ISCFMMT 2022, Batumi, Georgia

International School and Conference on Functional Materials for Modern Technologies

Program and abstract Booklet

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International School and Conference

on Functional Materials for Modern Technologies

ISCFMMT 2022

Batumi, Georgia

October 01-07, 2022

Ivane Javakhishvili Tbilisi State University

Batumi Shota Rustaveli State University

International School and Conference
on Functional Materials for Modern Technologies

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Program

October 1 **Arrival** **Opening**	
17:00-18:00 Lecture 1 (Opening talk)	**Gian-Luca Bona** From basic science to innovation in the market
Welcome reception	
October 2	
09:00-11:00 Lecture 2	**Tamar Tchelidze** Band theory, local and non-local states
11:00-11:20 coffee break	
11:20-13:20 Lecture 3	**Zaal Machavariani, Tamar Tchelidze** Low-dimensional structures
13:20-14:20 lunch	
14:20-16:20 Lecture 4	**Alexander Shengelaya** Superconductivity in nanostructures
16:20-16:40 coffee break	
16:40-17:10 Scientific Presentation	**Gian-Luca Bona** From bottom-up synthesis of graphene nanoribbons to new applications in (quantum) computing
17:10-17:40 Scientific Presentation	**Fabio La Mattina** Pulsed laser deposition of functional oxides
October 3	
09:00-11:00 Lecture 5	**Tamaz Kereselidze** Multiparticle effects, Harty-Fock and Thomas-Fermi approximations

11:00-11:20 coffee break	
11:20-13:20 Lecture 6	**Tamaz Kereselidze** Multiparticle effects, Harty-Fock and Thomas-Fermi approximations (continued, practical issues)
13:20-14:20 lunch	
14:20-16:20 **Lecture 7**	**Roman Kezerashvili** Application of few-body methods in condensed matter physics.
16:20-16:40 coffee break	
16:40-17:10 **Scientific Presentation**	**Roman Kezerashvili** Magnetoexcitons in isotropic and anisotropic monolayers, bilayers, and van der Walls heterostructures
17:40-19:40 Poster session	
October 4	
09:00-11:00 **Lecture 8**	**Zurab Guguchia** Muon Spin Rotation and Relaxation: method and applications
11:00-11:20 coffee break	
11:20-13:20 **Lecture 9**	**Fabio La Mattina** Impedance measurements and applications
13:20-14:20 lunch	
14:20-16:20 **Lecture 10**	**Igor Bondarev** Strongly correlated collective excitations in quasi-2D nanostructures Of metals and semiconductors
16:20-16:40 coffee break	

16:40-17:10 **Scientific Presentation**	**Zurab Guguchia** The time-reversals symmetry-breaking charge order and nodal pairing in a Kagome superconductor
17:10-17:40 **Scientific Presentation**	**Igor Bondarev** Magnetic-Field-Induced Wigner Crystallization of Charged Interlayer Excitons in van der Waals Heterostructures
19:00 Conference dinner	
October 5	
09:00-11:00 **Lecture 11**	**Teimuraz Mtchedlidze** The basic functional material in the modern production of integrated circuits.
11:00-11:20 coffee break	
11:20-13:20 **Lecture 12**	**Giorgi Japaridze** One-dimensional models of metal-insulator transitions
13:20-14:20 lunch	
14:20-14:50 **Scientific Presentation**	**Teimuraz Mchedlidze** Characterization methods for fully depleted silicon on isolator high-k metal gate stacks
15:20-19:00 excursion	
October 6	
09:00-11:00 **Lecture 13**	**Ramaz Khomeriki** Photonic Periodical Structures
11:00-11:20 coffee break	

11:20-13:20 **Lecture 14**	**Archil Ugulava** Brownian motion. Suspensions of magnetic nanoparticles
13:20-14:20 lunch	
14:20-16:20 **Lecture 15**	**Nugzar Ghomidze** Fundamentals of Medical Imaging
16:20-16:40 coffee break	
16:40-17:10 **Scientific Presentation**	**Ramaz Khomeriki** Ferroelectric-Vortex-Crystal Photonics
October 7	
09:30-11:30 **Lecture 16**	**Lali kalandadze** New challenges of spintronics
11:30-13:00	**Round table and conference closing**
13:00-14:00 lunch	

