**Bulgarian Academy of Sciences** 



Georgi Nadjakov Institute of Solid State Physics



# **BOOK OF ABSTRACTS**

# 20th Jubilee International School on Condensed Matter Physics

*Physics and Applications of Advanced and Multifunctional Materials* 

> September 3rd – September 7th , 2018 Varna, Bulgaria

Partially supported by the Ministry of Education and Science, Bulgarian National Science Fund (Grant No DPMNF 01/7 – 23.07.2018)





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## BULGARIAN ACADEMY OF SCIENCES GEORGI NADJAKOV INSTITUTE OF SOLID STATE PHYSICS

20<sup>th</sup> INTERNATIONAL SCHOOL ON CONDENSED MATTER PHYSICS "Physics and Applications of Advanced and Multifunctional Materials" September 3<sup>rd</sup> – 7<sup>th</sup>, 2018 – Varna, Bulgaria

Partially supported by the Ministry of Education and Science, Bulgarian National Science Fund (project number DPMNF 01/7 – 23.07.2018)

## **PROGRAMME**

## September 2nd (Sunday)

16:00-19:00	Registration
20:00	<b>Get Together Party</b>

## September 3rd (Monday)

09:00-09:20	Opening Ceremony
09:20-09:30	Honorary Chairman of event A.G. PETROV, "ISCMP: Twenty Issues of History"
09:30-11:00	Chair: H. Chamati
09:30-10:15	P. Ch. IVANOV, "The new field of network physiology: how statistical physics and nonlinear dynamics can help us understand organ network interactions and build the human physiolome" <i>Georgi Nadiakov Memorial Lecture</i>
10:15-11:00	I. MIHAILESCU, "Laser soft transfer, construction and reconstruction of thin layers of organic and inorganic materials for top technologies by pulsed laser techniques" <i>Milko Borisov Memorial Lecture</i>
11:00-11:30	Coffee break / Collective photo
11:30-12:50	Chair: S. Reynolds
11:30-12:10	E. GUZIEWICZ, "Mystery of electrical conduction of zinc oxide – from heavily n-type to p-type material"
12:10-12:30	M. GARTNER, "ZnO films prepared by physical and chemical methods for sensors and piezoelectric applications"
12:30-12:50	T. BABEVA, "Optical sensing of vapors and liquids using porous Bragg reflectors"
12:55-16:00	Lunch break
<b>16:00-17:20</b> 16:00-16:40	<b>Chair: D. Dimova-Malinovska</b> S. REYNOLDS, "Silicon thin-films: Functional materials for energy, healthcare and IT applications"

17:20-18:00	Chair: D. Nesheva
16:40-17:20	J.–P. KLEIDER, "Recent progress on the amorphous silicon / crystalline silicon interface"

# 17:20-18:00Chair: D. Nesheva17:20-18:00Five minutes presentations of posters of young participants

# September 4th (Tuesday)

<b>09:10-10:30</b> 09:10-09:50	<b>Chair: J. Genova</b> Y. A. ERMAKOV, "Electric fields at the membrane interfaces: from lipid models to biomedical applications"
09:50-10:30	A. IGLIČ, "Water polarization and asymmetric finite size of ions in electric double layer"
10:30-11:00	Coffee break
11:00-13:00	Chair: A. Iglič
11:00-11:40	S. KRALJ, "Topological defects and membranes"
11:40-12:20	O. BATISHCHEV, "Lipid membrane elasticity and protein-lipid interactions"
12:20-12:40	V. SOKOLOV, "The kinetics of binding of protons with bilayer lipid membrane"
12:40-13:00	R. MOLOTKOVSKY, "Adsorption of polylysines at the surface of lipid membranes: Theoretical analysis of electrokinetic data"
13:00-16:00	Lunch break
16:00-18:00	Chair: Y. A. Ermakov
16:00-16:40	B. RIZZUTI, "Disordered proteins as intrinsically multifunctional targets"
16:40-17:20	S. AKIMOV, "Raft boundary structure determines line activity and self- organisation of membrane inclusions into symmetric structures"
17:20-17:40	D. KHOMICH, "Phase transition of DMPS monolayers studied by molecular dynamics and X-ray reflectometry"
17:40-18:00	I. JIMÉNEZ-MUNGUÍA, "In vitro study of porphyrins as candidate photosensitizers in photodynamic therapy against cancer"
18:00-19:00	First poster session

# September 5th (Wednesday)

09:10-10:30	Chair: M. Sčepanovič
09:10-09:50	P. MONTGOMERY, "High resolution surface metrology using
09:50-10:30	microsphere assisted interference microscopy" P. PETRIK, "Monitoring of solid-liquid interfaces using ellipsometry"
10:30-11:00	Coffee break

11:00-13:00	Chair: P. Montgomery
11:00-11:40	M. SČEPANOVIČ, "Temperature-dependent Raman study of
	nanostructured and multifunctional materials"
11:40-12:00	V. DONCHEV, "Surface photovoltage study of GaInAsNSb layers for
	photovoltaic applications"
12:00-12:20	H. STROESCU, "Preparation and characterization of TiO <sub>2</sub> thin films for
	harvesting applications and optoelectronic devices"
12:20-12:40	R. GEORGIEV, "Mesoporous Ta <sub>2</sub> O <sub>5</sub> thin films as an active medium for
	pollution monitoring of air and water"
12:40-13:00	K. LOVCHINOV "Influence of deposition temperature on the structural
	and optical properties of electrochemically nanostructured ZnO films"
13:00-16:00	Lunch break
16:00-18:00	Chair: P. Petrik
16:00-16:40	F. BALESTRA, "NanoCMOS and Small Slope Switches for the end of
	the Roadmap"
16:40-17:20	PH. VANDERBEMDEN, "Type-II superconductors used as magnetic
	shields: distinguishing the effects related to geometry from those related
	to physics"
17:20-17:40	J. ČWIK, "Magnetic properties and magnetocaloric effect in low
	temperature ordered Tb <sub>1-x</sub> Dy <sub>x</sub> Ni <sub>2</sub> intermetallic compounds"
17:40-18:00	D. GAJDA, "High field pinning centers in NbTi wires and MgB2 wires"
18:00-19:00	Second poster session

# September 6th (Thursday)

09:10-10:30	Chair: Ts. Babeva
09:10-09:50	D. DIMOVA-MALINOVSKA, "Nanostructured ZnO films for application in gas sensors"
09:50-10:10	K. BUCHKOV, "Inter-granular effects at high magnetic fields of cuprate and iron chalcogenide superconducting materials"
10:10-10:30	S. KOLEV, "Semiconducting Graphene"
10:30-11:00	Coffee break
11:00-13:20	Chair: V. Donchev
11:00-11:40	B. SARUHAN-BRINGS, "Memrister type gas sensors for high sensitivity sensing at low temperatures"
11:40-12:20	S. BANERJEE, "Corralling Electrons in Vanadium Oxides: Implications for Neuromorphic Computing and Electrochemical Energy Storage"
12:20-13:00	S. BARANOVSKII, "Theoretical description of charge transport in disordered solids: to simulate or to think?"
13:00-13:20	L. UDACHAN, "Impact of substrate temperature on grain boundary reflection in chromium nanofilms"
13:20-16:00	Lunch break

<b>16:00-17:20</b> 16:00-16:40 16:40-17:20	<ul><li>Chair: A. G. Petrov</li><li>M. MICHAILOV, "Atomic scale design, structure and stability of quantum nanowires on epitaxial interfaces"</li><li>V. ČELEBONOVIČ, "Theoretically choosing multifunctional materials"</li></ul>
17:20-17:40	Coffee break
17:40-19:00	Chair: N. Ivanov
17:40-18:00	J. RICHTER, "Frustated quantum magnetism: The flat-band scenario"
18:00-18:20	L. SHIVA, "A study on nucleation, growth and grain boundary reflection in thin tin nanofilms"
18:20-18:40	G. LEWIŃSKA, "D-D-A ternary organic solar cells"
18:40-19:00	S. ŞEN, "Phthalimide derivative spun films for organic vapour sensing"
20:00	Farewell Dinner

