*Bulgarian Academy of Sciences*

*GEORGI NADJAKOV INSTITUTE*
*OF SOLID STATE PHYSICS*

**SOFIA, BULGARIA**

# BOOK OF ABSTRACTS

## 21st INTERNATIONAL SCHOOL ON CONDENSED MATTER PHYSICS

## *Progress and Perspectives in Functional Materials*

**August 31st - September 4th, 2020**
**Varna, Bulgaria**

Partially supported by the Ministry of Education and Science,
Bulgarian National Science Fund - Grant № КП-06-МНФ/2

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**GEORGI NADJAKOV INSTITUTE OF SOLID STATE PHYSICS**
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“Progress and Perspectives in Functional Materials”
August 31st - September 4th, 2020 – Varna, Bulgaria

Partially supported by the Ministry of Education and Science,
Bulgarian National Science Fund

## PROGRAMME

### August 30th (Sunday)

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|---|---|
| 16:00-19:00 | Registration |
| **20:00** | **Get Together Party** |

### August 31st (Monday)

| | |
|---|---|
| 09:00-09:30 | Opening Ceremony |
| **09:30-11:00** | **Chair: H. Chamati** |
| 09:30-10:15 | S. BALESTRA, “Challenges and possible solutions for the end of the nanoelectronic roadmap”<br>*Georgi Nadjakov Memorial Lecture* |
| 10:15-11:00 | Ph. VANDERBEMDEN, “Partial discharge measurements used as a tool to assess the quality of the electrode contact in flash sintering”<br>*Milko Borisov Memorial Lecture* |
| 11:00-11:30 | Coffee break / Collective photo |
| **11:30-12:50** | **Chair: H. Chamati** |
| 11:30-12:10 | I. MIHAILESCU, “Thin films fabrication for biomedical applications in: drug delivery systems, biosensors, advanced sensor coatings and antinosocomial infections” |
| 12:10-12:30 | N. KRASTEVA, “PEGylation of graphene oxide nanosheets modulate cancer cell mobility and proliferate ability” |
| 12:30-12:50 | K. ESMERYAN, “Anti-frosting performance of chemically functionalized super-nonwettable carbon soot coatings” |
| 12:50-16:00 | Lunch break |
| **16:00-18:00** | **Chair: D. Nesheva** |
| 16:00-16:40 | M. FABIAN, “Structural characterization of oxy-halide materials for solid state batteries” |
| 16:40-18:00 | Five minutes’ presentations of posters of young participants |

### September 1st (Tuesday)

| | |
|---|---|
| **09:10-10:30** | **Chair: J. Genova** |
| 09:10-09:50 | Y. A. ERMAKOV, “Lipid membrane interface - from electrostatics to molecular structure” |

| | |
|---|---|
| 09:50-10:30 | A. IGLIČ, “Plasma treated titanium nanostructures for modification of stents” |
| 10:30-11:00 | Coffee break |
| **11:00-12:20** | **Chair: J. Genova** |
| 11:00-11:40 | S. KRALJ, “Multifunctional topological defect-based soft materials” |
| 11:40-12:20 | O. BATISHCHEV, “Protein-lipid interactions in viral infections” |
| 12:20-16:00 | Lunch break |
| **16:00-18:00** | **Chair: J. Genova** |
| 16:00-16:40 | B. RIZZUTI, “Using model transport proteins to store, control and build functional materials” |
| 16:40-17:20 | S. AKIMOV, “Evolution of continuum models of membrane fusion” |
| 17:20-17:40 | S. PENIC, “Possible mechanisms of invaginations and endovesicles formation coupled to a global shape transformation driven by non-homogeneous lateral distribution of active force” |
| 17:40-18:00 | P. SANTOSH, “Phospholipid stabilized gold nanorods: Towards improved colloidal stability and biocompatibility” |
| **18:00-19:00** | **First poster session** |

**September 2nd** (Wednesday)

| | |
|---|---|
| **09:10-10:30** | **Chair: T. Hristova-Vasileva** |
| 09:10-09:50 | P. MONTGOMERY, “Spatially-resolved optical characterization of functional materials using coherence scanning interferometry” |
| 09:50-10:30 | P. PETRIK, “Development of methods for non-destructive materials characterization” |
| 10:30-11:00 | Coffee break |
| **11:00-12:20** | **Chair: T. Hristova-Vasileva** |
| 11:00-11:40 | G. ARZUMANYAN, “Ultrasensitive detection of analyte molecules at attomolar concentration by Raman spectroscopy“ |
| 11:40-12:00 | R. TODOROV, “Optical properties of thin Ag – In films prepared by interdiffusion in bimetallic nanolayered stacks” |
| 12:00-12:20 | T. HRISTOVA-VASILEVA, “Structural and optical properties of Au – In films for plasmonic applications” |
| 12:20-16:00 | Lunch break |
| **16:00-18:00** | **Chair: T. Hristova-Vasileva** |
| 16:00-16:40 | V. DONCHEV, “Dilute nitrides heterostructures grown by liquid phase epitaxy for solar cells applications” |
| 16:40-17:00 | K. LOVCHINOV, “Structural and optical properties of electrochemically deposited $ZrO_2$ layers on different substrate” |
| 17:00-17:20 | S. BOYADJIEV, “An optical excitation study of pure and Ru-doped $BI_{12}SiO_{20}$ crystals with graphene coating” |
| **18:00-19:00** | **Second poster session** |

**September 3rd** (Thursday)

| | |
|---|---|
| **09:10-10:30** | **Chair: A. Paskaleva** |
| 09:10-09:50 | M. LANZA, “Two-dimensional materials based resistive switching devices” |
| 09:50-10:30 | YAKIMOVA, “Towards 2D materials beyond graphene” |
| 10:30-11:00 | Coffee break |
| **11:00-12:20** | **Chair: A. Paskaleva** |
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| 11:40-12:20 | S. BANERJEE, “Neuromorphic materials by design” |
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| 18:00-18:20 | A. VARONOV, “Electric field effect of cleaved superconductors surface and the problem of effective mass of supefluid charge carriers” |
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|---|---|
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| 09:10-09:50 | Z. USATENKO, “Dynamics of polymer chains with complicated topology in confined geometries” |
| 09:50-10:10 | S. UDACHAN, “Infrared optical constants of chromium nano-films” |
| 10:10-10:30 | I. GORBACHEV, “Investigation of a nickel clusters growth dynamic under Langmuir monolayer of arachidic acid for creation of new conductive material” |
| **10:30-11:00** | **Closing Ceremony** |

# POSTER PRESENTATIONS

## 1. FIRST POSTER SESSION, September 1th (Tuesday)

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1.2. I. M. Dimitrova, V. I. Yordanova, R. I. Slavchov, Mixtures of quadrupolar liquids
1.3. G. R. Ivanov, I. D. Avramov, V. J. Strijkova, Y. G. Marinov, T. E. Vlakhov, E. Bogdanova, G. B. Hadjichristov, Mass sensitivity of Langmuir-Blodgett monolayer film coated surface acoustic wave resonators to volatile organic solvents
1.4. K. Koev, N. Donkov, N. Stancova, H. Naidenski, V. Kussovski, L. Avramov, Investigation of the antibacterial and antifungal effects of silver nanolayers on the ocular prosthesis coating after a two-year period
1.5. K. Koev, N. Donkov, N. Stancova, H. Naidenski, V. Kussovski, L. Avramov, Investigation of the antibacterial and antifungal effects of silver nanolayers on the hard contact lenses coating after one -year period
1.6. E. Belina, H. Kisov, I. Angelov, A. Gisbrecht, T. L. Dimitrowa, G. Dyankov, Thin layers of Hemin with sensing applications
1.7. A. Viraneva, A. Grigorov, N. Pankina, I. Iliev, T. Yovcheva, Effect of β-galactosidase immobilization on properties of chitosan/xanthan and xanthan/chitosan multilayers
1.8. S. Kasarova, N. Sultanova, Thermal variations of refractive and dispersive parameters of optical polymers
1.9. Y. G. Marinov, T. E. Vlakhov, G. B. Hadjichristov, G. R. Ivanov, I. D. Avramov, V. J. Strijkova, I. A. Gorbachev, A. G. Petrov, Phospholipid Langmuir-Blodgett films for detection of reactive gases and vapors at room temperature
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1.11. I. Bodurov, M. Marudova, A. Viraneva, T. Yovcheva, A. Grigorov, Investigation of polyelectrolyte multilayers deposited on corona charged composite polylactic acid / poly(ε-caprolactone) substrates
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1.14. G. Gentscheva, Kr. Nikolova, A. Pashev, Optical characteristics and chemical composition of high oleic sunflower oils with herbs oil additives
1.15. S. Milenkova, I. Manolov, M. Marudova, Curcumin loaded casein nanogels as drug delivery systems
1.16. T. E. Vlakhov, Y. G. Marinov, G. B. Hadjichristov, H. K. Koduru, N. Scaramuzza, Complex electrical impedance and dielectric spectroscopy of $Na^+$-conducting PEO/PVP/$NaIO_4$ solid polymer electrolyte with incorporated Graphene Oxide nanoparticles
1.17. T. E. Vlakhov, B. L. Martinov, A. D. Staneva, Y. G. Marinov, G. B. Hadjichristov, Complex electrical impedance and dielectric spectroscopy studies on reduced graphene oxide (rGO)/$ZnTiO_3$ nanocomposites
1.18. G. B. Hadjichristov, Y. G. Marinov, T. E. Vlakhov, H. K. Koduru, N. Scaramuzza, Solid polymer nanocomposite electrolyte complexes PEO/PVP/$NaIO_4$ with $TiO_2$ nano-additives: $Na^+$ ion conductivity and dielectric studies
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1.20. Z. Slavkova, N. Drinova, H. Chamati, J. Genova, Influence of carbohydrates on the phase behaviour of phospholipid systems
1.21. J. Genova, N. Drinova, H. Chamati, M. Petrov, Z. Slavkova, Influence of carbon nanostructures on the structural and thermal properties of lipid membranes
1.22. S. Panyovska, D. Dzhonova, I. Tsibranska, Comparative evaluation of approaches for CFD modeling of mass transfer in membrane filtration
1.23. M. T. Primatarowa, R. S. Kamburova, Soliton scattering on impurities with modified exchange interactions in anisotropic ferromagnetic chains
1.24. S. Varbev, I. Boradjiev, H. Chamati, Single-photon generation of entangled triplet states in an atomic spin dimer
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1.26. D. Yordanova, Modelling of multiple hollow cathode discharge
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2.4. T. Nurgaliev, M. Beshkova, Magnetic field effect in piezoelectric resonators with HTS electrodes
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2.8. S. Stankova, O. Volobujeva, Hr. Dikov, M. Ganchev, Solution deposition of ZnO thin films
2.9. B. L. Martinov, T. E. Vlakhov, A. D. Staneva, S. Slavov, Y. G. Marinov, G. B. Hadjichristov, Synthesis and characterization of nanosized $ZnTiO_3$ doped with of reduced graphene oxide (RGO)
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2.11. A. Atanasova, T. Hristova-Vasileva, R. Todorov, Influence of the molecular weight and concentration of PVP on the polyol synthesized silver nanoparticles

2.12. D. Dimitrov, I. Dionisiev, K. Buchkov, H. Dikov, V. Marinova, $WSe_2$ thin films and crystals
2.13. D. Nicheva, V. Ilcheva, R. Harizanova, I. Mihailova, T. Petkova, P. Petkov, Preparation and structural investigation of $BaTiO_3$
2.14. K. Lovchinov, G. Alexieva, B. Georgieva, M. Petrov, R. Gergova, B. Georgieva, Study of the sensitivity of electrochemically-deposited $ZrO_2$ on a quartz resonator
2.15. B. Georgieva, S. Kolev, K. Krezhov, Ch. Ghelev, D. Kovacheva, L.-M. Tran, M. Babij, A. Zaleski, B. Vertruyen, R. Closset, T. Koutzarova, Magnetic phase transitions in Zn2Y-type hexaferrites - the influence of substitutions
2.16. M. Beshkova, B. S. Blagoev, V. Mehandzhiev, R. Yakimova, B. Georgieva, I. Avramova, P. Terziyska, D. Kovacheva, V. Strijkova, Optimization of AlN films grown by atomic layer deposition
2.17. M. Beshkova, P. Deminskyi, C.-W. Hsu, I. Shtepliuk, H. Pedersen, R. Yakimova, Atomic layer deposition of AlN on different type of substrates
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2.19. Ts. Lazarova, D. Kovacheva, M. Georgieva, D. Tzankov, Physicochemical properties of nanosized $ZnFe_2O_4$ obtained by solution combustion synthesis and sonochemical synthesis
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2.31. S. Georgiev, V. Donchev, M. Milanova, Calculation of the bandgap of dilute nitride GaAsSbN alloys

# ABSTRACTS OF INVITED LECTURES

## Georgi Nadjakov Memorial Lecture

# Challenges and possible solutions for the end of the Nanoelectronic Roadmap

**Francis Balestra, Senior Member, IEEE**

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Future Nanoelectronic devices face substantial challenges, in particular increased power consumption and heating, saturation of performance, large variability and reliability limitation. In this respect, novel device architectures using innovative materials will be needed for Nanoscale FETs in the CMOS and Beyond-CMOS domains.

This paper presents promising solutions for the end of the roadmap in the CMOS and Beyond-CMOS fields. For NanoCMOS, MultiGate devices could be able to overcome most of the challenges for high performance and low power logic applications, using nanomaterial boosters, such as 1D (Nanowires, Nanotubes) or 2D (TMDs, BP, etc.) structures.

However, Beyond-CMOS solutions could be needed in the next decades, especially for ultra-low power applications and future autonomous Nanosystems, due to the limit of the subthreshold swing at 60mV/dec at room temperature for MOSFETs. In this respect, Steep Slope Switches Devices could allow to go beyond this red wall, for instance using tunnel transport (Tunnel FETs with alternative materials, Ge, III-V, 2D, etc.) or Ferroelectric materials (Negative Capacitance FETs with possible channel material boosters), or Hybrid structures (TFET/NCFET, FET with phase change materials or nanofilaments, etc.) [1-14].

These disruptive concepts will be able to reach the ambitious targets of the IRDS Roadmap for the next 2 decades [15].

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11. Z. Yu, IEDM 18, p. 524 (2018)
12. A. Saeidi, IEDM 18, p. 304 (2018)
13. E.A. Casu., IEDM 16, p. 19.3.1 (2016)
14. S. Lim, IEDM 16, p. 34.7.1 (2016)
15. International Roadmap for Devices and Systems, (2020)

**Milko Borisov Memorial Lecture**

# Towards 2D materials beyond graphene

**I. Shtepliuk[1], M. Beshkova[2], I.G. Ivanov[1], N. Pliatsikas[1],**
**T. Iakimov[1], K. Sarakinos[1], R. Yakimova[1*]**

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Two-dimensional non-graphene materials (2DNGMs) are paving the way to developing of conceptually new device technologies in electronics, sensorics and catalysis [1,2]. Compared to their bulk counterparts, 2DNGMs have more exotic electronic band structures and extremely large surface area, which enables non-conventional functionalities. Such material features provide key prerequisites of high-performance catalysis and ultrasensitive detection. Nevertheless, understanding synthesis and related physical properties of 2DNGMs is a challenging research task which requires incredibly special growth conditions including highly controlled surface energetics of the supporting template. Driven by these perspectives, we have scrutinized growth kinetics of extremely thin metal (Au, Ag) and nitride (AlN) films on graphenized surfaces of SiC. By estimating the diffusion and adsorption of film constituents as well as the behavior of early-stage nuclei, we discriminated the growth kinetics of gold on carbon-rich surface reconstruction of SiC (buffer layer, BL) and monolayer epitaxial graphene (MEG) and found that nm-thin gold films follow the Volmer−Weber growth mode on BL and quasi van der Waals-epitaxy on MEG, respectively. Weakly interacting MEG has also proved itself as SERS (Surface Enhanced Raman Scattering) substrate. By depositing 2-30 nm-thick plasmonically-active Ag nanofilms on MEG layer followed by thermal dewetting, we observed a strong tunable enhancement of the characteristic Raman modes of epitaxial graphene [3,4]. AlN thin layers were formed on epitaxial graphene by atomic layer deposition (ALD) technique using ammonia and trimethyl aluminum (TMA) as precursors. Based on morphology analysis and density functional theory (DFT) calculations, we propose a model describing the AlN growth mechanism We anticipate that combined in-depth experimental investigation and theoretical modelling presented here may bring us closer to reaching broad understanding of how to optimize synthesis of novel 2DNGMs and to manipulate their properties.

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# Thin films fabrication for biomedical applications in: drug delivery systems, biosensors, advanced sensor coatings and antinosocomial infections

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# Structural characterization of oxy-halide materials for solid state batteries

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Discovering new chemistry and materials to enable rechargeable solid state batteries with higher capacity and energy density are our priorities. The novel inorganic and thermally stable oxy-halide materials are potential substitutes for the toxic and flammable organic liquid electrolytes that are used in the Li-ion batteries. The oxy-halide glasses, are reported to show some of the highest $Li^+$ and $Na^+$ conductivities, $\sigma > 10^{-2}$ S cm$^{-1}$ at room temperature (25°C) [1,2]. We report the synthesis of Li-, Na- and K-ion based oxy halides materials with nominal compositions: $A_{3-2x}M_xO_{1+y}Cl_{1-2y}$ (where A=Li, Na, K; M=Ba, Ca, Mg; $0\leq x<1.5$; $0\leq y<0.5$) using wet-chemistry methods and maximum heat treatment limited to ~250°C. The samples have been characterized by neutron and X-ray diffraction, Raman spectroscopy, Differential Scanning Calorimetery and High Resolution Transmission Electron Microscopy (HRTEM).

In-situ neutron diffraction studies were performed on the PSD beamline at the 10 MW Budapest research reactor [3] at 100°C. The Rietveld *Fullprof* analysis and Reverse Monte Carlo simulation [4] of the neutron diffraction studies have been used to identify the crystalline phases and short-range structural properties such as alkali and alkaline ion co-ordination environments and the bond lengths. Neutron diffraction and Raman studies found that the investigated Li, Na and K-based samples are mostly crystalline with small amounts of amorphous phases. HRTEM studies show that the morphology of the Ba-$Li_3ClO$ and Ca-$Li_3ClO$ samples consists of nanograins of size < 10 nm. The study provides the structural characterization of alkali oxy-halide crystalline compounds doped with Ca, Ba and Mg, that have potential applications as electrolytes in the solid state batteries.

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# Lipid membrane interface - from electrostatics to molecular structure

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Electric charges on the membrane surface are involved in all structural rearrangements, and the ions of the medium participate in the charge at the interface and its screening by the diffuse part of the electric double layer. Therefore, most of the experimental work with a suspension of subcellular particles and liposomes is carried by electrokinetic methods. However, these methods are not suitable for analyzing the factors influencing the dipole component of the boundary potential, which is a convenient indicator of structural changes at the membrane-electrolyte interface. It has been found in our previous data with inorganic cations and polypeptides, and these structural changes have been associated with their biochemical applications [1,2]. The dipole potential was controlled by methods applied to planar bilayer lipid membranes (BLM). It was concluded that this component depends on the position of the adsorption plane of ions, charged molecules immersed in the polar region of the membrane, on the orientation of the dipole moments associated with phospholipids and water molecules. On the other hand, Langmuir monolayers demonstrate a direct relationship between boundary potential and the interface structure, especially in the case of negatively charged phospholipids with saturated carbon tails (DMPS) at their phase transition from liquid ordered (LO) to condensed (LC) state. Recently, it was found that the intensity of X-ray radiation scattered at different small angles from the lipid monolayer is sensitive to the difference in lipid packing of these states [3] and to the polymer layer on this surface [4]. The data on the charge distribution along the normal to the surface obtained by the X-ray reflectometry method are in good agreement with its distribution in these systems simulated by methods of molecular dynamics. It allows us to clarify some of the internal details of structure rearrangement at different lateral pressure and the contribution of various structural components of the system to the electric field [3].

