method is also used by MagTop’s researchers for deposition of ferromagnetic metals, which resulted in the invention [1], now employed by the PREVAC company.

[1] European Patent Application: EP22461556.7 (A. Glenz, A. K. Fronc, M. Chojnacki)

Identifying topological invariants in superconductors with machine learning – collaboration with BOSCH

One of the emerging fields of the deep-learning methods is the development of qualitatively new protocols for drawing relevant and unbiased information from ever increasing volume of experimental data. MagTop’s researchers in collaboration with other groups, particularly with Bosch Center for Artificial Intelligence, proposed a machine-learning approach for classifying the topological states of 2D chiral superconductors and insulators based on local density of states data [1,2] that can be obtained by scanning tunneling microscopy or possibly by nanoARPES. The developed new protocol can be applied to many experimental platforms that share qualitative features of the Shiba lattice models.

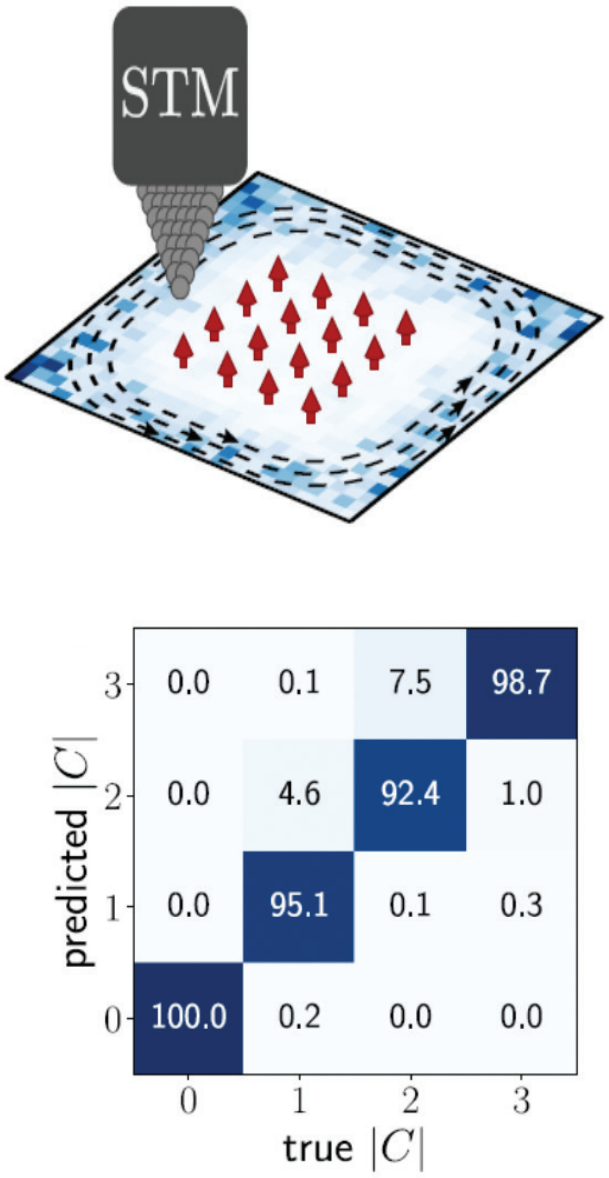

Figure: Scanning tunneling microscope provides LDOS data for the Shiba lattice (upper panel). Confusion matrix (lower panel) show accuracy of Chern number identification (in %) based on simulated LDOS data for a Shiba lattice model. All Chern numbers are predicted with the high accuracy (after [1]).

[1] P. Baireuther *et al.*, arXiv:2112.06777; under revision in SciPost Physics; [2] European Patent Application: EP21209049.2.

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Laboratory SL1: X-ray and Electron Microscopy Research

RESEARCH TOPICS

- X-ray absorption and photoelectron studies of the electronic structure of materials.
- XANES and EXAFS investigation of local structure in solids.
- Determination of crystal-structure parameters of bulk materials and nanostructures by X-ray and electron diffraction methods.
- Investigation of crystal defects by X-ray high resolution diffractometry and electron microscopy.
- Investigation of structural properties of crystals as a function of composition, temperature and pressure.
- Studies of strain and elastic properties of bulk materials and multilayers using X-ray diffraction methods.
- SIMS investigation of content and distribution of trace elements and kinetics of dopants.
- New methods for atomic and electronic structure studies of low dimensional materials used in technology of electronic devices.
- Rutherford backscattering spectrometry (analysis of sample composition) and ion channeling (measure of crystal structure).
- Ion implantation, energy 250 keV - 3 MeV.

RESEARCH RESULTS

New materials and nanomaterials important for modern technologies or bio-technologies are the subject of interest of researchers in the Laboratory.

Materials are characterized by applying electron, ion, and X-ray techniques. The real crystal structure parameters and crystallographic defects are investigated by high resolution X-ray diffractometry (averaged over some volume) and high resolution electron microscopy (locally). The chemical composition of new materials and character of chemical bonding are studied by X-ray emission and absorption spectroscopy, and X-ray and UV photoelectron spectroscopy (XPS and UPS). In depth dopant and element distribution are estimated by ion mass spectroscopy and XPS depth profiling. Moreover, Rutherford backscattering spectrometry (RBS) is supplementary used for analysis of single crystal composition and ion channeling for defect location. The materials can be implanted with ions of energies from 250 keV up to 3 MeV. UV-Vis and FTIR spectroscopy is routinely used for the quantitative determination of different components, such as transition metal ions, highly conjugated organic compounds, and biological macromolecules in solid and liquid states. In addition to static characterizations techniques, time-resolved experiments on time scales from seconds down to (sub)

picoseconds enable studies of the dynamics of physio-chemical processes, in particular structural transformations in condensed matter. The experimental methods are supplemented by theoretical modeling using advanced *ab initio* calculations.

TEM studies: Mapping of the strain fields in axial nanowires - measurements using scanning nano-electron beam diffraction (NBED), Geometric Phase Analysis (GPA) of the HR-STEM images, and Finite Elements Modeling (FEM).

A method was developed to precisely map the strains of highly lattice mismatched hetero-nanowires (NW) with very high spatial resolution. It has been proven that this method can be used even in the case of nano-twins and for large thickness gradients of the tested nanoobjects (nanoparticles, nanowires).

The mapping was performed using scanning electron nanobeam diffraction (NBED) on the example of an axial ZnTe/CdTe nanowire (characterized by a significant lattice mismatch >6%). The stress mapping technique was applied to nanowires with diameters below 100 nm with a resolution of about 2 nm, i.e., 10 times better than in synchrotron nanobeam

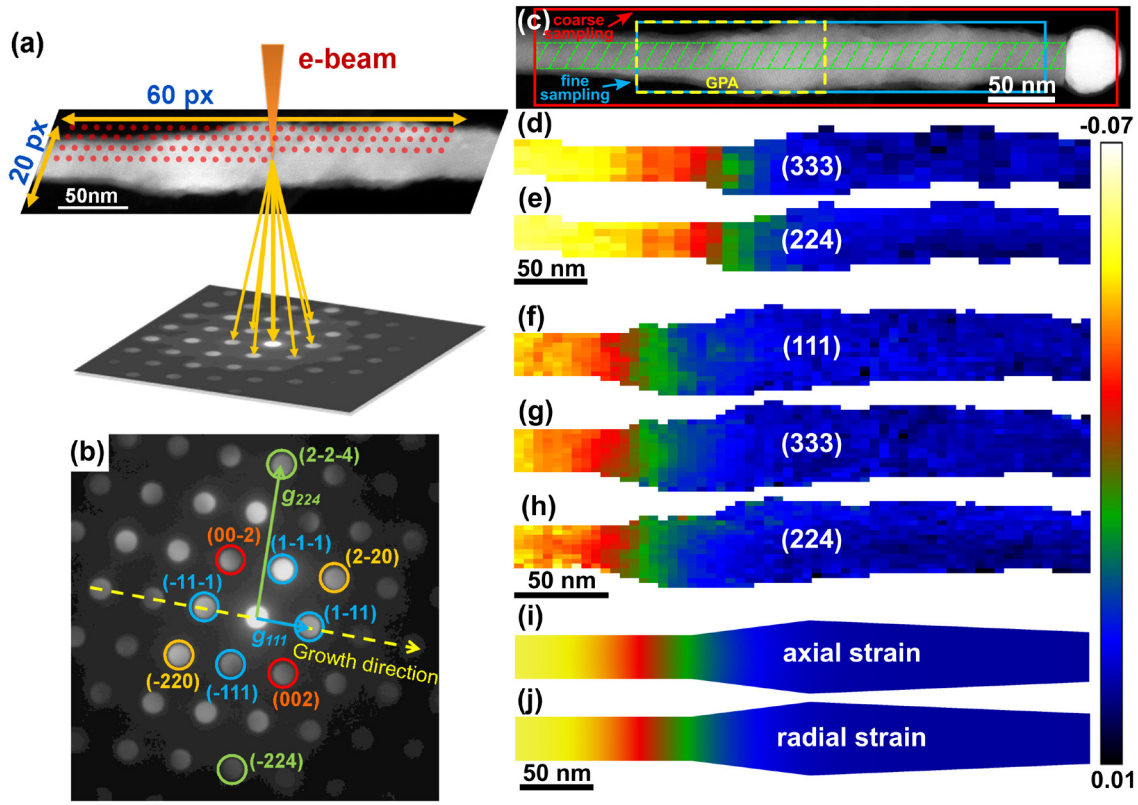

Fig. 1. (a) Diagram of the scanning nano-electron beam diffraction (NBED) experiment on an axial ZnTe/CdTe hetero-nanowire. (b) Obtained diffraction pattern. The yellow arrow indicates the NW growth direction. (c) STEM image of a part of the nanowire. The yellow rectangle indicates the region used for geometric phase analysis (GPA). (d), (e) Maps of relative lattice changes obtained with NBED using (333) and (224) reflections, respectively, for coarse sampling. (f), (g), (h) Maps of relative lattice changes obtained for (111), (333), and (224) reflections obtained with high spatial resolution. (i), (j) Simulated relative deformation maps obtained by FEM simulation in the axial and radial directions, respectively.

systems. Using an image processing algorithm based on the Hough transform and Sobel filtering allowed us to overcome difficulties in detecting the diffraction disk caused by the thickness gradient. In addition, the most probable three-dimensional distribution of elements and strains in the axial NW ZnTe/CdTe was reconstructed by fitting the experimental 2D strain map with the finite element method (FEM) [1].

[1] Serhii Kryvyi, Slawomir Kret, Piotr Wojnar, Precise strain mapping of nano-twinned axial ZnTe/CdTe hetero-nanowires by scanning nanobeam electron diffraction, Nanotechnology, 33(19), 195704 (2022)

Bio-Chemistry studies: Synthesis and structural studies of bioactive Cu(II) complexes with thiourea derivatives

One of the scientific goals of our team is the synthesis of novel bioactive compounds, related to the search for new and cheap potential antibiotics and potential drugs in the treatment of cancer. Therefore, in recent years, several series of Cu(II) complexes with 1,3-disubstituted thiourea derivatives have been designed, synthesized, and characterized by our group (Fig. 2, [1-5]). The obtained compounds possess high to moderate antibacterial activity [1-3] and strong anticancer potential against colon and prostate cancer [4,5]. Their biological activity depends on the type of substituents attached to the thiourea moiety. The complexes have been structurally characterized by ATR-IR, UV-Vis, and XAFS spectroscopies. These studies indicated that copper is in the +2 oxidation state and revealed that the initial thioureas act as N,S-donor ligands. Data obtained from experimental studies combined with DFT and XANES calculations allowed us to propose a three dimensional molecular structure of novel complexes. In these models, two thiourea ligands coordinate to the Cu(II) cation in bidentate fashion through thiocarbonyl S and deprotonated N atoms, having C_2 or C_i symmetry (see Fig. 1).