# September 7th (Friday)

<b>09:10-10:30</b> 09:10-09:50	<b>Chair: B. Rizzuti</b> M. FABIAN, "Bioactive glasses: structure characteristics and bone regeneration application"
09:50-10:30	Z. USATENKO, "Ring polymer chains in a slit geometry with mixed boundary conditions"
10:30-11:00	Coffee break
11:00-13:00	Chair: Z. Usatenko
11:00-11:40	A. BUKA, "Topological Defects in Liquid Crystals"
11:40-12:00	G. IVANOV, "Langmuir-Blodgett films from fluorescently labelled phospholipids deposited on surface acoustic wave devices and surface plasmon resonance substrates"
12:00-12:20	H. SOLUNOV, "On measuring the characteristic length of the cooperative molecular dynamic in glass-forming liquids"
12:20-12:40	Closing Ceremony
14:00	Social event/Visit of a historical place in the region, organized with the support of Varna Municipality

# **POSTER PRESENTATIONS**

# **1. FIRST POSTER SESSION, September 4<sup>th</sup> (Tuesday)**

- 1.1. V. Tashkin, V. Vishnyakova, A. Shcherbakov, H. Apell, V. Sokolov, Electrogenic transport of Na<sup>+</sup>, K<sup>+</sup> and H<sup>+</sup> ions in the cytoplasmic access channel of Na,K,ATP-ase studied by admittance measurements in model system.
- K. Hristova-Panusheva, M. Keremidarska-Markova, T. Andreeva, G. Speranza, D. Wang, M. Georgieva, G. Miloshev, N. Krasteva, Dose-dependent genotoxicity of ammoniamodified graphene oxide particles in lung cancer cells
- 1.3. C. Özkaya, R. Çapan, F. Yükrük, M. Erdoğan, A study of room temperature vapor sensing properties using perylenediimide thin film
- 1.4. Z. Özbek, F. Davis, R. Çapan, Electrical measurements of a Calix[4]acid/amine alternate layer Langmuir-Blodgett thin film
- 1.5. Y. Acikbas, C. Ozkaya, S. Bozkurt, G. Tetik, R. Capan, M. Erdogan, α-naphtol based monomer Langmuir-Blodgett thin films for vapor sensing applications
- 1.6. K. Zhelyazkova, B. Katranchev and M. Petrov, Surface plasmon resonance assisted with bilayer phospholipid membrane
- 1.7. J. Genova, I. Bivas, M. Fosnarič, A. Iglič and S. Penič, Influence of the stretching elasticity modulus on the thermal shape fluctuations of nearly spherical vesicles
- 1.8. Z. Slavkova, H. Chamati, J. Genova, Influence of gold nanoparticles on the elastic properties and phase behaviour of model lipid systems
- 1.9. D. Mitkova, G. Staneva, O.V. Batishchev and V. Vitkova, Bending elasticity of phosphatidylcholine membranes containing archaeal lipids
- 1.10. Y. Volkov, A. Tikhonov, B. Roshchin, V. Asadchikov, A. Nesterenko, D. Khomich, Y. Ermakov, Structural parameters of DMPS lipid monolayer during liquid/gel phase transition: X-ray reflectometry analysis
- 1.11. J. Halun, Z. Usatenko, Monomer density profiles for phantom ideal ring polymer chains in confined geometries
- 1.12. S. Şen, R. Çapan, Z. Özbek, M. E. Özel, G. A. Stanciu, F. Davis, CBAMINE LB films and the vapour detection of those against volatile organic compounds
- 1.13. S. Harkai, S. Kralj, Reconfigurable networks of nematic topological defects
- 1.14. G. Hadjichristov, Y. Marinov, Tz. Ivanov, H. Koduru, N. Scaramuzza, Electroanalytical survey of charge trapping in NaIO<sub>4</sub>:(PEO/PVP) ion-conducting polymer electrolyte
- 1.15. K. Danel, A. Wisła-Świder, T. Lemek, Benzyne based aryl cycloaddition and indenoannelation from a common starter
- 1.16. I. Bodurov, A. Viraneva and T. Yovcheva, Electret and dielectric properties of lyophilized polymer films
- 1.17. V. Velev, S. Salim, N. Arhangelova, Calorimetric studies on tensile stress-induced crystallization of amorphous poly (ethylene terephthalate) filaments
- 1.18. P. Kuterba, Z. Usatenko, Ring polymer chains with Dirichlet-Neumann boundary conditions in confined geometries
- 1.19. N. Ivanov and J. Schnack, Phase diagrams of Heisenberg chains with three-spin exchange couplings and different composite spins in the unit cell
- 1.20. M. Georgiev and H. Chamati, Model parameters and the spin trimer system  $A_3Cu_3(PO_4)_4$  (A = Ca, Sr, Pb)
- 1.21. S. Varbev, R. S. Kamburova and M. T. Primatarowa, Interaction of solitons with a qubit in an anisotropic Heisenberg spin chain
- 1.22. O. D'Huys, J. Rodríguez-Laguna, M. Jiménez, E. Korutcheva and W. Kinzel, Synchronization in fluctuating networks with delay interactions

- 1.23. E. Pisanova, Entropy and specific heat of a critical quantum system with long-range interaction
- 1.24. S. Varbev, R. Kamburova and M. Primatarowa, Soliton-impurity interaction in two coupled ferromagnetic chains
- 1.25. H. Hristova, S. Ognyanski, V. Steflekova, E. Dimova, Quantum-optical analogies
- 1.26. M. Milev, St. Minkova, Kr. Nikolova, Ir. Ivanova, N. Hristova-Akumuva, V. Hadjimitova, M. Kakalova, Comparative statistical analysis of Bulgarian red wines on the base of optical and chemical characteristics
- 1.27. R. Gergova, M. Sendova-Vassileva, G. Popkirov, G. Grancharov, V. Gancheva, Study of aged polymer bulk heterojunction solar cells by impedance spectroscopy
- 1.28. I. Angelova, C. Chiou, C. Fidanova, V. Marinova, S.Lin, D. Petrova, B.Blagoev and D. Dimitrov, Al -doped ZnO for flexible polymer dispersed liquid crystal devices
- 1.29. K. Temelkov, Y. Fedchenko, S. Slaveeva, T. Chernogorova, Theoretical study on some plasma parameters and thermophysical properties of gas-discharge plasma in various gas mixtures using new methods
- 1.30. G. Hadjichristov, Y. Marinov, A. Petrov, H. Koduru and N. Scaramuzza, Polymer(PEO)liquid crystal (LC E8) composites: The effect from the LC inclusion
- 1.31. H. Tonchev, A. Donkov, H. Chamati, Exact results for the energy spectrum of the Jaynes-Cummings model interacting with a spin chain

# 2. SECOND POSTER SESSION, September 5<sup>th</sup> (Wednesday)

- 2.1. E. Manolov, N. Nedev, V. Dzhurkov, D. Nesheva, J. Paz-Delgadillo, M. Curiel-Alvarez, B. Valdez-Salas, Investigation of resistive switching in SiO<sub>2</sub> layers with Si nanocrystals
- D. Nesheva, Ts. Babeva, M. Vasileva, B. Valdes-Salas, V. Dzhurkov, M. U. Grujić-Brojčin, M. J. Šćepanović, O. Perez, N. Nedev, M. Curiel, Ethanol adsorption in TiO<sub>2</sub> nanotubes anodically grown on Ti<sub>6</sub>A<sub>14</sub>V alloy substrates
- 2.3. S. Kansara, S. Gupta, Y. Sonvane, Two dimensional transition metals nanosheet for nitric oxide: A DFT study
- 2.4. S. Simeonov, A. Szekeres, M. Covei, D. Spassov, L. Predoana, H. Stroescu, M. Gartner, M. Zaharescu, Charge transport mechanism in Vanadium doped TiO<sub>2</sub> sol-gel films
- 2.5. S. Boyadjiev, S. Mihaiu, I. Atkinson, V. Georgieva, L. Vergov, P. Rafailov, I. Szilágyi, Solgel grown bare, Ni- and Li/Ni-doped ZnO thin films for gas sensor applications
- 2.6. V. Dzhurkov, Z. Levi, D. Nesheva, Room temperature sensitivity of ZnSe nanolayers to ethanol vapours
- 2.7. K. Lazarova, S. Boycheva, M. Vasileva, D. Zgureva, B. Georgieva and T. Babeva, Zeolites from fly ash embedded in thin niobium oxide matrix for optical sensing applications
- 2.8. D. Spassov, A. Paskaleva, T. A. Krajewski, UE. Guziewicz, T. Ivanov, Leakage currents in  $Al_2O_3/HfO_2$  multilayer high-*k* stacks and their modification by post-deposition annealing steps
- 2.9. M. Beshkova, R. Yakimova, Two-dimensional materials with focus on AlN-possibility of experimental growth and characterization by ellipsometry
- 2.10. T. Hristova-Vasileva, I. Bineva, R. Todorov, A. Dinescu, C. Romanitan, In-depth evolution of tellurium films deposited by frequency assisted thermal evaporation in vacuum (FATEV)
- 2.11. M. Ganchev, A. Katerski, J. S. Eensalu, R. Gergova, M. Sendova Vassileva, G. Popkirov, P. Vitanov, Influence of deposition parameters on opto-electronic properties of spin – coated SnO<sub>2</sub> thin films
- 2.12. M. Sendova-Vassileva, R. Gergova, Hr. Dikov, G. Popkirov, P. Vitanov, G. Grancharov, V. Gancheva, Alternative WO<sub>3</sub> hole transport layer for organic solar cells
- 2.13. A. Stoyanova-Ivanova, I. Ilievska, V. Petrunov, S. Cherneva, R. Iankov, V. Mikli, In-vivo study on titanium–niobium orthodontic archwires