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# Plasma treated titanium nanostructures for modification of stents

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Titanium and titanium alloys exhibit a unique combination of strength and biocompatibility, which enables their use in medical applications and accounts for their extensive use as implant materials. In cardiovascular applications, titanium stents are commonly employed to enlarge the lumen wall and to restore blood flow through the affected blood vessel. Although titanium alloys are extensively used for stent application they still lack desired biological responses. Namely, mostly due to restenosis. Therefore, the long term success of stent implantation depends mainly on avoiding the aggregation of platelets as well as on appropriate proliferation of endothelial cells and controlled proliferation of smooth muscle cells. The presented work provides an elegant solution for prevention of platelet and smooth muscle cell adhesion and activation on stent surfaces, while obtaining surface conditions to support the growth of human coronary artery endothelial cells. This was achieved by surface nanostructuring and chemical activation of the surface. Specific nanostructured surfaces of titanium were obtained by electrochemical anodization, while appropriate chemical properties were attained by treatment of titanium oxide nanotubes by highly reactive oxygen plasma. Our results show that a combination of nanostructuring and plasma modification of the surfaces is an effective way to achieve desired biological responses necessary for implantable materials, such as stents.

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# Multifunctional topological defect-based soft materials

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Liquid crystals (LCs) offer an ideal platform to design and realise diverse multifunctional devices. They combine a unique combination of simultaneous liquid and crystal order, optical anisotropy, softness (i.e., strong susceptibility to external stimulus), experimentally-tractable characteristic scales of time and spatial responses, and diversity of different phases and structures. Furthermore, numerous LC configurations are realized via continuous symmetry breaking transitions, which enable the existence of topological defects (TDs). They correspond to topologically protected localized regions within ordered media where the relevant order parameter field is frustrated. In singular TDs, at the defect origin, the continuum field, which describes defectless equilibrium configurations, is not uniquely defined. The key topological feature of a topological defect is its topological charge, which is a conserved quantity. Corresponding topological charge conservation laws regulate transformations (decomposing, merging, depinning) of defect configurations.

In our contribution, we illustrate numerically rich structural diversity in the nematic phase. The latter represents the simplest LC phase which exhibits in bulk equilibrium (defectless) spatially homogeneous structure possessing long-range order. We show that by confining nematic LC to simple plane-parallel geometry and appropriate surface treatment of one bounding plate one could establish conditions for which diverse competitive multistable defect structures exist. We demonstrate robust and reversible reconfigurability among these states, which in general exhibit different effective functionalities (e.g., optical appearance). This diversity of competing and reversible reconfigurable structures could be exploited for numerous applications, e.g., sensors, actuators, photonic units, light modulators, memory storage units, etc.

Furthermore, we show that these relatively simple and relatively easily observed and manipulated defect structures in confined nematic LC exhibit rich physics of interest for diverse other scientific fields. Namely, due to their topological origin, the physics of TDs exhibits several universal features, which are independent of microscopic details of a system. In nematics, confined within plane-parallel cells, we illustrate that TDs (i.e., “singularities” in orientational order) exhibit several phenomena that have analogs in electrostatics, particle-physics, and cosmology. We demonstrate the behavior of TDs analogous to the Faraday cavity effect in electrostatics, present nematic defect structures that resemble intriguing neutrinos, and quench driven coarsening dynamics of nematic defects which simulates events in the early universe.

# Protein-lipid interactions in viral infections

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The causative agents of almost all the most dangerous viral diseases are the so-called enveloped viruses – viruses, the genetic material of which is "hidden" in two envelopes: a protein scaffold and a lipid bilayer, into which the surface proteins of the virion are incorporated. Representatives of the enveloped viruses are such serious pathogens as human immunodeficiency virus (HIV), coronaviruses SARS, MERS, and SARS-CoV-2, hepatitis C, herpes, Ebola virus, influenza, etc. Despite significant differences in the clinical picture of the course of diseases caused by enveloped viruses, they themselves have a number of characteristic features that determine their commonality. Regardless of the method of penetration into the cell – by endocytosis or by direct fusion with the cell membrane – enveloped viruses bind receptors on the cell surface, fuse with the cellular lipid membranes and form fusion pores for release of their genome. Inside the infected cells newly expressed viral proteins should gather at the certain region of the outer (plasma) or intracellular membranes, combine with the genetic material of the new virus, and then, correlated in time and space, bud off from the cell membrane structures, forming a new viral particle. Matrix or capsid proteins that form the protein envelope of the virus play one of the key roles at different stages of the life cycle of viruses. Despite such an important function of these proteins, there are still many open questions about the mechanisms of their interaction with the lipid membranes of the cell and virus, the mechanisms of their self-organization during the assembly of new viral particles, as well as the reasons for the destruction of the viral protein capsid during infection. In this regard, capsid proteins, which are one of the most conserved proteins of enveloped viruses and constitute the bulk of proteins of any virus, are still not targets for antiviral drugs. Using different structural techniques, we investigated self-assembly and lipid membrane interactions for matrix and capsid proteins of influenza virus, HIV, and Newcastle disease virus at different stages of viral lifecycle. We found that these proteins use three main strategies of protein-lipid interactions to do the same thing: perform topological rearrangements of the membrane to entry the cell and to produce progeny virions.

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# Using model transport proteins to store, control and build functional materials

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Proteins are functional molecules essential for living organisms, and they can also be conveniently controlled and manipulated for nanotech applications due to their high versatility.

Proteins can be used as building blocks for the fabrication of microscopic objects with controlled morphologies and properties, especially by exploiting the self-assembly properties of their unfolded or misfolded states [1,2]. In particular, amyloid-based structures such as fibrils can be obtained by modulating a number of factors controlling the aggregation: protein type (sequence, concentration), solvent (including pH, ionic strength, presence of co-solutes), surface character (hydrophobic or hydrophilic), and other physico-chemical parameters (temperature, etc.).

One particularly important factor that can affect the behaviour of proteins is the presence of ligand molecules bound to them. For instance, small compounds can change the protein stability and affect the resistance to thermal denaturation [3,4]. In turn, proteins can be employed to control and store ligands. Again, this can be used in molecular nanotechnologies in a number of ways: stabilize or prevent degradation of a compound, detect or mask its presence, increase solubility or dispensability, or improve transport and routing to a specific target.

Common model transport proteins such as bovine β-lactoglobulin and human serum albumin have been long shown [5] to be particularly indicated to investigate the topics mentioned, as they are inherently designed by nature to store, protect and shuttle small molecules, and have been used in a number of different cases to build functional nanostructured materials. Other proteins able to transport a variety of additional molecular cargoes are currently studied for more advanced applications based on molecular recognition, including the development of sensor devices at the nanoscale.

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# Evolution of continuum models of membrane fusion

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Fusion of membranes is a key process in various phenomena of cell lifecycle. It is a necessary stage of fertilization, tissue growth, hormone secretion, synaptic transmission, and infection by enveloped viruses. The fusion process includes merger of membranes and combining of water volumes confined by them. This process requires fine topological rearrangement of membranes controlled by elastic properties of lipid bilayers. The elastic properties can be transformed to energy barriers and rate of the process in the framework of adequate theory of elasticity. For this reason continuum models based on theories of membrane elasticity are actively applied for the development of physical models of membrane fusion. These models evolved in parallel with advancement of theory of elasticity of lipid membranes. In the first theory developed by Helfrich in 1973 the membrane is considered as an infinitely thin film lacking any internal structure. This theory allowed for the first time to explain experimentally observed dependencies of fusion kinetics on lipid composition of merging membranes. The shortcomings of Helfrich theory of elasticity caused serious crisis of the theory of membrane fusion: it was shown that according to theoretical reasoning membranes should not fuse at all as the corresponding energy barriers are extremely high; however, membranes readily merged in experiments. The crisis was resolved by improvement of the elastic theory via introduction of additional deformational mode. The advanced theory of elasticity initiated a further development of numerous detailed models of membrane fusion that allowed predicting continuous trajectories of the whole process with molecular accuracy, starting from distant lipid bilayers and ending at the fusion pore. Modern approaches in this field allow continuum models of membrane fusion to stand shoulder to shoulder with molecular dynamics simulations and provide the deepest understanding of this process in multiple biological systems.

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# Spatially-resolved optical characterization of functional materials using coherence scanning interferometry

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The use of functionalized and complex surfaces and layers promises to lead to new functional materials with novel properties such as for example being able to detect and react to local stimuli or to detect biological properties. To achieve such functions, a growing challenge exists to characterize the physical properties of the individual microscopic components. Classical spectroscopy for measuring optical properties typically uses a large probing area over several mm$^2$. Recently, new techniques based on near field optical microscopy and hyperspectral imaging have been developed to perform spectral measurements on a local scale, in which the examination of large areas requires scanning in either the spatial or spectral domains. Another way of performing local spectroscopy is to use white light interference microscopy by means of Fourier transform processing of the polychromatic fringe signal combined with careful calibration of the optical system [1]. This approach captures the spectral information within the entire FoV in a single step, allowing rapid spectral mapping of spatially extended surfaces. In this work, we present some recent experimental results of local spectroscopy measurements using this latter technique, for example in measuring the local reflectivity of a gold layer on Si (Figure 1). The lateral mapping resolution is of a few µm$^2$, limited by the diffraction of the optical system, over a field of view that can reach up to 650x650 µm. We then discuss the potential of using microsphere-assisted microscopy combined with interferometry [2] to improve the lateral resolution even further.

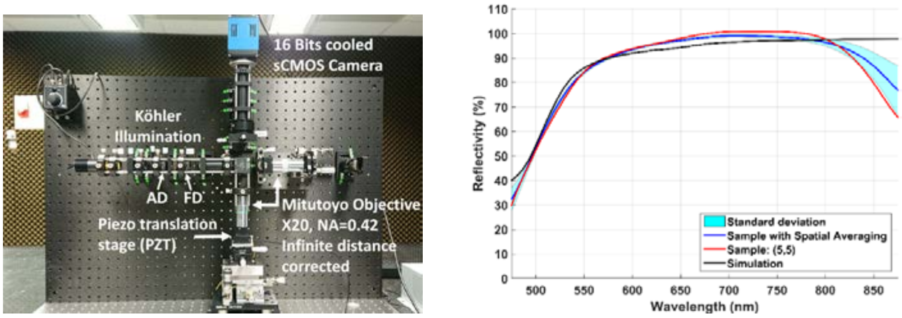

**Figure 1:** (Left) Interferometric microscope in Linnik configuration with Mitutoyo objective with large field of view. (Right) Local characterization of the reflectivity of Au layer deposited on Si with spatial and temporal averaging. The spatial resolution is a few µm$^2$.

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# Development of methods for non-destructive materials characterization

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Optical and magnetic measurement tools being developed at the Photonics Department [1] in the Centre for Energy Research of the Roland Eötvös Research Network and their applications in materials science will be discussed. The topics include the development of instrumentation for real time bioellipsometry [2] and large area mapping ellipsometry, Fourier scatterometry, waveguide interferometry, deflectometry, optical capillary bridge inspection, single particle scattering spectroscopy and surface mapping by magnetic adaptive testing. The talk will also include some related surface preparation techniques.

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2. http://www.ellipsometry.hu/

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# Ultrasensitive detection of analyte molecules at attomolar concentration by Raman spectroscopy

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Surface-enhanced Raman scattering (SERS) is a technique developed to detect extremely small quantities of molecules by determining their characteristic Raman signal. However, the adoption of SERS remains limited due to the difficulties in fabrication of highly sensitive and reproducible nanostructured plasmonic platforms. From this point-of-view, self-assembly techniques of SERS substrates formation allowing fabrication of highly branched dendritic silver nanostructures, to our opinion, are very promising for highly sensitive biosensensing applications.

We used so-called Ag corrosive deposition on a macroporous silicon (macro-PSi) template to grow 3D silver dendritic structure that demonstrated an unprecedented sensitivity in SERS spectroscopy. With the use of such substrates, it was possible for the first time to detect 4-MBA and DTNB acids molecules with very low concentrations of $10^{-16}$ M and $10^{-18}$ M, respectively.

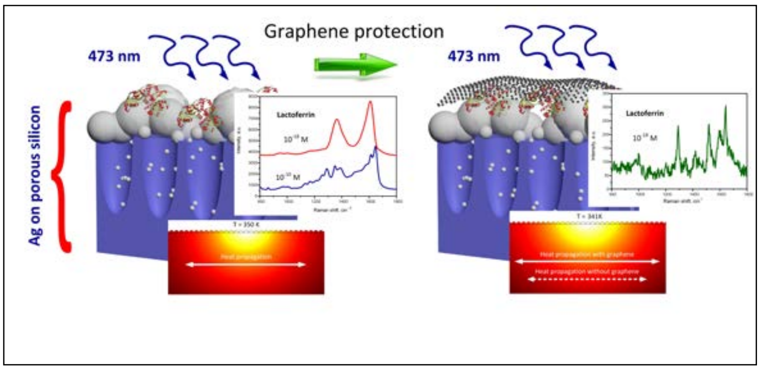

**Figure 1.** Schematic of the analyte molecule protection on the silvered por-Si with graphene

Besides, we examined SERS spectra of the human lactoferrin molecules adsorbed on a silvered porous silicon (P-Si) from $10^{-6}$–$10^{-16}$ M solutions. The SERS spectra of lactoferrin adsorbed from $10^{-6}$ M solution were rather weak but a decrease of the concentration to $10^{-10}$ M led to an enormous growth of the SERS signal. This effect took place as oligomers of lactoferrin were broken down to monomeric units while its concentration was reduced. Oligomers are too large for a uniform overlap with electromagnetic field from silver particles. They cannot provide an intensive SERS signal from the top part of the molecules in contrast to monomers that can be completely covered by the electromagnetic field. To prevent overheating the analyte molecules on the silvered por-Si were protected with graphene (Fig.1), which allowed the detection of lactoferrin adsorbed from the $10^{-18}$ M solution.

Thus, the SERS measurement results indicate the possibility of ultra-low analyte concentration detection, comparable to the concentrations of single molecules.

# Dilute nitrides heterostructures grown by liquid phase epitaxy for solar cells applications

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There has been great interest in dilute nitride III-V-N materials (such as InGaAs(Sb)N, GaAsSbN) during the last two decades, driven in part by their potential application in multijunction solar cells, which are expected to outperform single-junction devices. The research in this direction aims obtaining materials with a bandgap of the order of 1.0 - 1.2 eV, which are lattice matched to GaAs.

GaAsSbN layers and structures are grown by low-temperature liquid-phase epitaxy (LPE) on GaAs substrates and are characterized in view of the application of this material in solar cells. The GaAsSbN layers exhibit reproducible properties and good optical quality. X-ray diffraction, energy dispersive X-ray spectroscopy, atomic force microscopy, X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy are applied for investigation of the structural properties, surface morphology, local arrangement and chemical bonding of Sb and N in the obtained compounds. XPS spectra reveal clearly the Sb content (~7 at.%) and give indication for the presence of N (around 0.1 at.%) [1]. The band gap values at room temperature assessed from surface photovoltage (SPV) and photoluminescence (PL) measurements are in good agreement. They are 20-30 meV lower than those of reference GaAsSb layers and around 190-230 meV lower than the band gap of GaAs (1.42eV). PL spectra measured at different temperatures (10 - 300K) show a very weak S-shape-like behaviour of the PL peak energy position indicating minimal carrier localization. Electrical measurements have demonstrated that Mg is suitable dopant for obtaining from closely compensated to highly doped p-type GaAsSbN layers. Based on this result GaAs/GaAsSbN/GaAs p-i-n heterostructures, based on closely compensated GaAsSbN are grown for the first time by the LPE method. PL and SPV measurements reveal good optical quality of the structures with low concentration of localized states and photosensitivity red limit extended in comparison to GaAs down to about 1.2-1.24 eV [2]. Nearly the same IR photosensitivity behaviour has been revealed from external quantum efficiency measurements. Current-voltage curves are measured under standard test conditions (25°C, one sun AM1.5). A power conversation efficiency of 4.15 %, an open-circuit voltage of 0.44 V, short-circuit current of 17.31 mA/cm$^2$ and fill factor of 54.5 % are obtained for the cells without anti-reflection coatings and without rapid thermal annealing that has been used to achieve higher voltages for MOVPE and MBE grown materials. This is a very promising result for the first LPE grown GaAsSbN/GaAs solar cells, especially given that these cells are non-optimized, and the record of GaAsSbN/GaAs solar cell currently stands at just 6 % efficiency.

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# Two-dimensional materials based resistive switching devices

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Here we report the first realization of vertical MIM-like electronic synapses using 2D materials produced by chemical vapor deposition (CVD), which is a scalable method. By using multilayer hexagonal boron nitride (h-BN) sheets as RS medium, we have been able to implement both volatile and non-volatile RS simultaneously, which allows emulating several STP and LTP synaptic behaviours, including PPF, PPD, relaxation and STDP. The working regime can be selected by tuning the amplitude, duration and interval of the electrical stimuli. While until now all previous synaptic studies reported slow (0.1-100 s) erratic relaxation process during 0.1-100 s, here we show a fast (~200 µs) and stable relaxation during more than 500 cycles, with a very low variability. The power consumption of the synapses in volatile regime is 0.1 fW in standby and 600 pW per transition, and we find that the pulse voltage plays a more important role in the potentiation of the synapses than the pulse time/interval. These performances are enabled by a novel switching mechanism that combines characteristics from CBRAM and ReRAM. The volatile and non-volatile nature of the RS has been confirmed at the nanoscale via CAFM, demonstrating excellent potential for scalability.

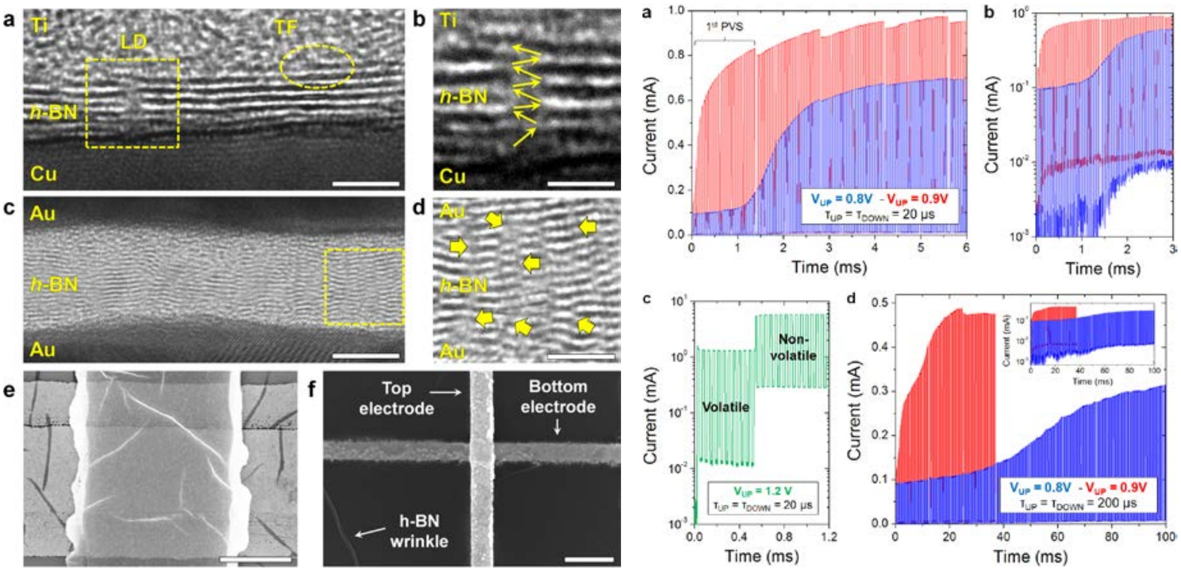

**Figure 1**: (Left) (a-d) Crsos sectional TEM images of the metal/h-BN/metal electronic synapses. (e-f) Top-view SEM images of the metal/h-BN/metal synapses with cross-point structure. (Right) (a-d) Potentiation of a h-BN based synapse applying pulsed voltage stresses with different height, duration and interval. Reprinted with permission from Y. Shi et al. Nat. Electron. 1, 458–465 (2018).

