IX PhD STUDENTS SYMPOSIUM

in Kazimierz Dolny nad Wisłą



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"Sapientia ducet ad astra"

Dear Fellow Participants, Professors, Doctors & Students,

Time flies! And indeed, with a summer days approaching, we're happy to announce 9th Students Symposium, which is held third consecutive year in a welcoming and cozy atmosphere of Kazimierz Dolny above the Wisła river.

We sincerely hope that these PhD Symposiums bring You positive experience and help to improve the presentation skills, deal with performing anxiety issues, surpass the English language barrier and learn about fascinating investigations performed in our Institute by fellow friends. Moreover, that you've a chance to meet new friends and spend good time)

Let's bring the Symposium to a higher level and enjoy every second of it together.

Sincerely,

Students Representative Council: M. Grzybowski, O. Chumak, K. Levchenko

Warsaw, IFPAN, 2017

CONTENT

G. P. Mazur, D. Sztenkiel, M. Foltyn, R. Adhikari, K.Kosiel, K. Gas, M. Zgirski, R. Kruszka, R.Jakieła, T. Li, A. Piotrowska, A. Bonanni, M. Sawicki & T. Dietl
Stretching Magnetism with an Electric Field in a Nitride Semiconductor
D. Kwiatkowski , L. Cywiński Entanglement Dynamics of NV Centers Coupled to a Bath of C-13 Nuclear Spins7
<i>M. Zięba</i> , <i>W. Wołkanowicz</i> , <i>B. Taliashvili</i> , <i>P. Dziawa</i> , <i>R. Minikayev</i> , <i>A. Reszka</i> , <i>K. Dybko</i> , <i>M. Sawicki</i> , <i>T. Story</i> Ferromagnetic and Structural Properties of Sn ₁ , Mn, Te Layers
<i>M. J. Grzybowski</i> , P. Wadley, K. W. Edmonds, R. Beardsley, V. Hills, R. P. Campion, J. S. Chauhan, B. L. Gallagher, M. Majewicz, T. Dietl, V. Novák, T. Jungwirth, F. Maccherozzi, S. S. Dhesi, M. Sawicki Towards Imaging Current-Induced Switching of Single Antiferromagnetic
Domains in CuMnAs
O.M. Chumak, A. Nabiałek, R. Żuberek, L. T. Baczewski, I. Radelytskyi, H. Szymczak, T. Yamamoto, T. Seki, K. Takanashi Magnetoelastic Properties of the Epitaxially Grown Layers of Co ₂ Fe _{0.4} Mn _{0.6} Si and Co ₂ FeGa _{0.5} Ge _{0.5} Heusler Alloys
Y. Konopelnyk , I. Radelytskyi, P. Iwanowski, D. J. Gawryluk, M. Berkowski, R. Diduszko, J. Fink-Finowicki & H. Szymczak Magnetic and Magnetocaloric Properties of Cobalt Substituted Fe ₇ Se ₈ Single Crystals
<i>A. Grochot</i> , <i>G. Springholz</i> , <i>A. Ney</i> , <i>G. Bauer</i> , <i>W. Jantsch & H. Przybylińska</i> Magnetic Properties of Ge1-xMnxTe – Multiferroic Semiconductor12
K. Karnas, A. Sawicki Universality of d-mode Gates
<i>J. Plachta</i> , M. Szot, A. Kaleta, A. Petruchik, L.T. Baczewski, G Karczewski, T.Wojtowicz, J. Kossut & P.Wojnar Growth and Properties of Type II ZnTe/CdSe Radial Nanowire Heterostructures14
K. Kalbarczyk, M. Foltyn, R. Adhikari, A. Bonanni, T. Dietl & M. Sawicki Electron Transport in GaN:Si/(Ga,Mn)N/GaN:Si Spin Filter Structures

R. Rudniewski, D. Śnieżek, M. Szot, M. Wiater, J. Wróbel, T. Wojtowicz Toward Spin Filter Based on Cd _{1-x} Mn _x Te Quantum Wells16
 P. Caban, R. Pietruszka, K. Kopalko, B. S. Witkowski, S. Gierałtowska, R. Jakieła, K. Gwóźdź, E.Płaczek-Popko, M. Godlewski p-ZnO/n-GaAs Heterojunction Solar Cells Fabricated by the ALD and RTP Methods
D. Śnieżek, K. Dybko, P. Dziawa, M. Szot, R. Rudniewski, M. Majewicz, M. Aleszkiewicz, M. Wiater, T. Wojtowicz, T. Story, T. Dietl & J.Wróbel Ballistic Transport of Topological Surface States in SnTe/CdTe Interface
K. Koroński, A. Kamińska, P. Strąk, A. Wierzbicka, M. Sobańska, K. Kłosek, Z. Żytkiewicz, E. Grzanka, J. Borysiuk, K. Sobczak, E. Monroy, S. Krukowski Optical Properties of GaN/AlGaN Multi-Quantum-Wells: Ambient And High-Pressure
Study
 M. Grabowski, P. Kruszewski, P. Prystawko, A. Nowakowska-Siwinska, M.Sarzynski & M. Leszczynski Properties of AlGaN/GaN Ni/Au Schottky Diodes on 2-off Silicon Carbide Substrates
K.Gibasiewicz , J. Kasperski, I. Makarowa, S. Grzanka, T.Suski and P. Perlin Practical Method of Fast Fabrication of 1µm diameter µLEDs21
D. Kalinowska, M. T. Klepka, A. Wolska, A. Drzewiecka-Antonik, C. A. Barboza, E. Heishman
Local Atomic Structure Investigation of Novel Coumarin Schiff Base Complex with Copper Ions
A. Sulich, E. Łusakowska, J.Z. Domagala, P. Dziawa, W. Paszkowicz Structural Properties of SnTe Films Grown on Miscut GaAs(001): XRD and AFM Studies
A.Kaleta, S. Kret, B. Kurowska, J. Sadowski Structural Investigations of Core-Shell III-V Semiconductor Nanowires by TEM Methods
<i>K. Morawiec, P. Dłużewski, S. Kret, M. Barańska, J. Sadowski</i> GPU Application for In-Line Electron Holography
<i>L. Kielesiński, A. L. Sobolewski, D. T. Gryko</i> Coumarines Photophysics – Still Challenge in XXI Century