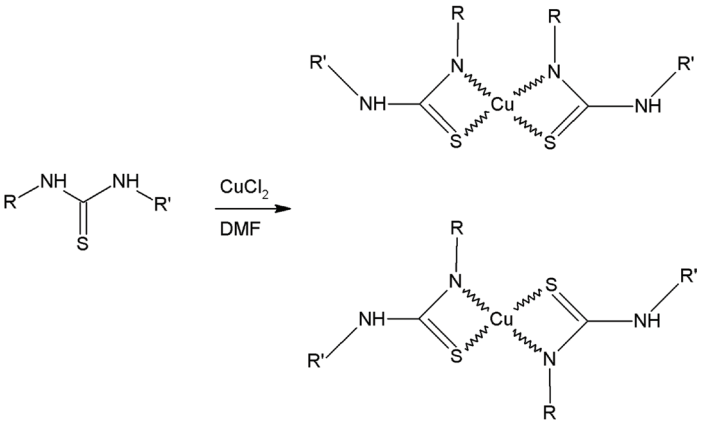

Fig. 2. Synthesis path of studied complexes. R, R'- aromatic substituents.

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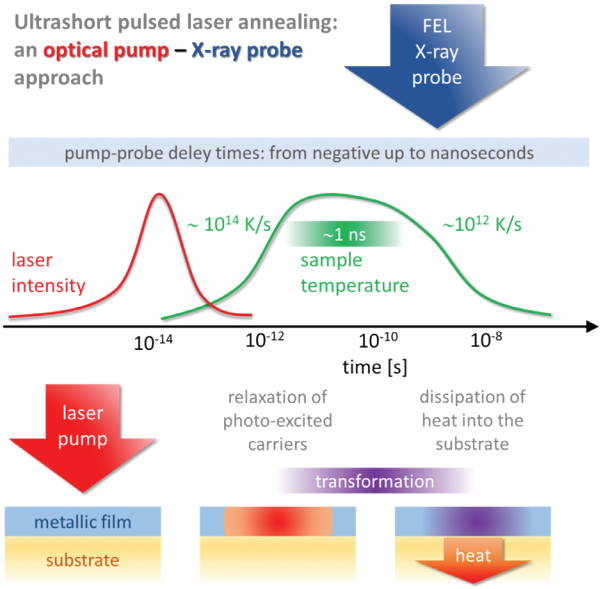
Time-resolved structural studies: Phase transitions in condensed matter

The aim of our research is to understand the process of melting followed by glass formation and/or crystallization in metals. Pure elements and alloys in form of nanostructures (mostly thin layers) are studied. We use ultrafast annealing methods with lasers to drive the samples out of the equilibrium. It is combined with structural characterization by a variety of experimental techniques involving optical,

X-ray, and electron scattering (including time-resolved measurements on ultrashort time scales of ps-ns), both with use of laboratory equipment available at our laboratory and large scale facilities (x-ray diffraction on synchrotron sources and free electron lasers) – see experimental scheme in the figure below. The work provides experimental data and analysis significant for understanding of the fundamental mechanisms responsible for melting, crystallization, glass formation, and solid-solid phase transitions.



X-ray Diffraction studies: high-complexity materials

One of such materials previously unknown is $Ca_{10.5-x}Ni_x(VO_4)_7$ with a whitlockite structure, the novelty of which is the introduction of nickel atoms into the original unit cell. In ref. [1] the solubility limit of Ni was determined as well as variation of the structure with temperature. The study demonstrated that Ni atoms preferentially occupy the M5 site (one of the five independent Ca sites, M1–M5). One of the results is the determination of the thermal expansion coefficient variation with Ni content and with temperature. For high Ni contents, a change in the thermal expansion anisotropy is observed at high temperatures (see Fig. 1).

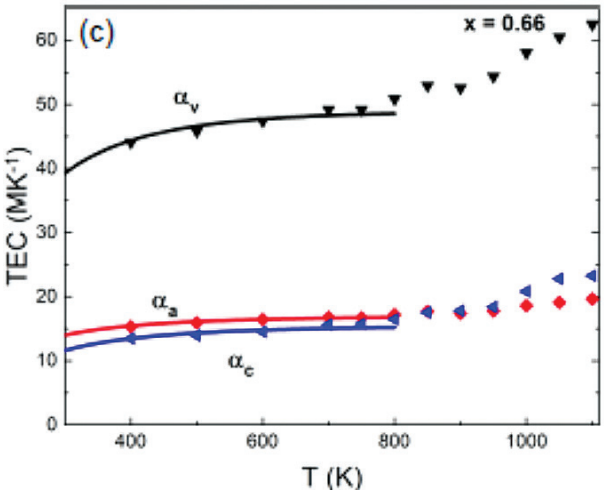


Fig. 1. Thermal expansion of $Ca_{10.5-x}Ni_x(VO_4)_7$ in the 300-1199 K range.

[1] Crystal Structure, Thermal Expansion and Luminescence of $Ca_{10.5-x}Ni_x(VO_4)_7$, H.S. Rahimi Mosafer, W. Paszkowicz, R. Minikayev, C. Martin, M. Kozłowski, O. Chukova, Y. Zhydachevskyy, S. Nedilko, Crystals 2023, 13, 853 (23 pp).

X-ray Diffraction studies: defects structure in thin films

The team conducts research on thin films and heterostructures determining, in particular, their defect structure. An example of such work is the analysis of heterostructures consisting of a layer of a topological insulator SnTe(001) of NaCl structure and a CdTe(001) buffer of zinc blende structure, deposited on a GaAs(001) substrate [2], see Fig. 2. The deformation of the crystal lattice and the degree of relaxation of both layers were studied in detail using high-resolution X-ray diffraction. The results showed almost complete relaxation of the CdTe crystal lattice and partial relaxation of SnTe. The relaxation mechanism was interpreted

as a process involving the formation of mismatch dislocations. Anisotropy of the spatial distribution of defects was found.

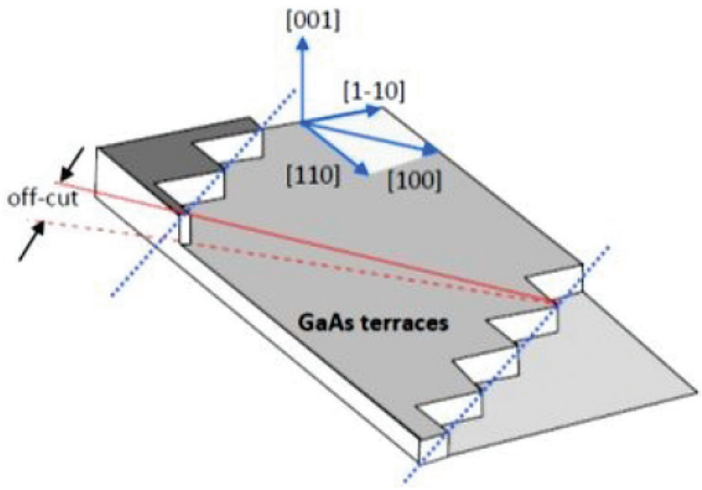


Fig. 2. Scheme of the studied heterostructure.

[2] A. Sulich, E. Łusakowska, W. Wołkanowicz, P. Dziawa, J. Sadowski, B. Taliashvili, T. Wojtowicz, T. Story, J. Z. Domagala, Unit cell distortion and surface morphology diversification in a SnTe/CdTe(001) topological crystalline insulator heterostructure: influence of defect azimuthal distribution, Journal of Materials Chemistry C, 10(8), 3139-3152 (2022)

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Laboratory SL2: Cryogenic and Spintronic Research

TOPICS AND METHODS

Since its foundation, the Laboratory of Cryogenic and Spintronic Research has remained at the forefront of experimental and theoretical research of spin-dependent phenomena in semiconductors at nanoscale, at ultralow temperatures, and in high magnetic fields, as well as in studies of superconductivity. The Laboratory has gained particular international recognition by elucidating the nature of dimensionality-dependent interplay of spin and quantum localization phenomena and the origin of ferromagnetism in semiconductors containing transition metals. Current interests, pursued together with a number of European and overseas research partners, including the groups of L. Molenkamp from Wurzburg University, J. Furdyna from Notre Dame (USA), S. Fukami from Tohoku University (Japan), and scientists from Aalto University (Espoo, Finland), are focused on:

(i) The development of material systems and device concepts for nanospintronics basing on dilute ferromagnetic semiconductors and antiferromagnetic materials, topological matter and hybrid ferromagnetic metal/semiconductor nanostructures. The core of the spintronics research is performed using two MPMS SQUID magnetometers from Quantum Design capable of establishing magnetic moment down to 10^{-8} emu, in magnetic fields of up to 5 and 7 Tesla and in temperatures between 1.8 and 400 K (or to 800 K using a special furnace fitting). Apart from standard magnetometry, both system have been modified to accommodate electrical connections allowing a direct detection of the modulation of the magnetization by electrical gating, Fig. 1. These abilities have led to the first ever direct magnetic detection of the electrical modulation of the Curie temperature in dilute ferromagnetic semiconductor (Ga,Mn)As [1]. This line of research has helped to settle the controversies regarding theoretical models describing ferromagnetism in magnetic semiconductors of the (Ga,Mn)As and (Ga,Mn)N families and to indicate directions to the practical applications of spintronics, including integrated circuits using ferromagnetic metals [2].

Fig. 1. Two MPMS SQUID magnetometers from Quantum Design. The left one is wired up for electrical-gating experiment.

(ii) The fabrication of meta-materials and hybrid structures for electromagnetic radiation coupling studies. The active element in such instruments will be micro-antenna arrays on insulating substrates or diffraction gratings, etched on layered structures with preset dielectric parameters. This effort is focused around a unique electron-beam lithography (EBL) system, based on Jeol 6400 scanning electron microscope and so-called interferometric stage (Raith) allowing for alignment with nanometer precision. As regards hybrid meta-materials, based on micro-antennas, they open up the possibility of designing active microcircuits with the ability to switch, modulate and slow down or accelerate terahertz waves [3]. Therefore, they can provide a platform for the construction of multifunctional photonic devices, including biochemical sensors, absorbers, filters and nonlinear switches. Works related to polariton laser are performed in cooperation with Warsaw University, fabrication of micro-antenna arrays is carried out in cooperation with the Military University of Technology. An example of a one-dimensional dielectric subwavelength grating is shown in Fig. 2.

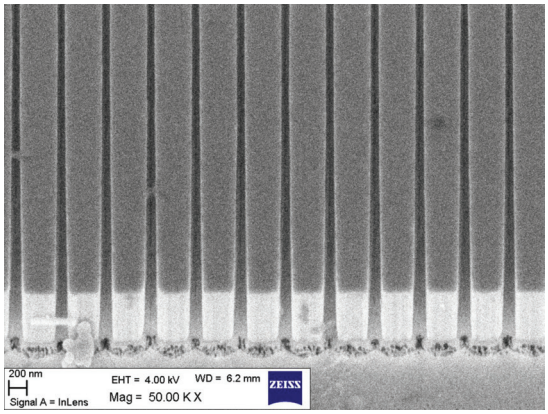

Fig. 2. Subwavelength grating on GaN substrate. Note the large aspect ratio, very smooth edges and sub-100 nm distance between etched lines. The device is intended as an active element of ultra-low threshold, tunable polariton laser operating at room temperature (Photo: D.Yavorskiy, Institute of Physics PAS, Institute of High Pressure Physics PAS).

(iii) Crystalline topological insulators from (Pb,Sn)Te family. We investigate classical magnetotransport in PbTe/SnTe junctions and describe it in the frame of so-called mobility spectrum analysis. This allows us to ascribe electron-like and hole-like maxima, observed in the mobility spectra, to a single-carrier transport in single topological band [4]. This work is carried out in cooperation the Military University of Technology in Warsaw using samples provided by ON1 and SL3 scientific divisions of Institute of Physics PAS.

(iv) Building and testing pioneering low temperature functional nanostructures with a special emphasis on superconducting devices. Our expertise involves fast time-resolved thermometry of nanostructures based on the probing of Josephson junctions with short current pulses. It allows us to trace the thermal transients, which appear in the response to a local dissipation, with a temporal resolution of a single nanosecond. We can directly investigate the dynamics of various energy relaxation channels at the nanoscale. Our another field of interest is vortex electronics. It involves building nanodevices for controlling and manipulating of superconducting vortices to present new functionalities *e.g.* memory cells and logical elements for application in quantum computing. Our low temperature measurements are performed in a bottom-loaded cryogen-free dilution refrigerator Triton 400 with a base temperature of 10 mK and 6-1-1 vector magnet, Fig. 3. We also use He^3 sorption cryostat Heliox, which offers cool-down from room temperature to a base temperature of 230 mK in only 45 minutes. Both devices originate from Oxford Instruments and were customized for dynamic testing of superconducting devices, involving probing with nanosecond electrical pulses and microwaves.