Table of Contents

From basic science to innovation in the market

Gian-Luca Bona*

Professor em. for Photonics, ETH Zurich and EPF Lausanne Director Empa - Material Science and Technologies, 2009 - May 2022

Advancements in science are driven through our curiosity to understand how our world functions and how we are embedded in a wider universe. What are the fundamentals of our existence as humans in an ever growing globalized world? Moreover, we all also want to improve our well-being and quality of life in our society. How can we take advantage of our basic discoveries and turn them into an innovation, i.e., into something that our society can take profit from or that a client is willing to pay for it. In this presentation we will show how the long path from basic scientific discoveries to a practical application can be accelerated by efficient transdisciplinary collaboration. Some recent examples of knowledge and technology transfer will be shown.

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From bottom-up synthesis of graphene nanoribbons to new applications in (quantum) computing

Gian-Luca Bona*

Professor em. for Photonics, ETH Zurich and EPF Lausanne
Director Empa - Material Science and Technologies, 2009 - May 2022

The "nanotech@surfaces" Laboratory team at Empa headed by Prof. Roman Fasel is working on the fabrication of novel low-dimensional carbon nanomaterials, such as graphene nanoribbons, with ultimate, i.e., atomic precision. This structural precision enables the development of completely new types of novel electronic devices based on quantum effects.

In recent years, Fasel's team has developed a novel "bottom-up" approach based on the surface-assisted self-assembly of molecular building blocks that enables the atomically precise fabrication of a wide variety of graphene nanoribbons. In such nanoribbons, all carbon atoms are in exactly the right place, according to the predefined "blueprint".

To verify the structural perfection of these nanostructures and to characterize their electronic properties, the highest resolution is required, which only scanning probe microscopy offers. The width and the structure of the long edges of these ribbons is what determines their quantum electronic properties. Although the nanoribbons designed and synthesized by Fasel's team only differ at the edges, they have fundamentally different electronic properties. They can be metallic, semiconducting or insulating, for instance. By slightly tweaking the shape of the ribbons, the Empa researchers thus create entirely new materials. Recently,

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they showed that by tweaking the shape, it is also possible to induce quantized spin magnetic moments and to control their interactions, thus obtaining graphene nanomaterials with quantum coherent magnetic ground states.

Thanks to these breakthroughs, the researchers have been able to develop methods and tools to construct complex nanoribbon structures with such precision that quantum effects can be harnessed and manipulated - at a level where a single atom makes a crucial difference. This has opened up concrete perspectives for carbon-based quantum devices and brings carbon-based nanomaterials a significant step closer to future quantum technologies.

[1] *S. Mishra et al.,* Nature Nanotechnology, **15** (2020) 22
[2] S. Mishra et al., Nature **598** (2021) 287