# Partial discharge measurements used as a tool to assess the quality of the electrode contact in flash sintering

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The measurement of phase-resolved partial discharge patterns is a well-established technique used in electrical engineering to study the degradation of electrically insulating materials placed at high voltage. The measured partial discharge (PD) signal gives information on the physics of the pre-breakdown mechanisms that may appear in this regime. In this talk, we show how this technique can also be applied to ceramics to better understand the so-called 'flash sintering' process, i.e. the sintering of ceramics under an applied electric field. We first recall the concept of phase-resolved partial discharge measurements and give details on the experimental system that was used to record simultaneously the partial discharge and the AC current. We then show results obtained on 3%mol yttria-stabilized zirconia (3YSZ) samples placed between planar electrodes and subjected to high electric fields up to 3.2 kV/cm [1]. The partial discharge signal is found to be much sensitive to quality of the contact between the platinum electrodes and the sample. The surface microstructure of the samples subjected to PD experiments exhibits various characteristics similar to those observed during dielectric breakdown.

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## Acknowledgements:

This study is supported by ERDF and the Walloon Region, in the frame of IMAWA – FLASHSINT research project (program 2014-2020). The authors thank M. Vedi Dupont from BCRC for the SEM observations.

# Influence of oxygen-rich and zinc-rich conditions on donor and acceptor states of zinc oxide

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For most of applications in electronics the control of electrical properties of zinc oxide is crucial. In the case of atomic layer deposition (ALD) the possibility of changing electrical conductivity of polycrystalline undoped ZnO films is surprisingly high, as it could be regulated up to three orders of magnitude only through growth temperature tuning between 100 and 200ºC. This effect has been reported by many groups, but its origin has never been investigated and addressed, which motivated our study.

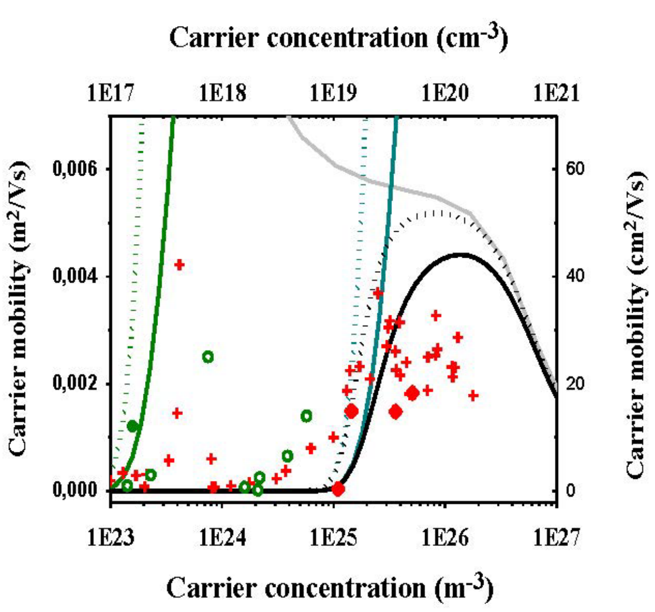

**Figure 1**: Hall mobility and concentration for ZnO-ALD films [2].

It has been shown that concentration of hydrogen, numbers of donors and its binding energies, relative ratio between donor and acceptors, deep states inside band gap, grain sizes with comparison to Debye length determine the final electrical properties of ALD layers. The above studies support the conclusion that the O-rich and Zn-rich growth conditions clearly influence not only deep defect states, which is widely believed, but also shallow donor and acceptor states as show Pl studies of the band-edge region. A number of donors, a ratio between donor and acceptor states as well as donors binding energies are clearly different for O-rich and Zn-rich growth conditions, which can be understood in terms of native-point-defects-hydrogen-impurity complexes that are created under O- and Zn-rich conditions [2].

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## Acknowledgements:

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# Neuromorphic materials by design

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Processing, storing, and transmitting information accounts for ~10% of global energy use; projections suggest that computational energy demands will be 10× higher than the projected global energy supply by 2040. Realizing solid-state analogs of neural circuitry, using ‘neuromorphic’ materials, holds promise for enabling a new energy-efficient computing paradigm. The metal–insulator transitions (MITs) of electron-correlated transition-metal oxides provide an attractive vector for achieving large conductance switching with minimal energy dissipation. In recent work, we have explored the intriguing electronic phase diagrams of low-dimensional ternary vanadium oxides with the formula $M_xV_2O_5$ where M is an intercalating cation and $x$ is its stoichiometry. Several of these compounds show colossal metal—insulator transitions and charge ordering phenomena. The talk will focus on mechanistic understanding of these transitions and their implications for the design of new “brain-like” vectors for computing (Fig. 1). If composition does not have to be structural destiny, a powerful new palette becomes available for tuning material properties.

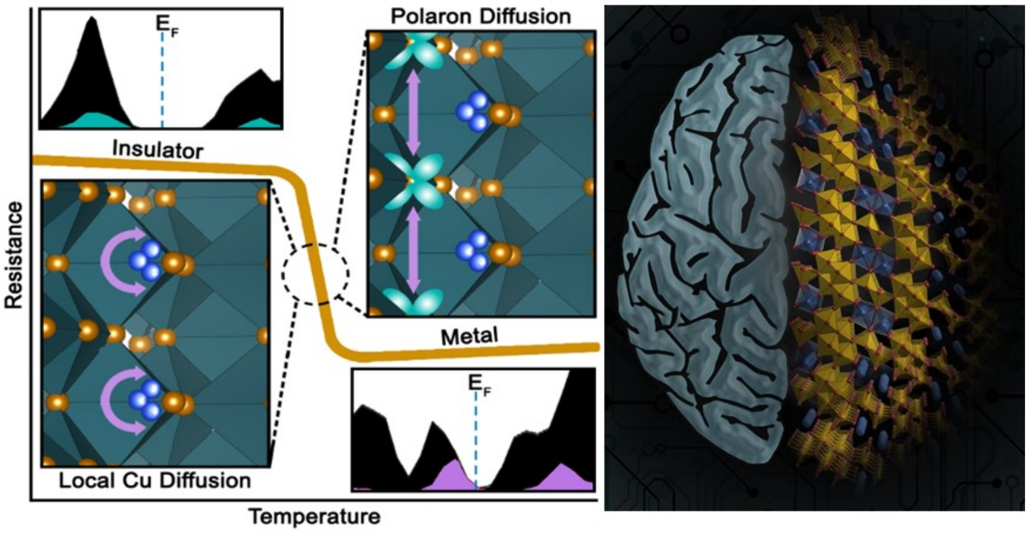

**Figure 1:** Cation shuttling and polaron oscillation in $\beta'$-$Cu_xV_2O_5$.

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# Strain-tunable conductivity and reflectivity of low dimensional systems within the Hubbard model

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The aim of this paper is to investigate the reflectivity of 1D and 2D systems under strain within the Hubbard model. The calculation discussed here is a distinct improvement compared to the previous paper on the same subject by the present author, where only the real component of the electrical conductivity was taken into account. In the calculation reported here both the real and imaginary components are taken into account. The final result is that the reflectivity is strain dependent, and that the dependence is approximately linear. Details depend on the material parameters. This dependence hints at the possibility of practical applicability of the results presented here.

# Electric oscillations generated by fluctuation cooper pairs

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We present computer simulations of the work of an electronic device for generation of electric oscillation by negative differential conductivity of a superconductor supercooled below the critical temperature. The superconductor is cooled below its critical temperature in the normal state at a small constant electric voltage. To simulate the device, we use formerly derived explicit analytical expressions for the conductivity of nanostructured superconductors supercooled below the critical temperature in an electric field. Computer simulations reveal that the negative differential conductivity region of the current–voltage characteristic leads to excitation of electric oscillations. We simulate a circuit with distributed elements as a first step to obtain gigahertz frequency. This gives a hint that a hybrid device of nanostructured superconductors will work in terahertz frequencies. If the projected setup is successful, we consider the possibility for it to be put in a nanosatellite (such as a CubeSat). The study of layered high-$T_c$ superconductors and EM waves emitted from them in space vacuum would be an important task for future space technology.

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# Dynamics of polymers with complicated topological structure in confined geometries

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Molecular Dynamics simulations of a dilute solution of ring polymer chains with different topological structures in a good solvent immersed in a slit geometry of two parallel walls with one adsorbing and the other one repulsive surface are performed. In our simulations we used a standard bead-spring model [1] of 360 beads. The polymer motion of polymer in a slit of two parallel walls was simulated using Langevin equation with the truncated Lennard-Jones 12-6 and 9-3 potentials. The monomer density profiles across the slit of ring polymer chains with different topological structures such as $0_1$, $3_1$, $6_1$, $7_1$, $9_1$, and twist knots with n={10,20} for different temperatures were obtained in the case of narrow and wide slits. In the case of low temperatures we observed that in narrow and wide slits increasing knotting of polymer reduces the monomer density near the adsorbing wall. At temperatures higher the adsorption temperature $T>T_{ads}$ the curves for monomer density profiles behave in a similar way for all knot types. With rising temperature the monomer density near the adsorbing wall decreasing quicker for wide slit than for narrow. The monomer density of ring polymer with topological structure $0_1$ in a slit geometry of two parallel surfaces with a different adsorbing and repelling properties in respect for monomers for all temperatures coincides with monomer density of linear polymer chain in the case of narrow as well as wide slit. This is in agreement with previous predictions obtained in [2] for the case of ring polymer chains in a slit of two parallel repulsive surfaces. Besides, the radius of gyration $R_g$, $R_{II}$ and $R_{\perp}$ of ring polymer chains with the above mentioned topological structures were calculated.

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# ABSTRACTS OF ORAL PRESENTATIONS

# PEGylation of graphene oxide nanosheets modulate cancer cell motility and proliferative ability

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Recently, graphene oxide (GO) has been increasingly investigated for its biomedical and biological applications, including cancer research [1,2]. Many data have demonstrated that PEGylation of nanoparticles (NPs) improves NPs solubility and stability in physiological solutions and can alter their reactivity toward cancer cells [2,3]. In this work, we have evaluated the effect of newly synthesized GO-PEG NPs on migratory and proliferation ability of melanoma cell line A375 used as a cancer cell model and have compared it to normal kidney MDCK cells. The successful PEGylation of GO was confirmed by IR spectroscopy. Both types of NPs, pristine and PEGylated GO, demonstrated inhibitory effect on cell proliferation and mobility of the cancer A375 cells while on normal MDCK cells the effect of GO was significantly weaker at 48 h of exposure suggesting that the cancer cells are more sensitive to GO and GO-PEG treatment. In general, PEGylation mitigated the inhibitory effect of GO on the growth and migratory ability of melanoma cells. Our results prove that the effects of both GOs NPs on cancer cell proliferation and mobility is dose-, NPs-type- and cell-type-dependent, hence providing a rational for future design and use of graphene-based nanomaterials for cancer research. The success of the last will be guaranteed by gathering deeper knowledge in the biology of graphene-cancer cell specific interactions.

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# Anti-frosting performance of chemically functionalized super-nonwettable carbon soot coatings

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The inherently hydrophilic surface of many heat exchanging industrial appliances, including air-conditioners, refrigerators or heat pumps, is a highly-beneficial platform for the accumulation of frost at negative surface temperatures, dramatically aggravating the heat transfer efficiency and energy consumption of these devices. In this proceeding, we present novel experimental data from systematic research on the frosting/defrosting performance of super-nonwettable soot coatings additionally functionalized with alcohols, fluorocarbon or silver hydrogen fluoride ($AgHF_2$)– one of the very few “smart” materials ensuring the required fabrication scalability of the synthesis approach, satisfactory mechanical durability, anti-icing and anti-bioadhesion properties. The subsequent analysis of the anti-frosting/defrosting activity of three groups of soot coatings reveals that the frost incipiency on the soot can be efficiently controlled by regulating its surface chemistry and porosity. In turn, the nonwettable thin films are capable of delaying the onset of vapor condensation and frosting to supercooling degrees of 8.4 °C and 15.8 °C, accordingly, and maintaining relatively large frost-free areas up to -20 °C. Moreover, the onset of soot defrosting is accelerated by a factor of 35 compared to a bare Cu substrate, demonstrating extremely low ice adhesion forces and strong potential for integrating the soot in passive icing protection systems of many cryogenic facilities.

**Keywords:** condensation frosting, hydrogen bonding, ice bridging, icephobicity, soot, superhydrophobicity

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# Possible mechanisms of invaginations and endovesicles formation coupled to a global shape transformation driven by non-homogeneous lateral distribution of active force

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Certain amphiphilic molecules can induce the formation of a large number of small spheroidal membrane invaginations, i.e. buds/endovesicles. Previous theoretical descriptions of invaginated (stomatocyte) red blood cell (RBC) shape transformation, based on the minimisation of the membrane bending energy, were able to explain only large stomatocyte invagination(s), but not also the large number of small membrane buds/endovesicles. By using Monte Carlo (MC) simulations, we suggest a possible mechanism of invaginations/buds formation coupled to a global shape transformation. It is shown that active force nanodomains/inclusions may partially control the shape of invaginations and the budding process. We also indicated that topological anti-defects may induce the rupture of thin membrane necks connecting the membrane buds (endovesicles) with the parent membrane.

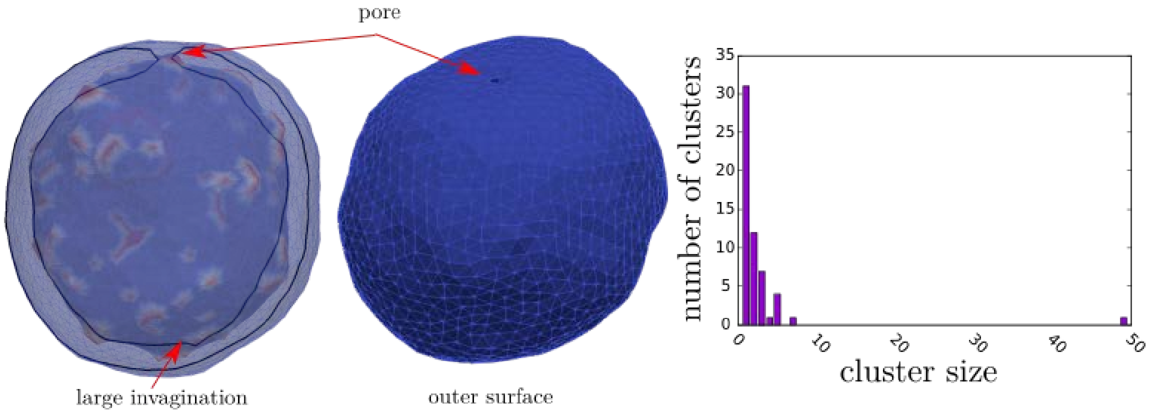

**Figure 1:** The Monte Carlo simulation of the RBC membrane transformation induced by mobile membrane inclusions with negative intrinsic curvature with negative active force acting on them. Concentration of membrane inclusions is 5%. The negative sign of force denotes that the nanodomains (inclusion) generated forces point to the vesicle interior. Red vertices on the mesh represents the locations of the membrane inclusions. The triangulated membrane surface is drawn semitransparent to uncover its interior shape.

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# Phospholipid stabilized gold nanorods: Towards improved colloidal stability and biocompatibility

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Biocompatible and colloidally stable gold nanorods (GNRs) of well-defined plasmonic properties are essential for biomedical and theranostic applications. The widely used seed-mediated method for the synthesis of GNRs uses a surfactant called as cetyltrimethylammonium bromide (CTAB) as a template, which is toxic to different cells. Biocompatible GNRs synthesized from known protocols are also reported to exhibit some extent of cytotoxicity and colloidal instability because of incomplete removal of CTAB. We report a facile method to overcome these difficulties and for the efficient removal of toxic CTAB molecules with 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) phospholipids, which are naturally present in cell membranes. The ligand exchange kinetics is studied using surfaceenhanced Raman scattering (SERS) and corroborated with matrix assisted laser desorption/ionization (MALDI) mass spectrometry. From colloidal stability studies using dynamic light scattering (DLS) and UV-Vis spectroscopy, the optimal lipid concentration and duration required for successful ligand exchange of CTAB by DMPC are reported. The 3-(4,5-dimethylthiozol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT) and lactate dehydrogenase (LDH) assays show that the surface modified DMPC-GNRs have significantly better biocompatibility compared to CTAB-GNRs. Studies on ligand exchange, colloidal stability and biocompatibility of DMPC-GNRs of aspect ratios in the range of 2.2 - 4.2 demonstrate the robustness of the proposed method. The results provide insight on the important factors to be considered to design biocompatible GNRs suitable for applications in nanomedicine.

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# Optical properties of thin Ag – In films prepared by interdiffusion in bimetallic nanolayered stacks

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The presence of interband transitions in noble metals, such as gold and silver, in the blue and ultra-violet (UV) parts of electromagnetic spectrum is a reason that these metals do not satisfy the needs of materials with high plasmonic activity in the UV spectral range. Thus an increasing interest in the transition metals and their alloys appears to produce new materials suitable for application in the high resolution spectroscopic methods, such as Plasmon-enhanced ultra-violet fluorescence and attosecond spectroscopies. Recently, an optical absorption dominated by a strong surface plasmon resonance (SPR) in the near UV for $In_{50}Ag_{50}$ clusters was reported [1].

The present work reports preparation, structural and optical properties of thin bimetalic films from the Ag-In system. Thin films with required compositions were prepared by annealing of Ag/In stacks. To achieve this aim, multilayered coatings consisted by 17 alternating Ag and In films were deposited. The silver and indium sublayers thicknesses in the stacks were chosen to produce thin layers with Ag/In ratio of 20:1, 10:1, 3:1, and 1:2. The chemical and phase composition, as well as the surface morphology of thin films were analyzed by energy dispersive X-ray microanalysis, X-ray diffraction (XRD) and atomic force microscopy, respectively. The analysis of the XRD patterns indicated that the silver-rich coatings are consisted mainly by Ag-based solid solution while the thin films with indium content higher than 25 at % In show alloying to crystalline phases of $Ag_9In_4$, $Ag_3In$ and $AgIn_2$.

The optical properties of the thin film coatings were characterized by UV-Vis-NIR spectrophotometry and spectroscopic ellipsometry. The dispersion of the complex permittivity, $\hat{\varepsilon} = \varepsilon' + i\varepsilon''$, was analyzed by the Drude – Lorentz model. The increase of the indium content increases the values of the imaginary part of the complex permittivity in the visible spectral region and decreases them in the ultraviolet spectral region. As a result, an increase of the quality factor for the excitation of the localized surface plasmon resonance, $Q_{LSPR} = -\varepsilon'/\varepsilon''$ in the spectral region of 3 – 6.5 eV was achieved.

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# Structural and optical properties of Au – In films for plasmonic applications

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In this work we present the preparation and investigation of structural and optical properties of thin films from the Au-In system.

The samples were prepared by thermal co-evaporation from the initial elements Au and In. The chemical and phase composition of the coatings were probed by X-ray microanalysis and X-ray diffraction, respectively. The resultant composition of the thin films was close to the expected one. The X-ray diffraction analysis revealed a good correspondence to the Au-In phase diagram. The thin films with low indium content (In < 20 at. %) contain $Au_3In$, Au and In. Presence of $Au_7In_3$ and AuIn phases was registered in the intermediate compositions, while the In-rich thin films appear as a mixture of the $AuIn_2$ compound and elemental In.

In the reflection spectra of thin films with indium content over 70 at. %, a minimum was observed in the spectral range of 1.4-2.0 eV, as its position shifts to the lower photon energies with increasing the indium content.

To clarify this behaviour, the dispersion of the complex permittivity was determined by ellipsometric measurements in the spectral range of 1.2-6.5 eV. The results showed that the real part, ε’ possess a maximum at photon energies of 1.5-2.0 eV, while the imaginary part, ε” is characterized by a maximum, whose position is in the spectral range of 2.2-3.0 eV and depends on the composition of the thin films – Figure 1.