- 2.14. J. Shah, M. Ranjan, S. K. Gupta, Y. Sonvane, Temperature-dependent thermal conductivity and viscosity of synthesized α-Alumina nanofluids
- 2.15. D. Nicheva, I. N. Mihailescu, G. Stan, I. Pasuk, G. Popescu-Pelin, C. Ristoscu, P. Petkov, T. Petkova, Structure investigation of thin films from Zn-cobaltite prepared by pulsed laser deposition
- 2.16. K. Garasz, M. Kocik, Experimental investigations on ultrashort laser ablation for micro and nanomachining of materials
- 2.17. I. Bliznakova, A. Daskalova, A. Zhelyazkova, L. Angelova, A. Trifonov, I. Bucharov, Femtosecond Laser surface of thin chitosan/ hydroxyapatite layers for biomedical applications
- 2.18. T. Yovcheva, S. Rusev, B. Pilicheva, A. Marinova, A. Viraneva, I. Bodurov, G. Exner, S. Sotirov, I. Vlaeva, Y. Uzunova, M. Marudova, Crosslinked chitosan/casein polyelectrolyte multilayers for drug delivery
- 2.19. V. Steflekova, D. Zhechev, Light induced nonselective effects in the negative glow
- 2.20. Y. Marinov, G. Hadjichristov, P. Rafailov, S. Lin, V. Marinova, A. Petrov, Optical, electrooptical, electrical and dielectric characterization of nematic liquid crystal (E7) layers doped with graphene and graphene oxide nanoparticles for electro-optics
- 2.21. G. Hadjichristov, T. Vlakhov, Y. Marinov, Impedance and dielectric spectroscopy study of graphene-doped liquid crystal E7
- 2.22. H. Nichev, N. Tyutyundzhiev, M. Petrov, K. Lovchinov, P. Petrov, Development of lowcost technology to obtain supercapacitors based on activated carbon
- 2.23. A. Vasev, P. Lilov, Y. Marinov, A. Stoyanova, D. Karashanova, G. Ivanova, D. Kovacheva, V. Mikli, A. Stoyanova-Ivanova, Electrochemical behavior of BSCCO cuprate ceramics in alkaline solution
- 2.24. N. Tyutyundzhiev, K. Lovchinov, M. Petrov, H. Nichev, P. Petrov, C. Angelov, Graphene/polyaniline flexible supercapacitors using non-metallic electrodes
- 2.25. R. Gegova, A. Bachvarova-Nedelcheva, R. Iordanova, Y. Dimitriev, Sol-gel synthesis and structural characterization of compositions in the system TiO<sub>2</sub>-TeO<sub>2</sub>-SeO<sub>2</sub>
- 2.26. G. Dyankov, K. Zhelyazkova, M. Petrov, B. Katranchev, H. Naradikian, Y. Marinov, T. Dimitrova, Surface plasmon for exploration the temperature dependence of hybrid cholesterc liquid crystal's pitch
- 2.27. İ. Çapan, M. Bayrakci, M. Erdogan, M. Ozmen, Fabrication of thin films of phosphonated calix arene bearing crown ether and their gas sensing properties
- 2.28. S. Reynolds, A. Houghton and D. Keeble, Electronic transport in methylammonium lead halide perovskite single crystals studied by transient photoconductivity
- 2.29. E. Iordanova, G. Yankov, V. Mihailov and N. Nedyalkov, LIBS analyses on glass materials doped with noble metal nanoparticles

# **ABSTRACTS OF INVITED LECTURES**

## The new field of Network Physiology: mapping the Human Physiolome

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The human organism is an integrated network where complex physiological systems, each with its own regulatory mechanisms, continuously interact to optimize and coordinate their function. Organto-organ interactions occur at multiple levels and spatiotemporal scales to produce distinct physiologic states: wake and sleep; light and deep sleep; consciousness and unconsciousness. Disrupting organ communications can lead to dysfunction of individual systems or to collapse of the entire organism (coma, multiple organ failure). Yet, we know almost nothing about the nature of the interactions between diverse organ systems and their collective role in maintaining health. Through the prism of concepts and approaches originating in statistical and computational physics and nonlinear dynamics, we will present basic characteristics of individual organ systems, distinct forms of pairwise coupling between systems, and a new framework to identify and quantify networks of interactions among diverse organ systems. We will demonstrate how physiologic network topology and systems connectivity lead to integrated global behaviors representative of physiologic states and functions. We will discuss implications for further theoretical developments and practical applications within the context of the emerging field of Network Physiology, where physicists have a key role in uncovering basic principles and mechanisms. The presented investigations are initial steps in building a first atlas of dynamic interactions among organ systems and the Human Physiolome.

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- 2. Bartsch RP, et. al. "Network physiology: how organ systems dynamically interact." PloS One (2015) 10(11): e0142143.
- 3. Ivanov PCh, et. al. "Focus on the emerging new fields of network physiology and network medicine." New Journal of Physics (2016) 18(10): 100201.
- 4. Liu KKL, et. al. "Plasticity of brain wave network interactions and evolution across physiologic states." Frontiers in Neural Circuits (2015) 9: 62.
- 5. Lin A, et. al. "Delay-correlation landscape reveals characteristic time delays of brain rhythms and heart interactions." Phil. Trans. R. Soc. A (2016) 374: 20150182.
- Ivanov PCh and Bartsch RP. Network Physiology: Mapping Interactions Between Networks of Physiologic Networks. In "Networks of Networks: the last Frontier of Complexity", edited by D'Agostino G and Scala A. Springer International Publishing Switzerland, Series Title 5394 Understanding Complex Systems, (2014): pp. 203-222
- Ivanov PCh, et. al. Network Physiology: From Neural Plasticity to Organ Network Interactions. In "Emergent Complexity from Nonlinearity, in Physics, Engineering and the Life Sciences", edited by Mantica G, Stoop R, and Stramaglia S. Springer Proceedings in Physics (2017) 191: pp. 145-165

## Laser soft transfer, construction and reconstruction of thin layers of organic and inorganic materials for top technologies by pulsed laser techniques

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Basic principles of laser pulses interaction with solid and liquid materials using advanced pulsed laser technologies are introduced and new recent results in synthesis of biomaterial layers are reviewed. The layers are optimized based upon the results of physical-chemical investigations, while biocompatibility, bioactivity and bio-degradation were assessed by dedicated in-vitro tests.