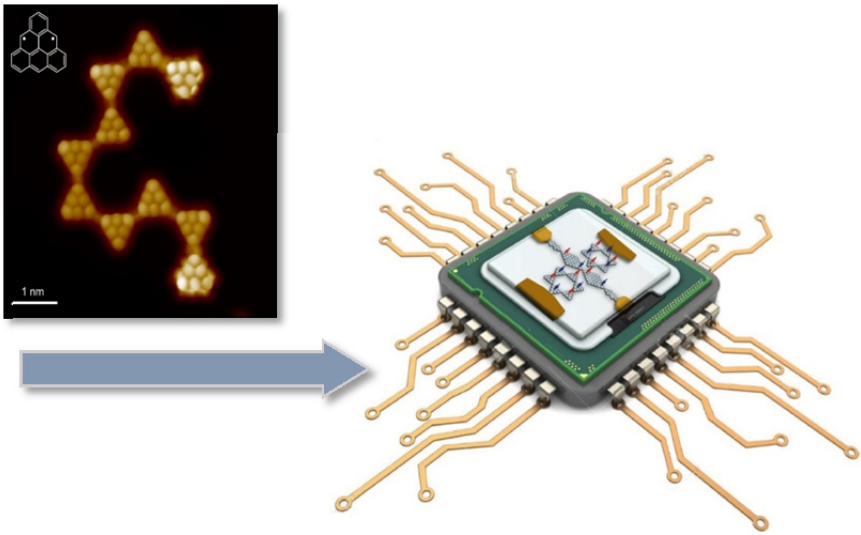

Fig. 1: vision of Carbon-based nanostructures for next generation quantum computers

Pulsed laser deposition of functional complex oxides

Fabio La Mattina*

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Transition metal (TM) complex oxides are intensively investigated for their enormous variety of physical properties and for their potential as next-generation electronic materials. Their property range includes high temperature superconductivity, piezoelectricity, ferroelectricity, ferromagnetism, multiferroic behavior, resistive switching behavior, ionic conduction, and catalytic properties. While the trend in scaling down Si-based devices approaches its limit, in contrast, the multifunctional character of transition metal oxides manifests unexpected properties related to the ultrathin limit. Some of these oxides can be stacked in multi-layer epitaxial heterostructures exhibitting an enhancement or even new properties with respect to the parent compounds. Among the various thin-film growth technologies, pulsed laser deposition (PLD) has several features that make it remarkably competitive in growing thin films of complex oxides. The ablation from a single target containing all the components allows a relative simple stoichiometric transfer onto the substrate, thus one could rapidly produce thin-films of nearly any oxide compound regardless of the complexity of the crystal chemistry. In this lecture, I will provide an overview of the PLD technique and show some results of recent investigations on several oxides currently under intensive study.

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Magnetoexcitons in 2D isotropic and anisotropic monolayers and van der Walls heterostructures

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Direct and indirect excitons in Rydberg states in 2D isotropic and anisotropic monolayers, bilayers, and van der Waals (vdW) heterostructures in an external magnetic field are studied within the framework of the effective mass approximation. We use both the Rytova-Keldysh and Coulomb potentials for charged carriers interaction to analyze the influence of the screening on the studied phenomena. We report the magnetic field energy contribution to the binding energies and diamagnetic coefficients for magnetoexcitons that depend strongly on the effective mass and effective mass anisotropy of electrons and holes. The comparative study of transition metal dichalcogenide (TMDC), transition metal trichalcogenides (TMTC) and phosphorene is given. In TiS_3, $TiSe_3$, and $ZrSe_3$ the excitonic binding energies and diamagnetic coefficients demonstrate the same kind of anisotropy as in phosphorene. In contrast, ZrS_3 has the opposite anisotropy to phosphorene. The tunability of the binding energy of direct and indirect magnetoexcitons by the external magnetic field and the possibility to control the binding energy of magnetoexcitons in vdW heterostructures by manipulation of numbers of hBN monolayers are demonstrated.

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Within a mean-field approach superfluidity of indirect excitons in TMTC vdWHs is studied. Our study demonstrates the angle-dependent superfluidity temperature in TMTC vdWHs: for a given density a maximum and minimum Tc of superfluidity occurs along chain and a-directions, respectively. We suggest an experiment for the observation of anisotropic superfluidity in TMTC vdWH.