Fig. 3. Triton 400 laboratory. Cryogen-free dilution refrigerator from Oxford Instruments. Samples are cooled to the base temperature of 10 mK in 12 hours with the bottom loading mechanism. Equipped with 6-1-1T vector magnet.

(v) Numerical simulations, modeling and symbolic computations. The codes developed here allow for simulations of magnetization and ferromagnetic resonance (FMR) in insulating dilute magnetic semiconductors using both quantum and classical approach [5], modelling of classical and quantum transport, which is necessary in analyzing electrical properties of semiconductor structures with reduced dimensionality [4], and topological insulators [6].

ACHIEVEMENTS

A new method for very high-sensitivity integral magnetometry

The shift in the interest of the magnetic studies towards layered structures comprising very thin layers of either antiferromagnetic materials or dilute magnetic materials prompted elaboration of means and experimental protocols assuring vastly increased detectability of the relevant minute magnetic signals buried underneath large signals from the bulky substrates or other housings on which these materials are provided for magnetic studies. The paper describes a pioneering approach of an *in situ* compensation method to alleviate this issue. Here, a sample abutting by sufficiently long strips made of material of matching magnetic properties to that of the substrate of the housing is shown to reduce its detrimental contribution by 20 to 30 times and to mitigate other issues which affect integral magnetometry such as various system instabilities and an inadequate data reduction. Practical solutions are exemplified in Fig. 4. Proper expressions to calculate the absolute values of the investigated moments are given. Their universal form allows the user to employ the suggested design in investigations of a broad range of specimens of different sizes, shapes and compositions. The method does not require any extensive numerical modeling, it relies only on the output data provided by the magnetometer. The solution has been successfully implemented in studies of antiferromagnetic materials [7,8], and constantly attracts interest from various laboratories worldwide. This compensational approach to volume magnetometry was later extended into shapeless and powdered materials which require encapsulation (a kind of plastic capsules) to perform the measurements [9], allowing in particular

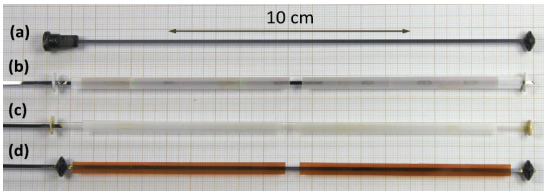

Fig. 4. Examples of assemblies allowing *in situ* compensation of unwanted flux of either the substrate or a bulk part of the sample. They are customized to work with Quantum Design MPMS magnetometers. In these assemblies the strips of the compensating materials (sapphire and GaP [7], respectively) differ from the material used for the supporting stick—Si, whereas inthe assembly (c) all parts are made of sapphire [11].

precise investigations of single-milligram samples of coordination compounds of pharmaceutical relevance [10].

K. Gas, M. Sawicki, *In situ* compensation method for high-precision and high-sensitivity integral magnetometry, Meas. Sci. Technol. 30, 085003 (2019).

How to measure temperature by flipping a coin?

We proposed and demonstrated experimentally a new type of time-resolved nanothermometry for testing the electron temperature (i.e. the population of quasiparticles) of nanostructures in thermal transients with unprecedented resolution of a single nanosecond. The method involves measuring the probability of transitioning of a Josephson junction from a superconducting to a normal state, which, from a mathematical perspective, is analogous to tossing a coin to determine the likelihood of getting heads. We can excite nanostructures with short heating pulses and trace their relaxation back to the thermal equilibrium. It allows to single out various fundamental processes responsible for the heat flow/dissipation at nanoscale. It is in contrast to the conventional steady state studies, which have been popular so far for the lack of fast time-resolved thermometers. Our approach allows to understand and optimize the thermal budget of low temperature nanostructures, and evaluate the role of dissipation on the functioning of various superconducting circuits, whose operation is known to be very sensitive on the population of quasiparticles. It is also an excellent tool for exploring an emerging field of experimental quantum thermodynamics, as our recent study shows. The method has been presented and developed in 5 consecutive Physical Review publications [12-16].

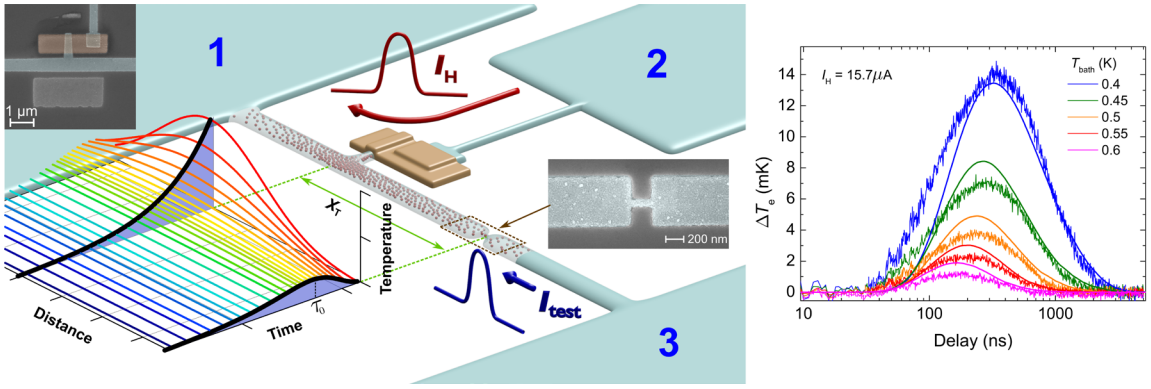

Fig. 5. The temperature dynamics of the superconducting nanobridge after creating nonequilibrium quasiparticles in copper island placed 60 μm away with a short 10 ns-long heating pulse. The hot electron signal peaks up ~300 ns after application of the heating pulse which well agrees with expected diffusion time across 60 μm long nanowire. One can observe the delay of ~40 ns between the heating pulse and the onset of the signal. This delay shows that switching current of the bridge depends on the local distribution (local temperature) of quasiparticles. This measurement is an example of the excellent temporal and temperature resolution of our pioneering approach.

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Laboratory SL3: Growth and Physics of Low Dimensional Crystals

RESEARCH TOPICS

- Optical properties of quantum wells, quantum wires, self-organized quantum dots, colloidal quantum dots, SiN quantum dots.
- Theory of electronic states in low dimensional quantum nanostructures (self-organized quantum dots, quantum wires, and quantum wells).
- Semimagnetic semiconductors.
- P-type and n-type doping.
- Semimagnetic p-i-n junctions and diodes.
- Trion states and charged excitons.
- Ferroelectricity of II-VI compounds.
- Electron/ion beam lithography.
- Cathodoluminescence.
- Thin film II-VI photovoltaic solar cell structures, novel quantum solar cell structures, and sustainable materials for photovoltaic applications.
- Ab-initio calculations of electronic and magnetic properties of solids: dopants, defects, and magnetism based on p-electrons.
- Colloidal synthesis of semiconductor quantum dots (QDs) and lanthanide doped up-converting nanoparticles (UCNPs).
- Spectroscopy of colloidal QDs, UCNPs, and 2D van der Waals semiconductors.
- Photoluminescence (PL) dynamics.
- Single QD spectroscopy.
- Magneto-photoluminescence of colloidal QDs.
- Spin polarization dynamics.
- Interaction between light emitters and surface plasmon polaritons.
- Density functional theory (DFT) calculations of electronic and magnetic properties of nanostructures.

Laboratory SL3 was created in 2002 as a specialized lab where by using ultra high vacuum epitaxial techniques low dimensional materials were to be prepared for use by researchers from the entire Institute. Since then, the members of the groups have developed also a scientific program of their own. Initially, the equipment consisted of a molecular beam epitaxy system aiming at fabrication of epilayers, quantum wells, and superlattices made of II-VI wide band gap semiconductors, often containing addition of magnetic Mn ions. Photoluminescence was employed as a main characterization method. Nowadays, we aim at growth of diverse low dimensional semiconductor structures including, apart from two dimensional structures already mentioned, also nanowires and quantum dots obtained in several ways. Emission of light from those structures

is studied in the context of, *e.g.*, single photon emission, application in spintronic devices, photovoltaics, to mention only a few topics. The equipment consists now of a two chamber MBE system, a chemical lab where quantum dots are grown by co-precipitation, measurement systems enabling single photon counting, microluminescence studies of single nano-objects, and photon correlation measurements. We share the electron beam lithography system with colleagues from SL2. At this moment, there are 8 young researchers working for their PhD. There is also a small subgroup of theoreticians specializing in numerical *ab initio* methods supporting the experimental efforts.

In the course of our work a new facility was developed for synthesis of colloidal light emitting nanostructures. The main research tool is the study of photoluminescence as well as photoluminescence dynamics. In particular, we developed a setup for temperature dependent studies of individual nanostructures. Currently, we are developing another setup, which will enable studies of single quantum dots at room temperature and, in particular, studies of the quantum nature of the emitters by means of photon correlation spectroscopy.

RECENT ACHIEVEMENTS

Carrier separation in type II quantum dots inserted in (Zn,Mg)Te/ZnSe nanowire

Semiconductor nanowires belong to the most intensively studied nanostructures in the last decade. They have drawn interest as a promising platform for nanoelectronics, light sources, and light detectors. The characteristic feature of these nanostructures is the greater flexibility to combine semiconductors with different lattice constants as compared to their planar counterparts. Moreover, different semiconductors can be merged either in the radial or axial direction depending on the growth direction. Axial heterostructures are investigated mainly in view of their possible applications for single photon emission. The latter effects are observed in nanowire quantum dots (NWQD), i.e., small optically active axial insertions of a low band gap semiconductor inside a nanowire composed of a large bandgap semiconductor forming zero-dimensional traps for electrons and holes.

The aim of this study is the fabrication of NWQD composed of II-VI semiconductor compounds. The uniqueness of our approach relies on the fact that the usual NWQD, consisting of an axial low bandgap insertion inside a large bandgap NW core, is coated with a radial shell made of a semiconductor forming a type II interface with the dot semiconductor. In effect, the electrons and holes are expected to be spatially separated in the radial direction. The intentional design of the band structure within this NW-heterostructure and the resulting effective control over the charge carrier wavefunctions on the nanometer scale may open the door towards novel applications. In particular, type II NWQD in which the electron wavefunction forms a ring around the dot could be especially well suited for the observation of the excitonic Aharonov-Bohm effect. This quantum interference effect raises interest due to its potential application in the field of quantum information storage.

Quantum dots consisting of axial ZnTe insertions inside large bandgap $Zn_{0.9}Mg_{0.1}Te$ nanowire cores are fabricated in a molecular beam epitaxy system by employing the vapor-liquid-solid growth mechanism. Additionally, this structure is coated with a thin ZnSe radial shell which forms type II interface with the dot semiconductor. The resulting radial electron-hole separation is evidenced by several distinct effects which occur in the presence of ZnSe shell,

including: the optical emission redshift of about 250 meV, a significant decrease of the emission intensity, the increase of the excitonic lifetime by one order of magnitude, and the increase of the biexciton binding energy. Controlling separately the electron and hole wavefunctions within a single NW heterostructure may result in novel functionalities which could be applied in the field of quantum information technologies, photodetection, and photovoltaics. In particular, the type II NWQDs with a radial electron-hole separation have a great potential to be used in quantum devices employing the excitonic Aharonov-Bohm effect. The latter effect has been recently observed in III-V semiconductor based NW heterostructure and might open novel opportunities in the frame of the quantum information storage.

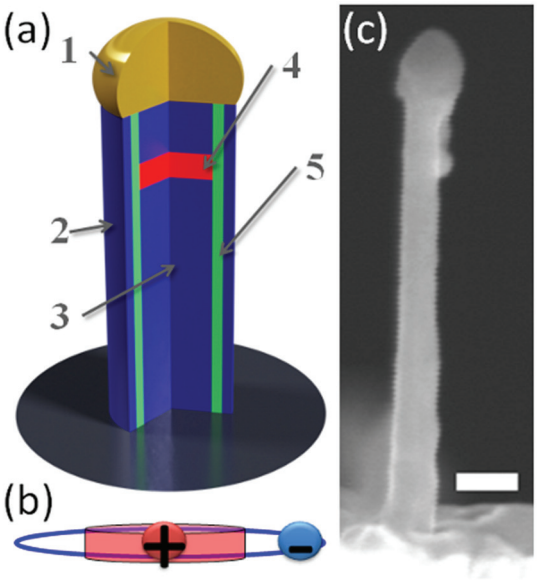

Fig. 1. (a) Scheme of investigated nanowire heterostructure 1 - Au/Si eutectic droplet, 2 - $Zn_{0.9}Mg_{0.1}Te$ outermost shell, 3 -$Zn_{0.9}Mg_{0.1}Te$ core, 4 - $Zn_{0.97}Mg_{0.03}Te$ low bandgap insertion, 5 - ZnSe internal shell. (b) Scheme representing spatial separation of electrons and holes occurring at NWQD/ZnSe shell interface. (c) Scanning electron microscopy of a typical nanowire heterostructure investigated in this work. Scale bar corresponds to 100 nm.