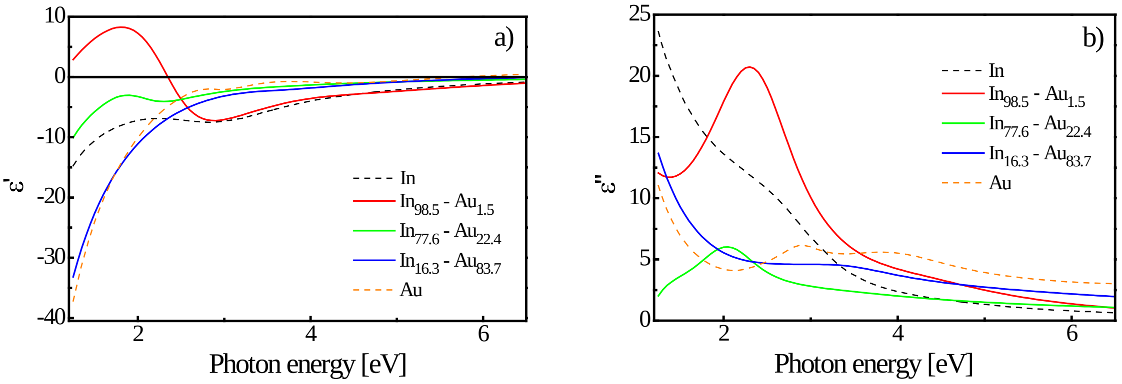

**Figure 1:** Real and imaginary parts of the complex permittivity of thin Au-In films.

Due to the fact that gold and silver have similar outer electron shell configurations (Ag – $4d^{10}5s^1$ and Au – $5d^{10}6s^1$), a comparison of the spectra of reflection of thin Au–In films with such from the Ag-In system, in the case of high indium content, was made. The role of the $AgIn_2$ and $AuIn_2$ crystals was discussed.

**Acknowledgements:** This work is financially supported by contract KP-06-N38/8 - 05.12.2019 with the Bulgarian National Science Fund (BNSF).

# Structural and optical properties of electrochemically deposited $ZrO_2$ layers on different substrate

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The work presents electrochemical deposition of $ZrO_2$ thin films on different substrates using a three-electrode system with a saturated calomel electrode as a reference electrode, in aqueous solution containing $ZrOCl_2$ and KCl. The structural and optical properties of the obtained $ZrO_2$ layers are investigated by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), UV-VIS-NIR and photoluminescence spectroscopy and optical profilometry. The XRD spectra show the polycrystalline nature of the films at all studied deposition substrate with the typical characteristic reflexes of the $ZrO_2$. The SEM micrographs show that the $ZrO_2$ films have a developed surface, with delayed different formations. Is presented and discussed the influence of the substrate on the reflectance and transmittance spectra and haze ratio of the ZnO layers. High values of the diffuse reflection and diffuse transmission in the 350 − 800 nm spectral range are observed; this type of thin films can be applied as rear contacts of thin films solar cells.

# An optical excitation study of pure and Ru-doped $Bi_{12}SiO_{20}$ crystals with graphene coating

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CVD-grown graphene was transferred onto polished crystal plates of pristine and Ru-doped bismuth silicate ($Bi_{12}SiO_{20}$:Ru), which are well known inorganic materials possessing very high carrier mobility and photo conductivity. The obtained heterostructures were investigated by ellipsometry, optical absorption and Raman spectroscopy. The influence of photoinduced phenomena in the crystal substrate on the graphene layer with possible implications for optical doping of graphene was examined.

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# Smart self-composing leaning system with functional restricted data learning from small datasets

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One of the main problem of the machine learning is the high dimensionality of the input raw data and the lack of independence between the inputs. The data although noisy and thus having the dimensionality of the embedding space, normally have lower but unknown dimension D. Using universal solving machines one can extract the information of the number of the data points should be of order at least $K^D$ (K of order 10). If the input data, the observations are in space with much higher dimension, $\Delta >> D$, and noisy, the problem can be solved just with huge amount of data.

If we consider an engineering, for example, if we observe T, p and V of some gas, seemingly it has three dimensions, but if we consider that the dependence RT=pV holds, then p and T will actually determine V, so the system is two-dimensional. (Figure 1).

In general considering a set of variables $x_1, x_2, \ldots x_\Delta$ and dependencies $f_i(x_{i1}, x_{i2}, \ldots, x_{iki}) = 0$, each dimension will, in general, diminish with one for each constraint $f_i(.)$. We can consider the f(.) as “molecules” that should be linked by learning the unknown dependencies between the different variables, say we know that $x_{im}$ and $x_{jn}$ is the quantity, that we can express as $\Sigma w_{r,im}\, x_{im} = 0$. If we are going to investigate or control natural system and we use different sources of information and in general, it is not know in advance the equivalence and the dependence of the variables.

As an example application, we consider a set of human physiological data – blood tests for metabolic problems. The complete blood tests are performed once every 6 months. It is possible to have one measurement per day, say blood pressure. The dimension of the problem is probably more than 7. This means that we need $10^7$ samples of blood tests, which is more than the life span. However, given that the deviations from normality occur in one or two regulation circuits, one can deduce rather precise model from just some 20-30 measurements instead of 10 million.

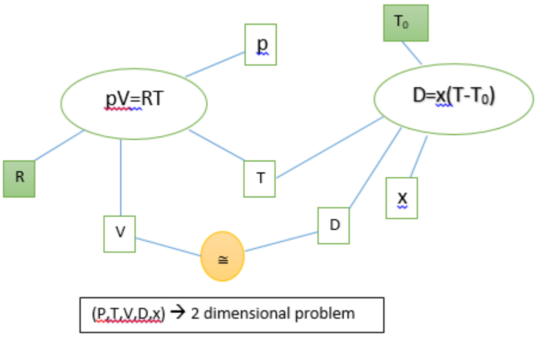

**Figure 1:** Schematic representation of the method. The derived model is learning by adjusting the yellow glue boxes, e.g. the unknown connections between the rules.

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# The magnetic properties of $Ni_4Mo_{12}$ molecular magnet: Theory and experiment

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The unusual magnetic behavior of molecular magnet $Mo_{12}O_{30}(\mu_2\text{-}OH)_{10}H_2(Ni(H_2O)_3)_4$ shortly denoted as $Ni_4Mo_{12}$ has attracted a lot of attention among the researchers [1–4]. The experimentally observed broadening of the cold peaks in the magnetic spectrum, non-equidistant steps and high-filed saturation in magnetization have posed a great challenge for the theory molecular magnetism.

Characterizing the origin of $Ni_4Mo_{12}$ magnetism we take into account the molecular orbital theory in conjunction with the multi-configurational self consisting field method and construct an effective spin-like Hamiltonian to capture all magnetic features predicted by the named method. The obtained theoretical results are in very good agreement with the experimental findings [5,6].

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# Electric field effect of cleaved superconductors surface and the problem of effective mass of supefluid charge carriers

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The determination of the effective mass of Cooper pairs is an open problem of the condensed matter physics. We analyze two alternative experimental methods both requiring cleaved surface of a superconductor to which the superconducting wave function can reach it. Both effects require electric field but in some sense they are inverse to each other: 1) in the first effect a strong electric field is applied to the surface of the superconductor which is in the vortex state at a constant magnetic field. In such a way the cleaved surface of the superconductor is one of the plate of a plane capacitor. At the capacitor is applied alternative sinusoidal voltage and the electric field at the interface with the insulation layer creates a surface magnetization, which can be measured. This effect (electric field induced surface magnetization of the Abrikosov phase) was theoretically predicted this year [1]. 2) In the second effect electric current density is excited at the surface of the superconductor by magnetic field or electric contacts and nanovolt range contact potential difference is measured by a lock-in voltmeter and low noise pre-amplifier. The contact potential difference (CPD) is proportional to the square of the current analogously to airplane wing lift force is proportional to the square of the velocity. That is why this second effect predicted by Fritz London in 1935 is also known as Bernoulli effect in superconductors [2]. The measurable values of these effect are parameterized by the effective mass of Cooper pairs and their study will lead to an effective Cooper pair mass spectroscopy. The proposed set-ups require standard electronics and the main difficulty is the technology of the cleaving of superconductor surface. Perhaps most appropriate material to start this research is $Bi_2Sr_2Ca_1Cu_2 0_8$ which has above liquid nitrogen critical temperature and simultaneously its surface can be simply cleaved by adhesive tape.

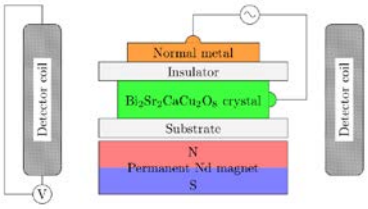

**Figure 1:** Surface magnetization

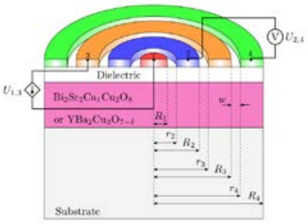

**Figure 2:** Bernoulli effect experiment

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# Infrared optical constants of chromium nano-films

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In the present work, nanofilms of chromium have been prepared by thermal evaporation in vacuum on to ultrasonically cleaned glass substrates held at room temperature (22 ºC). Films have been characterized by using X-ray diffraction (XRD) spectra, Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM) and Infra-Red (IR) spectra were used to examine the morphology and nano-structures to find out the cause. The transmission measurements were made on chromium films in the thickness range 5-60 nm for the incident photon energy of wave-length range, (2.5-4.5) µm. The optical transmittances of films have been found to decrease with increase in the film thickness in the entire IR spectral region of incident photon energy. In this case the optical constants like refractive index (n), absorption coeffient (a), extinction coefficient (k), real part (ε') and imaginary part (ε'') of relative permittivity are obtained from IR spectrum.

**Keywords:** chromium nanofilms, refractive index, extinction coefficient, absorption coefficient, real and imaginary parts of relative permittivity.

# Investigation of a nickel clusters growth dynamic under Langmuir monolayer of arachidic acid for creation of new conductive material

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Creation of new types of functional materials is an important task in modern science. One of the prospective ways for creation of high-ordered thin films is a Langmuir-Blodgett technology. This technology allows us not only to create a high ordered monomolecular film but also to modify them by incorporation of metallic ions. It is well known that Langmuir monolayers of fatty acids and lipid molecules could be bonded by metal ions of different valence. Research of the dynamics of such processes is important for applications in biology during the tissues biomineralization, physics of the conductive materials creation and chemistry for creation of templates for synthesis of nanoparticles. In the present work an influence of subphase temperature in the range of 10°C - 30°C on the formation process of $Ni^{2+}$ ion clusters growth in a Langmuir monolayer of arachidic acid was investigated. A simultaneous analysis of nickel arachidate compression isotherms and transferred film morphology makes possible to determine an influence of subphase temperature on the cluster growth process. The main influence is in a changing number of growth centers of nickel arachidate clusters under the Langmuir monolayer and area covered by them by the alteration of subphase temperature. So, an increase of subphase temperature leads to the increase of clusters growth centers and at the same time to decreasing of average area covered by each of them that is schematically shown in fig. 1.

The obtained results will be useful for deeper understanding of metallic clusters' growth dynamics under the Langmuir monolayer. Also, obtained data has a potential for possible application at the process of formation of organometallic coatings based on fatty acids and ions of transition metals.

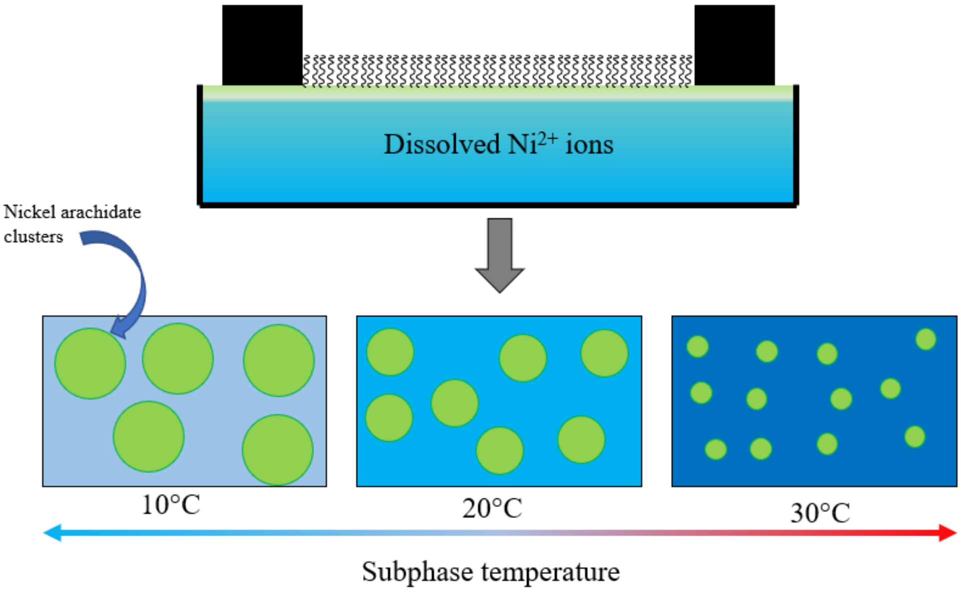

**Figure 1:** Schematically illustration of subphase temperature influence on the nickel clusters growth process

**Acknowledgements:** The reported study was funded by RFBR, project number 20-37-70021.

# ABSTRACTS OF FIRST POSTER SESSION

# 1.1. Effect of physicochemical characteristics of super-nonwettable carbon soot coatings on the freezing time delay and freezing temperature depression of sessile cooled water droplets

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The negative outdoor temperatures in winter seasons and/or cold climate regions cause many inconveniences in our routine daily-life, but the tremendous and nature-inspired development of physical, chemical and engineering sciences has promoted the launch of novel strategies for passively combating the atmospheric and condensation icing. The primary objective of this proceeding is to describe the icephobic properties of super-nonwettable carbon soot coatings with diverse physicochemical profile (i.e. morphology, chemistry and surface roughness) in order to establish the freezing mechanisms of cooled water droplets resting on the surface of these materials; a task that has not been implemented yet. For that purpose, a set of 10 μL and 50 μL water droplets are subjected to freezing events at constant negative temperature of -30 °C (freezing delay assessment) or progressively decreasing surface temperatures (freezing temperature assessment) on three groups of soot. The obtained experimental results hint that except the particle size, interfacial cracks, roughness profile, surface free energy values and solid-liquid contact area, the surface chemistry of the soot plays dominant role in controlling the freezing time delay and freezing temperature depression of the liquid droplets. This is a result of fundamental importance, allowing subtle control of the freezing events on soot coated surfaces, by tailoring their chemical composition, and revealing the strong potential of the soot for applications in cryobiology and cryogenics.

**Keywords:** freezing time delay, freezing temperature, icephobicity, soot, superhydrophobicity

**Acknowledgment:** This study was performed thanks to the financial support of Bulgarian National Science Fund within the frame of a research project entitled “Studying the impact of physicochemical characteristics of super-nonwetting carbon soot coatings on their icephobic properties” (grant № КП-06-Н37/7/06.12.2019).

# 1.2. Mixtures of quadrupolar liquids

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Quadrupolar liquids are continuous media which is build of molecules that possess large quadrupole moment (e.g. $H_2O$) or do not have any dipole moment ($CO_2$). Macroscopic characteristics of such kind of media are their dielectric constant $\varepsilon$ and quadrupolar length $L_Q$. Following Onsager [1] we have derived a theoretical relations between $\varepsilon$ and $L_Q$ and the molecular characteristics: molecular polarizability $\alpha_p$, dipole moment $p$, molecular quadrupolarizability $\alpha_q$, and quadrupolar moment $q$. Now we extend the theory to quadrupolar liquid mixtures. For example, for two component mixture knowing the parameters of both components we could predict the dielectric constant $\varepsilon$ and the quadrupolar length $L_Q$ of the mixture. Figure 1 illustrates $L_Q$ of $CH_4$ + $N_2$ mixture. The quadrupolar length of the mixture varies from approximately 0.30 Å to 0.70 Å with increasing the nitrogen mole fraction $x_{N2}$. That compares well with previously obtained values of $L_Q$ for pure methane (0.15-0.30 Å) and pure nitrogen (0.40-1.10 Å) [2].

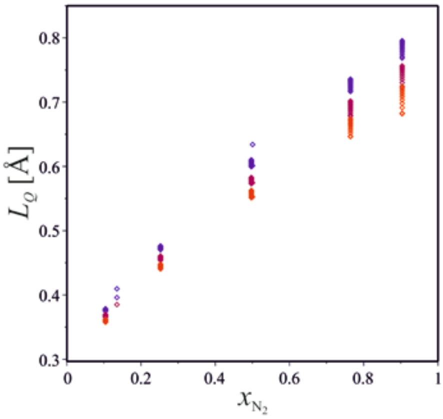

**Figure 1:** Quadrupolar length $L_Q$ of methane + nitrogen ($CH_4$+$N_2$) mixture as a function of nitrogen mole fraction $x_{N2}$. The dispersion of the points is due to different temperatures and pressures they are calculated for.

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# 1.3. Mass sensitivity of Langmuir-Blodgett monolayer film coated surface acoustic wave resonators to volatile organic solvents

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Langmuir-Blodgett (LB) monolayer films from Dipalmytoyl Phosphatidyl Ethanolamine head labelled with Nitrbenzoxadiazole (DPPE-NBD) have been studied. Because of its biomembrane molecules' mimicking properties, it is expected that DPPE-NBD molecules can serve as an excellent matrix for the incorporation of selectively reacting with the analyte under study proteins or enzymes while preserving their function. This combination can act as an active layer in chemical biosensor applications for operation in either gas or liquid environments. Newly discovered effects for this molecule can be used to enhance biosensor sensitivity and selectivity [1]. In this study, LB monolayers from DPPE-NBD were deposited on Rayleigh Surface Acoustic Wave (RSAW) resonant devices working at 440 MHz and simultaneously on ultra-flat Si wafer substrates for Atomic Force Microscopy (AFM). Depositions with very slow compression and substrate withdrawal to eliminate kinetic effects were carried, both at a very low surface pressure of 3.8 mN/m, where the liquid-expanded phase dominates, or at a very high pressure of 35 mN/m, where the liquid-condensed (solid) phase dominates. AFM topography reveals the liquid and solid phase coexistence as well as 3 - 30 nm high 50 - 1000 nm in diameter 3D cylinders. In a vapor sensing experiment, the RSAW devices were exposed subsequently to saturated vapors of 7 solvents including water. The most significant resonant frequency shift of 225 kHz which corresponds to 11,41 ng mass change was observed with chloroform vapors when the substrate with the solid phase LB monolayer was used as a sensing layer. Adsorption and desorption of the vapors were reversible and the resonance frequency was found to return within a few seconds to the baseline after removing vapor exposure. The higher-pressure deposited LB film demonstrates a higher sensitivity to all solvents. Mechanisms for this behavior are discussed. The authors believe that these results are a step forward to more complex nano-biosensor developments, where a SAW resonant device is the most promising method for the transduction of the sensor signal.

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## Acknowledgements:

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# 1.4. Investigation of the antibacterial and antifungal effects of silver nanolayers on the ocular prosthesis coating after a two-year period

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Long-term use of ocular prostheses causes frequent ocular infections with a number of adverse effects.The antibacterial and antifungal activity was investigated of Ag-doped $Al_2O_3$ nanolayers deposited by radioactive magnetron sputtering on ocular prostheses after a two-year period. A microbiological study was performed to determine the antibacterial action of the nanocomposite $Ag/Al_2O_3$ nanolayers against gram positive and gram negative bacteria, and an antifungal action against Candida albicans. From the conducted microbiological studies we have found the preservation of the antibacterial and antifungal action of the $Ag/Al_2O_3$ nanocoating of the eye prostheses after two years. The results of microbiological studies show that antibacterial and antifungal activity has the same full inactivation by intensity for the reference period. Experimental studies show a very promising application of such antibacterial and antifungal $Ag/Al_2O_3$ nanocoating to reduce ocular infections in the placement of ocular prostheses over a prolonged period of use.