Structures with compositional gradient are obtained by Combinatorial-MAPLE (C-MAPLE) by the simultaneous laser vaporization of two targets. Synchronized MAPLE of levan and oxidized levan cryogenic targets is applied in order to transfer under protection and assemble a twocompound biopolymer film structure. FTIR micro-spectroscopy confirmed the existence of a composition gradient along the length of the sample. In-vitro cell culture assays illustrate characteristic responses of cells to specific surface locations. Cells attached along the gradient are in direct proportion with oxidized levan concentration. C-MAPLE is applied to synthesize crystalline gradient thin films with variable composition of Sr-substituted hydroxyapatite (Sr-HA) and Zolendronate modified hydroxyapatite (ZOL-HA). The inhibitory action of ZOL on osteoclast viability and activity is more efficient than that of Sr, which plays a greater beneficial role on osteoblast proliferation and viability. C-MAPLE allows to modulate the composition of the thin films and hence the promotion of bone growth and the inhibition of bone resorption. We demonstrate the use of C-MAPLE to the in-situ synthesis of Poly-dl-lactide (PDLLA) and fibronectin (FN). Confocal and FTIR microscopy evidence FN packages embedded in the polymeric matrix. The composition of PDLLA and FN is preserved after C-MAPLE as demonstrated by protein staining and FTIR. Our conclusion is that the thin films prepared by pulsed laser techniques are identical in chemical composition, structure, morphology, and most likely functionality resembling the base material, as proved by physical-chemical characterization and invitro testing. C-MAPLE opens the possibility to combine and immobilize two or more organic materials on a substrate in a well defined manner by laser evaporation under protection.

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## Mystery of electrical conduction of zinc oxide – from heavily *n*-type to *p*-type material

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Because of a wide band gap, high exciton binding energy and feasibility to form a wide range of nanostructures, zinc oxide is a perspective material for many applications and conductivity control is crucial for most of them.

Without any external doping zinc oxide is n-type semiconductor in which the level of electron concentration can vary from  $10^{16}$  till  $10^{20}$ /cm<sup>3</sup> depending on the method and parameters of the growth. Recent studies show that an observed doping level can be attributed to interaction of native defects with impurities unintentionally introduced during the growth process. P-type doping, although possible, has been found to be extremely difficult because of the ZnO band structure with the valence band maximum placed far below the Fermi level. In the paper we present structural, electrical and optical studies on thin ZnO films obtained by Atomic Layer Deposition in temperature range  $100 - 200^{\circ}$ C. I will show that varying the growth conditions from oxygen- to zinc-rich results in a dramatic change of electron concentration even without external doping. Acceptor doping can be achieved by appropriate tuning of growth conditions in order to induce a successful interaction of nitrogen with native defects and hydrogen.



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# Silicon thin-films: Functional materials for energy, healthcare and IT applications

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Amorphous and microcrystalline silicon emerged as useful thin-film electronic materials in the 1970s and 80s. Since then our understanding of their properties and ability to modify and optimise them has improved markedly, and applications including LCD TFT backplanes, photovoltaics and flat-panel x-ray imagers are now worldwide industries. The number and diversity of proposed applications continues to grow, with water-splitting, flexible electronics, biomedical implants, thermoelectric generation and THz, IR and UV detectors showing particular promise. Their technology impact thus spans energy, healthcare, IT and consumer goods sectors, demonstrating that thin-film silicon represents a 'case-study' functional electronic material. Here we briefly review the physics and technology legacy of the past 50 years, before discussing and evaluating a selection of more recent developments.

### Recent progress on the amorphous silicon/crystalline silicon interface

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While crystalline silicon (c-Si) has been studied and developed since the 1950's for both microelectronics and photovoltaics, studies on hydrogenated amorphous silicon (a-Si:H) are more recent, and have led in the 1980's to the development of LCD display applications, while thin film a-Si:H solar cells only reached a very small part of the PV market that is largely dominated by c-Si technologies. The two worlds of amorphous and crystalline matter have gone their own way with their own physics until the Sanyo laboratories demonstrated that a-Si:H/c-Si interfaces could replace the traditional diffused junctions in c-Si photovoltaics and lead to very high energy conversion efficiencies. As a matter of fact, the highest efficiency reached so far for a c-Si based solar cell employs an n-type c-Si substrate with bottom electron and hole extracting contacts built on (i) a-Si:H / (n) a-Si:H and (i) a-Si:H / (p) a-Si:H layers, respectively.

A lot of work has been devoted to the study of the a-Si:H/c-Si interface. The (i) a-Si:H layer used as a buffer layer between the doped a-Si:H layer and the c-Si wafer in solar cell applications is known to work as an excellent passivation layer. However, the interface states density could never be measured, and the quality of the device is generally assessed through the open circuit voltage of the cell or the effective lifetime in the c-Si wafer, measured from various techniques like photoluminescence or photoconductivity decay. In this presentation, I will give a short review of our knowledge of the a-Si:H/c-Si interface, emphasizing the role of strong inversion (Fig. 1). I will present some recent approaches developed in our laboratories to quantify interface defect densities through modelling based on the defect-pool model in a-Si:H, combined modulated photoluminescence and planar dark- and photoconductivity measurements, and I will also present a new approach for high efficiency heterojunction solar cells, namely the homo-heterojunction solar cell, where a thin implanted doped crystalline layer forms the junction (Fig. 2), while the a-Si:H layers are still useful for the passivation.



Figure 1: Band diagram of the (p) a-Si:H/ (i) a-Si:H/(n) c-Si heterojunction.

**Figure 2:** Sketch of the usual silicon heterojunction cell (left) and advanced homo-heterojunction concept (right)

# **Electric Fields at the Membrane Interfaces: From Lipid Models to Biomedical Applications**

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Lipid matrix of biological membranes consist from phospholipids with headgroups that can be uncharged (PC, PE etc.) or have a negative charge (PS, CL). Ionized polar groups make a significant input to potential drop at the membrane interface, boundary potential,  $\varphi_{\rm b}$ . Two components of this electric field have a different physical nature. Diffuse part of the electrical double layer (EDL) located close to membrane surface corresponds to a surface potential,  $\varphi_s$ , and consists of hydrogen dissociated from headgroups and inorganic ions of the media. Dipole moments of lipid moieties together with associated water molecules are oriented at the membrane-water interface and create the dipole component of boundary potential,  $\phi_d$ . Generally, some ions and small charged molecules may penetrate to the polar area of the membrane and contribute to this component as well. Several experimental techniques shortly presented in the review used to control both components of  $\varphi_b$ : electrokinetic measurements sensitive to  $\varphi_s$ , technique of planar lipid membranes and Langmuir monolayers detected any changes in the total  $\varphi_b$ . Their difference reports on  $\varphi_d$  component and reflects some structure reorganization in lipid bilayers induced by various membrane active agents, especially, by multivalent cations or positively charged polypeptides (i.e. polylysine). Gouy-Chapman model of EDL supply the quantitative description of electrostatic phenomena in simple systems with inorganic ions. The analytic model for charged macromolecules adsorbed at membrane surface currently developed in our laboratory. Our previous studies considers the significant changes of dipole potential (up to 150 mV) by adsorption of  $Gd^{3+}$  and  $Be^{2+}$ cations with a high-affinity to lipid membranes, if the negatively charged phosphatidylserine (PS, CL) presents in their composition. These observation correlate with data of calorymetry and compressibility of lipid monolayers detected a lateral condensation of PS in the presence of multivalent cations. Molecular dynamic simulations visualized this phenomenon at the molecular level and show micro-cluster of PS formation by adsorbed multivalent cations and polypeptides, which participate in the lateral compressibility of lipid membrane. So, it well explain the blocking effect Gd<sup>3+</sup>on mechanosensitive channels of *E.coli* reconstituted into artificial lipid membrane composed from the mixture of PS/PC [1]. Tight coordination between neighbor PS molecules follows from MD simulations in the presence of Be<sup>2+</sup>. Experiments with artificial PS-coated silica beads or aged erythrocytes suggest that Be<sup>2+</sup>can displace Ca<sup>2+</sup> from headgroups of PS. This effect may mask them from  $Ca^{2+}$ -mediated recognition by PS-receptors that potentially prevent normal phagocytosis [2]. It seems to be significant for initial steps of membrane transformation in apoptotic cells and may results in some dangerous chronic inflammation.