9th PhD Students Symposium, Kazimierz Dolny, 2017

R. Oldziejewski, K. Rzążewski Quantum Measurement of two Bosons
D. Pęcak, M. Gajda and T. Sowiński Experimentally Accessible Invariants Encoded in Interparticle Correlations of Ultra-Cold Fermions
J. Mikulski, B. Sikora, K. Fronc, P. Wojnar, P. Aleshkevych, Ł. Kłopotowski, J. Kossut Colloidal Quantum Dot Doped with Copper
<i>K. Wolek, and M. Cieplak</i> Assembly and Aggregation of Thermally Denaturated Protein Complexes in Coarse- Grained Models
 P. Kowalik, D. Elbaum, K. Fronc, J. Mikulski, A. Borodziuk, I. Kamińska, M. Szewczyk, K. Zajdel, G. Gruzel, P. C. Morais, E. Mosiniewicz-Szablewska, M. Pawłyta, R. Minikayev, T. Wojciechowski, A. Sienkiewicz, M. Łapiński, P. Stępień, W. Paszkowicz, M. Frontczak-Baniewicz, A. Gardias, J.Rybusiński, J. Szczytko, A. Twardowski, P. E. de Souza, R. B. Nunes, F. H. Veiga-Souza, B. Sikora Biological and Medical Application of Up-Converting Rare-Earth Ions Doped NaYF4 Nanoparticles and Magnetic Fe₃O₄ Nanoparticles
<i>NOTES</i>

Stretching Magnetism with an Electric Field in a Nitride Semiconductor

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Interplay between magnetic and electric properties of magnetic layers is of a considerable interest owing to possibility of low--power information storage and processing. Several different ways have been exploited for agile control of magnetization vector by an electric field including gating of thin ferromagnetic layers [1], electric and magnetic coupling in multiferroics [2] or strain in hybrid magnetic/piezoelectric devices. In this paper we show that the application of an electric field along a polar axis in a wurtzite magnetic semiconductor leads to a sizable change of its crystalline magnetic anisotropy via the inverse piezoelectric effect. We investigate this new phenomenon experimentally and theoretically in an insulating paramagnetic wz-Ga_{0.975}Mn_{0.025}N as a function of temperature, magnetic, and electric field, see **Fig. 1**.



Fig. 1: Left panel: Sample structure and set-up for magnetization measurements in phase with an applied electric field. Right panel: Changes in magnetization ΔM_E induced by an electric field of 0.47 MV/cm applied to (Ga,Mn)N at selected temperatures as a function of the magnetic field applied along the hard axis. Red curves depict results of theoretical modeling employing known values of the piezoelectric constant and parameters of single-ion Mn³⁺ anisotropy. To take into account ferromagnetic Mn-Mn interactions, simulations have been performed for lower temperatures (shown near curves). Inset shows a decrease of ΔM_E with temperature.

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Entanglement Dynamics of NV Centers Coupled to a Bath of C-13 Nuclear Spins

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The ms = 0 and ms = 1 levels of nitrogen-vacancy (NV) center in diamond form a qubit that can be initialized, controlled, and read out at room temperature, and which is intensively researched in the context of nanoscale magnetic imaging applications [1]. The main source of decoherence of this qubit is its interaction with the bath of C-13 nuclei. Recently, entanglement between two NV centers (separated by ca. 20 nm) was created [2]. We present an extension of calculation of decoherence due to the nuclear bath (using the state-of-the-art Cluster-Correlation Expansion method [3,4]) to the case of two qubits. We also include the presence of magnetic field gradient which is helpful for separate addressing of the two qubits, but which modifies the nuclear dynamics.

Entanglement of two-qubit Bell states calculated in pure-dephasing approximation is simply related to two-qubit coherences $\rho 01;10$ and $\rho 00;11$. When two qubits interact with a partially common bath (as is the case for two nearby NV centers), the decay of these coherences can be slower or faster than the decay of product of single-qubit coherences, depending on whether the bath is source of correlated/anticorrelated noise, respectively.

We investigate the nature of effective magnetic field noise generated by the bath of nuclear spins coupled by dipolar interaction. Flip-flopping nuclear spin pairs can either accelerate or slow down the two-qubit decoherence, depending on their position and orientation relative to the two qubits. For moderate NV-NV distance (10 nm) the decoherence acceleration dominates, but at shorter distances the noises experienced by the two qubits become correlated, and decoherence is suppressed.



Fig. 1: Coherence for: (a) single qubits - Wi and entangled pair - W12 for centers 5 nm apart. (b) $\Lambda = W12/(W1W2)$ for NV-NV distances: 2.5 nm, 5 nm (dashed) and $\Lambda = 1$ line

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Ferromagnetic and Structural Properties of Sn1-xMnxTe Layers <u>M. Zięba¹</u>, W. Wołkanowicz¹, B. Taliashvili¹, P. Dziawa¹, R. Minikayev¹, A. Reszka¹, K. Dybko¹, M. Sawicki¹, T. Story¹

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 $Sn_{1-x}Mn_xTe$ is a IV-VI diluted magnetic (semimagnetic) semiconductor exhibiting ferromagnetic, spin glass or paramagnetic properties depending on conducting hole concentration and Mn content [1]. In bulk crystals grown by the Brigdman method the thermodynamic solubility limit of Mn in rock-salt SnTe crystals is x=0.12. The corresponding ferromagnetic Curie temperature is about 20 K for optimal hole doping [1]. In the early studies of thin $Sn_{1-x}Mn_xTe$ layers grown by molecular beam epitaxy (MBE) the single crystal rock-salt phase was observed only for quite low Mn content x≤0.04 [2]. Recent renewal of interest in SnTe-based semiconductor alloys is related to the discovery of topological crystalline insulator states at (001) and (111) surfaces of bulk SnTe crystals [3], with a variety of new theoretical proposals concerning ultrathin SnTe layers and SnTe-based materials with nonzero magnetization [4]. In this work, we study the growth of Sn_{1-x}Mn_xTe layers by MBE under various stoichiometry regimes known to determine carrier (hole) concentration and magnetic properties.