Time-reversal symmetry-breaking charge order in a kagome superconductor

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The kagome lattice, the most prominent structural motif in quantum physics, benefits from inherent nontrivial geometry to host diverse quantum phases [1-4], ranging from spin-liquid phases, topological matter to intertwined orders, and most rarely unconventional superconductivity. Recently, charge sensitive probes have suggested that the kagome superconductors AV_3Sb_5 (A = K, Rb, Cs) [4] exhibit unconventional chiral charge order. However, direct evidence for the time-reversal symmetry-breaking of the charge order remained elusive. We utilized muon spin relaxation to probe the kagome charge order and superconductivity in KV_3Sb_5 and RbV_3Sb_5 [5,6]. We observe an enhancement of the internal field width sensed by the muon ensemble, which takes place just below the charge ordering temperature and persists into the superconducting state. Remarkably, the muon spin relaxation rate below the charge ordering temperature is substantially enhanced by applying an external magnetic field. We further show the nodal nature of superconducting gap in KV_3Sb_5 and RbV_3Sb_5 and that the T_c/λ^{-2}_{ab} ratio is comparable to those of unconventional high-temperature superconductors. Our results point to unprecedented time-reversal symmetry breaking charge order (Fig. 1) intertwining/competing with unconventional superconductivity in the correlated kagome lattice. While low-temperature time-reversal symmetry-breaking superconductivity has been discussed for many systems, high-temperature time-reversal symmetry-breaking charge order is extremely rare, and finds a direct comparison with the fundamental Haldane and Varma models.

[1] Z. Guguchia et. al., Nature Communications 11, 559 (2020).
[2] Y. Zhou et. al., Rev. Mod. Phys. 89, 025003 (2017).

[3] Ortiz, B. et al. Phys. Rev. Lett. 125, 247002 (2020).
[4] Y.-X. Jiang,..., Z. Guguchia, et. al., Nature Materials 20, 1353 (2021).
[5] C. Mielke III et. al., and Z. Guguchia, Nature 602, 245-250 (2022).
[6] Z. Guguchia et. al., arXiv:2202.07713 (2022).

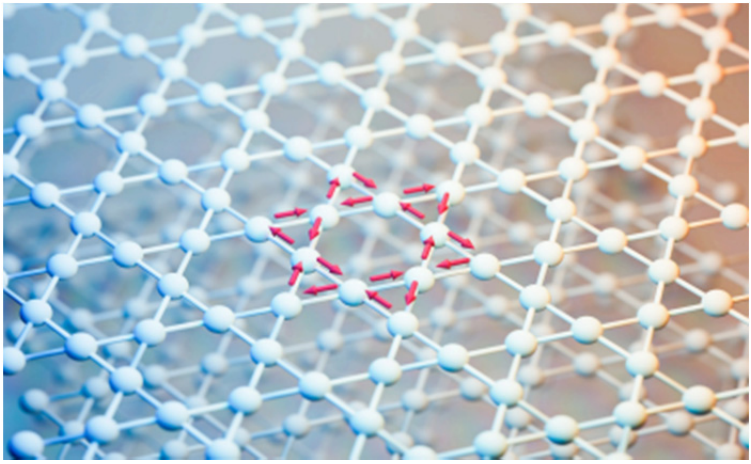

Fig. 1: The discovered time-reversal symmetry-breaking fields suggest the presence of long-theorised 'orbital currents', where charge flows spontaneously in loops around the unit cells of the kagome lattice.

Magnetic-Field-Induced Wigner Crystallization of Charged Interlayer Excitons in van der Waals Heterostructures

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We develop the theory for the magnetic-field-induced Wigner crystallization of charged interlayer excitons (CIE) [1] discovered recently in transition-metal-dichalcogenide (TMD) heterobilayers [2]. We derive the ratio of the average potential interaction energy to the average kinetic energy for the many-particle CIE system subjected to the perpendicular magnetic field of an arbitrary strength at zero temperature. We analyze the weak and strong field regimes and obtain the critical temperature for the 'cold' crystallization phase transition in the strong field regime where the lowest Landau level alone is occupied. We also generalize the effective g-factor concept previously formulated for interlayer excitons [3], to include the formation of CIEs under electrostatic doping of heterobilayers in the strong perpendicular magnetic field. We show (see Fig.1) that magnetic-field-induced Wigner crystallization and melting of the many-particle system of CIEs can be detected and monitored in magneto-photoluminescence (PL) experiments that measure the effective g-factor of excited TMD bilayers under controlled electrostatic doping [1]. The CIE crystal-

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liquid internal energy difference is estimated to be ~0.3 meV for a typical case of the AA-stacked MoSe2/WSe2 heterobilayer.