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# Water polarization and asymmetric finite size of ions in electric double layer

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Electric double layer is described within a lattice statistics approach by taking into account the orientational ordering of water molecules and the asymmetry of the anion and cation size [1]. Since water is a polar molecule with its own dipole moment [2], its total dipole moment arises from the internal and external contributions, the latter modified by the cavity field of neighbouring molecules. It is shown that due to orientational ordering of the water dipoles near the charged surface the relative permittivity is locally strongly decreased [1, 2]. Analytical expressions for the space dependence of relative permittivity are derived [1, 2]. Asymmetric camel-like shape of the voltage dependence of the differential capacitance is studied within the model [1, 2].

Bikerman-Wicke-Eigen model of electric double layer [3,4] is derived as a limit case of the presented more general model of electric double layer [1]. The Wicke-Eigen equation [4] taking into account finite size of ions, was in some publications named after Bikerman who first studied the role of finite size of ions and water polarization in electric double layer properties [3]. However, cation and anion distribution functions and the corresponding volume charge density for finite size of ions were first derived by Wicke and Eigen in 1952 [4], while in the Bikerman's paper [3] they do not appear. Therefore, it seems correct to give to the model of electric double layer which takes into account the symmetric finite size of cations and anions the name Bikerman-Wicke-Eigen model and not just Bikerman model.

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#### **External field and confinement controlled topological defects**

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Topological defects (TDs) are an unavoidable consequence of continuous symmetry breaking phase transitions [1]. They appear at all scales of physical systems, including particle physics, condensed matter and cosmology. Due to their topological origin they display several universalities that are independent of the systems' microscopic details. For example, they might even explain the stability of "fundamental particles" via topological protection if fields represent a fundamental entity of nature [2]. Furthermore, by invoking curvature inhomogeneities in spacetime [3], they could explain the nature of "dark matter" and "dark energy".

It is of interest to find system where TDs are relatively easy accessible. For this purpose, liquid crystal (LC) phases [4] represent an ideal testing ground owing to their extraordinary and unique combination of optical anisotropy, fluidity and softness. Furthermore, they possess a rich variety of different phases and configurations that contain practically all qualitatively different TDs from a symmetry perspective. Consequently, LCs could be exploited as a convenient window into the fundamental behavior of TDs. In addition, TDs in LCs could be employed in diverse electro-optical applications.

In this presentation we present our studies of diverse thermodynamically stable controllable assemblies of TDs in orientationally ordered nematic LCs [4,5,6]. We show how one could manipulate their key characteristics and positions by geometry and appropriate external electric fields. We demonstrate how such configurations could be exploited for various nano-based functional devices.

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### Lipid membrane elasticity and protein-lipid interactions

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The protein-lipid interactions play an essential role in topological rearrangements of cellular membranes, vesicle traffic and signal transduction in living cells. Usually they require coordination of a wide range of proteins and associated lipids, thus complicating their investigation and experimental modeling. However, in the case of viral infection, the total number of participants can be quite limited. Fusion of enveloped viruses with the target cell membrane and budding of the virions from the host cell plasma membrane is achieved by a single or very few proteins Enveloped viruses, e.g., HIV, hepatitis, influenza virus, share certain important commonalities. All of them are wrapped in an envelope consisting of two layers: an outer lipid membrane and the inner protein layer. The inner layer is a scaffold of matrix proteins interacting both with the lipid bilayer and with the nucleocapsid of the virus. These proteins play an important role both in the release of the genetic material of a virus inside the host cell, and in production of the progeny virions in the infected cell. The protein matrix serves several purposes: protecting the integrity of the virus, enabling controlled release of the genetic material, and assembly of new virions in the infected cell. In all these processes, matrix proteins interact with lipid membranes, and the molecular mechanisms underlying these interactions are far from being fully understood. In the present work, for the case of influenza virus matrix protein M1 we have studied the role of matrix proteins and their lipid interactions both in the process of initiation of viral fusion and release of genetic material and at the last stage of the viral lifecycle, assembly and budding of progeny virions. Using combination of atomic force and confocal microscopy with fluorescent techniques and theoretical investigations we have shown that the M1 protein utilize membrane elastic properties to be an active participant at the most significant stages of viral infection.

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## Disordered proteins as intrinsically multifunctional targets

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Proteins are the basic molecules of life, and they are widely investigated to address various topics that include the fundamental functional mechanisms in biological organisms, up to advanced nanotech applications. In fact, knowledge of their behaviour is increasingly exploited in soft- and condensed-matter physics for the design of bio-inspired materials with tailored properties.

Intrinsically disordered proteins (IDPs) form a specific class of proteins that do not have a stable fold (i.e., secondary or tertiary structure, see Figure 1) throughout their amino acid sequence or in most regions, but they exist as an ensemble of rapidly inter-converting conformations. Because of their plasticity, disordered proteins act as hubs in interaction networks carrying out several functions in recognition and regulation processes, and they are often involved in diseases.



Figure 1: Example of a transient and unfolded structure of an intrinsically disordered protein.

Computational techniques are especially important to investigate IDPs, because they provide details on their structure and dynamics that cannot be captured in the experiment. A number of examples (including the studies [1-3]) show how *in silico* approaches can be combined with different *in vitro*, *in cellulo* and *in vivo* experiments for investigating IDPs, to solve biologically relevant questions that range from basic science research to applied pharmacology.

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# Raft boundary structure determines line activity and self-organization of membrane inclusions into symmetric structures

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Cell plasma membrane is laterally inhomogeneous due to formation of domains referred to as rafts. The domains are rich in sphingomyelin and cholesterol. Lipid in such domains is in liquidordered state, while the surrounding membrane is liquid-disordered. Substantial part of membrane proteins predominantly distributes into rafts, and liquid-ordered environment appears crucial for normal function of the proteins. In vivo investigation of rafts is challenging because of their small (sub-optical) size and, probably, short lifetime. Micron-sized long-living domains can be formed in model lipid membranes, which lipid composition resembles that of plasma membranes. The domains result from phase separation induced by temperature drop; they are used as a model of cellular rafts. Model domains are usually bilayer. They are more rigid (possess larger elastic moduli) than the surrounding membrane, and their bilaver is thicker than the surrounding membrane. Recently, we have shown that that coupling of monolayer domains to bilayer raft may take place by two mechanisms. Higher bending rigidity if the ordered monolayers leads to hindering of thermal shape fluctuation of the membrane in the ordered regions. Coupling of the ordered monolayer domains to bilayer rafts is favorable as it allows maximizing the area accessible for thermal fluctuations. Besides, elastic membrane deformations arise at the domain boundary in order to compensate thickness mismatch. The energy of deformations is shown to be minimal when the boundaries of monolayer domains are relatively shifted by about 2-4 nm. Specific structure of the deformations favors predominant distribution of any membrane inclusions possessing non-zero spontaneous curvature (e.g. gangliosides, amphipathic peptides, etc.) into the transitional zone between the monolayer domain boundaries. Accumulation of such inclusions at the domain boundary leads to crucial drop of the boundary line tension due to relaxation of elastic stress in the transitional zone. In turn, the drop results in alteration of equilibrium size distribution of the domain ensemble. Such mechanism allows explaining a phenomenon of line activity of some membrane components, which are capable of substantial decrease of the line tension being presented in the membrane in very low concentration (fractions of mole percent). Moreover, out model predicts the line activity for any membrane inclusion possessing non-zero spontaneous curvature. Line tension provides approximately circular shape of the domains. Thus, membrane inclusions distributing to the domain boundary become organized to symmetric circular structure. We hypothesize that such self-organization of fusion proteins is substantial for process of membrane fusion induced by enveloped viruses.

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# High resolution surface metrology using microsphere assisted interference microscopy

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In the development of new advanced and functionalized materials, high resolution characterization is a challenge due to the features often being sub-micrometer in size and involving homogeneous and/or fragile materials. The use of classical techniques such as MEB and AFM are often essential in order to check the exact details but their use is not always possible since they can be destructive or time consuming. There is therefore a need for new high resolution techniques [1]. Microsphere-assisted microscopy is just such a new technique, in which a small glass microsphere (10  $\mu$ m to 50  $\mu$ m in diameter) placed on the sample in front of the objective allows an increase in lateral resolution by a factor of up to 4 to 5 times [2]. Examples are given of resolving silicon gratings and features on a microprocessor using a x50 objective (NA = 0.55) in combination with a 24  $\mu$ m diameter microsphere. A grating period as small as 200 nm, i.e.  $\lambda/3$ , is resolved through the microsphere, giving an equivalent numerical aperture of 1.5 in air, which is not visible directly by the objective. While the theoretical resolution of the objective alone has a value of 560 nm, in practice this is closer to 850 nm in white light. The increase in resolution provided by the microsphere in this case is therefore a factor of 4.25 times.