 $Sn_{1-x}Mn_xTe$ monocrystalline layers with the Mn content x \leq 0.09 and the thickness about 1 micron were grown by MBE on fresh cleaved and epi-ready BaF2 (111) substrate. Apart from SnTe and Mn fluxes we used additional Te flux to control variation from stoichiometry in layers. The X-ray diffraction analysis of the layers (x \leq 0.05) revealed the expected (111) growth direction and the rock-salt crystal structure with the lattice parameter following the Vegard law. For the layer with the highest Mn content (x=0.09) additional diffraction peaks were found and assigned to inclusion of $Sn_{1-x}Mn_xTe$ with (001) crystal orientation and inclusions of anti-ferromagnetic MnTe. Magnetic properties of the layers were examined over temperature region T=3-300 K by electron paramagnetic resonance (EPR), SQUID magnetometry and anomalous Hall effect measurements. The layers grown under close to stoichiometry regime revealed Curie-Weiss paramagnetic properties with the EPR angular dependence indicating only a weak magnetic anisotropy effects. For Sn_{1-x}Mn_xTe layers grown under excess tellurium regime a ferromagnetic transition was observed at helium temperatures.

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Towards Imaging Current-Induced Switching of Single Antiferromagnetic Domains in CuMnAs

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Antiferromagnetic materials are of increasing interest for potential applications in spintronics. Their zero net magnetic moment, resulting from alternating directions of neighboring moments, makes them insensitive to quite strong external magnetic field. However, magnetic order in antiferromagnets can be manipulated by staggered current-induced fields resulting from relativistic spin-orbit coupling in materials with local inversion asymmetry, which was shown for CuMnAs [1]. A study of electrical switching of CuMnAs thin film devices with simultaneous electrical (anisotropic magnetoresistance – AMR) and photoemission electron microscopy (PEEM) measurements was reported [2]. Together, the applied techniques allow observation of the domain pattern of the material, identification of pronounced changes of the domains under the influence of current-induced torques, and determination of the dependence on current magnitude. The spatial inhomogeneity of the effect is observed. Here, we present experiments leading to the observation of single antiferromagnetic domain switching, showing the current status of the work, challenges to overcome and perspectives.



Fig.1 PEEM image of CuMnAs surface with domain structure visible.



Fig.2 Micrograph of the 1.5 μ m size cross shaped device defined by separation trenches (dark regions) etched down to the substrate

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Magnetoelastic Properties of the Epitaxially Grown Layers of Co₂Fe_{0.4}Mn_{0.6}Si and Co₂FeGa_{0.5}Ge_{0.5} Heusler Alloys

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The out-of-plane magnetocrystalline anisotropy and magnetoelastic properties of series of epitaxially grown layers of $Co_2Fe_{0.4}Mn_{0.6}Si$ (CFMS) and $Co_2FeGa_{0.5}Ge_{0.5}$ (CFGG) Heusler alloys thin films [1] deposited on MgO with chromium buffer layer were investigated by means of the ferromagnetic resonance, SQUID magnetometer and by the strain modulated ferromagnetic resonance technique [2].

The change of the anisotropy is caused mainly by the surface effects [3]. However, for some of the samples series the change of chemical ordering with the change of the magnetic layer thickness was also observed. An additional silver buffer layer influence on the properties of the laver magnetic was also investigated. For all three of the investigated series of the Heusler alloys, i.e. CFMS without Ag, CFMS with Ag and CFGG, the experimentally observed magnitude of the magnetoelastic constant [4] increases with the increase of the magnetic layer thickness.



Fig. 1: Magnetoelastic constants of the three series of CFMS or CFGG samples studies at room temperature, as a function of the inverse of magnetic layer thickness.

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Magnetic and Magnetocaloric Properties of Cobalt Substituted Fe₇Se₈ Single Crystals

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The main purpose of this research is to determine magnetocaloric efect (MCE) in iron selenide Fe_7Se_8 (3c type) single crystals doped with 2% of cobalt atoms. The single crystals have been grown applying modified Bridgman's method. Magnetization measurements have been carried out using magnetometer SQUID MPMS 7XL. MCE has been determined based on M(H,T) measurements.

The compound is ferrimagnetic metal with high Neel temperature. The 3c type structure derives from the hexagonal (NiAs-type) by introducing ordered Fe vacancies. The first order phase transition of the spin reorientation type from easy c-axis to easy c-plane has been observed near the temperature $T_r \approx 132$ K. Conventional magnetocaloric effect related to the metamagnetic transitions has been found above T_r while below T_r inverse MCE was identified. The magnetization and magnetic anisotropy as a function of temperature have been measured and discussed in relation to the observed rotational magnetocaloric effect.

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Magnetic Properties of Ge_{1-x}Mn_xTe – Multiferroic Semiconductor A. Grochot¹, G. Springholz², A. Ney², G. Bauer², W. Jantsch², and H. Przybylińska¹

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Amongst single phase multiferroics, materials which are simultaneously ferroelectric (FE) and ferromagnetic (FM) are very rare. One of them is $Ge_{1-x}Mn_xTe$, a multiferroic semiconductor, in which FE and FM orders coexist at low temperatures up to Mn content of x = 0.5. As demonstrated previously with use of ferromagnetic resonance (FMR), in MBE grown $Ge_{1-x}Mn_xTe$ layers deposited on (111) BaF_2 substrates the ferromagnetic and ferroelectric moments are coupled to each other, leading to reversal of ferroelectric polarization under relatively low externally applied magnetic fields [1].

In the present study we demonstrate that magnetic field induced ferroelectric polarization reversal can be even entirely suppressed in the presence of exchange bias. A series of 500 nm thick $Ge_{1-x}Mn_xTe$ layers (with x ranging from 0.18 to 0.3) grown at the same conditions as those used in **Ref. 1** but terminated with a thin Te/Se cap layer to prevent sample degradation (Mn out diffusion and oxidation) was investigated using the FMR technique. In contrast to previous studies where two FMR signals were observed,

corresponding to two FE domains differing by rotation of oblique <111 > axes by 180° around the [111] growth direction, in the capped samples only one dominant FMR signal is detected. Also, whereas previously the intensities of the FMR signals could be switched between the two domains by appropriate rotation of the magnetic field, in the capped layers no domain switching occurs. At the same time, in all layers we detect a significant (exceeding 300 G at 3 K) internal, unidirectional magnetic field Hint. This field is tilted with respect to the [111] growth axis (which is the easy magnetization direction in the investigated Ge_{1-x}Mn_xTe composition range) and points towards the substrate. The tilt angle depends on Mn composition x and temperature T. A similar exchange field, but oppositely directed (out of the layer surface) is observed for Ge_{1-x}Mn_xTe grown on a 20 nm thick PbEuSe buffer. We attribute Hint to exchange field induced by uncompensated and pinned Mn spins at the interface between the antiferromagnetic (AFM) cap (or buffer) and ferromagnetic Ge_{1-x}Mn_xTe layer.