**Keywords**: $Ag/Al_2O_3$ nanolayers, antibacterial and antifungal action, ocular prostheses coating, two-year period

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2. K. Koev, Donkov N., Stankova N., Najdenski Hr., Nurgaliev T., Nikov R. and Avramov L. Application of silver antibacterial nanolayers for hard contact lenses coating IOP Conference Series: Materials Science and Engineering 2019

# 1.5. Investigation of the antibacterial and antifungal effects of silver nanolayers on the hard contact lenses coating after one-year period

**Krasimir Koev[1]*, Nikolaj Donkov[1], Nadya Stancova[1],**
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The paper reports on antibacterial properties of Ag-doped $Al_2O_3$ nanolayers deposited by RF reactive magnetron sputtering on hard contact lenses after one-year period. The coatings were deposited on hard contact lenses by RF magnetron co-sputtering of Ag and Al under the following conditions: frequency 15 MHz; working pressure in the vacuum system ~ 5.5 Pa and the optimal mixture of Ar and $O_2$. The study has been provoked by the need of suppressing the infections caused by pathogenic microorganisms following the placement of hard contact lenses. There is a risk of developing bacterial keratitisc and conjunctivitis when wearing contact lenses (1-3). The microbiological experiments was carried out to determine the antibacterial properties of the coating considered in suppressing Gram-positive and Gram-negative bacteria after a two-year period. The following strains were used: *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa and Candida albicans*.

Our experimental findings suggest a very promising application of such antibacterial and antifungal $Ag/Al_2O_3$ nanolayers regarding the reduction of eye infections when the hard contact lenses are used after one-year period. The antimicrobial properties of the surface of Ag doped Al oxide coated products are very promising for many biomedical applications.

**Keywords:** $Ag/Al_2O_3$ nanolayers, antibacterial and antifugal action, hard contacts lenses coating, RF reactive magnetron sputtering, one-year period

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# 1.6. Thin layers of Hemin with sensing applications

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Biosensors play an important role in advanced diagnostics. For this reason, high accuracy, specificity and real-time registration of analytes are required. Such type of detection is provided by Surface Plasmon Resonance (SPR) method.

Hemin (ferric protoporphyrin IX chloride) is an iron-containing porphyrin, formed from a heme group, which is found in the hemoglobin of human blood. It is widely used for the treatment of porphyria attacks and in antimalarial drugs. In compound, hemin has a great potential as a recognition element of DNA in electrochemical sensing devices [1, 2]. However, hemin alone is very difficult to dissolve, which determines the main limitation in its application. In this work, we report for efficiently immobilized thin layers of hemin on an SPR chip gold surface. The layers are biologically active and resistant over time, which makes them applicable for sensory purposes. The properties of these recognition layers deposited on the surface of a highly sensitive optical sensor open up new possibilities for fast and accurate diagnostics.

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# 1.7. Effect of β-galactosidase immobilization on properties of chitosan/xanthan and xanthan/chitosan multilayers

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Polyelectrolyte multilayers (PEMs) deposited on non lyophilized and lyophilized polylactic acid (PDLA) substrates were investigated. The substrates were charged in a corona discharge. The charging of the substrates in a corona discharge was carried out by means of a conventional corona triode system consisting of a corona electrode (needle), a grounded plate electrode and a grid placed between them. Positive or negative 5 kV voltage was applied to the corona electrode and 1 kV voltage of the same polarity - to the grid. The dependences of the normalized surface potential on the storage time for positively and negatively charged non lyophilized and lyophilized PDLA substrates were studied. The results obtained show that the values of the normalized surface potential of non lyophilized substrates decay faster than those of the lyophilized ones. For multilayer build-up layer-by-layer (LbL) deposition technique was used. The first built-up layer always possesses an electric charge opposite to that of the substrate. PEMs with different number of layers (4 or 8 layers) were obtained. In the polyelectrolyte multilayers obtained the enzyme β-galactosidase were immobilized. The enzyme activity of each multilayer configuration was measured. The experimental results show that, in case of enzyme immobilization in multilayer films with 8 layers the efficiency of immobilization is considerably better compared to ones with 4 polyelectrolyte layers.

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# 1.8. Thermal variations of refractive and dispersive parameters of optical polymers

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Temperature dependence of refractive and dispersive parameters of principal and some trade-marks of optical polymers has been studied. Refractive indices have been measured at several spectral lines in visible light at different temperatures between 0 and 50 °C. Thermo-optic coefficients have been determined and compared.

Our previous studies on refraction and normal dispersion of optical polymers in visible and near-infrared regions on base of refractive index measurements at more than 20 spectral lines have shown that Cauchy-Schott and Sellmeirs's approximations give accuracy better than $10^{-5}$ if 6 dispersion coefficients are applied [1]. In case of the single-oscillator model of Wemple and DiDomenico [2], the accuracy is much lower but two parameters – single oscillator energy and dispersion energy, could be determined. These two quantities are related to the structure, charge distribution and chemical bonding of the material.

In this paper, oscillator and dispersion energies of polymethyl methacrylate, polycarbonate, polystyrene, styrene acrylonitrile, Optorez 1330, cyclo olefin polymer Zeonex E48R and styrenic material with low molecular weight (S-low styrene) are calculated. Correlation of these energy parameters to the dispersion properties of polymers is established. Variations of the two oscillator parameters with temperature are studied. The established thermo-optic coefficients vary with the polymer material but are fairly constant in the considered thermal region. Almost linear dependence of oscillator and dispersion energies with temperature is obtained. Gradients are negative with higher values for the dispersion energies.

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# 1.9. Phospholipid Langmuir-Blodgett films for detection of reactive gases and vapors at room temperature

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This work addresses the experimental investigations of Langmuir-Blodgett (LB) films from phospholipid for sensing of gases and vapors, such as acetone, chloroform, ethanol, methanol, hexane, dichlormethane, dimethylformamide, trichloroethylene and other, at relatively low concentration in the air, lower than the maximum allowable their concentration according to the European Union Directive. For the purpose, LB molecular monolayers of phospholipid dipalmitoyl-phosphatidyl-ethanolamine (DPPE) were employed [1] at room temperature. In view of practical applications, the gas sensing with DPPE LB films was electrically achieved by means of electrical impedance approach in the frequency range 0.1 Hz – 1 MHz. Due to the presence of gases/vapors, the electrical response of the DPPE LB films was changed, and the electrical conductivity of the films is increased. The electrical measurements were performed in longitudinal geometry (in the plane of the LB film). The obtained results show that in this way one can reliably detect volatile organic compounds by lipid monolayers.

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# 1.10. Effect of pH and ionic strength of chitosan/casein and casein/chitosan multilayers on curcumin release

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In the present paper the effect of pH and ionic strength on the immobilisation and release of curcumin from chitosan and casein polyelectrolyte multilayers (PEMs) was investigated. The investigated PEMs were deposited on polylactic acid (PLA) substrates. The PLA substrates were charged in a corona discharge system, consisting of a corona electrode, a grounded plate electrode and a grid placed between them. The substrate was charged for 1 minute at room temperature. Positive or negative 5kV voltage was applied to the corona electrode and 1 kV voltage with the same polarity was applied to the grid. Chitosan solutions with different pH and ionic strength were prepared. Layer-by-Layer (LbL) deposition technique was used for the multilayer build-up. For the deposition process was ensured that the first deposited layer always possessed an opposite electric charge to that of the substrate. An investigation of the water uptake properties of the deposited PEM multilayers was carried out. Curcumin was immobilised in the resulting polyelectrolyte multilayers. The release of the immobilised curcumin from the multilayers in saline buffer was investigated and the effects of the different pH and ionic strengths of the chitosan solutions were determined.

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# 1.11. Investigation of polyelectrolyte multilayers deposited on corona charged composite polylactic acid / poly(ε-caprolactone) substrates

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In the present study chitosan and casein polyelectrolyte multilayers (PEMs) deposited on composite polylactic acid (PDLA) / poly(ε-caprolactone) (PEC) substrates were investigated. The substrate's morphology was investigated using polarized light microscopy and their degree of crystallization was studied by the application of differential scanning calorimetry. The substrates obtained were charged in a corona discharge system, consisting of a corona electrode (needle), a grounded plate electrode, and a metal grid placed between them. Positive or negative 5 kV voltage was applied to the corona electrode. 1 kV voltage of the same polarity as that of the corona electrode was applied to the grid. The dependences of the normalized surface potentials on the storage times of positively and negatively charged substrates were studied. Layer-by-layer (LbL) technique was used for multilayer deposition on the substrates. PEMs with different number of layers (4 or 8) were obtained. An investigation of the water uptake properties of the PEMs was carried out. A model drug Benzydamine hydrochloride was loaded in the casein layers in order to evaluate the effect of the kind of substrate on the drug immobilization and release. A study of the drug release kinetics in saline buffer was carried out and the amount of the released drug was calculated spectrophotometrically. It was shown that the experimental results fit to the Weibull model with a very good level of correlation and the model parameters differ depending on the used substrate.

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# 1.12. Langmuir-Blodgett nano-thin monolayers of phospholipids: electrical response to Cadmium ions

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Langmuir-Blodgett (LB) nano-thin molecular monolayers of phospholipid dipalmitoyl-phosphatidyl-ethanolamine (DPPE) [1] were deposited from aqueous subphase. The DPPE LB films were with a thickness of ~ 3 nm. They were studied as biosensor platform for detection of Cadmium ions ($Cd^{2+}$). The change of the electrical response of the DPPE LB films due to the presence of $Cd^{2+}$ ions was characterized by means of electrochemical impedance spectroscopy in the frequency range 1 Hz – 3 MHz, as well as with linear sweep and cyclic DC voltammetry. The electrical measurements were performed by applying a micropipette-drop technique. The obtained results show that in this way one can reliably detect $Cd^{2+}$ by lipid monolayers. The applied electro-analytical methods have potential to be used for detection of $Cd^{2+}$ contamination of water, e.g., $Cd^{2+}$ at concentration level of 1 µg/L.

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# 1.13. A clustering of red wines based on physicochemical and optical properties

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Sixty three samples of red wines, produced in different regions of Bulgaria, Chile and South Africa from the Merlot (42 samples) and Cabernet Sauvignon (21 samples) grape varieties are characterized by 13 physicochemical and optical properties. The physicochemical characteristics (antioxidant activity and anthocyanin content) have been obtained spectrophotometrically, and the antioxidant activity (AOA) has been measured by using both DPPH and ABTS methods. At an excitation wavelength of 265 nm by dividing of the fluorescence spectra [300nm; 800nm] into ten regions (each region with a width of 50 nm) and using the capabilities of the Mathematica system, for each sample we have calculated ten integral fluorescence intensities – optical characteristics. Based on a hierarchical cluster analysis with average linkage algorithm, the studied wines from grape variety Merlot as well as these from grape variety Cabernet Sauvignon, according to their antioxidant activities (AOA ABTS and AOA DPPH) and anthocyanins content are grouped into three generalized groups. When the integral fluorescence intensities are added as a factor, for the wines from grape variety Cabernet Sauvignon there isn't difference in their grouping, and for these ones from grape variety Merlot the only difference is that one sample of wine pass to the first cluster. It could be concluded that the integral fluorescence intensities have a minimal effect on the grouping of wines. The resulting clusters are associated with the geographical areas of the wine production. The results obtained from the clustering procedure are presented graphically by dendrograms.

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# 1.14. Optical characteristics and chemical composition of high oleic sunflower oils with herbs oil additives

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Optical characteristics and chemical composition of cold-pressed sunflower oleic oils with addition of oils from: 1) basil (Ocimum basilicum), 2) rosemary (Rosmarinus officinalis) and 3) oregano (Origanum vulgare) were studied.

The aim of the study is to compare chemical composition of cold pressed oil with and without addition of different plant oils. The concentrations of some elements (essential and toxic) in oil was determined by using inductively coupled plasma mass spectrometry (ICP-MS) after microwave digestion. Infrared spectroscopic experiments (ATR and transmittance) are used to study the fatty acid profile of the analysed oils. The fluorescence spectra for investigated samples are obtained at excitation wavelength 390 nm. They show a peak between 741 nm and 746 nm range, which is due to pigments different from chlorophyll and a chlorophyll peak at about 683 nm. The spectroscopic data as transmission and adsorption coefficient are determined and used for calculating the content of pigments as β- carotene and chlorophyll.

Adding herbs to the sunflower oil increases the content of polyunsaturated fatty acids, β-carotene and chlorophyll and leads to the decreasing of an oxidation stability.

So oils mixtures could change the properties of base oil in order to suit different applications – food industry, cosmetics, pharmacy.

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# 1.15. Curcumin loaded casein nanogels as drug delivery systems

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Hydrogels from natural polyelectrolytes possess many important features such as low toxicity, biocompatibility, biodegradability and hydrophilicity (1). These properties make them very suitable applications such as immobilization and controlled release of drugs and other types of biologically active molecules (2). In the present study nano-sized hydrogels made from casein by ionotropic gelation are investigated. For this purpose, two types of crosslinking agents are used at different pH conditions. In order to characterize these nanogels, their sizes, chemical structures and thermal stability are examined by dynamic light scattering (DLS), FT-IR and Differential Scanning calorimetry (DSC) respectively. To prove their immobilization ability, active compound, namely curcumin, will be captured is immobilized in the hydrogel~~s~~ structures. The loading efficiency of the nanostructures together with the curcumin release kinetics are evaluated and modelled mathematically.

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# 1.16. Complex electrical impedance and dielectric spectroscopy of $Na^+$-conducting PEO/PVP/$NaIO_4$ solid polymer electrolyte with incorporated Graphene Oxide nanoparticles

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Being of significant interest as electrolytic materials for mini-mobile energy storage devices, we have studied solid-state polymer-based electrolytic systems - nanocomposites, in particular, $NaIO_4$ salt-complexed poly(ethylene oxide) (PEO)/polyvinyl pyrrolidone (PVP) polymer blends doped with Graphene Oxide (GO) nanoparticles-nanosheets. The GO monolayer average size and thickness were 5 µm and 2 nm, respectively. In the PEO/PVP polymer blend, the PEO:PVP ratio was 70:30 weight percent (wt.%), the concentration of the salt sodium metaperiodate $NaIO_4$ was 10 wt.%. The GO nanosheets were dispersed with concentration of 0; 0.2; 0.4 and 0.6 wt.%. Thin films (150 µm) of GO/PEO/PVP/$NaIO_4$ $Na^+$ ion-conducting nanocomposites were produced by solution casting technique. They were studied by complex electrical impedance and dielectric spectroscopy in the frequency range 0.1 Hz – 1 MHz of the applied electric field. The ion conductivity, the complex dielectric function, dielectric loss and AC conductivity of GO/PEO/PVP/$NaIO_4$ at various concentration of GO were analyzed, and the effect from the GO nanofillers was estimated. The results from dielectric analysis were interrelated to the macroscopic properties and ionic conductivity of the studied nanocomposite solid polymer electrolytes. At concentration 0.6 wt.% GO, the enhancement of dielectric permittivity of GO-doped PEO/PVP/$NaIO_4$ can reach a factor of 60, as compared to undoped PEO/PVP/$NaIO_4$ electrolyte. The electrical conductivity and dielectric properties of the produced $Na^+$ ion-conducting nanocomposites with GO nanodopants are promising for ion electrolytic applications and energy-storage devices.

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# 1.17. Complex electrical impedance and dielectric spectroscopy studies on reduced graphene oxide (rGO)/$ZnTiO_3$ nanocomposites

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We studied nanocomposites (NCs) produced from Zinc titanate ($ZnTiO_3$) doped with nanoparticles (NPs) of reduced graphene oxide (rGO) nanosheets with mean thickness ~ 2 nm. $ZnTiO_3$ ceramics and their NCs, are of current interest as innovative materials for photoanodes in quantum-dot-sensitized solar cells and photocatalytics, litium storage in Li-ion batteries, as well as for microwave electronics (ultra-high frequency, UHF) and dielectric applications [1,2]. In the presented work, the rGO/$ZnTiO_3$ NCs were produced by ultrasonically assisted precipitation technique and prepared in forms of disk tablets with diameter 1 cm and thickness 2 mm. In them, the concentration of the incorporated rGO NPs was varied from 1 wt.% to 20 wt.%. The electrical and dielectric characteristics of a series of rGO/$ZnTiO_3$ samples were determined by means of complex electrical impedance and dielectric spectroscopy in the frequency range 0.01 Hz – 3 MHz of the applied electric field. By analysis of the frequency spectra of complex impedance and complex dielectric permittivity, useful new information on the structural, electronic, electrical and dielectric properties of the studied NCs was obtained, as depending on the concentration of rGO nanodopants. In particular, we estimated that the value of electrical conductivity of rGO/$ZnTiO_3$ can be considerably increased upon addition of rGO NPs. At some concentration of rGO, in our case close to 10 wt.%, the electrical conductivity was found to be optimal. Further, we established that the dielectric properties of rGO-doped $ZnTiO_3$ were also enhanced by increasing concentration of rGO. The observed effects show that the prepared rGO/$ZnTiO_3$ ceramics are promising materials for electronic and dielectric applications, and most likely – in energy storage devices, e.g., supercapacitors.

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# 1.18. Solid polymer nanocomposite electrolyte complexes PEO/PVP/$NaIO_4$ with $TiO_2$ nano-additives: $Na^+$ ion conductivity and dielectric studies

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The effects of $TiO_2$ nano-additives on electrical conductivity and dielectric properties of the nanocomposite solid polymer electrolyte (NCSPE) system PEO/PVP/$NaIO_4$/$TiO_2$ were investigated in order to asses its competence for ion-electrolytic applications. The examined NCSPEs for sodium-ion conduction were based on binary polymer blend formed from poly(ethylene oxide) (PEO) and polyvinyl pyrrolidone (PVP), with added sodium metaperiodate ($NaIO_4$) at concentration of 10 wt.% [1,2] and nanoparticles of Titanium oxide ($TiO_2$) of average size ~ 10 nm. $TiO_2$ was included at concentrations 1, 2, 3, 4 and 5 wt.%. As depending on the concentration of $TiO_2$ nanoparticles, the electrical conductivities and dielectric properties of thin films (150 µm thick) of the salt-complexed polymer-ion NCSPE PEO/PVP/$NaIO_4$/$TiO_2$ were studied by complex electrical impedance and dielectric spectroscopy in the frequency range 1 Hz – 1 MHz. Compared to additive-free samples, the incorporation of nano-sized $TiO_2$ into the PEO/PVP polymer matrix increased both electrical conductivity and dielectric permittivity of PEO/PVP/$NaIO_4$/$TiO_2$ NCSPEs by more than one order of magnitude at concentration 3 wt.% of $TiO_2$. The results from dielectric analysis were related to the macroscopic properties of the examined ion-conductive NCSPEs and show their ability for $Na^+$ ion-conducting applications.

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# 1.19. Photo-electrical response of nanocomposites of single-walled carbon nanotubes incorporated in tris(*keto*-hydrozone) discotic mesogen

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We report an experimental study of novel photoresponsive nanocomposite (NC) system based on mesogen LTTH-6 (L-long arm, T-trialkoxy, TH-tris-hydrazone core, with 6 carbon atoms in the tails) – star-shaped macromolecular structure with three branches. In this discotic liquid-crystalline material (the host) were incorporated semiconducting single-walled carbon nanotubes (SWCNTs) at concentration of 1 wt.%. Thin layers (thickness 3 μm) of the SWCNTs/LTTH-6 NCs were characterized by optical absorption spectroscopy, differential scanning calorimetry (DSC), thermo-optical studies, polarizing optical microscopy and electro-optical measurements at variation of temperature of the layers. The electrical properties of the produced SWCNTs/LTTH-6 layers were studied by current-voltage measurements under static electric field, as well as by electrical impedance spectroscopy in the frequency range from 1 Hz to 1 MHz of the applied electric field. Upon illumination of the SWCNTs/LTTH-6 layers with a low-intensity light in the visible spectral range, in them was found a significant photo-electrical effect that leads to a decrease in their electrical conductivity. The photo-electrical response of the studied NCs at room temperature was linked to their structural and macroscopic properties, and explained. The observed photo-induced effect and considered functional NCs can be used in organic electronics and for sensorics.

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# 1.20. Influence of carbohydrates on the phase behaviour of phospholipid systems

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Phospholipids are essential for cell differentiation, proliferation and regeneration, as well as for the transport of molecules across membranes. They control membrane-dependent metabolic processes inside the cell and in the intercellular space, maintain and stimulate the activity and activation of membrane bounded proteins such as enzymes. Sugars have another important characteristic, beside their biological importance- source of energy. They are cryoprotectors- preventing the cells from freezing. With the development of tissue storage technologies, knowledge of different sugars and their effect on lipid membranes is becoming increasingly important. The present work is focused on the influence of sucrose on SOPC (1-stearoyl-2-oleoyl-sn-glycero-3-phosphocholine) lipid systems. Differential scanning calorimetry is an appropriate method to study the phase behaviour of organic compounds because of its high sensitivity. Research reveals that the addition of sucrose has effect on, both, mechanical and physico-chemical characteristics of the systems. There are tangible differences in the bending elasticity moduli, temperature and enthalpies of the phase transitions with the addition of sucrose.