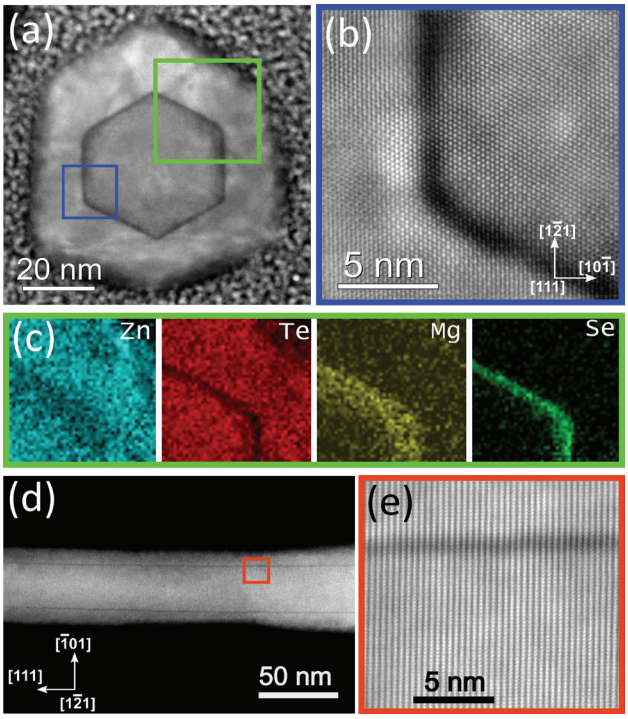

Fig. 2. Morphology and elemental composition of a $Zn_{0.9}Mg_{0.1}Te/ZnSe/Zn_{0.9}Mg_{0.1}Te$ core/double-shell NW heterostructure. (a) STEM image of nanowire cross-section revealing the shape and the thicknesses of both shells. (b) close-up indicating an epitaxial relation between the core and the shells marked in (a) with dark-blue frame. (c) EDS maps revealing the distribution of Zn, Te, Mg, Se atoms within the area marked in (a) by the green frame. (d) side view of a typical NW shown in [1-21] zone axis. (e) close-up of the area marked in (d) with orange frame confirming NW epitaxial relation observed from side view.

Reference: Piotr Baranowski, Małgorzata Szymura, Anna Kaleta, Sławomir Kret, Maciej Wójcik, Rosen Georgiev, Sergij Chusnutdinow, Grzegorz Karczewski, Tomasz Wojtowicz, Lech Tomasz Baczewski and Piotr Wojnar, Nanoscale 15, 4143-4151 (2023).

Nonradiative Energy Transfer and Selective Charge Transfer in a WS_2/$(PEA)_2PbI_4$ Heterostructure

Two-dimensional (2D) layered materials have been in the scientific spotlight for more than a decade. The seminal work of Geim and Novosolov on graphene was followed by the rediscovery of transition-metal dichalcogenides (TMDs), the recent explosion of the field of 2D perovskites, and other emerging layered materials. While initially the investigations of electronic properties were limited to monolayers within a particular group of materials, recently, the engineering of van der Waals stacks has attracted tremendous attention. The inherently weak van der Waals interaction between the 2D crystals facilitates the stacking of a variety of different layers into hetero- or homostructures with new functional properties. The encapsulation of TMDs with h-BN results in superior electrical and optical quality. Stacking two different TMDs leads to a plethora of new properties, including long-lived interlayer excitons, which can be controlled by an electric or magnetic field, and the formation of moiré patterns, which can lead to exotic crystal phases.

These functional properties strongly depend on the nature of the spatial excitation transfer between the layers, which can rely on charge transfer and/or energy transfer. For example, the type-II band alignment in TMD stacks favors charge transfer, which leads to the formation of interlayer excitons with new exotic properties. On the other hand, stacks of 2D semiconductors, in principle, form an ideal platform to explore energy transfer (nonradiative transfer of the excitation). This is due to the large oscillator strength and ultimate proximity of the functional layers (in the range of single to a few dozens of Å), essential for nonradiative energy transfer of the Förster or Dexter type. The energy transfer can be the dominant process if the direct interlayer charge transfer is strongly suppressed. This can be achieved, for example, by separating TMD layers with an insulating sheet of h-BN. The incorporation of different numbers of h-BN layers allows us to control the mechanism of excitation transfer from direct charge transfer to energy transfer.

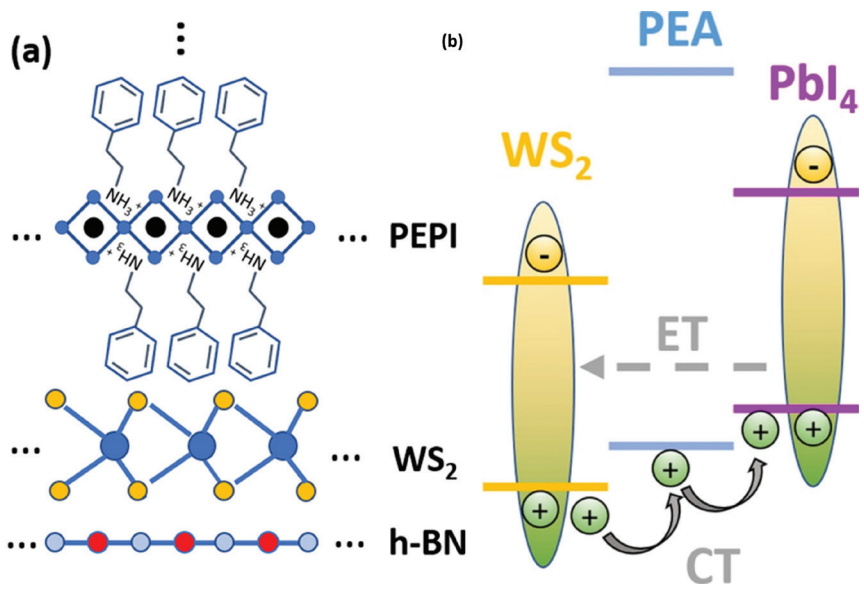

Fig. 3.
(a) – Schematic atomic structure of PEPI/WS_2 van der Waals stack along the stacking axis. (b) – Proposed band alignment in PEPI/WS_2 stack based on the DFT calculations. The charge transfer (CT) and energy transfer (ET) paths are indicated by grey curved and dashed arrows, respectively.

Recently, we proposed a novel approach to control the excitation transfer process, using a hybrid heterostructure built from a TMD monolayer and a 2D perovskite $(PEA)_2PbI_4$ (PEPI). The 2D perovskite provides a charge blocking layer in the form of organic spacers. As we have shown, such a stack can provide a rather unique band alignment, not achievable in TMD-based van der Waals heterostructures. Taking into account the plethora of available organic spacers that can be incorporated into the 2D perovskites, this new approach to heterostructure design provides greater flexibility in the band alignment, together with the possibility to engineer the excitation transfer mechanism. The efficient energy transfer can be used to sensitize the photoresponse of one layer (for example, TMD) using the other layer (2D perovskite), without reduction of the overall photoresponse yield characteristic for the interlayer charge transfer and weak interlayer emission.

Reference: M. Karpinska, M. Liang, R. Kempt, K. Finzel, M. Kamminga, M. Dyksik, N. Zhang, C. Nodlseder, D. K. Maude, M.Baranowski, Ł. Kłopotowski, J. Ye, A. Kuc, and P. Plochocka, ACS Appl. Mater. Interfaces 2021, 13, 28, 33677–33684.

Low-Temperature Photoluminescence Dynamics Reveal the Mechanism of Light Emission by Colloidal $CuInS_2$ Quantum Dots

Colloidal quantum dots (QDs) constitute an exciting family of nanostructures with potential applications ranging from bioimaging and biosensing, via photovoltaics, to display technologies. Among the QD materials, the most widely studied are cadmium and lead compounds. However, the inherent toxicity of Cd and Pb ions complicates industrial scale applications of these materials. Thus, in recent years, a lot of attention was devoted to studies of Cd- and Pb-free alternatives.

Copper indium sulfide ($CuInS_2$) QDs offer several advantages over the lead and cadmium compound QDs. For example, $CuInS_2$ QDs can accommodate much higher off-stoichiometries and higher degrees of alloying. These features afford additional handles for tuning the optical properties and achieving photoluminescence (PL) quantum yields in the 75%–95% range. Moreover, the PL spectra of these QDs exhibit giant global Stokes shifts in excess of 0.3 eV, which reduces reabsorption losses. As a result, $CuInS_2$ QDs are ideal fluorophors for applications in luminescent solar concentrators. Furthermore, the PL lifetimes of $CuInS_2$ QDs are usually longer than 200 ns, and PL energies can be tuned to the near-infrared biological window. These properties make $CuInS_2$ QDs excellent candidates for time-gated bioimaging, biodetection, and intracellular temperature sensing. Finally, full width at half-maximum (FWHM) line widths of $CuInS_2$ QD PL are usually larger than 300 meV. The broad emission spectra together with high PL quantum yields offer an application possibility in light sources.
Despite the great progress in synthetic tailoring of the optical properties, the mechanism underlying the PL of $CuInS_2$ QDs is still a matter of debate. Two pathways are considered. In the free-to-bound mechanism, a delocalized conduction band electron ($1S$) recombines with a hole localized on the copper cation. In the excitonic mechanism, the hole is delocalized on a P-symmetry state and the PL is due to a parity-forbidden $1S$–$1P$ transition. The poor understanding of the nature of the luminescent excited state limits further development of these materials toward existing and emerging applications.

In our work, we established the PL mechanism in core-only $CuInS_2$ QDs and revealed the fine structure of the luminescent excited state. To this end, we employed a tool which proved instrumental in explaining the PL mechanism in Pb and Cd chalcogenide QDs. Namely, we investigated temperature and magnetic field dependencies of the carrier and spin dynamics - a subject largely unexplored in the context of $CuInS_2$ QDs. We cast the experimental results against the expectations of excitonic and free-to-bound recombination models and drew conclusions based on four observations: (i) The PL decay rate increases with the temperature faster for long decay components than for short ones. (ii) The PL lifetimes are independent of the magnetic field. (iii) The spin relaxation times are 2–3 orders of magnitude longer than for CdSe QDs. (iv) The equilibrium spin polarization exhibits a peculiar temporal decay. We argued that neither of the four effects is compatible with the excitonic PL mechanism. On the other hand, all four are consistent with the recombination of a delocalized electron with a Cu-localized hole, whereby the luminescent excited state is composed of a lower energy dark triplet and a higher energy bright singlet. Our results allowed us to evaluate the singlet–triplet energy splitting and determine the impact of the Cu position within the QD volume on the PL properties of $CuInS_2$ QDs.

Reference: M. Szymura, M. Duda, M. Karpińska, T. Kazimierczuk, R. Minikayev, K. Sobczak, M. Parlińska-Wojtan, and Ł. Kłopotowski, J. Phys Chem. C 2023, 127, 14, 6768–6776

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Laboratory SL4: Biological Physics

RESEARCH TOPICS

Molecular biophysics

- Prevention and control of infectious diseases by selectively blocking pathogens in aquaculture, based on intrinsically disordered protein studies (research within the European consortium PathoGelTrap)
- Biomolecular regulatory switches involved in cellulosome function (research within the European consortium CellulosomePlus)
- Protein conformational dynamics and hydrodynamic properties in the context of intermolecular recognition, cellular regulatory processes, and extracellular biomineralization
- Nascent protein chain folding on the ribosome, knots formation and mechanical stability for better understanding of molecular interactions, native and neurodegenerative diseases, as well as biomedical applications
- Protein-protein and protein-RNA complexes involved in eukaryotic gene expression regulation and silencing
- Development of new models of intrinsically disordered proteins
- Coarse-grained and all-atom molecular dynamics modelling of proteins, their complexes, and virus capsids

Nanobiotechnology

- Design, synthesis, and optimization of luminescent and magnetic up-converting nanoparticles for biomedical applications
- Biofuctionalization of the nanoparticles, characterization of their properties, interactions with living cells, and toxicity in the context of medical theranostics
- Investigation of biomineral crystal structure and growth governed by coral acid-rich proteins; spherulites formation

RESULTS AND ACHIEVEMENTS

Protein Structural Dynamics

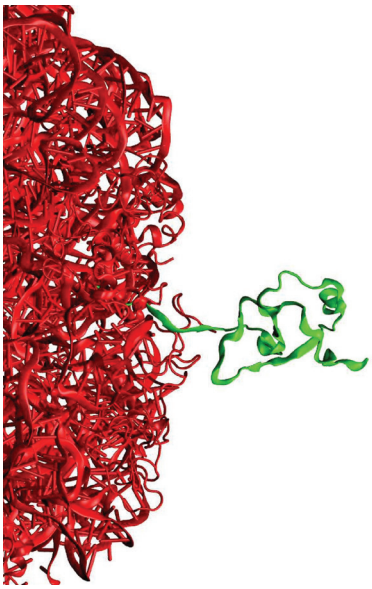

Fig. 1. On-ribosome folding of YibK protein.