In contrast to typical FM/AFM structures, where the direction of the bias field can be set by cooling below the Néel temperature in an applied magnetic field, in the studied samples the exchange field appears spontaneously with no field cooling and its direction cannot be reversed with field cooling up to 1 T available in the experimental setup.

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Universality of d-mode Gates

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We consider the problem of deciding if a set of quantum d-mode gates $S = \{g_{1,-}, g_k\} \subset G$ is universal, i.e. if the group generated by S, which we denote by $\langle S \rangle$, is dense in G, where G is either the special unitary group SU(d) or the special orthogonal group SO(d). In other words we ask if every d-mode gate can be constructed with an arbitrary precision using the elements of S. Such a set is called universal.

In order to answer this question we assign to every gate $g_i \in S$ the orthogonal matrix Ad_g that is the image of g under the adjoint representation $Ad: G \to SO(Lie(G))$, where Lie(G) is the Lie algebra of G. As we have shown using theory of Lie groups and Lie algebras, the necessary condition for the universality of S is that the only matrices that commute with all the matrices Ad_{g_i} are proportional to the identity. Next we will briefly present the conditions for S providing that $\langle S \rangle$ is an infinite group. Using these results we provide a simple algorithm that allows deciding the universality of any set of d-mode gates in a finite number of steps. and present it on examples of universal and non-universal sets of 2-mode gates.

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Growth and Properties of Type II ZnTe/CdSe Radial Nanowire Heterostructures

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The most common design of a quantum well involves a band alignment providing a potential minima for holes and electrons in the same part of a sample, so the probability of recombination is maximized. This configuration is often called type I junction, as opposed to type II (**Fig 1a**), where both conduction and valence band of one semiconductor are situated energetically below (or above) the other one. This layout allows for charge separation and is commonly found in p-n diodes. Thanks to such a band alignment, an "indirect" (in real, not momentum space) exciton is formed after an excitation. The behavior of such an "indirect" exciton exhibits several interesting properties and grants access to some emission energies, which would not be available with ordinary bandgap engineering.



Fig. 1 a) type I versus type II band alignment; b) normalized emission from an as-grown nanowire sample as a function of excitation power. Excitation powers were 1;4;12.5 mW from left to right, T=10K, λ_{ex} =473nm

This kind of structure was realized in a radial ZnTe/CdSe nanowire heterostructure capped by (Zn,Mg)Te or (Cd,Zn)Se shell. ZnTe and CdSe are nearly lattice matched, so it is almost strainfree. The nanowires were grown by molecular beam epitaxy (MBE) in vapour-liquid-solid (VLS) mode. They were about 1.5um long and 60-70nm in diameter. CdSe layer is estimated to be less than 10 nm.

The chosen band alignment should result in a near infrared emission, at approximately 1.1eV. This emission has indeed been observed in as-grown nanowires as well as the reference sample containing a quantum well (QW). Emission from nanowire samples and a QW exhibit a strong (tens of meV at 5K) blueshift as a function of excitation power increase (**Fig 1b**). This effect is due to coulomb interaction between same sign charges, which raises the energy of the transition with a charge buildup [1]. Another interesting feature of the indirect transition is a lower probability of recombination because of a charge separation. This results in a longer exciton lifetime and a different decay characteristics [2]. For radial structures

where charge is separated, yet another effect has been predicted – an optical Aharonov-Bohm effect, observation of which is the main motivation directing this research. It was initially investigated in columnar quantum dot ensemble [3] and quantum rings [4]. Our plan is to check if it can be observed in nanowires as well.

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Electron Transport in GaN:Si/(Ga,Mn)N/GaN:Si Spin Filter Structures K. Kalbarczyk¹, M. Foltyn¹, R. Adhikari², A. Bonanni², T. Dietl^{1,3,4,5}, and M. Sawicki¹

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In our project we want to verify experimentally theoretical prediction about large spin filtering capabilities of spin filters and resonant tunneling diodes involving insulating ferromagnetic barriers. The tunneling spin-filter effect in a metal/ferromagnetic insulator/metal tunnel junction takes place when electrons with randomly oriented spins tunnel from the Fermi level of the nonmagnetic metal through the spin-dependent barrier. The spin-split conduction band of the ferromagnetic part creates a lower barrier height for spin-up electrons (\uparrow) and higher barrier height for spin-down electrons (\downarrow), giving rise to a highly spin-polarized current, as depicted in **Fig. 1a** [1].



The barrier material which we use is (Ga,Mn)N - a ferromagnetic insulator whose long range ferromagnetic ordering has been confirmed at the low end of cryogenic temperatures [2]. In our first fabrication attempt to prepare the spin filter structure a few hundred micrometers contacts were defined. Such structures turned out to be good conductors and showed linear IV characteristics. It was concluded that the structures were shorted by highly conductive sapphire-GaN misfit-related threading dislocations (TDD). Two solutions have been proposed to eliminate the detrimental influence of TDD: i) a use of structures grown homoepitaxially on GaN substrates, and ii) a reduction of the structures to a submicrometer size. While the former structures have not been obtained yet, the latter approach has been exercised recently very intensively. **Fig. 1b** shows an example of a test structure of e-beam lithography obtained Au "air bridge" – an vital element of the structure required to connect a micrometer size vertical structure with external experimental setup. This technological effort is the first step towards elaboration of fully operational submicrometer devices.

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9th PhD Students Symposium, Kazimierz Dolny, 2017

Toward Spin Filter Based on Cd_{1-x}Mn_xTe Quantum Wells <u>R. Rudniewski</u>¹, D. Śnieżek ¹, M. Szot ¹, M. Wiater¹, J. Wróbel ^{1,2}, T. Wojtowicz ^{1,3}

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Generation of pure spin current is one of the important steps during engineering of new semiconductor devices leading to development of spintronics and quantum computing. I concentrate on creating spin filters as a devices based on electron spin splitting and separation of flowing electrons into two oppositely polarized branches. One way to realize this kind of device is to produce "Y" shape nanostructure [1,2] from semiconductor quantum structure using multi-step electron beam lithography, etching and metallic gate deposition. In this presentation I will focus on demonstrating how to modify edge states using quantum point contacts and to fulfill condition necessary for spin filtration. I will show first result on sample preparation and magnetotransport measurements at mK temperatures.