We emphasize that magnetic-field-induced 2D Wigner crystallization in the strong perpendicular magnetostatic field is a universal phenomenon. In this regime, the only internal parameter that remains there to control the properties of the system is the cyclotron frequency, which exceeds all other internal parameters including crystal lattice vibrational frequencies and interparticle coupling strength. Hence, any many-particle (or quasiparticle) system with repulsive interparticle interactions, be it fermionic or bosonic, be it charged such as electrons, holes and CIEs, or even neutral such as interlayer excitons, will experience the Wigner crystallization phase transition (which we will give the full account of elsewhere) when the external magnetostatic field is strong enough to isolate the lowest Landau level and make the cyclotron frequency the leading parameter of the system. Despite this universality, however, only for CIEs the Wigner crystallization effect can be detected and monitored in the effective g-factor measurement experiments we discuss, as the features we predict for the g-factor are all coming from the additional magnetic moment of the CIEs that is associated with their rotational angular momentum in the crystallized phase.

Work supported by the U.S. Department of Energy under award No.DE-SC0007117 (I.V.B.) and by the RFBR grants No. 20-02-00410 and No. 20-52-00035 (Yu.E.L.). Yu.E.L. is supported by the Basic Research Program at the National Research University HSE. I.V.B. acknowledges discussions with Luis Jauregui (UC Irwine), Andrew Joe (Harvard), and Philip Kim (Harvard) at the beginning of this work.

[1] I.V. Bondarev and Yu.E. Lozovik, *E-Print: arXiv2112.13995, to appear in Communications Physics (Nature)*

[2] L.A. Jauregui, A.Y. Joe, K. Pistunova, D.S. Wild, A.A. High, Y. Zhou, G. Scuri, K.De Greve, A. Sushko, C.-H. Yu, T. Taniguchi, K. Watanabe, D.J. Needleman, M.D. Lukin, H. Park, and P. Kim, Science 366, 870 (2019)

[3] P. Nagler, M.V. Ballottin, A.A. Mitioglu, F. Mooshammer, N. Paradiso, C. Strunk, R. Huber, A. Chernikov, P.C.M. Christianen, C. Schüller, and T. Korn, *Nature Communications 8, 1551 (2017)*

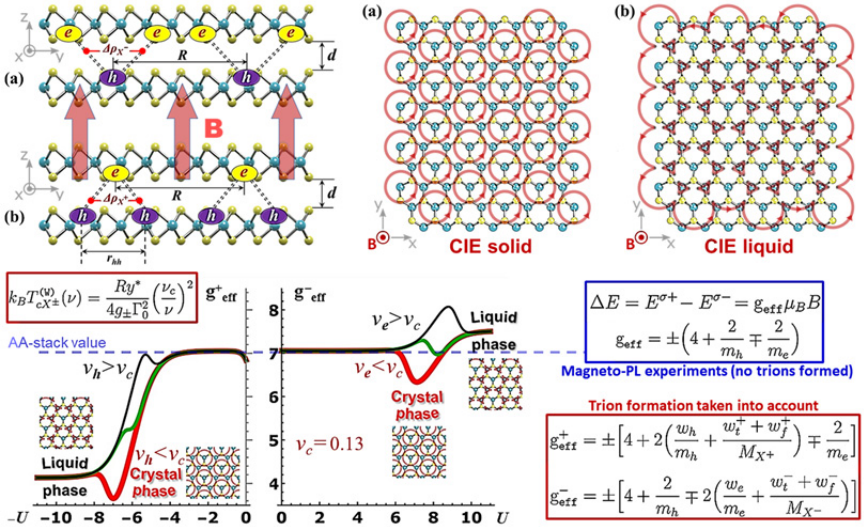

Fig. 1. *TOP LEFT*: Schematic of the TMD bilayer under study, with negative (a) and positive (b) CIE complexes subjected to a perpendi-cular homogeneous magnetostatic field. *TOP RIGHT*: Top view of the crystal phase (a) and liquid phase (b) for the negative CIEs in the strong magnetic field directed upward. *BOTTOM:* The effective g-factor behavior as predicted by the CIE Wigner crystallization model for the positive (left) and negative (right) CIEs in a generic AA-stacked TMD heterobilayer with the doped carrier energy U and initial filling factor $\bar{\nu}_{e,h}/\nu_c = 0.9, 1.0, 1.1$ in the strong field (line thickness increase indicates stronger field, $\nu_c = 0.13$ is the critical filling factor value).