## Acknowledgements:

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# 1.21. Influence of carbon nanostructures on the structural and thermalproperties of lipid membranes

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Studies of carbon nanostuctures, incorporated in phospholipid bilayers show a strong effect of these admixtures onthe local structure and dynamic properties of biomembranes, as well as ontheir toxicity and ability to promote trans-membrane channel formation depending on their size, shape, and surface modification. However, the dominant forces of the influence of these structures on the conformational states and functions of biomembranes remain not clarified.

The main goal of our study is the investigation of the thermal and conformational structure characteristics of 1-stearoyl-2-oleoyl-sn-glycero-3-phosphocholine (SOPC) phospholipid at variation of carbon nanostructures in various concentrations. For that purpose, we use the methods differential calorimetric analysis and Fourier transform Infrared (FT-IR) spectroscopy. In the present work we study the influence of incorporated in the membrane carbon nanostructures(pristine or amide functionalized single wall nanotubes and nanoparticles) on the phase transition temperatures and enthalpies of SOPC phospholipid and discuss the possible physical mechanism driving the energetic and structural states of the bio-nano-composites.

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# 1.22. Comparative evaluation of approaches for CFD modeling of mass transfer in membrane filtration

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This work is part of a research on integrated bioreactors with membrane separation. Membrane filtration plays an important role in modern life, and has grown from a specialised laboratory tool into a widespread industrial process with significant industrial, economic and environmental importance. Computational Fluid Dynamics (CFD) is a strong tool to study the processes in the filtration modules. It reveals the distribution of the flow parameters in the calculation domain, showing a detailed hydrodynamic picture. The modeling of the selective permeability of the membrane is a complex task and different types of approaches are reported in literature. They accept different formulation of the boundary conditions at the membrane surface.

The aim of the present study is to do comparative evaluation of approaches for modeling of mass transfer in filtration cell by CFD, based on experimental data from literature. A simple geometry of membrane cross-flow filtration is chosen to reduce the computational time. It consists of a two-dimensional (2D) slit with a height h=0,001m and a length l=0,020m, the bottom wall being a membrane. The upper wall is impermeable. The numerical simulation uses the tools of ANSYS Fluent R13. The present work complements previous information from literature by comparing the predictions with experimental data for one and the same mode of operation by using different modeling approaches for the mass transfer at the membrane on the retentate side.

**Keywords:** CFD modelling, mass transfer, numerical simulation, membrane filtration

## Acknowledgements:

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# 1.23. Soliton scattering on impurities with modified exchange interactions in anisotropic ferromagnetic chains

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The soliton propagation in an anisotropic ferromagnetic chain where the exchange interactions of an impurity spin with its neighbours are modified is investigated. We considered easy-axis anisotropy of the chain where the soliton solutions are of bell type. The character of the soliton-impurity interaction is different when the exchange coupling of the spin is modified in the x,y-plane or in the z-direction. Our results show that the action of the defect depends on the soliton wave number in a complicated manner and for large velocities becomes significant. A comparison with the soliton dynamics in the presence of point defects is made.

## Acknowledgements:

This work is supported by the Bulgarian National Science Fund under Grant No. КП-06-Н38/6 from 05.12.2019.

# 1.24. Single-photon generation of entangled triplet states in an atomic spin dimer

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We show that entanglement between two atomic spins, coupled via XY interaction, can be produced with the aid of a single photon in a controllable manner. Given that the spin-photon coupling is constant two different cases are considered – excitation with a constant and with a linear time-dependence of the photon frequency. These problems reduce to the study of the well known Jaynes-Cummings and Jaynes-Cummings-Landau-Zener model, respectively, where the two-level system is formed by the zero-momentum mode states of the dimer. Having the exact solutions of both models, by tuning the relevant parameters, one can design and coherently control the dynamics of the excitation process. For instance, one can adiabatically switch from a spin system initialized in a state with S=1, S_z=-1 to the maximally entangled triplet state.

**Acknowledgements:**

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# 1.25. Finite-size scaling and bulk critical behavior of a quantum spherical model with a long-range interaction: entropy, internal energy and specific heat

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The entropy, the internal energy and the specific heat of one infinite $d$-dimensional quantum system are studied close to its zero-temperature quantum critical point ($T = 0$, $g = g_c$) in the context of the finite-size scaling (FSS) theory [1]. The corresponding FSS forms, in which the universal scaling functions are expressed in terms of the scaling function of the singular part of the free energy, $f_s$, are presented. We have shown that the critical exponent $\alpha_{\delta g}$, obtained by the FSS form of the susceptibility $\chi_{\delta g} = \partial^2(\beta f_s)/\partial(\delta g)^2$ ($\beta = 1/T$ and $\delta g$ measures the deviation from $g_c$), which at $T = 0$ and close to the quantum critical point $g_c$ behaves as $\chi_{\delta g} \propto |\delta g|^{-\alpha_{\delta g}}$, satisfies the hyperscaling relation and $\alpha_{\delta g}$ is the specific heat exponent of the equivalent classical problem in $(d + z)$ dimensions, where $z$ is the dynamical critical exponent [2]. In the example of a quantum spherical model with a long-range interaction [3], for the special case $d = \sigma$, where $0 < \sigma \leq 2$ is a parameter controlling the decrease of the long-range interaction, the universal scaling functions of the entropy, the internal energy, the specific heat and the susceptibility $\chi_{\delta g}$ are obtained in an explicit form. The asymptotic behaviors of these functions as well as the leading critical behaviors of the corresponding quantities in both the renormalized classical and the quantum disordered regions are given.

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# 1.26. Modelling of multiple hollow cathode discharge

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The laser tube configuration for sputtering metal vapour lasers [1] is studied. The construction consists a main hollow cathode and a few hollow cathode holes (CH’s). The design is schematically presented in Figure 1. Inside the main cathode the optimal conditions for laser oscillation are realised, while in the side CH's the current density is higher and the discharges that occur in the cathodes holes can be used as additional sources of metal atoms, obtained by sputtering. The main cathode and the cathode holes can be made by a different metal which gives the possibility for simultaneous laser oscillation on different metals in the same active volume. To study the processes in the discharge and the capabilities of the construction the PLASIMO modelling platform [2] is used.

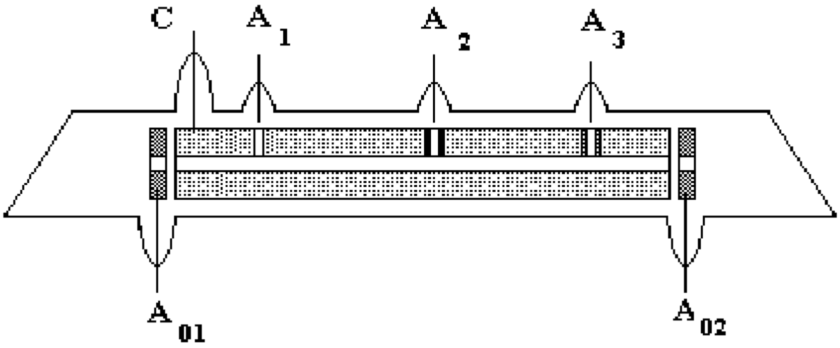

**Figure 1:** The case study of the design

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## Acknowledgements:

This work was supported by the Bulgarian Ministry of Education and Science under the National Research Program “Young scientists and postdoctoral fellows” approved by DCM#577/17.08.2018.

# 1.27. Interaction of solitons with a qubit in an anisotropic Heisenberg spin chain with first and second-neighbor interactions

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The interaction between soliton, propagating in Heisenberg spin chain with first and second-neighbour interaction and a spin 1/2 particle is studied. The spin chain has single-ion anisotropy. The spin 1/2 particle (qubit) is modeled by a two level quantum system. The system of equations for the components of the Bloch vector of the qubit are obtained and numerically solved. The role of the parameters responsible for the qubit-soliton interaction and second-neighbor interaction for the evolution of the qubit are investigated.

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# 1.28. Random walkers on deformable media

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We consider random walkers that deform the medium (RMDM) as they move, enabling a faster motion in regions which have been recently visited. This induces an effective interaction between walkers mediated by the medium, which can be regarded as a space metric. Such an effect gives rise to a statistical mechanics toy model for gravity, motion through deformable matter or adaptable geometry. In the strong deformability regime, we find that diffusion is ruled by the porous medium equation, thus yielding sub diffusive behaviour of an initially localized cloud of particles, whose global width will grow like $t^{1/3}$, though the sample-to-sample width average will sustain a $t^{1/4}$ or $t^{1/2}$ growth, which can be explained through ergodicity breaking. Indeed, random walkers present anti-persistence and strong memory effects, which we explore indirectly through the fluctuations of the center of mass of the cloud.

Our model is built from of $N_p$ random walkers on a chain. Any particle standing on site i has a certain probability per unit time $J_{i,i-1}$ of hopping to site i -1, and $J_{i,i+1}$ of hopping to site i + 1. We will assume these probabilities are symmetric and the system starts with uniform hopping rates, $J_i = J_0$ for all i. Furthermore, whenever a particle jumps across a link (i; i + 1) the hopping probability is updated, $J_i \rightarrow J_1$ higher or equal to $J_0$. If no walker crosses the link during the subsequent time-steps, its hopping probability will decay towards the relaxed value $J_0$ in a time of order $t_0$ (Figure 1).

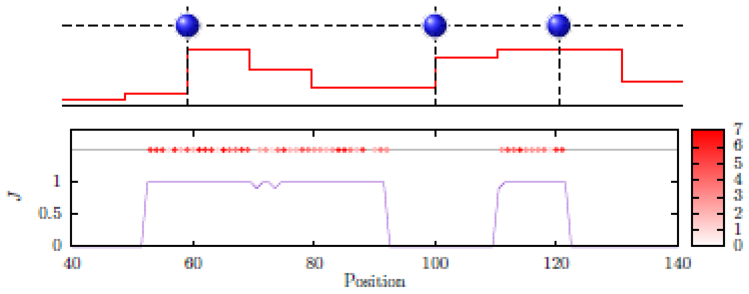

**Figure 1:** Top: Illustration of our RWDM model. Walkers occupy integer positions of a chain, and hopping probabilities between neighboring sites can be different. Bottom: A configuration for $J_0 = 10^{-6}$, J1 = 1, $t_0 = 10$ and $N_p = 100$ particles on L = 200 sites, after $T = 10^9$ time-steps. Notice that most hopping probabilities are near $J_0$ or $J_1$, and that the particles are neatly divided into two blocks.

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# 1.29. Origin of exchange interactions: localized vs. delocalized electrons

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Attracting the researchers attention for decades, exchange interactions have become the most widely used type of interactions when studying the microscopic origin of magnetism. Thus, different techniques and models have been applied and tested in many occasions over time [1–4], emphasising the interrelationship between theory and experiments.

In the present study we discuss how magnetism in non-conductive compound may originate form the exchange symmetry that the constituent electrons obey and what variety of mechanisms of electrons' exchange and the effective exchange interactions they correspond to. Respectively, we demonstrate how the spin coupling in the Heisenberg model derives and what is the difference in its physical interpretation regarding the cases of localized and delocalized electrons.

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## Acknowledgments

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# 1.30. Separation of glucose, other reducing sugars and phenolics from natural extract by nanofiltration: effect of pressure and cross-flow velocity

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Aquatic plants are still less studied from biorefinery viewpoint than the terrestrial plants. *Myriophyllumspicatum* is one of the major invasive aquatic weeds of natural habitats all over the world but still remains unstudied as resource of valuable chemicals, sugars and phenolics. The aim of this work was to derive carbohydrates and phenolics from this aquatic weed and then to fractionate the complex liquor obtained by nanofiltration. For this purpose we first subjected the plant material to hydrothermal pre-treatment and then post-enzymatic hydrolysis was carried out to accomplish cellulose degradation. This two–step treatment resulted in full recovery of water soluble phenolics and conversion of bioenergy carbohydrates to glucose. By applying nanofiltration as a separation tool of fractionation of this complex liquor we aimed at glucose permeation through the membrane and retention of other reducing sugars and phenolics. For this purpose we used Mycrodyn Nadir NP030 P membrane which previously showed good permeability with respect to compounds resembling glucose in its molecular weight. The nanofiltration experiments were carried out on a MaxiMem cross-flow filtration system (PS Prozesstechnik GmbH). The influence of the process parameters – transmembrane pressure and cross-flow velocity was studied and their effect on the permeate flux and rejection was described. The rejection behavior of glucose, other reducing sugars and total phenolics was followed analytically and checked by the mass balances of the filtration unit. The nanofiltration conditions were evaluated with respect to the permeate flux and better glucose permeation through the membrane, as well as the retention and concentration of the other biologically active substances.

# 1.31. Bound soliton - defect spin states in anisotropic ferromagnetic chain

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The interaction of soliton with an impurity spin in a discrete anisotropic ferromagnetic chain is studied. The defect spin in our model is characterized by modification of the exchange interaction with its neighbors. A perturbed nonlinear Schrödinger (NLS) equation for spin amplitude is derived on the basis of a semiclassical and a continuum approximation. Specific feature of this type defects is that it leads to perturbations to all terms of the NLS equation. Localized soliton-defect spin solutions are obtained for the case of dark and bright solitons and their stability is analyzed.

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# 1.32. Discrete dynamics of energy and momentum transfer

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Quantum mechanics is considered as one of the greatest achievements in theoretical physics [1–3]. It stands as an invaluable tool for interpreting experimental findings from the nano-scale world and thus being a ground for vast number of researches accounting for different atomic and subatomic processes.

Whether one studies problems in the field of fundamental or applied quantum mechanics, defining the Hamiltonian is a key point in understanding the system's dynamics characterized by all processes of energy and momentum transfer. However, within its continuous time framework, the Hamiltonian approach does not provide enough information for the rate at which these processes take place over time, a knowledge that at some point may strongly enrich the study. In order to explore the dynamics of energy and momentum transfer more closer and search for a possible discreteness in time an additional investigation about the observables such as the mechanical power that a certain interaction generate and the applied forces is required.

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## Acknowledgments

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# ABSTRACTS OF SECOND POSTER SESSION

# 2.1. Graphene based optical light modulators

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Multilayer graphene, grown by Chemical Vapor Deposition (CVD) method and transferred on rigid and polyethylene terephthalate (PET) substrates have been used as transparent conductive layer for optical modulators. For flexible substrates, sheet resistance stability during bending of large area graphene is studied. Graphene/PET retains its low sheet resistance, even after continuous bending of up to 1000 times. Several graphene-based optical modulators has been assembled and demonstrated.

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# 2.2. Atomic layer deposited Al-doped ZnO thin films for flexible display applications

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The rapid growth of transparent electronics and electro-optical devices on flexible supports call for the development of the transparent electrodes prepared by methods with low thermal budget and precise controllable thickness and conformality. Here we demonstrate transparent and conductive functionality of Aluminum-doped zinc oxide (AZO) thin films deposited on flexible mica substrates by using Atomic Layer Deposition (ALD) technique. AZO thin films possess high optical transmittance at visible and near-infrared spectral range and electrical properties competitive to commercial Indium Tin Oxide (ITO) layers. AZO layers deposited on mica demonstrate stable sheet resistance over 1000 bending cycles, proved by AFM and SEM analysis before and after the bending. Based on the performed optical and electrical characterizations several possible applications of ALD AZO as transparent conductive layer are envisaged. The electro-optical operation of AZO/mica based flexible Polymer Dispersed Liquid Crystal (PDLC) devices are shown as a representative example.

**Acknowledgements:** This work is supported by the Bulgarian National Science Fund project КП-06-КП 28/8. Research equipment from the distributed research infrastructure INFRAMAT (part of the Bulgarian National roadmap for research infrastructures), supported by the Bulgarian Ministry of Education and Science under contract D01-284/17.12.2019, was used for AFM measurements.

## 2.3. Correlation between optical basicity, chemical bonding, and optical characteristics of glasses in the $TeO_2$-$V_2O_5$-$MoO_3$ and $TeO_2$-$V_2O_5$-$Bi_2O_3$ systems.

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Glasses with wide range of compositions in the $TeO_2$-$V_2O_5$-$MoO_3$ and $TeO_2$-$V_2O_5$-$Bi_2O_3$ are prepared using a conventional melt quenching method. The polarizability approach based on the Lorentz-Lorenz equation is applied. The optical basicity and the oxide ion polarizability are estimated. The theoretical refractive index and the energy gap of the glasses are also estimated. The chemical bonding of the glasses is elucidated on the basis of the interaction parameter and the single bond strength of an average cation-oxide ion (M-O) bond. It is found that the samples possess relatively high values of the optical basicity and the electronic oxide ion polarizability, relatively low values for the average single bond strength and low values of the interaction parameter. The refractive index based third order nonlinear optical susceptibility of the glasses is established using generalized Miller's rule and three-photon model. The glasses possess comparatively high third order nonlinear optical susceptibility. These results indicate for the presence of weak chemical bonds which are formed between $TeO_3$, $TeO_4$, $BiO_6$, $MoO_3$, $VO_4$ and $VO_5$ groups confirmed by IR analysis. Structural model containing these groups is proposed.

# 2.4. Magnetic field effect in piezoelectric resonators with HTS electrodes

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Aliminuim Nitride (AlN) is characterized by low losses, excellent piezoelectric characteristics and is attractive for use in microwave resonators, filters and sensors based on the resonance effect. Although such devices mainly function at ambient temperatures, attempts to make their cryogenically cooled versions are also important because it can reduce electrical losses in the devices. For example, AlN piezoelectric-on-silicon resonators functioning at 77 K and demonstrating high quality factors were reported in [1]. The use of high temperature superconducting (HTS) elements in such resonators at low temperatures leads to a significant decrease in the limit value of the quality factor caused by losses in the electrodes [2]. On the other hand, the application of external magnetic field or the injection of electric current cause a change of the characteristics of the HTS components and can lead to some adjustment of the device parameters. In this paper the magnetic field effect on the characteristics of the piezoelectric resonators with HTS electrodes are modeled and analyzed in view of importance of such devices for different applications.

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# 2.5. Electric properties of new composites materials based on RGO, nanosized ZnO and Cu nanoparticles

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Graphene nanostructures combine properties that make them attractive material at the same time for various technical applications. The objectives of this study is to obtain a series composites based on RGO, nano-sized ZnO and Cu nanoparticles. Reduced graphene oxide (RGO) is synthesized by modified Hammer`s method and chemical reduction after sonication. ZnO nanoparticles are obtained by Sol-Gel method. The composites are phase and structural characterized by XRD, SEM, TEM, EDX analysis (Fig. 1). It is shown that ZnO is monophasic with a particle size of 48 nm. A series of composite materials based on RGO, ZnO and Cu nanoparticles was obtained by ultrasonic treatment. Electrical and dielectric properties are measured by Impedance analyzer and RLC bridge. For comparative conductivities for 100% RGO of 309.513 S/m and 100 % Cu nanosized of 0.0056 S/m, it should be initially concluded that increasing the RGO in the mixture will increase the conductivity and increasing Cu nanosized will decrease it. The presence of cluster regions with different conductivity was found: 1) nano grains of conductive copper and 2) partially or completely surrounding low-conductivity shells of copper oxide and a minimum number of RGO. The present work is promising for future research in which to create promising new composite materials with controlled shape and size of copper oxide - RGO clusters. Dielectric measurements for RGO/ZnO composites have been made in range from 5 mass% to 100 mass% content of RGO, the composites are more or less conductive. For lower concentration of RGO selected samples are dielectrics.