Our material, modulated doped $Cd_{1-x}Mn_xTe$ quantum wells, is particularly well suited to successfully realize this project because of the strong exchange interaction between spins of localized magnetic ions and spins of high mobility two-dimensional electron gas, resulting in a very large electron g-factor [3]. Large g-factor allows to obtain a large spin splitting at the Fermi level already at low external magnetic fields, favorable for effective spin separation.

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p-ZnO/n-GaAs Heterojunction Solar Cells Fabricated by the ALD and RTP Methods

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Fabrication of the p-ZnO/n-GaAs heterojunction solar cells was the aim of this research. Photovoltaic structures were prepared with the use of ALD and RTP methods.

Both GaAs single crystal (100) substrates chosen for this test were mainly characterized by their low resistivity as well as low donor concentration that was of 10^{15} [cm⁻³] for the undoped GaAs and 10^{17} [cm⁻³] for GaAs doped with tellurium. After the bottom contact structure Ni/Ge/Au/Ni/Au was evaporated, the GaAs wafers underwent the ALD process of n-ZnO layer deposition at 200°C. Then the obtained n-ZnO/n-GaAs structures were annealed (RTP) in the one of five different temperatures within the range of 550-750°C. High temperature of annealing resulted in enhanced arsenic diffusion from the substrate into the n-ZnO layer, what in turn changed its native conductivity type to the opposite one. Such p-ZnO:As converted layers effectively created p-n heterojunction solar cells structures with the underlying gallium arsenide substrates within most of the applied annealing temperatures.

We observed clear photovoltaic effect for such devices with the highest efficiencies gained for annealing temperature of 650°C. In particular efficiency of 2.3% was reported for the undoped GaAs substrate, while the highest one for the GaAs:Te reached 0.73%. Performance of such designed solar cells can be further improved by optimization of top and bottom contact, thickness of ZnO layer and GaAs substrate, temperature and time of annealing as well as by optimizing their electrical properties.



Fig. 1: Comparison of the currentvoltage light characteristics between the p-ZnO/n-GaAs (green and red curves) and n-ZnO/p-GaAs solar cell structures. Symmetry with respect to the X=0 axis points that if the devices on the left side are based on n-p junction then the ones on the right side work on the basis of p-n junction (consequently it also indirectly proves the p-ZnO layer existence).

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9th PhD Students Symposium, Kazimierz Dolny, 2017



Ballistic Transport of Topological Surface States in SnTe/CdTe Interface

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In the last years, IV-VI semiconductor materials are actively studied because many of them belong to a new class of the so-called 3-dimensional topological crystalline insulators (3D TCI) [1,2]. This state of matter is characterized by the presence of conducting surface states, which are protected against backscattering by the symmetry of the crystal lattice. However, transport studies of 2D surface states in this system are strongly hindered by the intrinsic p-type conductivity of bulk material. In order to separate both contributions, we have performed the non-local transport measurements on multi-terminal Hall bar structures, patterned from CdTe/SnTe/CdTe quantum well. Another approach is to measure capacitance of surface states. By utilizing gate to limit bulk carriers it is possible to probe primarily the top surface [3].

Our devices have been prepared from a 20 nm thick SnTe epilayer that was grown on (100) GaAs substrate with 4 μ m CdTe buffer and then covered by 100 nm cap of CdTe. Hall bar samples have been patterned using the low-temperature electron beam lithography method [4]. Additionally we prepared three gated samples dedicated to capacitance measurements. Each one was covered with 160 nm thick SiO₂/Si₃N₄ layer under 50 nm Cr/Au gate. First one is 6-terminal Hall bar with channel of size 1000 μ m x 60 μ m. Second one with the same structure is with channel divided into stripes of size 1000 μ m x 2 μ m to facilite control of carrier density. The last one is 8-terminal microstructure with channel 7 μ m x 3 μ m.

We have analised the local- and non-local quantum transport using a low-frequency lock-in technique and compared it to what was reported in [5,6]. We have observed a very strong non-local magnetoconductance signal for several current-voltage contact configurations. Moreover we plan to control carrier density and probe capacitance of surface states with gates samples. The measurements have been performed in 3He cryostat at temperatures down to 250 mK and magnetic fields up to 7 T.



Fig. 1: Microscope picture of one sample dedicated to capacitance measurements. The area under the gate was divided into long stripes of width 2 μ m and depth 155 nm

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Optical Properties of GaN/AlGaN Multi-Quantum-Wells: Ambient and High-Pressure Study

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In the presentation the results of spectroscopic study of GaN / AlGaN multi- quantum wells series with the same geometry and different Al content in the barriers will be shown. The structure of the samples was determined using X-ray diffraction and transmission electron microscopy imaging. The characterization of optical properties of the samples was made using a variety of optical methods. The influence of high pressure on the quantum confined Stark effect and the internal electrical fields resulting from spontaneous and piezoelectric polarization will be discussed.



Fig. 1. Dependence of photoluminescence energy and photoluminescence pressure coefficient on Al content in the barriers

Properties of AlGaN/GaN Ni/Au Schottky Diodes on 2-off Silicon Carbide Substrates

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The current–voltage characteristics of planar Ni/Au Schottky diodes fabricated on top of AlGaN/GaN structures with two different surface miscut, 0.5 and 2°-off, were measured at elevated temperatures of up to 580 K and then discussed. The Schottky contact parameters, such as ideality factor (*n*) and barrier height (φ_b), were extracted by a commonly used thermionic emission approach, combined with Norde's method. In this study, we show that the temperature shift of the Schottky barrier height for a structure with 0.5°-off is equal to 0.5V/100 K, which is close to the value obtained for the temperature dependence of the energy band gap for GaN. We found that for both types of structures the ideality factor decreases with the temperature increase, while the barrier height increases. Finally, we observed some differences in the leakage current mechanism and thermionic behavior, which we attribute to differences in surface homogeneity of diodes fabricated on different surface miscut.