The theoretical part of the group at the Laboratory of Biological Physics focuses on the research of both structured proteins and IDPs. The studies were initiated by Marek Cieplak and are now continued in several directions. One of them is the protein confinement, in particular the process of formation of knots and cavities in structured proteins. A public server called SPACEBALL (http://info.ifpan.edu.pl/~chwastyk/spaceball) has been established, which made it possible to describe cavities in most of the structures deposited in the Protein Data Bank [1]. The same approach was used to analyse the properties of the interior of the ribosomal exit tunnel and to describe the nascent polypeptide chain folding of structured proteins. This allowed for a better understanding of protein folding and knotting processes [2]. An example of a nascent protein folding on the ribosome is shown in Figure 1.

The second area of interest is related to the molecular mechanism of the cellulosome activity responsible for cellulose degradation into sugar molecules [3]. The architecture of cellulosome machinery is based on very strong non-covalent binding of proteins like dockerins and cohesins. Dockerins are very diverse but all share the same motif of two parallel and symmetric helices that bind to a cohesin. The helices share similar sequences so their position in the macromolecule could be switched and most dockerins could bind to cohesins in two similar modes (Figure 2). The experimental results showed the exact proportion between both modes. The theoretical contribution of Michał Wojciechowski was to propose an efficient method for estimation of proportion between the modes, sensitive to mutation of the helix sequences. The method was based on Monte Carlo sampling of the dockerin near the cohesin and use of external (FoldX) approach to estimate the energy of rigid protein complexes. This improved estimation of the free energy allowed differentiating the proportion of the modes depending on the helix mutations.

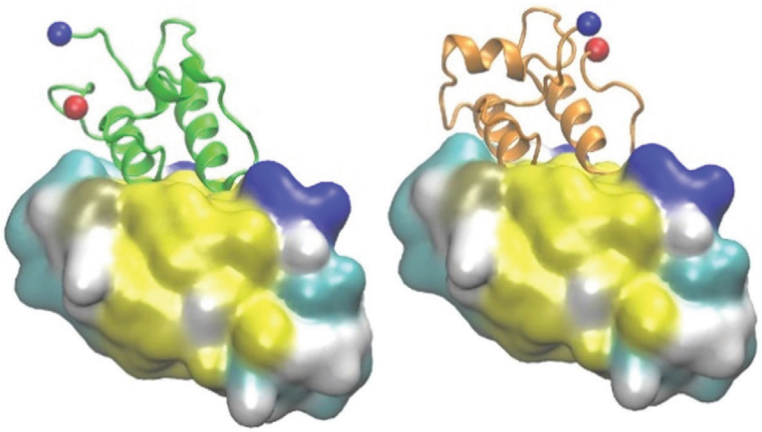

Fig. 2. The cohesin-dockerin complex (PDB: 1OHZ); cohesin is shown as a surface, and dockerin in a cartoon model. The dockerin could be bound in two positions (left and right panels); N- and C- termini of dockerin are marked by blue and red spheres, respectively.

The theoretical group was also involved in studies of IDPs that are associated with human neurodegenerative diseases. The most important tool used here is an in-house created program for molecular dynamics simulations of IDPs [4]. The methods and approaches developed by the group have also allowed contribution to the response to the global threat of COVID-19. In collaboration with his co-workers, Mateusz Chwastyk has described the mechanostability of coronavirus spike proteins [5]. Currently, the group focusses on research within a European project aimed at the prevention and control of infectious diseases by selectively blocking fish pathogens in aquacultures.

The experimental part of the group at the Laboratory of Biological Physics focusses on the studies of the IDPs that regulate crucial biological processes in living organisms: gene

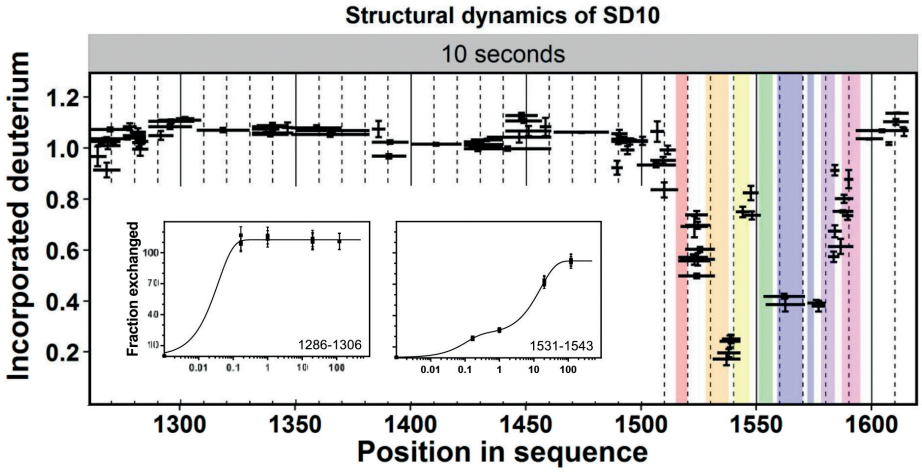

Fig. 3. Hydrogen-deuterium exchanged fraction of peptic peptides of GW182 silencing domain (horizontal black bars), corrected for back-exchange, after deuteration by 10 s. Insets: (left) the CIM1 peptide belonging to the intrinsically disordered region of GW182 that undergoes immediate exchange and (right) a peptide from the RRM domain that displays attenuated double exponential exchange kinetics.

expression and biomineralization. During the microRNA-mediated gene silencing, the targeted mRNA is selectively degraded only when the tryptophan- and glycine-rich protein of 183 kDa mass (GW182) brings together a multiprotein complex at the mRNA 3' terminus. The interactions among over a dozen of proteins are enabled by a large, scaffolding GW182 molecule. Anna Niedźwiecka and her co-workers proved by means of hydrogen-deuterium exchange mass spectrometry that the silencing domain of GW182 is completely unstructured except for the RRM domain, which is folded, but conformationally unstable and can exist in equilibrium of open and closed forms [6].

The studies of IDPs' molecular interactions needed, however, a closer analysis of their hydrodynamic properties. Since IDPs are described by a large configurational state space, a new method avoiding time-consuming molecular and Brownian dynamics simulations was necessary. The possibility of precise estimation of the experimentally relevant long-time diffusion coefficient of elastic macromolecules was elaborated by Anna Niedźwiecka and her co-workers [7].

Multifunctional Opto-Magnetic Nanoparticles

The aim of the work is to create multifunctional opto-magnetic nanoparticles (NPs) based on $NaYF_4$ [8-10] and Gd_2O_3 [11] matrices doped with rare earth ions (*e.g.*, Er^{3+}, Yb^{3+}, Nd^{3+}) for a future use in cancer theranostics. Nanoparticles exhibit up-conversion, i.e., anti-Stokes emission. It is an optical process in which an ion in a transparent matrix absorbs a few photons of low-energy radiation (*e.g.*, near-infrared, NIR) and emits one high-energy photon from ultraviolet (UV) to infrared (IR). These NPs can be used for diagnostics and phototherapy. The magnetic properties of these NPs can be used as contrasts in MRI imaging and for therapy by inducing magnetic hyperthermia. All these methods can be combined in one NP. The NP can be biofunctionalized with specific antibodies for cancer, allowing use in targeted therapy and for the detection of circulating tumour cells responsible for metastases in the blood. The research involves the production, physical characterization of nanomaterials, and the study of their interaction with biological materials (cells, tissues). Another direction of research conducted in the laboratory is the use of technology for obtaining Gd_2O_3

nanoparticles doped with Er^{3+}, Yb^{3+}, and Mg^{2+} as new types of sensory materials for use in temperature memory coatings.

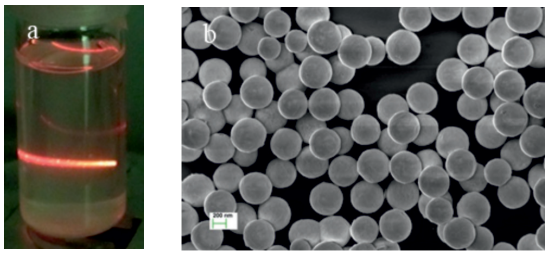

Fig. 4. a) Luminescence of Gd_2O_3: 1%Er^{3+}, 18%Yb^{3+}, 5%Zn^{2+} NPs in DMSO. Excitation: 980 nm (cw laser); b) SEM image of Gd_2O_3: 1%Er^{3+}, 18%Yb^{3+}, 1% Nd^{3+} NPs.

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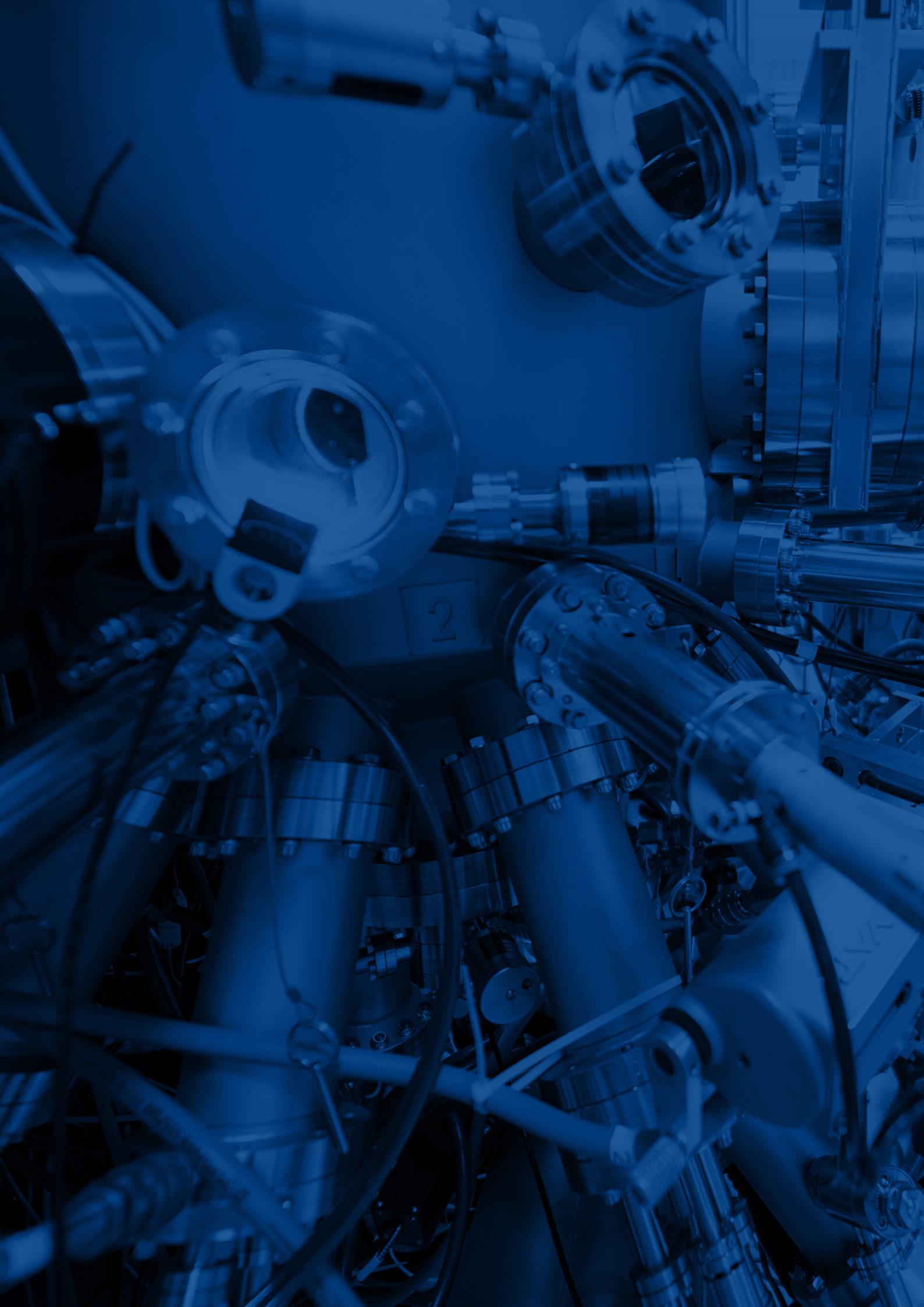