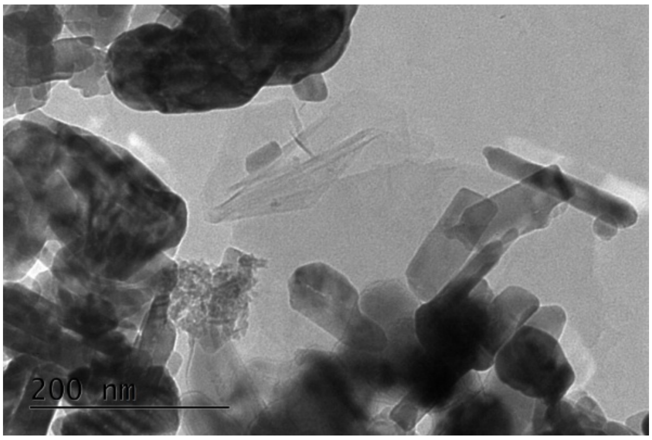

**Figure 1**: TEM analysis of composite RGO/ZnO - 50/50 mass %.

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**Acknowledgements:** Authors acknowledge the financial support of the National Science Fund of Bulgaria, Project КП-06-Н27/17 17.12.2018.

# 2.6. Dielectric properties of monophase polycrystalline bismuth titanate pyrochlore ($Bi_2Ti_2O_7$) ceramics and glass-ceramics

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Bismuth titanate ceramics containing $SiO_2$ and $Nd_2O_3$ were synthesized in the $Bi_2O_3$-$TiO_2$-$SiO_2$-$Nd_2O_3$ system using the melt-quenching method. The phase composition of selected samples was determined by X-ray diffraction (XRD) analysis and the microstructure was observed by scanning electron microscopy (SEM). As a result, the preparation of mono-phase polycrystalline materials was cocluded. Infrared Fourier-transformed spectroscopy (FTIR) was applied in order to identify the structure. The conductivity, conductivity activation energy, as well as the dielectric losses and dielectric constants of selected samples were determined, and the influence of the phase composition on the dielectric characteristics was evaluated.

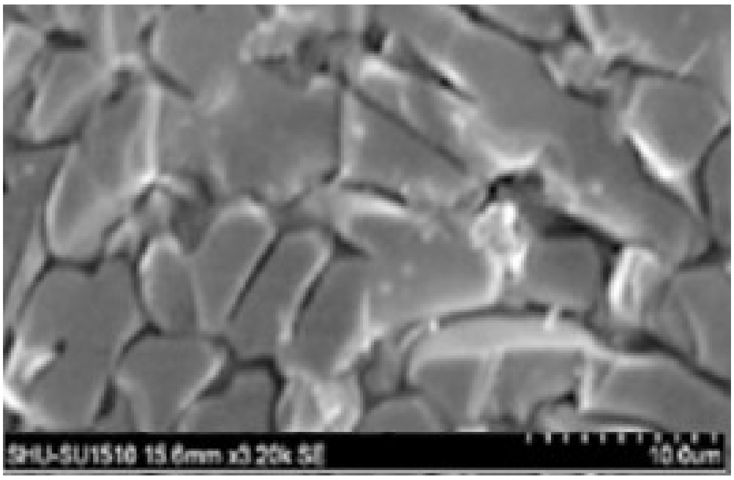

**Figure 1**: SEM analysis of $19Bi_2O_3$-$66TiO_2$-$8SiO_2$-$7Nd_2O_3$.

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# 2.7. Synthesis and characterization of tunnel-type $Na_4Fe_3(PO_4)_2P_2O_7$ as cathode material in Sodium-ion batteries

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Lithium-ion batteries are widely used as sources of energy for portable electronics due to their high energy density. Globally, the sources of lithium are depleted and the price of lithium is constantly rising. In this regard, sodium-ion batteries are considered as an alternative to lithium-ion batteries because of their low cost and wide availability of sodium resources. Polyanionic materials with 3-D frame structures attract a lot of attention due to their high durability of the structure with repeated $Na^+$ insertions /extractions and the strong inductive effect that increases the working voltage. The researchers have focused their attention on cathode polyanionic materials such as phosphates, fluorophosphates and pyrophosphates.

In this contribution we report data on the preparation and characterization of a tunnel-type $Na_4Fe_3(PO_4)_2P_2O_7$ which is very promising electrode material due to the presence of three channels for fast reversible $Na^+$ diffusion in its structure. This mixed phosphate-pyrophosphate salt is obtained by a new soft chemistry method. It is based on the formation of a freeze-dried Na-Fe-phosphate-formate precursor with the needed Na:Fe:P molar ratio, followed by precursor thermal decomposition and further annealing. In order to increase the electron conductivity, a composite with conductive carbon black Super C/65 is prepared by ball milling procedure. The structure and morphology of both pristine $Na_4Fe_3(PO_4)_2P_2O_7$ and its composite are characterized by the powder XRD, IR spectroscopy and SEM. The capability of $Na_4Fe_3(PO_4)_2P_2O_7$/C to intercalate reversibly sodium ions is tested in model two-electrode sodium cells of the type: Na| NaTFSI+5%$NaPF_6$/PC | $Na_4Fe_3(PO_4)_2P_2O_7$/C.

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# 2.8. Solution deposition of ZnO thin films

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Zinc oxide is a popular material with variety of applications, depending on size and shape of the grains, preferred orientation and relative disposition of the faces and especially with its specific chemical and electro-physical properties. The fields of use include catalysers, gas sensors, surface acoustic wave devices etc. In thin films photovoltaics it serves as passive optical antireflection coatings [1], buffer or conductive windows (in chalcopyrite and Kesterite solar cells) [2] and mesomeric electron selective material in organic solar cells [3]. Solution deposition technique serves as suitable approach to deposit nano-structured films with tailored geometric shape and aspect ratio, electrical conductivity and high optical transmittance on large working surfaces at lower cost. Depending on the solution composition, temperature of the deposition and post deposition treatment we describe deposition of thin films of intrinsic ZnO with well defined hexagonal wurtzite structure and with high optical transmittion in the visible region. Deposition of doped layers of ZnO:Al with aluminium concentration up to 3 $_{wt}$% does not cause degradation of the wurtzite structure and sheet resistance of the films is near $8.0*10^{2}$ Ω / □. After thermal annealing absorption edge gets sharper and optical band gap is found to be near 3.26 eV for direct transitions. Addition of the ethanol on the aqueous deposition solution leads to formation of ZnO nanostructured films with triclinic configuration.

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# 2.9. Synthesis and characterization of nanosized $ZnTiO_3$ doped with of reduced graphene oxide (RGO)

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Composite materials based on nanosized zinc titanate ($ZnTiO_3$) doped with reduced graphene oxide (RGO) were obtained by means of ultrasonically assisted precipitation. In these composites, the concentration of RGO nanopartiles was varied from 1 wt.% to 20 wt.%. Initially, the starting components, RGO and $ZnTiO_3$, were synthesized and characterized. The $ZnTiO_3$ ceramic was produced by sol-gel method. Analyses by X-ray diffraction (XRD) demonstrated that the $ZnTiO_3$ was single-phase with a particle size of ca. 6 nm. RGO was prepared by a modified Hammers method and subsequent chemical reduction with sodium borohydride. Structural and phase characterization of the fabricated composites was performed by XRD, scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) at room temperature. It was established that for all of the studied samples of the RGO/$ZnTiO_3$ series, the two principal phases are uniformly distributed over the observed areas, which proves the formation of homogeneous nanocomposite materials. The electrical properties of the series of RGO/$ZnTiO_3$ samples were characterized by complex electrochemical impedance spectroscopy (EIS) in the frequency range from 0.1 Hz to 1 MHz. The results obtained by EIS for the electrical conductance of RGO-doped $ZnTiO_3$ as a function of the concentration of RGO nanoparticles were correlated with the data from structural studies. Corresponding conclusions were done.

**Keywords:** RGO, $ZnTiO_3$, composites, electrical properties,

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# 2.10. Thermally stabilized soot for supercapacitors

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Soot is used as an electrode material for possible supercapacitance applications. The carbonaceous product is collected from a domestic heating system and possesses a naturally developed high surface area, which is one of the key requirements for such applications. The low molecular weight compounds in the soot are evaporated and carbonized by heat treatment of the samples in the range 400 – 800 °C. The different temperatures cause different degrees of carbonization, functional groups removal and samples stabilization. The capacities are compared of capacitor prototypes with electrodes made from materials treated at different temperatures. The prototype samples are investigated by FTIR and TEM, revealing consequently removed functional groups and a variety of carbon structures, such as graphene sheets, monocrystalline carbon particles, onion like structures.

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# 2.11. Influence of the molecular weight and concentration of PVP on the polyol synthesized silver nanoparticles

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In the present work the synthesis of silver nanoparticles by the polyol method is investigated. The self-seeding polyol process was chosen from the number of variations of this method. In this approach $AgNO_3$ was used as a precursor, poly (N-vinylpyrrolidone) (PVP) as capping agent and ethylene glycol as solvent and reducing agent. We investigated the influence of the molecular weight of PVP on the microstructure of the particles considering a polymer with molecular weight Mw = 58 and 360 K by changing the molar ratio of PVP/$AgNO_3$ for both polymers. The molar ratios were varied from 0.5 to 2.5. The as prepared nanoparticles were characterized by microscopic and structural methods. The shape and the size distribution were characterized by Transmission Electron Microscopy and Diffractive Light Scattering. The crystal structure of the nanoparticles was studied by X-ray Diffraction and Selected Area Electron Diffraction. Due to their plasmonic properties, the silver nanoparticles find application for improvement of the efficiently of the solar cells, substrates for surface-enhanced Raman and florescence spectroscopies. All these applications require the frequencies of the localized surface plasmon resonance (LSPR) to appear at an exact position. Therefore, we indicated the wavelength of the LSPR of the as prepared nanoparticles trough the transmittance spectra. A variation between 400 and 650 nm was observed.

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# 2.12. $WSe_2$ thin films and crystals

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Transition metal dichalcogenides (TMDs) are a family of layered materials that show unique properties (different from their bulk counterparts) when thinned down to nanoscale thickness. The 2D $WSe_2$ is important for future application in nanoelectronics, spintronics and valleytronics devices. Besides having a direct band gap which is in favour of electronic and optoelectronic applications, particularly the monolayer $WSe_2$ has the largest spin splitting and longest valley coherence time among all known monolayer transition-metal dichalcogenides (1). Therefore, significant efforts are underway to obtain large scale and with controlled number of layers' materials.

In our experiments two different approaches for preparation of 2D $WSe_2$ are used: synthesis of bulk crystal by Chemical Vapor Transport (CVT) method and synthesis of thin films by Chemical Vapor Deposition (CVD) and thermal-assisted conversion of pre-deposited W films. The production of $WSe_2$ mono or few-layers from bulk crystals is usually accomplished through top-down micromechanical exfoliation, as was first explored in graphene (2). CVD thin film samples were prepared by selenization of magnetron-sputtered W film – thermally assisted in $Ar/H_2$ gas mixture flow. The bulk crystals and thin films were characterized structurally by mono and powder XRD as well as XPS methods to obtain the crystal quality and chemical composition and stoichiometry. Optical and electrical properties are further examined towards device applications.

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# 2.13. Preparation and structural investigation of $BaTiO_3$

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Perovskite materials, based on barium titanate are subject of intensive research in the recent years due to their interesting electrical and magnetic properties and the possibility for application in electronics, environmental monitoring and energy storage. It is a challenge to create a material with desired structure and properties (electric and magnetic), which can be easily controlled by changing the composition, synthesis method and heat treatment conditions.

The objective of our work was to prepare $BaTiO_3$ powder by three different techniques: sol-gel, hydrothermal method and solid state synthesis. The influence of the preparation method on the structure of the resulting material was studied and discussed. The structure of the samples was investigated by X-ray diffraction, Fourier transform infrared spectroscopy, scanning electron microscopy and X-ray photoelectron spectroscopy. The thermal properties were examined by differential thermal analysis. It was established that the structure of the sol–gel samples depends on the subsequent heat treatment, i.e. crystallization at 900 ºC results in cubic structure, while the thermal treatment at 1100 ºC leads to formation of tetragonal phase of $BaTiO_3$. The structure of the samples, obtained by hydrothermal and solid-state method, is cubic at the synthesis conditions. The infrared spectra of the prepared powders show absorption bands, characteristic for Ti-O bonds, $CO_3{}^{2-}$ and OH groups. $BaTiO_3$ particles obtained by sol gel have a relatively wide size-distribution and mostly possess round shape with a tendency to agglomerate. The particles obtained by the hydrothermal method are noticeably agglomerated as well. The surface of the sol-gel sample, annealed at 900 ºC was studied by X-ray photoelectron spectroscopy. $Ti_{2p}$, $Ba_{3d}$ and $O_{1s}$ photoelectron peaks were deconvoluted and analyzed. The $Ti_2$ peak displays the presence of $Ti^{4+}$ in the synthesized $BaTiO_3$ while the $Ba_{3d}$ peak indicates the occurrence of $Ba^{2+}$ in both $BaTiO_3$ and $BaCO_3$. The $O_{1s}$ spectrum reveals the presence of oxygen in $BaTiO_3$, $CO_3^{2-}$ ions and C-O groups.

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# 2.14. Study of the sensitivity of electrochemically-deposited $ZrO_2$ on a quartz resonator

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This work presents sensitivity of electrochemically-deposited $ZrO_2$ on a quartz resonator. The nanostructured $ZrO_2$ layers are deposited by electrochemical method on the Au electrodes of the quartz crystal micro-balance resonators (OCM). The deposition of the electrochemical layers of $ZrO_2$ is carried out in aqueous solution of $ZrOCl_2$ ($5\times10^{-3}$ M) and KCl (0.1 M) at 70 °C and –900 mV (vs SCE) using a three-electrode electrochemical cell. The structure of the $ZrO_2$ layers deposited on the polished QCM surface is studied by X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM), and optical profilometry. The influence of the quartz roughness on the $ZrO_2$ sorption properties is investigated. The results are compared to the corresponding data obtained for the QCM before $ZrO_2$ growing. The sorption ability of the $ZrO_2$ thin layers is defined by measuring the resonant frequency shift ($\Delta f$) of the QCM-$ZrO_2$ structure in the presence of different acetone concentration (500 – 5000 ppm).

# 2.15. Magnetic phase transitions in Zn2Y-type hexaferrites - the influence of substitutions

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We report studies on the effect of substituting the magnetic $Fe^{3+}$ cations with non-magnetic $Al^{3+}$ cations in Y-type hexaferrite $Ba_{0.5}Sr_{1.5}Zn_2Fe_{11.92}Al_{0.08}O_{22}$ powders on their magnetic properties and especially on the magnetic phase transitions responsible for observing the magnetoelectric effect. In this research, the Y-type hexaferrite ($Ba_{0.5}Sr_{1.5}Zn_2Fe_{11.92}Al_{0.08}O_{22}$ and $Ba_{0.5}Sr_{1.5}Zn_2Fe_{12}O_{22}$) powders were synthesized by citric acid sol-gel auto-combustion. After the auto-combustion process, the precursor powders were annealed at 1170 °C in air to obtain the Y-type hexaferrite materials. The effects of Al substitution on the structural, microstructural properties and phase content were investigated in detail using X-ray powder diffraction and scanning electron microscopy. Hysteresis measurements were performed by a physical-property-measurement-system (PPMS) (Quantum Design) at 4.2 K and at room temperature. The *ac*-magnetization was measured in an ac-magnetic field with an amplitude of 10 Oe and frequency of 1000 Hz to determine the magnetic phase transitions. The *dc*-magnetic measurements of the temperature dependence of the magnetization at magnetic fields of 50 Oe, 100 Oe and 500 Oe were used to determine the influence of the applied magnetic field on the magnetic-phase transition temperature. We demonstrated that the helical spin state can be modified further by varying the magnetic field.

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# 2.16. Optimization of AlN films grown by atomic layer deposition

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Aluminum nitride (AlN) which is the III-V family compound offers unique combination of material properties including wide and direct band gap of 6.2 eV, high thermal conductivity (320 W/mK at 300 K) and high sound velocity (up to 6000 m/s) which make it a suitable candidate for UV detectors, high power electronics and surface acoustic wave devices (SAW) for harsh environments [1].

Atomic layer deposition (ALD) is a special type of low temperature chemical vapor deposition which offers excellent conformality and scale-up potential combined with precise thickness control.

However, some difficulties, such as deposited III-nitrides films being non-stoichiometric are often reported [2].

In this study AlN thin films (~25 nm) have been grown with a Beneq TFS-200 ALD reactor on Si (111) substrates. TMA (trimethylaluminum) and $NH_3$ were used as precursors while nitrogen ($N_2$) was used as the carrier gas. The substrate temperature was 330°C, ALD cycles were 550.

To study the stoichiometry of AlN film TMA and $NH_3$ dose were varied from 60 to 180 ms and from 60 to 90 ms, respectively.

X-ray diffraction (XRD) data showed that the AlN films have an amorphous character.

Chemical composition and bonding states were investigated by X-ray photoelectron spectroscopy. High resolution Al 2p and N 1s spectra confirmed the presence of AlN with peaks located at 73.02 and 396.0eV, respectively for all layers. The atomic concentration of Al is about 2.5 times higher than that of N, only for the AlN film grown at a dose of TMA and $NH_3$ 180 and 90 ms, respectively. Al/N ratio is close to the stoichiometric value (1:1), which is important when applying AlN films to SAW devices [3].

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# 2.17. Atomic layer deposition of AlN on different type of substrates

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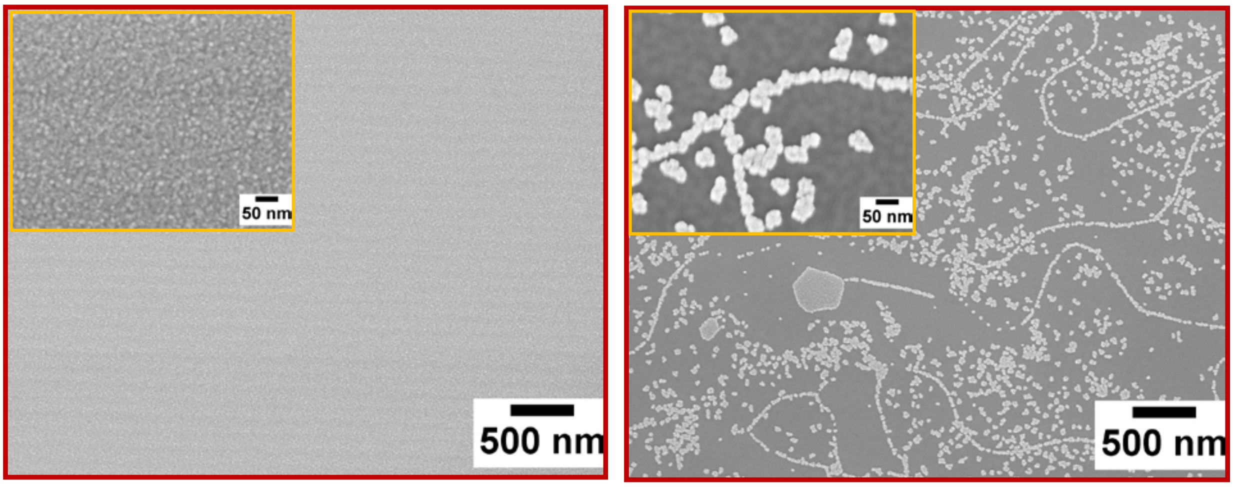
AlN thin films with thickness ~5 and 10 nm have been grown with a Picosun R-200 ALD (atomic layer deposition) reactor on different type of substrates. Type I were on axis 4H-SiC (0001) and Type II was on axis 4H-SiC with a seed layer of monolayer (ML) graphene grown by sublimation method [1]. TMA (trimethylaluminum) and $NH_3$ were used as precursors and the substrate was cleaned in-situ by $H_2$ and $N_2$ plasma. The surface morphology was studied for the films grown in the temperature range of 400-450°C. The results of scanning electron microscopy (SEM) revealed grain morphology for films grown on Type I substrate and mesh morphology for films grown on Type II substrate, Fig.1 a and b, respectively.

Chemical composition and bonding states were investigated by X-ray photoelectron spectroscopy. High resolution Al 2p and N 1s spectra confirmed the presence of AlN with peaks located at 73.02 and 396.0 eV, respectively for all layers. The films deposited on 4H-SiC (0001) with graphene sublayer had 3 times lower concentrations of Al and N, which reveals preconditions for fabrication of two-dimensional AlN (2D-AlN) [2].



a) b)

**Figure 1.** Top view SEM images of AlN films deposited at 400°C, 40 ALD cycles a) on 4H-SiC(0001) and b) 4H-SiC(0001) with a seed layer of monolayer (ML) graphene.