Practical Method of Fast Fabrication of 1μm diameter μLEDs <u>K.Gibasiewicz¹</u>, J. Kasperski¹, I. Makarowa², S. Grzanka¹², T.Suski¹ and P. Perlin^{1,2}

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Nitride optoelectronics is currently the most important and the fastest developing branch of semiconductor optoelectronics. Its economical impact consists among other factors achievements related to efficient emission of the white light and in an opportunity of demonstrating LED-type emitters. In our work we are focusing on two matters. First is answer to a question: if we could make modern LED even more efficient by varying third dimension. Second: if by proper change in third dimension we could fabricate device with completely new properties, like single photon emission.

In this work we applied top-down strategy to MOVPE grown, efficiency-wise optimized LED structures (**Figure 1: A**). Later by application of different approaches: photo-, electronolitography (**Figure 1: C,D,E**), hard masking with nanoparticles (**Figure1:B**), we prepare our sample for RIE plasma etching through upper layers down to n-contact. After etching, our microcolumns can be exposed to various agents which goal is to improve outside surface of our columns. After this stage we planarize and isolate etched columns by applying Spin-On-Glass, which has other advantage that our sample gains rigidity. Also difference in refractive indexes allows our μ LEDs to have some light guiding properties. Last step is to fabricate upper electrical contact.

So far we were able to obtain single, columnar, micro LED with diameter about $\sim 1.5 \mu m$ and characterized it electrically and optically (**Figure 2**). They show diode IV curve with opening voltage around 3 volts which is typical for bulk structure. Spectrum also does not show any deviations from bulk LED s. This conclude that we were able to achieve one of our goals. Next step will be to measure how fast our micro LED can be and if by simply reducing dimensions we could produce very fast device. We believe small and fast devices would find application in communication market.



Fig. 1: Schematic showing various approaches to fabricate µLED and Characterization of single columnar µLED

Local Atomic Structure Investigation of Novel Coumarin Schiff Base Complex with Copper Ions

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Coumarin is a naturally occurring organic compound having a broad spectrum of biological activity. Thereby it can be used in the design of synthetic compounds that exhibit extensive pharmacological activity, i.e. anti-inflammatory, antioxidant, anticoagulants, antiviral, antibacterial, antihyperlipemic, hepatoprotective and anticarcinogenic or cytotoxic [1]. Schiff bases are the condensation products of carbonyl compounds and primary amines often used in the design of new therapeutic substances due to the formation of stable complexes with metal ions [2]. Their complexes with transition metals are the subject of interest due to antimicrobial as well as anticancer activity [3]. Particularly complexes with copper ions exhibit cytotoxic activity against tumor cells. By use of suitable chelating compounds of copper ions the control of angiogenesis, tumor growth and metastasis may be achieved [4, 5].

The unique properties of these compounds make their complexes perfect as potential pharmacological agents. Knowledge of their structure is extremely important in the planning of chemical reactions, intended to obtain the compounds of the assumed physical and chemical properties. However, quite often it is impossible to obtain a complex in a crystalline form. The use of aggressive solvents, in order to force crystallization, may cause structural changes. Therefore, to determine the geometry of complexes X-ray absorption spectroscopy (XAS) technique is needed. This method gives information about the local structure around the specific element and is ideal to study compounds regardless of their crystal form or state.

Our studies were focused on a novel bioactive complex of copper synthesized from 7hydroxy-8-[1-(4-methoxyphenylimino)ethyl]-4-methyl-2H-chromen-2-one and copper(II) chloride. XAS measurements at Cu K-edge were performed at XAFS beamline of the Elettra storage ring (Trieste, Italy). Spectra were collected using transmission detection mode. EXAFS analysis (performed using Demeter software) gave information about the type and quantity of atoms around the copper cation as well as the average distance between absorbing and the neighboring atoms. In our case it revealed that the mononuclear complex is formed and the first coordination sphere of Cu is composed from five oxygen atoms. These information were used to construct structural models of studied complex. Next models were optimized with DFT algorithms (available in the Turbomole version 7.0 software) and XANES calculations were performed (with FEFF 9.6 code).

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9th PhD Students Symposium, Kazimierz Dolny, 2017

Structural Properties of SnTe Films Grown on Miscut GaAs(001): XRD and AFM Studies

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SnTe is one of currently studied topological crystalline insulators [1-4]. For our studies we selected the samples with SnTe(001) film grown on 2° miscut GaAs(001) substrate and investigated them by mean of XRD and AFM techniques.

The obtained results shows that the surface of the samples is shaped into ridge-andvalley structures. The studied structures exhibit orientations close to the two possible crystallographic directions: <110> or <100>, despite the fact, that all of the samples have the same GaAs miscut direction and comparable layers misorientation. We suppose that the differences between the grooves directions are related to Te/SnTe molecular flux ratio which is considered to be a factor influencing the SnTe layer growth mechanism.

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Structural Investigations of Core-Shell III-V Semiconductor Nanowires by TEM Methods

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Nowadays semiconductor nanowires offer a promising technological solution for a wide range of devices in many fields starting from bio-medicine and ending with electronics. the nanowires (NWs) combining the ferromagnetic metals with Particularly. semiconductors are now very interesting nanostructures [1] which can be used, for example in the nonvolatile memory devices containing magnetic information storage. We report the transmission electron microscopy (TEM) analysis of the core-shell semiconductor/intermetallic hybrid NWs with ferromagnetic properties. The NWs were produced using a molecular beam epitaxy (MBE). Firstly, the wurtzite (WZ) structured (Ga,In)As cores were grown on the GaAs(111)B substrates with Au catalyst, then they were covered by (Ga,Al)As, (Ga,Mn)As (or (Ga,Al)As again) and the low temperature (LT) GaAs shells (Fig. 1a,b) [2]. Subsequently, the NWs were annealed at high temperatures (450 °C or 600°C) inducing formation of hexagonal MnAs precipitations (Fig. 1 c,d,e,f). The (Ga,Al)As and LT-GaAs shells were used to confine holes to the (Ga,Mn)As shell, moreover the (Ga,Al)As shells also acted as diffusion barriers for manganese and determined the size and the shape of the MnAs nanocrystals. In this research we investigated the crystal structure quality of as grown NWs by High-Resolution TEM (HRTEM), High-Resolution Scanning TEM (HRSTEM), Energy Dispersive X-ray spectroscopy (EDX) and Geometric Phase Analysis (GPA).