For 3D surface metrology, while interference microscopy has nm axial resolution, the theoretical lateral resolution is limited by diffraction to around 300 nm in air. Recently, several teams succeeded in combining microsphere-assisted microscopy with interferometry to greatly improve the lateral resolution in surface roughness measurement [3-5]. Experimental results are presented of high resolution measurements fine pitch etched gratings, nanotextured stainless steel using femtosecond lasers, and Ag nanodots on Si. Other results are also presented of simulations of 2D and 3D imaging which help in the understanding of image formation.

The technique has the potential for being a powerful nanometrology technique, since it conserves all the advantages of far field imaging in terms of being non-invasive and rapid. Nonetheless, several challenges remain in order for the technique to become more widely used. For example, there is a need to better understand the imaging process using microspheres as well as reducing the measurement artifacts that are known to be present. Technological challenges also exist, such as developing new ways of supporting and adjusting the microsphere or arrays of microspheres in front of the microscope objective. These are the subjects of our future work in the field.

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### Monitoring of solid-liquid interfaces using ellipsometry

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Interface processes are of primary importance in both physical and chemical studies. Most bioprocesses in our bodies take place at solid-liquid interfaces. These systems are mainly characterized by optical methods. Besides the high sensitivity and speed optical tools like microscopy, waveguide sensing or ellipsometry [1] are capable of real time monitoring which is a key to understand the kinetics and the dynamics of the processes. Ellipsometry is a kind of interferometry in which the reference beam is "built in the system" in form of the perpendicularly polarized light. This fact is important, because it provides a high sensitivity without the requirement of a coherent source that enables a relatively easy realization of spectroscopic instrumentation. The large number of complex, phase-sensitive, spectroscopic data allows the construction of complex optical models, and the determination of numerous parameters of the investigated systems, also during real time monitoring. The application of ellipsometry in biology goes back to the '40s, but the number of application started to increase significantly in the middle of '80s (Figure 1). In this work a short summary is given on the developments of ellipsometry for solid-liquid interface characterization, with emphasis on the most recent advancements.



Figure 1: Number of articles with the words of "ellipsometry" and "bio\*" in the title, abstract or keywords.

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# Temperature-dependent Raman study of nanostructured and multifunctional materials

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Variable-temperature Raman scattering measurements are of great help in the analysis of structural, electronic and magnetic properties, as well as phase transitions of large number of materials that are in the focus of modern research in condensed matter physics. Two classes of such materials, nanomaterials and iron-based compounds, are in the scope of the present paper. Temperature-dependent Raman spectra of nanomaterials give lot of information about their thermal stability and other properties affecting the shape, shift and linewidth of characteristic Raman modes, as most of these properties (such as phase composition, nanocrystallite size distribution, strain, defects and non-stoichiometry) strongly depend on temperature [1]. The Raman results presented and analysed here are related to TiO<sub>2</sub> nanopowders (with dominant anatase [2] and brookite phase) and Zn<sub>x</sub>Cd<sub>1-x</sub>Se single layers. The influence of the antiferromagnetic order, ferromagnetism, and magnetic fluctuations on the Raman spectra of several iron-based materials is also reported. These materials can have not only superconducting but also low-dimensional magnetic properties (forming spin chains, spin ladders, spin dimers, etc.). The Raman spectra of iron-based selenides (BaFe<sub>2</sub>S<sub>3</sub> and BaFe<sub>2</sub>Se<sub>3</sub>, belonging to the family of the iron based S = 2 two-leg spin-ladder compounds [3]), layered iron oxychalcogenide BaFe<sub>2</sub>Se<sub>2</sub>O [4], and alkali-doped iron selenides (superconducting  $K_xFe_{2-\nu}Se_2$  and non-superconducting  $K_{0.8}Fe_{1.8}Co_{0.2}Se_2$  [5]) are measured and analysed in a wide temperature range. A physical model, including thermal expansion of the crystal lattice and the contribution from phonon-phonon scattering (lattice anharmonicity), is used to quantitatively analyse experimentally obtained temperature dependence of energy and linewidth of the Raman modes characteristic for investigated nanostructured and iron-based materials.

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## NanoCMOS and Small Slope Switches for the end of the Roadmap

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We are facing many challenges for future nanoelectronic devices in the next two decades dealing with power consumption, computing performance, variability and reliability. With respect to the substantial reduction of the static and dynamic power consumption of future high performance/ultra low power terascale integration logic and autonomous nanosystems, new materials and novel device architectures are mandatory for Nanoscale MOSFETs and Small Slope Switch Nanoelectronics Devices [1-4].

This paper presents the most promising solutions for the end of the roadmap using ultimate Multigate NanoCMOS and Nanowire FETs, Tunnel FETs and FeFET, and Hybrid Nanoscale Transistors such as Fe TFET, Phase Change Tunnel FET and Metal Filament MOSFET. To boost their electrical properties, these innovative device architecture will be combined with alternative materials, including ultra-thin Si-Ge-III-V/OI, 2D layers (phosphorene, transition-metal dichalcogenides, etc.), 1D semimetals, and Heterostructures using strained Si, Ge and III-V materials [5-16].

#### Acknowledgements

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# Type-II superconductors used as magnetic shields: distinguishing the effects related to geometry from those related to physics

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Based on their unique ability to carry resistanceless electric currents at cryogenic temperature, superconductors are able to act as efficient magnetic shields. The magnetic shielding phenomenon in a type-II irreversible superconductor arises from the pinning of individual flux lines (vortices) by defects or, equivalently, from high amplitude shielding current loops flowing in the sample and opposing to the external magnetic field. This behaviour is markedly in contrast with the magnetic shielding provided by high-permeability ferromagnetic materials. In this talk the difference between the magnetic shielding properties of superconductors and ferromagnets will be explained and illustrated, with the emphasis placed on how effects related to geometry can be distinguished from those related to the physical properties of the materials. The talk will be illustrated with magnetic measurement data [1,2] obtained recently on various high temperature superconducting (HTS) magnetic shields. The factors that are relevant to the design of an efficient magnetic shield for practical large scale applications will also be discussed.

In the second part of the talk, the possibilities offered by the EIT (European Institute of Innovation and Technology) KIC (Knowledge & Innovation Communities) funded project "Magnetometry network" (<u>http://magnetometry.cnrs.eu</u>) will be presented, together with scientific and training activities related to magnetometry.

Acknowledgements: We thank the EIT KIC Raw Materials through the "Magnet" project.

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## Nanostructured ZnO films for application in gas sensors

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ZnO is a material widely used in industry from decades, which goes through a scientific and technical renascence in the last few years. Zinc oxide has been recognized as one of the most important semiconductor materials for optoelectronics, solar cells, piezoelectricity, gas sensing, bio-applications etc. ZnO has been an object of intensive investigation, particularly in its low dimensional structures – thin layers with nanometer sized crystallites, nano-wires, nano-rods or nano-tubes, nano-bells and others. Nanostructured ZnO possessing interesting structural and optical properties offers challenging opportunities for innovative applications. Because of its sensitivity to different adsorbed gases, high chemical stability, amenability to doping, nontoxicity and low cost ZnO attracted much attention as gas sensor. The sensitivity of nano-grain ZnO gas elements is comparatively high because of the grain-size effect. Application of nanostructured ZnO films deposited by magnetron sputtering and electrochemical method for gas sensors is described and demonstrated.