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# 2.18. Quantum-optical analogy for constructing of new devices: Sagnac-type polarization independent optical isolator

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Recently, the mathematical resemblance in the equations describing evolution of quantum systems and light transfer processes rise to investigation of quantum-optical analogies with possible realization as simulation tools or as new techniques for manipulation of light signals. Based on quantum-optical analogy some optical devices, constructed with commercially available optical elements, were theoretically investigated and experimentally demonstrated [1,2].

Here we propose a design for a polarization-independent optical isolator using Sagnac-interferometer-like configuration. We construct a prototype using a Faraday rotator in combination with quarter-wave plates to achieve nonreciprocal conversion with zero polarization rotation in one direction and 90° rotation in the other. The performance of the suggested device was tested with different input polarization states of the light.

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# 2.19. Physicochemical properties of nanosized $ZnFe_2O_4$ obtained by solution combustion synthesis and sonochemical synthesis.

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Spinel ferrites have been intensively investigated due to their versatile physical and chemical properties and due to their technological applications in magnetic sensors, biosensors, photocatalysts, nanoelectronics, biomedical. Bulk zinc ferrite have the normal spinel structure with $Zn^{2+}$ ions occupying tetrahedral (A) site and $Fe^{3+}$ ions being occupied in octahedral (B) site and is antiferromagnetic material having Neel temperature around 10 K.

Nanosized $ZnFe_2O_4$ was obtained by two methods of solution combustion synthesis and sonochemical synthesis. The obtained samples were thermally treated at different temperatures. Structural characteristics of $ZnFe_2O_4$ were studied by powder X-Ray diffraction (XRD). The results show the formation of single-phase samples with different particle sizes. Morphological characteristics of $ZnFe_2O_4$ were studied by Scanning electron microscopy (SEM), transmission electron microscopy, infrared electronic microscopy. Magnetization curves were measured at room temperature (RT) using vibrating sample magnetometer (VSM) in fields up to 6 kOe.

**Keywords:** $ZnFe_2O_4$, solution combustion synthesis, sonochemical synthesis magnetization curves.

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# 2.20. Niobium oxide sol-gel Bragg stacks for acetone sensing with optical read-out

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Nowadays tailoring properties of different materials is a focus of intensive research activities worldwide aiming to adjust their characteristics to one's needs and thus overcome numerous disadvantages of conventional materials. Often the increased requirements to the devices necessitate more complex structures or geometries of the constituent materials. Such structures are commonly applied as optochemical sensors as they allow low power consumption, fast response and naked-eye detection.

In the current study Bragg stacks of $Nb_2O_5$ have been tested as an active medium for acetone sensing with optical read-out. To create the low refractive index medium in the structure, porosity has been generated using commercially available Pluronics PE6800 and PE6200 as soft templates. The thicknesses and the refractive indices of the two media have been determined by nonlinear curve fitting method of reflection spectra of single dense (without organic template) and porous niobium oxide films deposited on silicon substrates. The porosity generated in the films has been estimated by Bruggeman effective medium approximation. The stacks have been deposited by spin-coating of alternating dense and porous $Nb_2O_5$ films. The reflection / transmission spectra of the stacks before and after acetone vapours exposure have been measured. The stacks have been studied in reflection and transmission regimes due to different advantages and disadvantages of the two approaches. Possible application and integration of those structures as a sensor for all kind of volatile organic compounds has been discussed.

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# 2.21. Properties of ZnSe nanocrystalline thin films prepared by thermal evaporation

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Zinc selenide is an important material, which finds applications in various electronic and optoelectronic devices, such as lasers, transistors, photodetectors, optical windows, etc. but the investigations on the gas sensitivity of ZnSe are rather limited. Our recent study on nanocrystalline ZnSe films of various thicknesses, prepared by thermal evaporation in vacuum, revealed good sensitivity to ethanol vapours at room temperature [1]. Higher sensitivity was obtained for the thinner films. In this study ZnSe films with thickness of 30 nm and 50 nm were prepared on Corning 7059 glass substrates at room temperature by applying periodically interrupted physical vapour deposition of ZnSe at different deposition rates. All as-deposited films were annealed at 200$^{o}$C and a part of them were further annealed at 400$^{o}$C. Results from spectroscopic ellipsometry have shown that the porosity of the films, which is important for the ethanol sensitivity decreases with increasing deposition rate and annealing temperature. The porosity changes caused by the films annealing at 400$^{o}$C are accompanied with roughness and thickness decrease.

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# 2.22. Effect of infrared laser irradiation on electrical conductivity and ethanol sensitivity of sol gel ZnO thin films

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Laser irradiation is a new alternative method which can be applied to change the structure and surface morphology of sol gel ZnO thin films. In this study two types of films were prepared on silicon wafers with oxidized surface by sol gel “spin coating technique” and post-deposition heat treatment at 140$^{o}$C and 400$^{o}$C. The influence of application of warm air stream during the film preparation is investigated. X-ray diffraction measurements show that both types of films, annealed at 140$^{o}$C and 400$^{o}$C, treated with warm air during preparation are crystalline with wurtzite structure. Spectroscopic ellipsometry results show that the film thickness is affected by both annealing temperature and warm air application. The observed thickness changes are related to effusion of organic molecules or parts of them which incorporate during the film deposition. The effect of laser irradiation for different times by infrared nanosecond pulse laser with a fluence of 90 mJ/cm$^2$ on the electrical conductivity and ethanol sensitivity of samples from all types is also studied. The film prepared by applying warm air stream and annealed at 400$^{o}$C show good sensitivity to ethanol vapors at room temperature.

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# 2.23. Effect of high temperature annealing on the electrical properties of Metal/$SiO_x$/Si structures

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Thin $SiO_x$ layers with $x = 1.15$ and 1.3 were deposited by thermal evaporation of SiO in vacuum on (100) n-type Si with resistivity of 4 – 6 Ω cm. Two sets of samples were investigated, with nominal thickness of the $SiO_x$ layer of 50 and 100 nm determined by quartz crystal microbalance. All samples were annealed at 250 $^{o}$C for 30 min in an argon atmosphere for stabilization and then split in several groups. The first group annealed at 250 $^{o}$C was used as control samples, while the other groups were additionally annealed at 600, 700, 800 or 1000 $^{o}$C for 60 min in a nitrogen atmosphere. High temperature annealing at 700 $^{o}$C leads to formation of amorphous Si nanoparticles in a $SiO_x$ matrix with $x \sim 1.7$, while annealing at 1000 $^{o}$C leads to a complete phase separation and formation of Si nanocrystals in a stoichiometric $SiO_2$ matrix [1,2]. For electrical characterization of the $SiO_x$ layers MOS structures were formed by thermal evaporation of top Al contacts with diameter of 0.5 mm and thickness of ~300 nm. Thick Al layer was deposited for back contact. The fabricated MOS structures were characterized by current-voltage (I-V) and capacitance-voltage (C-V) measurements. Results for the effect of annealing temperature on the electrical properties of the $SiO_x$ layers will be presented. A discussion for possible applications of such MOS structures will be carried out.

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# 2.24. Effect of blocking and tunnel oxide layers on the charge trapping properties of MIS capacitors with ALD $HfO_2/Al_2O_3$ nanolaminated films

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The fabricated by atomic layer deposition ALD nanolaminated $HfO_2/Al_2O_3$ or Al-doped $HfO_2$ films have attracted lately the researchers interest as charge-trapping media for the charge-trapping non-volatile memory cells. Recently, we have reported promising charge-trapping characteristics of ALD $HfO_2/Al_2O_3$ nanolaminates [1]. It was noticed, however, that down scaling of the thickness results in somehow worsening of the charge trapping effect (mainly the electron trapping). Thus, the impact of the dedicated blocking (BO) and tunnel oxide (TO) layers on the electrical characteristics and charge trapping of nanolaminated $HfO_2/Al_2O_3$ metal-insulator-silicon (MIS) structures were studied. The ALD $HfO_2/Al_2O_3$ dielectric (16.5nm) was obtained at low deposition temperature (135 °C). Two different TO films – 3.5nm thermal $SiO_2$ and 3nm ALD $Al_2O_3$ were investigated; as BO 20nm ALD $Al_2O_3$ was employed. It is demonstrated that the introduction of BO and TO layers substantially improves the charge trapping into $HfO_2/Al_2O_3$ multilayer dielectric (Figure 1). The $SiO_2$ tunnel layer was found to provide better characteristics in terms of electron trapping and retention.

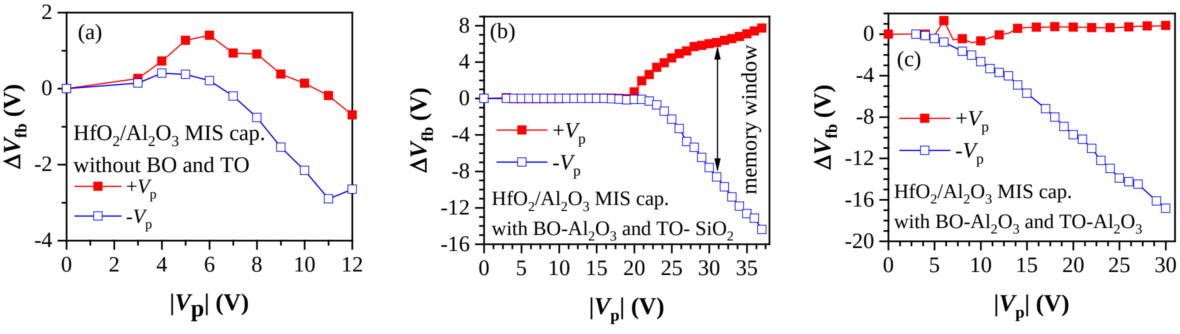

**Figure 1:** Flat-band voltage shifts ($\Delta V_{fb}$) resulting from the charge trapping under voltage pulses with duration of 1s and different polarity and magnitude.

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# 2.25. Influence of ZnO nanopraticles as electron transport material on the performance and shelf-life of P3HT:PCBM bulk heterojunction solar cells

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ZnO has been widely used as electron selective material in P3HT:PCBM organic solar cells to enhance the extraction of electrons and block the collection of holes at one electrode. In this work we use impedance spectroscopy to investigate the influence of ZnO nanoparticles electron transport layer (ETL) on the performance and stability of P3HT:PCBM based organic solar cells. A series of devices of standard architecture glass/ITO/P3HT:PCBM/ZnO/Ag were prepared in ambient environment with magnetron sputtered silver contacts and were compared with devices deposited under similar conditions but without ZnO. Their degradation after storage in the dark was monitored by measuring the J-V characteristics and the impedance spectra at regular time intervals. The impedance spectra were taken as a function of applied bias under illumination in order to reveal more information about the degradation mechanisms. Results of degradation studies under real outdoor conditions will also be presented.

# 2.26. Experimental results on photovoltaic heat pump with PCM/water thermal storage

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In nowadays, the sector of HVAC equipment has been influenced strongly by the photovoltaic (PV) technology. The growth of sector implies an increase of electricity consumption for room heating and cooling and demands for more energy generated by renewables. The concept of PV building integration has been developed further in smart houses, smart buildings and smart cities. However, to date, there is a room for optimization of electrical and thermal performance of small household AC devices (air-water heat pumps).

This study presents experimental results on design, assembling and performance of 12 BTU heat pump driven by solar electricity. The heat pump system has been assembled using standard components and new electronic units in order to facilitate the end-user and to show him universal methodology how to transform a commercial system with grid-only supply to a solar-energy driven cooling/heating system.

In this hybrid PV/Thermal system the concept for energy efficiency improvement in cooling/heating cycle is further extended with embedding of thermal storage unit. The 120 liter water tank due to its higher thermal capacity tends to smooth the variations of indoor temperatures due to outdoor solar irradiation variability in partially cloudy days. Phase change materials (PCM) are used to test and to improve thermal efficiency of the system. During the summer 2020 the developed PV/Heat pump system is tested in real conditions. The values of main Key Performance Indicators (KPI) : Performance ratio(PR), Energy Efficiency ratio(EER) were calculated. The first results indicate that during summertime PV modules with 700 Wp total installed power are enough - to generate approx. 6.5 kWh per day to supply the equipment for the daytime and to ensure thermal comfort for 4 hours after sunset.

# 2.27. Development of cost-efficient wireless network for solar UV irradiation monitoring in Bulgaria

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Researches in the last decades have identified exposure to solar UV radiation as one of the most important problems for human health. Possible consequences of UV over-exposure are skin tanning, sun burning or even skin cancer in humans. The absorption of UV–A radiation by the water content of cells may cause ionization and may produce free radicals.  The UV-B radiation has higher energy per photon and may provoke direct collision with DNA molecules. The proteins are found also to absorb strongly in the UV–C region with a maximum around 280 nm.

Fortunately, ozone in the atmosphere prevents the most harmful UV-C radiation from reaching the biosphere. Aerosols, water drops and cloud cover are other factors that play a dominant role in the variability of UV irradiation. These optical and abssorbtion effects have to be monitored carefully in order to prevent people from extraordinary risk. The deeper penetration, easy maintenance of UV sensor equipment and dense disperse of UV monitoring points will improve further the accuracy of UV forcasting and will convince the citizens in the responsibility of researchers and their work.

The goal of this study is to present recent success in UV monitoring in the frame of INTERGA_UV project (No. КП 06 /24Н - 2018 of National Research Fund of Bulgaria)  by development of a network of sensors, remote databases and UV monitoring center. The developed UV monitoring system differs from conventional equipment with a flexible structure, upgradability, higher temporal resolution of measurement for multiple points (<1min) due to implementation of open-source Python applications, embedding of open-source Influxdb database and Arduino-based platforms of hardware.

The collected data graphs from high-mountain locations reveal underestimated dangerous UV peaks during summer days with dispersed clouds. In urban locations a shift in the maximum of UVA and UV-B irradiation compared to visible sunlight is observed. The collected database during one-year field measurements is intended for development of deep-learning algorithms for short-term UV forecasting.

# 2.28. Cost-effective selective absorber for solar tower application

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A new type of energy generator “Solar Thermal Plant” (STP) is designed and investigated. This facility uses a large area solar collector to heat the air at the bottom of a chimney. The air is accelerated by the “chimney effect” and propels an electric generator via mechanical turbine. The amount of energy produced depends critically on the area of the solar collector and its efficiency.

This study presents experimental results on optimization of the solar collector by developing an efficient absorber of the solar irradiation. The absorber consists of a metal plate (base), which is painted by a coating with specific optical properties. A low cost paint, containing silicon particles and appropriate binder, is developed for the purpose. The aim is to obtain a “selective absorber” that has a high absorption in the spectral region of solar irradiation (visible and near IR range), as well as a low radiative emission in the far IR range (i.e. low radiative loses). Thus, the metal plate can reach higher temperatures due to minimization of the radiative loses that are dominant at temperatures around 100 °C.

# 2.29. Magneto-optical characterization of ZnO / Transition Metal Oxides nanolaminates obtained via Atomic Layer Deposition

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The magneto-optical (MO) properties of ZnO and Co, Fe and Ni transition metal oxide (TMO) nano-laminate structures prepared by Atomic Layer Deposition (ALD) have been investigated. Using a MO Kerr effect microscopy, we have studied the local magnetic coercivity and its distribution and mapping for the ZnO/TMO nanolaminates on a microscale level. Taking into consideration the preparation details, structural and morphological data, possible vacancy effects and overall influence of the magnetic elements (Co, Fe and Ni), we have comparatively analysed the inhomogeneous coercivity dispersion and the values of the Kerr polarization rotation for the different films.

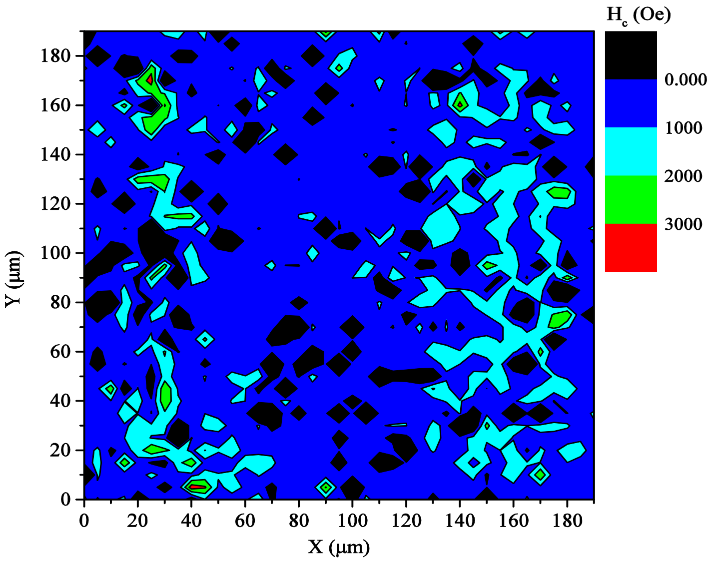

**Figure 1:** Coercivity map of ALD ZnO/Fe nanolaminate on a microscopic level.

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# 2.30. Environmental radiation monitoring at BEO Moussala

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The scope of research at the Basic Environmental Observatory (BEO) Moussala (2925 m a.s.l.), Rila Mountain, comprises studies of the aerospace and terrestrial environments. The global climate change, natural hazards and anthropogenic pollutions are natural parts of these investigations. In this respect, the real-time measurement of various types of radiation being conducted at the BEO is an important field of research. Thus, the natural and technogenic radioactivity of air aerosols has been monitored at the BEO since 2006. A detector, part of the SEVAN worldwide network, is in operation at the observatory as well, measuring the intensity of the secondary cosmic rays particles with three counting channels – low-energy (electron-photon component), neutral (mainly neutrons) and high-energy particles (mainly muons). The Muon Telescope at BEO consists of eight water Cherenkov detectors and has been in operation for more than 12 years. Furthermore, a large-volume NaI(Tl) scintillator is being used to monitor the intensity and energy distribution of energetic cosmic particles. In the paper we discuss the performance and setup of the systems along with the results obtained. The equipment employed at BEO include also a broadband Kipp&Zonen pyranometer for measuring the solar global horizontal irradiation; a Liulin-6MB (developed in Bulgaria) silicon-diode-based radiation dosimeter for radiation monitoring at high-altitude observatories; and two AIRDOS M dosimeter units (developed in the Czech Republic) for measuring low-intensity mixed ionizing radiation fields, which are operating simultaneously. Also, the ambient equivalent radiation dose is measured by an IGS421B1 gamma probe. We present analyses of the energy spectra thus obtained to complete the set of studies on the environmental conditions. As an important example, we show data from gamma-ray background monitoring during the Fukushima accident. The analysis of the results demonstrate that the background radiation is within acceptable limits.

**Keywords:** Gamma-spectrometer, NaI detector, secondary cosmic rays

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# 2.31. Calculation of the bandgap of dilute nitride GaAsSbN alloys

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Dilute nitrides are semiconductor alloys, obtained from the conventional III-V compounds by incorporating a small amount of nitrogen. The interest in these compounds is due to their potential to alter the energy band gap and the lattice constant, which creates additional flexibility desired in many applications such as multijunction solar cells, heterojunction bipolar transistors, lasers, and high-speed photodetectors.

In this work, we focus on GaAsSbN considered as a perspective material for incorporation in multijunction solar cells. Nitrogen creates a localized level inside the conduction band continuum. The interaction of this level with the conduction band is usually described by the single band anti-crossing (BAC) model [1]. The double BAC model of GaAsSbN [2] considers both the N and the Sb localized levels in the conduction and the valence band, respectively.

We calculate the bandgap energy of GaAsSbN employing the single and double BAC model for different concentrations of Sb and N. Parameters of the BAC model taken from different literature sources [3–6] are used in the calculations and their influence on the final result is explored. Finally, the calculated bandgap energies are compared to experimental data of GaAsSbN layers grown on n-GaAs substrates by low-temperature liquid phase epitaxy. These data include the optical absorption edge of the material determined by surface photovoltage spectroscopy and the energy position of the photoluminescence peak at room temperature.

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