Fig. 1: a) Schematic visualization of the NW cross-section before annealing b) STEM– HAADF image in [0001] zone axis (ZA). c) Scheme of the NW cross-section after annealing d) HRTEM image in [0001] ZA – in circles MnAs nano-participations. e) HRSTEM image in [11-20] ZA with visible MnAs nano-participations and f) magnification of the hexagonal MnAs precipitattion.

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GPU Application for In-Line Electron Holography K. Morawiec¹, P. Dłużewski¹, S. Kret¹, M. Barańska¹, J. Sadowski^{1,2,3}

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Due to the electron-optic aberrations present in transmission electron microscope a single image does not allow for direct interpretation of the investigated structure. In order to recover exact information about the specimen structure some additional image refinement needs to be done. By combining a series of differently defocused images (i.e. focal series) it is possible to recover both amplitude and phase of the exit electron wave. This problem is known as the in-line electron holography or exit wave reconstruction (EWR) and (when connected with correction of aberrations) it allows for expanding the image resolution and verifying the specimen structure. The in-line electron holography can be a complementary method for off-axis holography in terms of determination of magnetic field distribution in the sample. In this case two focal series from the same area are required, each one recorded at the same electric, but different magnetic conditions.

By adapting the parallel architecture of GPU we were able to significantly accelerate the computations needed for solving the EWR problem. The procedure known as the IWFR (iterative wave function reconstruction) was implemented in the in-line electron holography software and applied to focal series of two different specimens: (1) ~100 nm in size amorphous acrylic polymer particles, and (2) MnAs nanocrystals (~20 nm in size) embedded in GaAs matrix. In the former case the EWR refinement revealed the core-shell structure of amorphous particles, see **Fig. 1b**. In the latter case two focal series were recorded in order to determine phase changes related to nano-objects' magnetic state. Phase image restored from one of those focal series (**Fig. 1f**) shows a great improvement in contrast and resolution in comparison with the experimental image (**Fig. 1d**).



Fig. 1: Experimental TEM images (a,d) and the results of in-line electron holography, including restored amplitude images (b,e) and restored phase images (c,f), for two kinds of specimens

Coumarines Photophysics – Still Challenge in XXI Century <u>L. Kielesiński^{1,2}</u>, A. L. Sobolewski¹, D. T. Gryko²

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Aromatic oligoamides are intensively explored since they form an amazing variety of discrete architectures such as helixes, tapes and molecular electrets. The main driving force responsible for the stacking of such systems was dipol-dipol and π - π interactions. The mode of tethering in that cases was always head-to-head i.e. D-A-linker-A-D. There is no case of floding of the aromatic compound where moieties or linked in A-D-linker-A-D fashion, which may result in a large polarization of the system.

Recently, it was theoretically predicted, that in ferroelectric columnar assemblies the exceptionally high polarizability of the structure provides a driving force for the splitting of excition and the separation of the electric charge [1]. Such mechanism could potentially be used to construct photovoltaic devices made of organic ferroelectric structures [2-4]. Such ferroelectric assemblies have not been investigated yet in respect to the possibility of charge separation and its influence of the structure. We wanted to design and synthesis a dye built of two, structurally similar coumarin units linked with amide bond as a model chain of the simple ferroelectric system (Scheme 1).



Scheme 1: Synthesis of coumarin dimer.

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Quantum Measurement of Two Bosons

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We observe a remarkable progress in experiments with ultra cold gases. In all of them a measurement of properties characterizing gaseous ensemble is based on atom-light interactions i.e. light absorption. Present theoretical description does not fully accounts for the influence of spatial and temporal properties of a light beam in diagnosing a many-body state of cold atoms. We present a simple theoretical model concerning these issues. Within our model we show how an analysis of statistical properties of an ultra cold gas like density fluctuations and higher order correlation functions may be biased by using a light beam improperly.

Experimentally Accessible Invariants Encoded in Interparticle Correlations of Ultra-Cold Fermions

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A system of two species of fermions of different masses (m \uparrow and m \downarrow) trapped in a onedimensional harmonic potential of frequency ω is studied with an exact diagonalization approach. The Hamiltonian of the system of N \uparrow and N \downarrow particles interacting via δ -like contact potential reads:

$$H = \sum_{i=1}^{N_{\downarrow}} \left[-\frac{\hbar^2}{2m_{\downarrow}} \frac{\partial^2}{\partial x_i^2} + \frac{m_{\downarrow}\omega^2}{2} x_i^2 \right] + \sum_{i=1}^{N_{\uparrow}} \left[-\frac{\hbar^2}{2m_{\uparrow}} \frac{\partial^2}{\partial y_i^2} + \frac{m_{\uparrow}\omega^2}{2} y_i^2 \right] + g_{1D} \sum_{i,j=1}^{N_{\downarrow},N_{\uparrow}} \delta(x_i - y_j).$$

We show how to filter out the center of mass excitations (see left and middle panel of **Fig. 1**) from the spectrum of the total Hamiltonian which was presented in [1]. Then we show how to experimentally determine and classify internal excitations by calculating appropriate pair-correlation function. In this way, we define the quantity I which depends only on the relative excitations, i.e., it is insensitive to the excitations of the center of mass of the system.



Fig. 1: The mass imbalanced $(m\uparrow/m\downarrow=40/6)$ system of N $\uparrow=2$, N $\downarrow=1$ particles. The spectrum of the Hamiltonian after (left) and before (middle) filtering out the excitations of the center of mass motion.

Right: pair-correlation functions for two different many-body eigenstates of the Hamiltonian with the same state of the center of mass and different relative excitations. Although the pair correlations seem to be the same, the quantity I calculated straightforwardly is completely different.

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Colloidal Quantum Dot Doped with Copper J. Mikulski¹, B. Sikora¹, K. Fronc¹, P. Wojna¹, P. Aleshkevych¹, Ł. Kłopotowski¹, J. Kossut¹

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Colloidal nanocrystal semiconductors are a class of materials with great potential for applications in low-cost optical, magnetic and electrical signal processing devices (e.g., photovoltaic cells, light emitting diodes, as well as new advanced equipment making use of "zero-threshold" optical gain). Nickel, manganese, cobalt are the most common ions used as magnetic dopants. From this point of view the possibility of using copper remains relatively unexplored.