Miscellanea

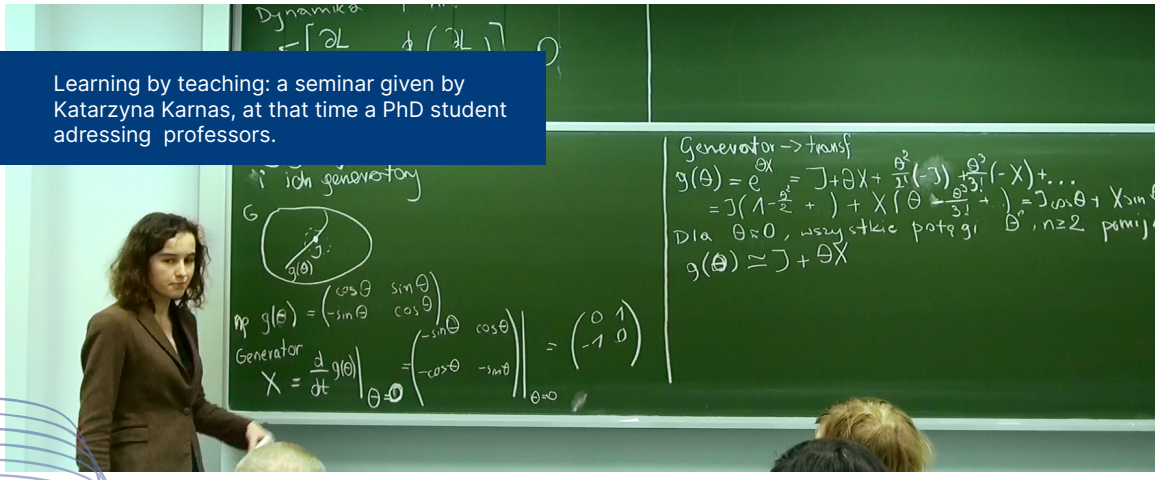
Education - PhD from the Institute

Educating young scientists is one of the most important tasks carried out at the Institute of Physics of the Polish Academy of Sciences. Naturally, the science community needs continuous influx of new talents who may become researchers in the future. The Institute educates PhD students and bestows doctoral degrees already for over half a century. At present, the PhD education takes place in the framework of the Warsaw Doctoral School in Natural and Biomedical Sciences, Warsaw-4-PhD, which involves nine scientific institutions of the Polish Academy of Sciences.

The average number of doctoral students remained at a stable level of about 80-90 in recent years. Doctoral scholarships are financed mostly from national and international research projects, some doctoral scholarships are also funded from the Institute's statutory budget. About one fifth of our present doctoral students are Polish nationals, the large majority stems from India, Pakistan, and far- and middle-east countries. Although male students represented a majority in the past years, these days quite a large fraction of the students are women.

The Institute educates doctoral students in three main specializations: condensed matter physics which includes also material science, quantum physics covering atomic and molecular phenomena, and biological physics. The above specializations, however, do not exhaust the available topics of doctoral studies. This gives PhD students a wide range of choice of their research profiles. The formal education of PhD students includes lectures, specialization classes, seminars, workshops and, for experimentalists, of course daily activities in laboratories.

For more information visit www.ifpan.edu.pl/edukacja/szkola-doktorska.html



Learning by teaching: a seminar given by Katarzyna Karnas, at that time a PhD student adressing professors.

Kwasi - a student from far away

My name is Kwasi Nyandey, I was born in Ghana and received both Bachelors and Master of Science Degrees in Physics in 2010 and 2019 respectively from University of Cape Coast, Cape Coast, Ghana. Upon application and acceptance I was offered a full scholarship to pursue a PhD program at the Warsaw PhD School in Natural and BioMedical Sciences. I was accepted to work – under the supervision of Daniel Jakubczyk – on the project: "Investigation of thermodynamics of evaporation of multi-component micro-droplets – distillation at micro scale", at the Institute of Physics, Polish Academy of Sciences. Apart from the difficulty I encountered to obtain a visa appointment at the Polish Embassy in Nigeria and a place to stay while in Nigeria, all other arrangements such as travel to Poland, accommodation, and school documentation were made easy with the help of my supervisor. After joining the school in December 2020, I was able to do the required medical examination immediately after the 10-day COVID 19 quarantine and started my experimental work afterwards. As a result of the fast processing of the needed documentation, I started receiving my student scholarship at the end of December 2020. I must state here that I was able to start my courses before joining the school in person because the lectures were conducted online.

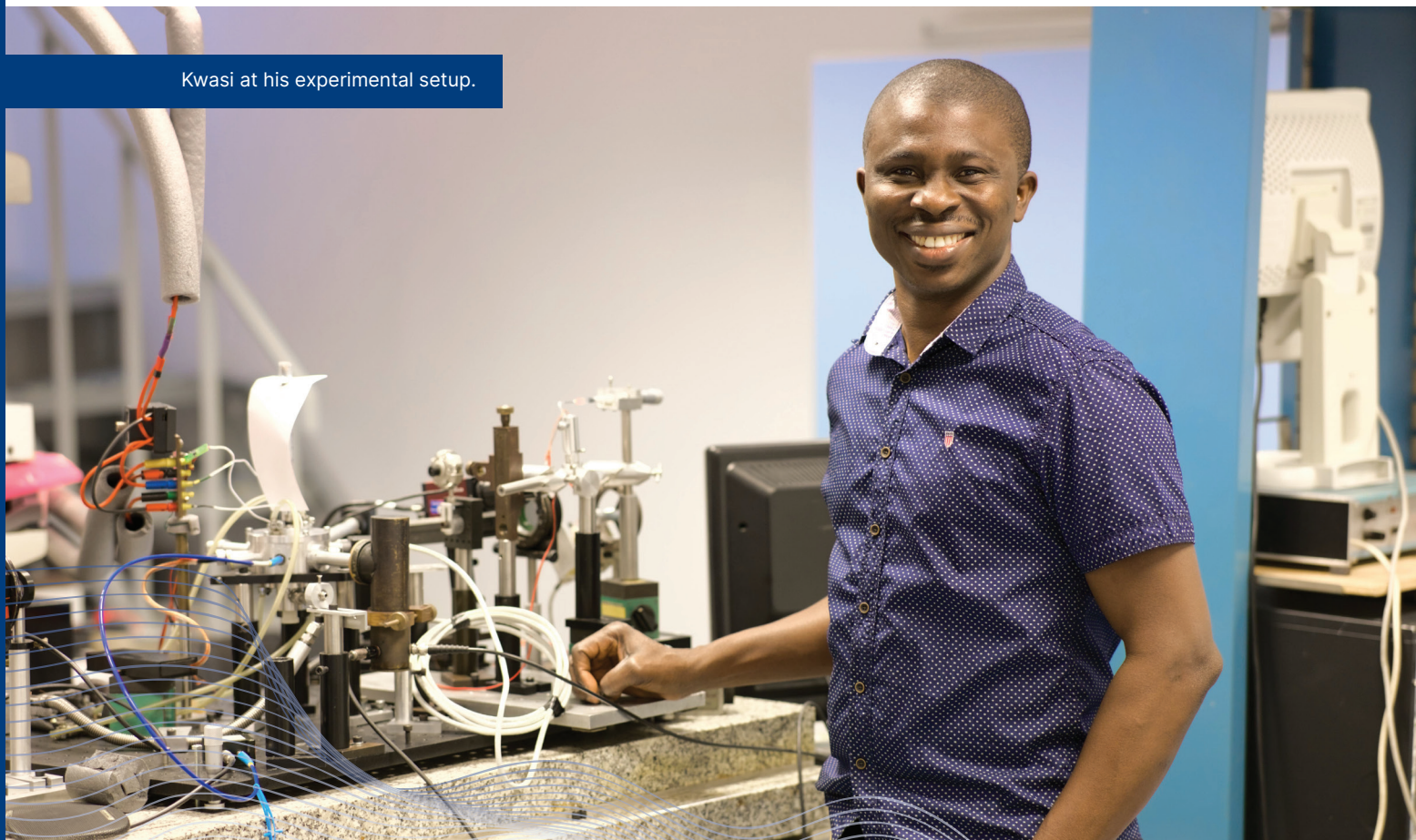
After getting acquainted with the group's experimental procedures – I was motivated to assist in the recording of data in the ongoing experiment, which resulted in a publication (Luminescent nanoparticles in a shrinking spherical cavity–probing the evaporating micro-droplets of colloidal suspension–optical lattices and structural transitions). During that period I also collaborated with my group in an experiment to measure the chromatic dispersion and thermal coefficients of the group's experimental liquids. On matters related to my project, I investigated the possibility to directly link coherent light scattering patterns (speckles) from milk (as a natural colloidal suspension) to their fat content categories using convolutional neural network. Consequently, an extended abstract was produced from preliminary results which I presented at the 13th International Conference Series on Laser-light and Interactions with Particles, Optical Particle Characterization follow-up (LIP2022) organized at the Institute.

After these few endeavors and discussions with my supervisor I progressed by combining electrodynamic trapping and machine learning to build an optical-numerical system for fast characterization of micro-droplets of clean liquids and suspensions. This meant that I was going to need a fast computer with memory capabilities to handle large data. However, I was faced with the well-known problem of procurement delays in all public institutions. At the moment I am using two computers, thanks to the fast response from my supervisor, to carry out this task while waiting for the dedicated computer. Now I can breathe a sigh of relief because I have been informed that the computer has now been purchased and is going through final preparation for use. This and similar problems alike are not uncommon in life since my colleagues PhD students have also complained to me about similar problems

after my candidacy and election into the office of the PhD Students' Representative for Scientific Council of Polish Academy of Sciences. These problems are faced by Professors and Postdocs alike but for PhD students (as one may have experienced) it turns into a nightmare when we think about completing our programs of study in four years.

Outside research and study, I collaborated with Krzysztof Pawlowski (Centre for Theoretical Physics, PAN) and other PhD students to conduct a few popularization of science workshops at selected high schools in Warsaw. I am in my third year of study and live (currently) in the Institute's hotel with other PhD students, which for me is very affordable and convenient compared to my former apartment. There are other systems/structures in IFPAN designed to help foreign students and employees. The Welcome Centre (launched in June 2021 as part of the „Welcome to Poland" project of the National Agency for Academic Exchange) is one such to oversee foreign students and employees in indirect matters. Matters such as administrative issues, residence permits, visa applications, integration trips *etc.* are conducted in Polish language. The state health and accident cover as well as the private health cover (PZU; basic cover paid by the Institute) are other systems worth mentioning. However, for foreign students and employees, the small number of English speaking doctors causes unnecessary delays in booking appointments. Also the Welcome Centre has been very helpful in accompanying students to non-English speaking doctors but personally, I have not asked for this support because I want to keep my medical records private.

I wish to conclude by stating that the Institute has provided several platforms such as scientific group seminars, journal club, fundamentals of physics seminars and student symposiums for students to advance not only their scientific careers but also their writing, reporting and presentation skills. I encourage my colleagues students to utilize such platforms since I have benefited from such provisions.