Characterization methods for fully depleted silicon on isolator high-k metal gate stacks

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Fully depleted (FD) silicon-on-insulator (SOI) high-k metal gate (HKMG) field-effect transistors (FET) are becoming a mainstream of semiconductor technology [1], [2]. We propose a method for the electrical characterization of the FDSOI HKMG stack. The method is based on assessing low field carrier mobility and trap density distributions for front and back gate interfaces of a FET. These characteristics are obtained from current-voltage measurements in a near subthreshold swing (STS) regime at various temperatures. The previously reported trap density characterization method [3] allows an estimation of averaged trap densities separately for the front and the back interfaces of a channel. Performing STS measurements at several temperatures allowed the extraction of the energy distributions of the interface trap densities $D_{IT}(E_{IT})$ for both interfaces and obtaining other essential characteristics of the stack. Assessing the value of the low-field mobility (μ_0) for a stack from measurements in the STS regime at several temperatures allows specifying the impact of various carrier scattering mechanisms on the total stack mobility. Further, the application of double-gate operation in the optimal coupling mode for the FET allows analysis of the impact of the gate interface on mobility.

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From our study, it appeared that interface trap densities and trap mobilities should be assessed from STS measurements on FETs with non-similar geometry. Namely, FETs with channel dimensions $L_{CH}\times W_{CH} \approx 100\times150$ nm^2 were found optimal for $D_{IT}(E_{IT})$ estimations, while larger channels with $L_{CH}\times W_{CH} \approx 500\times1000$ nm^2 appeared optimal for assessing $\mu_0(T)$. Such difference can be attributed to the specifics of the carrier scattering in FDSOI HKMG stacks [4], [5].

Further possibilities for the analyses and characterization followed from a comparison of the results obtained during $D_{IT}(E_{IT})$ and $\mu_0(T)$ data for the same stacks and comparision of area distribution maps of the measured parameters. The method can be used in the monitoring of stack quality and in the design and development of stack fabrication processes.

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[3] T.Mchedlidze and E. Erben, *Phys. Status Solidi A* **217**, 2000625 (2020).
[4] B. Qui, Z. Tian, A. Vallabhaneni, B. Liao, J. Mendoza, O. Restrepo, X. Ruan and G. Chen, EPL journal **109**, 57006 (2015).
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Ferroelectric Vortex-Crystal Photonics

R. Khomeriki*

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In this talk, I will concentrate on the development of linear response theory and dispersion characteristics for a very recently observed THz collective dynamics in ferroelectric vortex lattice which is a promising candidate for the realization of high-speed and low-energy-power devices. Analytical approach and a numerical code are developed in order to verify our model and make reliable predictions for future experiments. The point is that, according to our estimates, nonlinear coefficient is several orders higher than in widely promoted silicon medium and thus, the system could allow the excitation and propagation of low-power band-gap solitons, which could serve as digital information carriers in all-optical devices.

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Investigation of electronic structure at the SrTiO3/YBa2Cu3O7-δ interface

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Structural and electronic reconstruction at interface of epitaxial perovskite complex oxides is under intense investigation due to the emerging novel transport properties observed in selected heterostructures. We present investigation of interface phenomena between high-temperature superconductor $YBa_2Cu_3O_{7-\delta}$ (YBCO) and high dielectric constant material $SrTiO_3$ (STO). We use soft-X-ray angle-resolved photoelectron spectroscopy (SX-ARPES) to access electronic states at buried of STO/YBCO interface. We studied for the first time by SX-ARPES the fermi surface of YBCO thin film and its modification due to STO interface. Additionally, investigation by means of resonant photo-emission spectroscopy across the Ti $L_{2,3}$ absorption edge was performed to study electronic states of the insulating STO near the YBCO interface.