Here we report on the synthesis of colloidal based zinc oxide and cadmium selenide nanoparticles doped with copper ions. The synthesis used chemical co-precipitation from homogeneous solution. The sizes (as measured by absorption edge position at room temperature after the first stage of the reaction) are below 10 nm. Then, during the second stage of the growth process nanoparticles were covered by shells composed of materials having small mismatch of lattice parameters, also by precipitation. In the case of CdSe samples checked with x-ray diffraction we observed clear peaks corresponding to the zinc blende shells. In the case of ZnO samples we did not see any clear signals corresponding to the shells because they were either identical with those of wurtzite cores or because their thickness was too small.

An attempt was made to observe the electron paramagnetic resonance and from those measurements it was deduced that Cu in as grown ZnO nanocrystals is in the second oxidation level while in CdSe nanocrystals – in the first oxidation level. We did not observe any changes of the charge state of Cu ions by illumination with blue light, as sometimes suggested in the literature.

The bandgap is determined from the edge of the absorption band position, which in the case of nanocrystals strongly depends on particle size. Photoluminescence spectra of the nanoparticles with various concentration of Cu doped were examined. In both cases, ZnO and CdSe, increasing the copper content leads to quenching of the luminescence originating in the interband transitions.

The results of luminescence measurement of copper-doped nanoparticles in the magnetic field are unequivocal. The key issue here seems to be related to the way of embedding the copper ions into the host crystal lattice (or in their charge state) which, in the end, results in a material either exhibiting either strong or weak magnetooptical properties.

Assembly and Aggregation of Thermally Denaturated Protein Complexes in Coarse-Grained Models

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The ability to self-organize is a very important feature of biological structures. It makes possible to create very complex structures within living organisms or organisms themselves. Sometimes, molecules appear to create complexes in improper way. It can be dangerous for organisms especially when the formed aggregates are more stable than proper complexes.

Here, we focus on the study of the self-organization and aggregation of virus capsids. They are typical examples of the formation of large structures from single simple proteins. In our studies, the simulations are performed using the structure-based coarse-grained model of virus proteins [1] and it has been applied to the virus capsids with well known structure [2].

We have studied thermal denaturation of virus capsids phenomena and their ability to return to the native state in presence and absence of genetic material. First, we have performed simulation in order to characterize the thermal stability of full capsid and then separate capsid proteins. Based on obtained results, we conclude that proteins in capsids and capsids itself are more stable at high temperatures than the single proteins, especially the transition from globular structure to random coil is observed at higher temperatures for capsids.

However virus capsid requires longer time to self-organize even in the low temperature range, but the aggregated non-native structures are also observed in high concentrations. Especially, when additional non-native contacts are introduced to our model. Results of self-organization of capsids and aggregation of capsid proteins will be presented.

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Biological and Medical Application of Up-Converting Rare-Earth Ions Doped NaYF4 Nanoparticles and Magnetic Fe3O4 Nanoparticles P. Kowalik¹, D. Elbaum¹, K. Fronc¹, J. Mikulski¹, A. Borodziuk¹, I. Kamińska¹, M. Szewczyk^{2,3}, K. Zajdel⁴, G. Gruzel⁵, P. C. Morais^{6,7}, E. Mosiniewicz-Szablewska¹, M. Pawlyta¹², R. Minikayev¹, T. Wojciechowski¹, A. Sienkiewicz^{8,9}, M. Łapiński¹⁰, P. Stępień^{2,3,11}, W. Paszkowicz¹, M. Frontczak-Baniewicz⁴, A. Gardias¹⁴, J.Rybusiński¹⁴ J. Szczytko¹⁴, A. Twardowski¹⁴, P. E. de Souza⁶, R. B. Nunes⁶, F. H. Veiga-Souza¹³, B. Sikora¹ ¹ Institute of Physics PAS, Al. Lotników 32/46, PL- 02668 Warsaw, Poland ² Institute of Genetics and Biotechnology, Faculty of Biology UW, Pawińskiego 5a, Warsaw. ³ Institute of Biochemistry and Biophysics PAS, Pawińskiego 5a, Warsaw ⁴Mossakowski Medical Research Centre PAS, Pawińskiego 5, Warsaw ⁵Institute of Nuclear Physics PAS, ul. Radzikowskiego 152, 31-342 Krakow ⁶Instituto de Fisica, Universidade de Brasilia, Brasilia DF 70919-970, Brazil ⁷College of Chemistry and Chemical Engineering, Anhui University, Hefei 230601, China ⁸Laboratory of Physics of Complex Matter, EPFL, Station 3, CH-1015 Lausanne, Switzerland ⁹ADSresonaces, CH-1028 Préverenges, Switzerland ¹⁰ Institute of Optoelectronics, Military University of Technology, Gen. S. Kaliskiego 2, Warsaw ¹¹ Centre of New Technologies, 'Ochota' UW, S. Banacha 2c, Warsaw ¹² Institute of Engineering Materials and Biomaterials, Silesian University of Technology, ul. Konarskiego 18A, Gliwice 44-100, Poland ¹³Faculty of Ceilandia, Universidade de Brasilia, Brasilia DF 70919-970, Brazil. ¹⁴ Institute of Experimental Physics, Faculty of Physics UW, ul. Pasteura 5, Warsaw Contact e-mail: pkowalik@ifpan.edu.pl

The main aim of our research was to create multifunctional system based on connecting of two types of nanoparticles – NaYF4 nanocrystals doped with rare-earth ions with up-converting properties and Fe_3O_4 nanoparticles with superparamagnetic properties.

The proposed system allows to prepare nanomaterials for theranostic applications (diagnostics and therapeutics). Optical part of the nanoconstruct, using near-infrared light as a excitation source, has potentially huge applications in biological studies because of relatively low absorption by water and low autofluorescence level of organic components in this region. In addition, the nanomaterials can be applied in photodynamic therapy as an energy donor for organic molecules able to generate on demand toxic Reactive Oxygen Species. The surface modification of the nanoparticles can be used as targeting factor in cancer diagnosis (to identify the location and area of tumor, occurrence of circulating tumor cells). Second type of material – iron oxide nanoparticles – is suitable for magnetic hyperthermia. Superparamagnetic nanoparticles, exposed to alternating magnetic field, generate heat thus lead to damage of cellular membrane. Additionally, the nanoparticles could be used as a contrast agent for Magnetic Resonance Imaging.

Coating presented materials in a single silicon oxide shell further expands possibility for their surface modification thus generation of biologically specific, multitask materials.

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