## Memrister type gas sensors for high sensitivity sensing at low temperatures

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A sensor configuration having top-bottom Pt-electrode (TBE) and yielding Memrister sensing mechanism is described. These TBE-sensors display high sensitivity H<sub>2</sub> and NO<sub>2</sub> sensing with undoped and Cr-doped TiO<sub>2</sub> SE at RT and 200°C, respectively. The improved sensing properties are observed with a wide range of gas concentrations in contrast to the sensors fabricated with classical interdigitated electrodes (IDEs). The sensors with TBE-TiO2:Cr layers showed highest NO<sub>2</sub>-sensor responses at 200 °C with negligible drift and noise. The substitution of trivalent Cr<sup>3+</sup> (0.755 Å) within Ti<sup>4+</sup> (0.745 Å) lattice modified the electronic structure of TiO<sub>2</sub> yielding ptype semiconductor sensor response. As for H<sub>2</sub>-sensing, high sensitivity RT-detection of a few hundred ppm H<sub>2</sub> was possible without the use of any heater. These sensors consume extremely low energy during operation and are capable of being constructed as self-powered sensors. By means of impedance spectroscopic studies, sensing mechanism is predicted and the processing related influences on the sensing are correlated by means of microstructural (GDEOS, SEM/EDX and XRD) analysis. The impedance equivalent circuit modelling identified the contributions of the Ptelectrodes, sensing layer and interface between them. The gas sensing tests of TBE based sensors by covering the Pt-electrode surfaces revealed that the gas reaction beneath Pt-TE is dominating. Moreover, the interfaces between SE layer with the bottom and top Pt-electrodes contributes individually and significantly in the sensing mechanism.

# Corralling Electrons in Vanadium Oxides: Implications for Neuromorphic Computing and Electrochemical Energy Storage

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The binary vanadium oxides  $VO_2$  and  $V_2O_3$  have long been canonical examples of compounds showing pronounced electronic instabilities underpinned by the interplay of electronphonon coupling and strong electron correlation. The precise control of lattice and electronic instabilities within such materials through size control and doping has allowed us to develop thermochromic glazing ("smart windows"). In recent work, we have furthermore explored the intriguing electronic phase diagrams of low-dimensional ternary vanadium oxides with the formula  $M_x V_2 O_5$  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 "braininspired" vectors for computing. The insulating phases of these compounds are characterized by the stabilization of small polarons. The stabilization of polarons and their eventual melting to form delocalized metallic phases has interesting implications for the design of Mott field-effect transistors and memristors. The discovery of novel topochemical intercalation routes has provided access to a vast metastable phase space wherein correlation strengths and the extent of covalency can be precisely tuned. If *composition does not have to be structural destiny*, a powerful new palette becomes available for tuning material properties. I will demonstrate the application of this  $M_x V_2 O_5$ palette to two specific problems: (a) the design of cathode materials for multivalent insertion batteries; and (b) the design of photocatalysts for the water oxidation reaction.



**Figure 1:** Schematic depiction of an energy landscape with metastable polymorphs (left) and a metastable  $\zeta$ -V<sub>2</sub>O<sub>5</sub> phase allows for reversible intercalation of multivalent ions (right).

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## Theoretical description of charge transport in disordered solids: to simulate or to think?

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Disordered materials, such as amorphous organic and inorganic semiconductors, chalcogenide glasses and ionic glasses, are commercially used in electrophotography, smartphone displays, solar cells, field transistors, optical memories, light-emitting diodes, solid batteries, etc. . Charge transport properties are decisive for all these applications. Therefore, understanding the charge transport mechanisms is of vital importance for device applications of disordered materials.

Intensive study of disordered materials is driven not only by their usefulness for valuable devices, but also by the interest of researchers in fundamental properties of such systems. Theory of charge transport has been for many years confined to crystalline solids. University courses and textbooks offer theories based essentially on the long-range atomic order. The lecture at 20th ISCMP will present theoretical concepts developed for description of charge transport in solids without translational symmetry.

Theoretical research on charge transport in disordered solids is often essentially focused on computer simulations. Many deficinceies of numerical simulations will be highlighted in the lecture. Computer simulations are useful, and sometimes unavoidable to check the ideas, but computers are not yet capable to take the full responsibility for theoretical research.

# Atomic scale design, structure and stability of quantum nanowires on epitaxial interfaces

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Metal nanowires excite remarkable academic curiosity as physical systems with confined geometry, reduced dimensionality and peculiar quantum properties. They also hold special attention in contemporary nanoscale material science because of the large number of important technological applications. The exotic quntum features of the nanowires are strongly dependent on their size, shape and morphology and therefore detailed knowledge of the nanowire fine atomic structure is indispensable. In the present lecture we overview the problem of structural stability, spontaneous breakdown and complete disintegration of metal monatomic nanowires (monatomic chains) as a result of random thermal fluctuations of their atoms. We discuss in detail the nanowire rupture and its total decomposition in several cases: (i) free-standing nanowire in vacuum not affected by any external forces, (ii) homoepitaxial nanowire grown on atomically smooth crystalline surface and (iii) nanowire located on heteroepitaxial interface. Finally, we consider the breakdown of twodimensional flat nanowire consisted of several monatomic chains. We develop a general atomicscale scenario of nanowire breakdown grounded on vacancy-mediated multi-step rupture mechanism. The implemented physical model accouns for the impact of essential physical quantities on the nanowire stability including system temperature, lattice mismatch, nanowire/substrate commensurability, interface anisotropy and entropy. The atomistic simulations data reveal unexpected oscillatory behaviour of nanowire lifetime as a result of the weakening of the strength of atomic interactions between the atoms in the chain. The consecutive step-down of the attractive interatomic forces give rise to large non-monotonic variation of the nanowire lifetime depending on the nanowire rigidity, flexibility and wave-shaped atomic morphology. This phenomenon is considered as a "stick-like" to "polymer-like" transition in the nanowire atomic structure as a result of the interaction energy variation. The presented physical and computational models open up a way of new type atomic-scale design of epitaxial interfaces, giving insight into thermal stability, breakdown mechanism and fine tuning of the structural, morphological and thermodynamic properties of metal nanowires on crystalline surfaces.

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# Theoretically choosing multifunctional materials

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Multifunctional material are defined as materials which, due to their chracteristics, can perform multiple functions within a system. They can posess a particular set of parameters either naturally, or as a result of a theoretical prediction and then wise chemical synthesis.

In this paper we shall discuss the possibilities offered by a particular theoretical model (the Hubbard model) in predicting the characteristics of multifunctional materials. The paper will be based on previous results of the present author [1].

This study was performed within the project 171005 of the Ministry of Education, Science and Technological Development of Serbia.

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## Bioactive glasses: structure characteristics and bone regeneration application

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Development and optimization of Ca and P containing bioactive glasses which, due to their composition, structure and mechanical properties, are suitable for biomedical application. A study of the structure and bonding configuration of the bioactive glasses by neutron diffraction, NMR and Raman spectroscopy will be presented.

The studied system: SiO<sub>2</sub>-Na<sub>2</sub>O-CaO-P<sub>2</sub>O<sub>5</sub> with the 0-5 mol % P<sub>2</sub>O<sub>5</sub> phosphate content range were prepared by melt-quench technique. For the study of the short- and intermediate range order were performed neutron (ND) diffraction experiments. ND measurements were carried out at the 10 MW Budapest research reactor using the PSD diffractometer [1] and at the 7C2 diffractometer in LLB/Saclay [2]. Reverse Monte Carlo simulation [3] was applied to generate reliable 3-dimensional atomic configurations and to calculate the partial atomic pair correlation functions, coordination number and bond angle distributions. The glasses were analyzed using Stokes Raman spectra, measured at 514.5 nm Argon ion laser (50 mW) on Renishaw In Via-Reflex Micro-Raman spectrometer. Nuclear Magnetic Resonance experiments were recorded on the 600 MHz Varian NMR System equipped with the 3.2 MAS probe installed in the Slovenian NMR Centre in Ljubljana.

The results show well-defined first neighbor distances for the Si-O at 1.60 Å, P-O at 1.58 and 1.95 Å where the intensity of the second peak increase with the P content, Ca-O at 2.3(6) Å and Na-O at 2.25(6) Å, distributions. For several glasses, it was found that the basic network structure consists of tetrahedral SiO<sub>4</sub> and PO<sub>4</sub> units. Significant intermediate-range correlations have been revealed for the second neighbor distances, indicating a stable and well-defined network.es in the inter-tetrahedral SiO<sub>4</sub> units with  $P_2O_5$  increase, it is surprising that even 1mol % can make difference.