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Fast Synthesis of $La_{1.84}Sr_{0.16}CuO_4$ Superconductor by Light Irradiation

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The effect of a photostimulated solid state reaction (PSSR) was investigated in $La_{1.84}Sr_{0.16}CuO_4$ samples. Starting pellets of oxide mixtures were irradiated by light during 2 minutes in the temperature range of 850°C – 1100°C. Light irradiation was performed by either halogen or UV lamps in order to study the effect of the spectral composition on the samples synthesis process. The obtained samples were studied by X-ray diffraction for structural characterization and magnetization measurements to estimate the superconducting volume fraction. It was found that at the same synthesis temperature the solid-state reaction rate of $La_{1.84}Sr_{0.16}CuO_4$ is strongly enhanced under light irradiation as compared with the usual heat treatment in a furnace. Moreover, it was observed that UV lamp irradiation is much more effective compared to halogen lamps. This indicates that some nonthermal processes take place during PSSR where the photon energy plays a significant role.

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Spark Plasma Sintering of Tungsten Oxide $WO_{2.9}$: Structural and Transport Properties

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Oxygen reduced tungsten oxide samples with a composition $WO_{2.90}$ were prepared by spark plasma sintering (SPS). Powder X-ray diffraction indicates that the obtained material mainly consists of $WO_{2.90}$ with Magneli phase together with a few percent of other tungsten oxide phases. Microstructure analysis by scanning electron microscope showed that the sintered pellets are very dense, allowing reliable measurement of transport properties. Temperature dependence of electrical resistivity measured in the 4-300 K range indicates metallic behavior of $WO_{2.90}$ samples.

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Excitonic complexes in one dimensional nanostructures

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Over the last few decades, the optical properties of nanoscale objects have been intensively investigated. The reason for this is the size dependence of electronic structure and connected to this the possibility of engineering optical parameters in a wide range. The excitons are main intrinsic emitters in short wavelength region in semiconductors and therefore, optimization of excitonic emission is very important for emitting device fabrication. Gallium oxide is very promising for optical-electronics material due to its ultra-high band gap. We present a theoretical approach to calculate the electronic state of excitons and biexciton in gallium oxide nanowires (NW) and nanotubes in the framework of the effective-mass model using the Born-Oppenheimer approximation. We consider the formation of excitons and biexcitons under the action of both the lateral confinement and the Coulomb potential. The analytical expressions for the binding energy and eigenfunctions of the excitons and biexciton are obtained in dependence on system geometry. The approach is based on the fact that the confinement effect is stronger than the Coulomb term. The Coulomb term is significant only along nanowire/nanotube axes (z-axes). That is why to calculate exciton states in the presence of space confinement we averaged the Coulomb potential over the lateral (perpendicular to nanowire/nanotube axes) wave functions of electrons and holes. This procedure reduces the dimensionality of

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Coulomb potential to one, and the 1D Schrödinger equation is solved in the frame of variational technique. Having known single exciton states biexciton states are calculated using Born-Oppenheimer approximation. The calculations reveal strong dependence of binding energy of excitons and biexcitons on geometrical size for nanowires as well as for nanotubes.

Transmission Spectra of GaN Grown By Reactive Magnetron Sputtering

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In this research is presented optic transmission spectra of GaN received by reactive magnetron sputtering. For formation III nitride semiconductor materials have been proposed many technologies such as: Molecular Beam Epitaxy (MBE) [1], Metalo Organic Chemical Vapor Deposition (MOCVD) [2], Hydride Vapor Phase Epitaxy (HVPE) [3] and others. Some of them are high temperature tecnologies, others require expensive technological equipment and special laboratory enviroments for toxic reagent gases and toxic waste products. All this circumstances effect on the price of the fabricated materials and devices based on them.