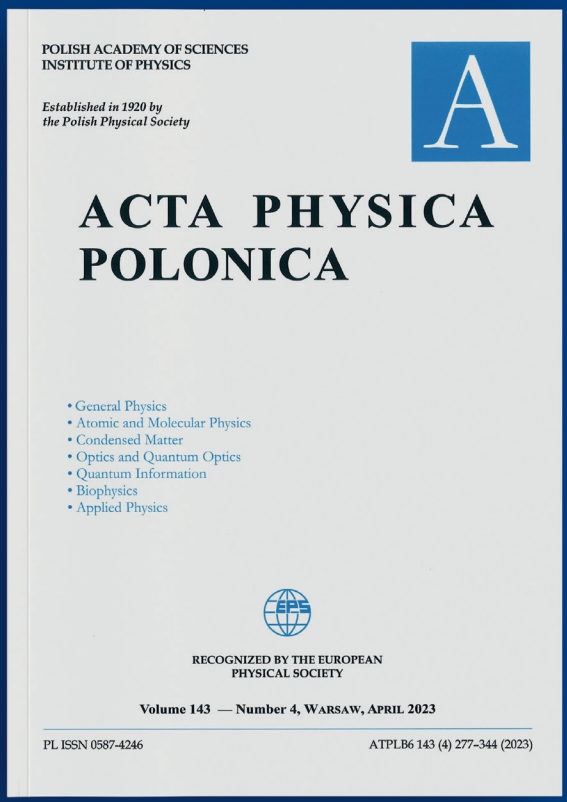


Kwasi at his experimental setup.

Acta Physica Polonica A

Institute of Physics of the Polish Academy of Sciences is the publisher of Acta Physica Polonica A, a journal specializing in research papers in physics.

The history of the journal dates back to 1920, when the newly established Polish Physical Society founded its journal, initially under the name „Reports and Works of the Polish Physical Society" („Comptes Rendus des Séances de la Société Polonaise de Physique"). In 1932, the name of the journal was changed to Acta Physica Polonica. The journal operated in this form until 1939, the beginning of the Second World War.



The journal was revived soon after the war, the first post-war volume was published in 1947. In 1970, Acta Physica Polonica was divided into two parts, A and B. Thus the journal will soon celebrate a centennial of its active existence. Acta Physica Polonica A publishes papers related to condensed matter physics, optics, atomic and molecular physics, while part B is devoted to nuclear physics, elementary particle physics, and gravity.

Part A, since 1991 has been published by the Institute of Physics of the Polish Academy of Sciences while part B continues to be published by the Jagiellonian University in Kraków. Both journals retain the original numbering of volumes. The Editors-in-Chief of Acta Physica Polonica A were: Wiesław Czyż (1973–1991), Jerzy Prochorow (1991–2006), Witold Dobrowolski (2006–2019), Jan Mostowski (2019–). Twelve issues are published each year, every issue contains at least ten original scientific articles. The authors are from all over the world. In the years 2016–2022, Acta published 14 volumes with a total number of 15 878 pages. In recent years, due to the pandemic, the number of published articles has slightly decreased, but hopefully it has a chance to increase to the pre-pandemic level.

The main objective of Acta Physica Polonica A has not changed in the last 30 years. Original research papers constitute the majority of published material. In addition to original articles, Acta Physica Polonica A also publishes review papers and post-conference materials. All published papers are reviewed prior to publication. All of them are of the „open-access" type. It should be noted that Acta does not charge for publications, which is not typical for fully open-access journals. Older issues of Acta Physica Polonica A are available in scientific libraries; papers published after 1990 are also accessible on the internet.

Jan Mostowski
The Editor-in-chief

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Centre of Technology Transfer (CTT) - „Science for Society”

The CTT group led by Marek Godlewski concentrates on promotion of a number of key solutions prepared by the scientists from the Institute. Generally they are aimed at health protection and environment-friendly applications (“green energy”).

Below we list some of the application--directed topics studied by scientists in the Institute:

1. health care – markers for early detection and therapy of cancer
2. health care – functional coatings for implants
3. health protection – methods of supplementation of microelements
4. health protection – antibacterial layers and varnishes
5. health protection – meshes to accelerate tissue regeneration after surgery
6. „green energy” – a new generation of silicon and organic photovoltaic (PV) cells
7. „green energy” – energy-saving windows.

Our solutions have been secured by numerous patents, mainly in Poland but also in Europe, including UK, France, Germany, Belgium, Switzerland.

CANCER MARKERS

Scientists in the Institute developed a new generation of fluorescent markers for early cancer detection. The developed markers are based on biocompatible nanoparticles (NPs) ZnO, ZrO_2 or Y_2O_3 activated with rare earth ions. Such NPs can penetrate various barriers in living organisms, including the blood-brain barrier. After modification, the same markers act as contrast agents in MRI, allowing the detection of internal tumors.The possibility of using our markers not only to detect cancer but also to treat it was demonstrated to increase the effectiveness of the therapy. The key to the invention is the patented ecological production of biodegradable conjugates of oxide nanoparticles with drugs. Thus, the new generation of biocompatible markers not only allows for early detection of tumors (through characteristic fluorescence or MRI), but also increases the chances of successful therapy. The selectivity of 100% has been demonstrated for lung cancer. The marker technology is protected by several of our patents and patent applications.

SUPPLEMENTATION

The main target was to develop a safe and efficient method of supplying organisms with appropriate micronutrients. The effectiveness of the developed method was verified by tests on laboratory animals. This solution has been secured by several

patents concerning the used technology and the method of manufacturing the zinc-containing micronutrient supplement.

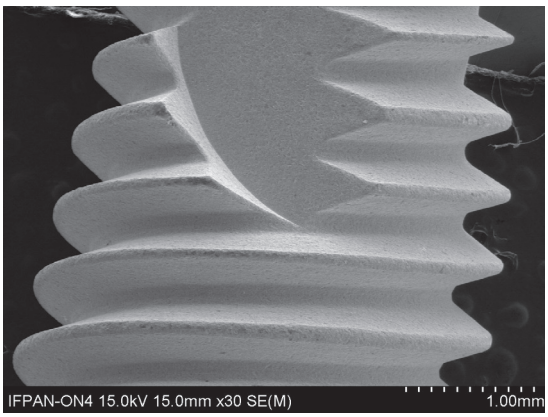
ANTIBACTERIAL LAYERS AND VARNISHES

The technology for coating with thin layers (in the Atomic Layer Deposition (ALD) process) was developed, allowing coating substrates sensitive to high temperatures, such as fibers, fabrics, paper, foils, polymers, and other materials used in hospitals. The developed coatings show antibacterial properties. The tests were carried out for typical materials used not only in hospitals but also in food industry (packaging) and in 3D printing.

IMPLANTS

Currently, a wide range of implants is used, which are mainly made of metals. The biofunctionality and biocompatibility of these metals is important. These two factors are crucial when choosing materials for medical applications and should be thoroughly tested. In addition, other properties should also be considered, such as corrosion resistance, the role of oxides formed on the surface of metals, time stability (if they remain in the body for a long time) and antibacterial activity. To avoid or minimize medical problems, the surface of metal implants should be biofunctionalized. The coating of the implant is used to block the penetration of metals from the implant into the tissues. The coating developed at the Institute not only allows improved implant compatibility but also accelerates bone formation.

The use of ALD technology enables uniform coverage of structured surfaces, such as various types of screws used in dentistry. It was proven that the developed coating accelerates tissue regeneration.



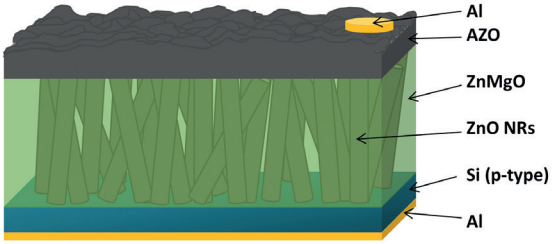
MESHES TO ACCELERATE TISSUE REGENERATION AFTER SURGERY

A technology for covering meshes placed on wounds has been developed in order to provide anti-bacterial protection and accelerate tissue regeneration. The meshes were tested on living organisms.

A NEW GENERATION OF SILICON AND ORGANIC PHOTOVOLTAIC (PV) CELLS

The main direction of works was to reduce the costs of currently produced PV panels. Our solutions leading to the reduction of costs (cells/panels) include changing the top metallization from Ag paste to aluminum, replacing ITO, which becomes more and more expensive, with an AZO layer (made in ALD technology), and developing an innovative concept of top structured electrodes in cells to improve the light collection. We proposed a significant simplification of PV cells (Si, GaAs,...) by introducing a new architecture of these cells (several European patents).

In the latest works, a new, very cheap technology of CuO layers was developed. These layers can replace Si and CdTe layers in PV cells.



ENERGY-SAVING WINDOWS

One of the recently undertaken research directions were thermally isolating coatings for windows. Researchers in the Institute have developed thin oxide coatings with optical performance similar to that of commercial coatings but significantly higher durability, even without a protective atmosphere. These coatings have a high transmission of visible light and at the same time they effectively block infrared transmission, stopping thus the flow of heat. Coatings can be applied as well to new glass panes as to foils that can be glued to already installed windows, which significantly extends the commercialization possibilities of the solution.

Recently, the above-mentioned activities were supported by the Innovation Incubator 4.0 program run by the Ministry of Education and Science. The activities within this program are described below.

INNOVATION INCUBATOR 4.0 PROGRAM

The aim of the program is to support the process of managing the results of scientific research and to help to undertake commercialization efforts. The implementation of the program aids promotion of scientific achievements, increases their impact on the development of innovation and strengthens cooperation between the scientific community and the industrial environment. To realize the program a consortium consisting of the Institute and NanoTechIP company was formed. The aim was as follows:

- conducting pre-implementation works adapting the invention to the needs of the potential industrial partner,
- preparation of commercialization projects for the results of scientific research carried out at IPPAS,
- initiating and strengthening cooperation between the scientific community and the industrial environment, promoting the technological offers and participation in exhibitions and the „science to business" fairs,
- promoting activities of Innovation Brokers acting as intermediaries between the scientific community and the industrial environment.

Anna Reszka and Agnieszka Krochmal-Węgrzyn from CTT promoting Institute's innovations at one of the fairs

The program financed 8 pre-implementation projects:

- Software for the analysis of exponential kinetics with additional analytical functions and an extensive graphical presentation layer.
- Diode detectors for a dedicated spectral range.
- Optimization of the parameters of infrared detectors based on PbTe/CdTe heterostructures operating at room temperature.
- Manufacturing technology of UV detectors based on oxide nanostructures.
- Nanocoatings for implantology applications for patients with osteoporosis.
- Optimization of the parameters of ZnO layers doped with Al for use as thermal insulation coatings for glass panes.
- A method of modifying paints and varnishes to obtain antibacterial properties.
- PA-MBE manufacturing technology of GaN nanowires on metallic buffer layers for high efficiency light emitting diodes.

Marek Godlewski
Head of CTT

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Large Scientific Projects at the Institute of Physics

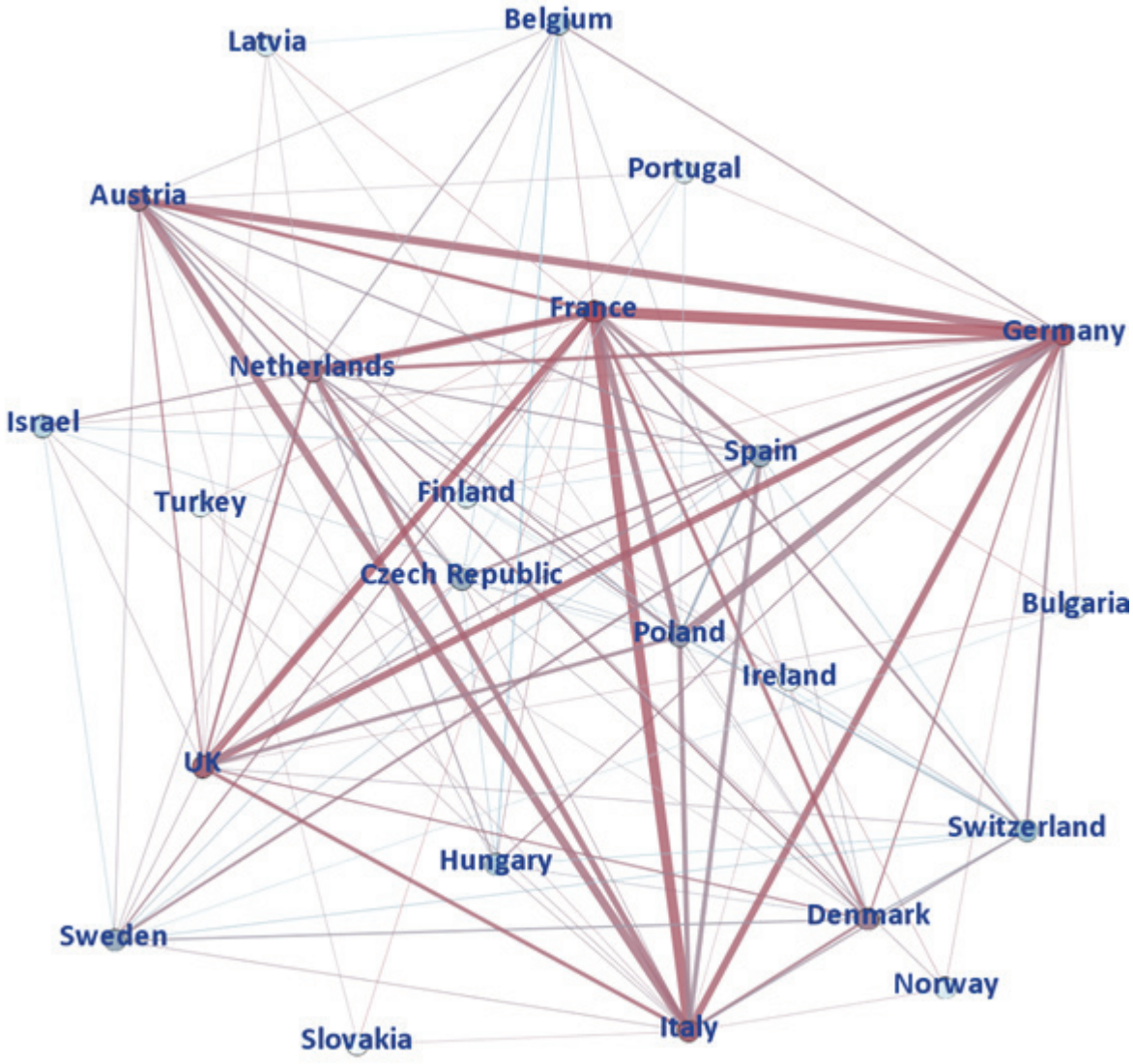
The Institute of Physics of the Polish Academy of Sciences continuously carries out a number of research projects. Over 80 projects funded by the Ministry of Education and Science, National Science Centre, and National Centre for Research and Development are currently being run. They allow for our daily scientific activity, partly financing laboratory equipment and participation in conferences. All our doctoral students work on their doctoral theses as part of the projects implemented at the Institute.

Several projects are funded by the European Union. Within the program Horizon 2020 we carry out the project PathoGelTrap – "New blue revolution through a pioneering pathogen blocking technology by bio-selective hydrogel forming proteins". Our scientists are responsible for the theoretical part of the project which is aimed at inventing a technology for selective blocking of pathogens directly in water. Within the Horizon 2020 RISE program we also participate in the grant ThermaSMART "Smart thermal management of high-power microprocessors using phase-change". ThermaSMART is an international and cross-sectoral network of organizations working on a joint research program in the area of phase-change cooling of microprocessors and high-power electronic devices. The grant is oriented towards supporting the mobility of researchers.

The knowledge and experience of our scientists in the field of quantum technologies resulted in participation in six different projects funded under the QuantERA Programme. The QuantERA Programme is an ERA-NET co-fund from the European Union's Horizon 2020 Research and Innovation Programme. The programme supports excellent Research and Innovation in Quantum Technologies and is a leading European network of 39 public Research Funding Organisations from 31 countries.

The Institute's research facilities, training capabilities, and international collaboration have been considerably expanded recently, in particular, owing to the International Centre for Interfacing Magnetism and Superconductivity with Topological Matter. MagTop is a newly formed constituent of the Institute of Physics. It operates within the International Research Agendas Programme of the Foundation for Polish Science, and is funded by EU and national programmes to a sum of 10 m. EUR. Another grant: „Manufacturing technologies of materials and structures used for X and gamma radiation detection, using low-defect uniform (Cd,Mn)Te crystals with high resistivity to radiation caused defects" (INNDEX) was financed within the National Centre for Research and Development TECHMATSTRATEG programme by a sum of 13 m. PLN. We also participate in four other grants under the TECHMATSTRATEG programme as consortium member.

Participation in international research infrastructure projects is an important opportunity for scientists in their work. This is possible thanks to funding from the state budget (Ministry of Education and Science) under the „Support for participation of Polish research teams in international research infrastructure projects" programme. The Institute is a member of three consortia supported by this programme.



European collaboration of the Institute. Thickness of the connecting network lines shows the intensity of the collaborations.

- The Institute coordinates Poland's participation in the European Synchrotron Radiation Centre (ESRF) in Grenoble, France. The aim of the activity is to provide Polish scientists with access to ESRF. Polish scientists and technologists gain access to a unique device enabling research and education of scientific staff at the highest world level.

- We coordinate also participation of Polish scientific units in the international AEgIS (Antihydrogen Experiment: Gravity, Interferometry, Spectroscopy) experiment conducted at the European Organization for Nuclear Research CERN. The main goal of the AEgIS experiment is to directly and very accurately measure the acceleration of a neutral antihydrogen atom in the Earth's gravitational field. Thus, an attempt will be made to precisely check the so-called weak equivalence principle for objects made of antimatter.

- The Institute is a member of the consortium „XFEL Centres of Excellence Network". The aim of the project is to support the Polish scientific community in the use of the European X-ray Free Electron Laser (EuXFEL) for the implementation of innovative scientific research. The Institute of Physics is responsible for the implementation of the scientific programme of the project.

Krystyna Jabłońska has initiated formal access of Polish scientists in European Synchrotron Radiation Facility in Grenoble, France.

Magdalena Załuska-Kotur
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Outreach and popularization of physics

The Institute of Physics of the Polish Academy of Sciences (IP PAS) has consistently prioritized the accessibility and engagement of physics for all. We have actively pursued the popularization of physics to the public for many years. The institute's involvement extends to major events such as the Science Picnic and the Science Festival. Additionally, we conduct popularization lessons for students and teachers, organize workshops for children and youth, including those from the National Fund for Children, and offer summer internships for students. As a co-organizer, the IP PAS contributes to various physics competitions such as the Physical Trails, Young Physicists' Tournament, and Physics Competition. Furthermore, the institute's employees contribute to the popularization of physics through a series of articles in esteemed magazines like Delta, Postępy Fizyki, and Wiedza i Życie. To reach a wider audience, the IP PAS has its own YouTube channel (https://www.youtube.com/@instytutfizykipolskiejakad6047) featuring over 140 lecture videos covering significant topics in contemporary physics.

The Institute of Physics actively engages in prominent events like the Science Picnic and the Science Festival. The Science Festival, initiated in 1997 by scientific community, has been hosting open lectures and workshops organized since 1998. The Science Picnic, on the other hand, was introduced through the collaboration of Łukasz Turski, Tadeusz Skośkiewicz, and employees of Polish Radio, including Krystyna Kępska-Michalska and Robert Firmhofer. The inaugural Science Picnic, known as the Science Picnic of Polish Radio BIS, took place on June 14, 1997, at the Market Square of Nowe Miasto. At this event, the IP PAS showcased a booth with liquid nitrogen, captivating visitors with frozen roses, which subsequently became an iconic symbol of the Science Picnics that followed.

Our highly attended booth at the 2019 Science Picnic of the Polish Radio and the Copernicus Science Center.

The Institute of Physics of the Polish Academy of Sciences offers popularization lessons that aim to promote physics education among students and teachers. These lessons are conducted in the form of engaging demonstrations. Marek Fołtyn delivers a

lecture on the history, techniques, and properties of materials at low temperatures, including superconductivity and superfluidity. Andrzej Wiśniewski's lecture focuses on the fundamental properties, microscopic theory, and applications of superconductivity, accompanied by a captivating magnet levitation demonstration. Marek Godlewski offers several lectures that cover a range of topics, including the history of light sources and the importance of modern and efficient lighting, innovative applications of lasers in medicine for bloodless surgery, cancer detection, and therapy, as well as the challenges posed by population growth, energy, water, food supply, pollution, poverty, and climate change. Moreover, these lectures provide inspiring examples of pro-ecological activities. The „Thursdays with Physics at IP PAS" workshops cater to preschool and school-age children (ranging from 4 to 19 years old) and are led by Beata Brodowska and Izabela Kudelska. These workshops are thoughtfully designed to align with the participants' age group, incorporating elements of playful learning and hands-on engagement through conducting simple physical experiments. The topics covered in the workshops, as well as their duration, vary to suit the specific needs and interests of each age group. The level of each workshop is carefully adjusted to match the perceptual abilities of the participants, ensuring an optimal learning experience for all.

The Institute's range of popularization activities also includes guided visits to laboratories, where participants can explore various fascinating aspects of scientific research. Piotr Dziawa provides insights into the MBE technique, explaining the preparation process for growing semiconductor layers and ensuring material purity. Wojciech Wołkanowicz discusses the structure and operational principles of SEM microscopes, covering image interpretation and chemical composition determination. Students have the opportunity to observe familiar objects under the microscope. Tomasz Wojciechowski delves into SEM construction, operation, sample preparation, and image interpretation, showcasing electron microscopy research. Marta Aleszkiewicz demonstrates scanning probe microscopy techniques, highlighting their working principles and surface property analysis, with a focus on STM. Bartłomiej Witkowski and Monika Ożga showcase the production of zinc oxide nanorods using a regular induction cooktop, examining the results with a scanning electron microscope. They emphasize the applications of nanotechnology and the simplicity of nanostructure production. Izabela Kamińska, Bożena Sikora, Krzysztof Fronc, and Anna Borodziuk provide a laboratory demonstration covering various topics. They showcase methods of synthesizing nanoparticles, quantum dots, and core/shell structures in the Biological Physics Laboratory. The optical and magnetic properties of these structures are explored, and participants have the opportunity to witness the luminescence (upconversion) of nanoparticles in organic solutions and nanopowders.

Beata Brodowska showcasing aspirin crystals grown by workshop participants under a microscope connected to a laptop during workshops for children and teenagers.

The potential applications of these structures, including hyperthermia, photodynamic therapy, and MRI imaging, are also highlighted. Moreover, students get to observe different cell lines (such as cervical cancer (HeLa), breast cancer (4T1), and others) under an optical microscope during the lesson.

The Institute also organizes workshops specifically tailored for youth recipients of the National Fund scholarship. These workshops attract talented students from across Poland who compete for a 5-day internship at the Institute. Each year, 6-8 research topics and qualification tasks are meticulously prepared for these aspiring physics enthusiasts. Successful participants are given the opportunity to collaborate with the team responsible for the chosen topic, engaging in small group learning and utilizing state-of-the-art equipment, thus acquiring valuable research methodology skills. The workshops culminate in a seminar where the groups present their findings. Additionally, the Institute offers summer internships for high school students who are keenly interested in physics. The Institute of Physics actively collaborates in the organization of several physics competitions, namely the Physical Trails, Young Physicists' Tournament, and Physics Competition. The Young Physicists' Tournament, overseen by Leszek Gładczuk, is a competition for high school students jointly organized by the Polish Physical Society, the Institute of Physics of the Polish Academy of Sciences, and the Teaching Department of Experimental Physics at the University of Wrocław. The Physical Trails Competition, chaired by Andrzej Wiśniewski, caters to primary and high school students and is organized by the National Centre for Nuclear Research and the Institute of Physics. The Physics Competition, coordinated by Jan Mostowski, holds the distinction of being the oldest subject competition in Poland, commencing in the 1951/1952 academic year. Poland played a pivotal role in establishing the International Physics Competition, with the inaugural edition taking place in Warsaw in 1967. The competition is organized by the Polish Physical Society.

It is imperative to acknowledge the contributions to popularization activities of retired professor Grzegorz Grabecki. Grabecki's extensive involvement encompasses various initiatives, such as organizing the Institute's exhibition stand at the Science Picnic, delivering engaging interactive lessons during the Science Festival, and coordinating Open Days. He has conducted captivating experiments at the Institute and visited schools, showcasing his popularization programs. Additionally, his role as a co-organizer and esteemed jury member has been instrumental in the Institute's competitions. As Deputy Director, Professor Grabecki has effectively supported staff in promoting physics through diverse channels. His unwavering dedication to advancing the dissemination of scientific knowledge stands as a cornerstone of the Institute's accomplishments.

Grzegorz Grabecki conducting an interactive demonstration lesson on mechanics during the Science Festival.

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