Magnetron sputtering technology developed and industrialized in late 1980s. Magnetron sputtering is able to effectively eliminate poisoning of targets and, therefore, is possible to produce multilayer films including metal, non-metal, ceramic, insulating, conducting and semiconducting films can be deposited in this way. Many authors work on magnetron sputtering technology. Some of them investigate influence of different frequency modes as a source of magnetron sputtering, total pressure, N_2:Ar ratio, substrate temperature, target-to-substrate distance, substrate and

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substrate orientation on the properties of the deposited films [4-6]. Main disadvantages of reactive magnetron sputtering technology is that by this technology it is impossible to grow (> 1 μm) thick materials due to its unprofitability (long deposition time). But, if we use its main drawback in nanotechnologies, which means obtaining nanoscale (10 ÷ 100 nm) materials; it is possible to get cheap, simple and cost-effective technology.

One of the key issues in the creation of optoelectric devices is the study of the optical properties of gallium nitride. The present paper discusses the technological processes on the basis of which the GaN release spectrum characteristic is improved. It is shown the trends of improving the optical properties of this material. Analysing transmission spectra showed good relevance with growth temperature and band gap of GaN, which can be calculated from the transmission spectra. With increasing formation temperature of GaN increases the accuracy of transmitted light wavelength to be around 361nm, which corresponds to the band gap 3.4 eV. The slope of the initial graph tends to be 90^0 with increasing growth temperature of the GaN.

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Thermodynamic analysis of Nitrogen and Magnesium Doping of Gallium oxide - Comparative Study

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Gallium oxide Ga_2O_3 has gained much attention because of its unique properties such as ultra-wide bandgap (~ 5eV), high breakdown field, which makes it very promising for application opto- and power electronics. However, in gallium oxide, like other semiconductor oxides, obtaining low ohmic hole conductivity is still challenging. The difficulty is connected to low hole mobility caused by the big effective mass of holes, high ionization energies of native and impurity acceptors, compensation processes (appearance of hole killer defects) stipulated by high band-gap, and low lying valence band. Nitrogen and magnesium substituting oxygen and gallium respectively are expected to lead to p-type conductivity.

We fulfilled the thermodynamic analysis of the concentration equilibrium for nitrogen and magnesium doped gallium oxide using the Kroger method of quasi-chemical reactions, which gives one possibility to find the dependence of concentrations of defects and free carriers on growth/processing parameters and impurity concentration, and correspondingly to find their optimal values. The analysis was carried out for the system Ga_2O_3 doped samples – vapor of components. In Mg-doped samples, the main defect which can compensate hole conductivity must be oxygen vacancy or interstitial gallium. The concentration of

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interstitial Mg atoms, which also can be compensating donors is expected to be very low because of the big atomic radius. High enough oxygen partial pressure is needed on the one hand to suppress the formation of compensating donors and on the other hand, the provides the room for substitutional Mg atoms. The analysis shows that the hole concentration increases with increasing oxygen pressure and at some critical value holes and substitutional magnesium become dominant spices (for T=800 K, P_{cr}=0.7 atm). However further increase of oxygen pressure does not affect significantly hole concentration. P_{cr} decreases with temperature, but it does not depend on the total concentration of impurity atoms. For nitrogen hole doping we took into account the formation of the nitrogen molecule, which is expected to reduce the effect of doping. The formation energy of nitrogen molecules is quite high – 9.756 eV. In Gallium oxide taking into account dielectric screening with local field correction, dissociation energy turned out to be approximately 2 eV. Thermodynamic analysis shows that, for nitrogen doping, the dependence on oxygen pressure still exists, but it is less pronounced. The critical pressure above which negatively charged acceptors and holes are dominant spices is again around 1 atm. Based on these results one can conclude, that for Mg doping of gallium oxide, as well as for N doping the native donors - oxygen vacancy or Gallium interstitial are responsible for p-conductivity compensation. Remarkably, in both cases, the expected hole concentration exceeds the one observed in undoped samples [1].

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