To test the bioactivity of the glasses, samples were treated in the Stimulated Body Fluid (SBF) for different soaking times (3h, 3days, 7days, 21 days). After three hours all P containing samples exhibited a Ca and P rich layer on their surface, which proves the bioactivity of the glasses. At the same time, on the surface of the P-free glass a silica layer was formed. The bioactive layer formed in 3h, 3d and 7d experiments is highly fractured and peels off after complete drying, while the 21d experiments provided a stable layer on the glass surface.

Details of the structural characteristics and biocompatibility will be presented.

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### Ring polymer chains in a slit geometry with mixed boundary conditions

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The behaviour of a dilute solution of phantom ideal ring polymer chains and ring polymer chains with excluded volume interactions in a good solvent confined in a slit geometry of two parallel walls with mixed boundary conditions which corresponds to the case of one repulsive and the other one inert wall is discussed. The calculation of the respective dimensionless depletion interaction potentials and the depletion forces and the monomer density profiles were performed in the framework of the massive field theory approach at fixed space dimension d<4 up to one loop order. The density – force relation in the case of phantom ideal ring polymer chains confined in a slit of two parallel walls with mixed boundary conditions is analyzed and the respective universal amplitude ratio is calculated. The obtained results indicate that ring polymer chains due to the complexity of chain topology and because of entropical reason demonstrate completely different behaviour in confined geometries than linear polymer chains. The depletion force in the case of mixed boundary conditions becomes repulsive in contrast to the case of linear polymer chains [1]. The presented results indicate the interesting and nontrivial behaviour of ring polymers in confined geometries and give possibility better to understand the complexity of physical effects arising from confinement and chain topology. The possibility of using ring polymer chains for production of new types of nano- and micro-electromechanical devices is analyzed.

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# **Topological Defects in Liquid Crystals**

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In confined liquid crystal (LC) systems, geometrical frustrations play an important role in the formation of various topological states. For example, it is well known that nematic (N) materials show unique structures in a spherical droplet or shell geometry bounded by an interface with a certain anchoring condition, because a geometrical frustration occurs in such a spherically confined state. Spherical-cap geometries, such as a N LC droplet placed on a flat solid substrate, are a little more complicated, because the N LC is now confined by two different boundary conditions.

In addition to the boundary conditions, elastic anisotropy also plays an important role. For example, spherical droplets with strong planar anchoring often exhibit the so-called 'Bipolar' state, in which the N director field has two surface point defects. On the other hand, it can be transferred into the so-called 'Axial' state with a central line defect, depending on the ratio of splay and bend elastic constants . In addition, weak twist elasticity (low twist elastic constant) allows the system to be twist-preferred. Helix formation through the spontaneous twist deformation has been well known even in N LCs of achiral molecules.

We study LC droplets in contact with glass and air for nematic, smectic A and nematic twist- bend states.







Figure: Droplets in polarizing optical microscope
# **ABSTRACTS OF ORAL PRESENTATIONS**

### ZnO films prepared by physical and chemical methods for sensors and piezoelectric applications

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In recent years ZnO nanostructures have attracted much attention due to their exceptional physical, chemical, optical, and electrical properties and their use in multifunctional applications. ZnO is used lately in piezoelectric applications in order to replace PZT which is a toxic material due to the presence of lead in its composition.

Extension of the application domain of the proposed materials can be achieved by forming ordered nanoporous structures, nanorods, nanotubes, nanospheres and thin films with controlled morphology and porosity. Hydrothermal technique (HT) is the most appropriate method to obtain such nanostructured films (as nanowires, nanorods, nanotubes). It offers a very easy control of the particle shape and size of the films, easiness to embed the dopants, combined with a low process temperature. To improve the adherence and the crystallinity of the layers (in our case Mn doped ZnO) a previous seed layer is recommended. A precise control of such seed layers can be obtained by Atomic Layer Deposition (ALD).

The aim of this work is the study of doped (with 1, 2 and 5% Mn) nanostructured ZnO films prepared by combining these two methods to obtain a performant piezoelectric material, used in MEMS systems for harvester applications.

First, we obtained the desired properties of ZnO-ALD layers studying their correlations with deposition technological parameters (as type and orientation of the substrate, deposition temperature) and the films thickness. They were very smooth, with small roughness (1-5 nm measured by AFM), which improved the adherence of the next ZnO-HT layer, grown on top of it. At the same time XRD has shown that the ALD films are crystallized in wurtzite phase which induces a high crystallinity of the upper layer.

The ZnO-HT final films deposited on ZnO-ALD layers contain a structure formed by nanorods with hexagonal cross section of 50 nm and length which varies from 30 to 300 nm. EDX and XRF showed the existence of Mn in all samples, even in those with 1% Mn. The dopant concentration influences the sample morphology (evidenced by SEM) and leads to the decrease of the grain size of the upper layer.

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#### Optical sensing of vapors and liquids using porous Bragg reflectors

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Bragg reflectors are multi-layered structures comprising alternating low and high refractive index media with quarter-wavelength optical thickness ( $nd = \lambda_c/4$ , *n*-refractive index, d – thickness,  $\lambda_c$  –operating wavelength). Owing to the phenomenon of constructive interference of multiple reflected waves a high reflectance band appears centred at  $\lambda_c$ . Because the position of reflectance band is extremely sensitive to the alterations of *n* and *d* of the constituent layers, a wavelength shift is observed when one or both parameters change due to the influence of external stimuli. Thus by appropriate selection of the reflector's building blocks and monitoring of the wavelength shift, liquids / vapors responsive structures could be prepared and utilized for optical sensing applications.

In the present study porous Bragg reflectors are investigated where the porosity is generated by three approaches. In the first one mesoporous  $Nb_2O_5$  films with low refractive index and different thicknesses are deposited on top of silica / silicon nitride Bragg stack, while in the second and third approach the same films with quarter-wavelength optical thicknesses or thin films of nanosized zeolites are implemented as low refractive index building blocks of  $Nb_2O_5$  Bragg reflectors.

Thin Nb<sub>2</sub>O<sub>5</sub> and zeolite films are prepared by sol-gel and spin-coating methods, respectively, and functional porosity is introduced in the oxide films by the method of evaporation induced selfassembly using commercially available Pluronic copolymers as soft templates. The optical and sensing properties of single films and Bragg reflectors are studied by reflectance measurements at normal light incidence prior to and after exposure to analytes (organic liquids and volatile organic compounds). Further information about the sensing mechanism is obtained from ellipsometric measurements and calculation of optical constants (refractive index and extinction coefficient) and thickness of each layer in the structure. The application of porous Bragg reflector for selective optical sensing of vapors and liquids is demonstrated and discussed.

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#### The kinetics of binding of protons with bilayer lipid membrane

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The kinetics of proton binding with bilayer lipid membrane (BLM) has been studied by measuring the changes of its capacitance and electrostatic potentials initiated by fast release of protons on the surface of the membrane. It was achieved by photolysis of "Caged-H<sup>+</sup>" - 2-methoxi-5-nitrosulphate (MNPS) bound on the surface of the membrane. The adsorption of anions of MNPS on BLM leads to change of the boundary potential measured rather by Inner Field Compensation (IFC) method developed by us earlier [1] or as the change of (-potential of liposomes measured by dynamic light scattering method. The stepwise increase of the proton concentration during illumination of BLM with bound MNPS leads to change of the capacitance of the membrane and the surface potential on the membrane/water interface measured either as a fast shift of open circuit potential measured by electrometer or as the boundary potential shift measured by IFC method. This boundary potential shift is assigned partially to decrease of the amount of the MNPS anions bound on surface of BLM due to their light induced damage, partially – to binding of liberating protons with the membrane. The shifts of the boundary potential and the membrane capacitance were depressed by increase of the concentration of buffer in the solution. The restoration of the membrane capacitance and boundary potential after the light flash took about ten seconds. The light induced changes of the membrane capacitance and surface potential were observed not only on BLM formed from phospholipids (phosphatidyl choline or phosphatidyl serine) but also on BLM formed from neutral lipid glycerolmonooleate. These results indicate that the binding of protons with the membrane leads to forming of a long lived state, involving, perhaps, binding of protons with water molecules oriented on the membrane/water interface.

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# Adsorption of Polylysines at the Surface of Lipid Membranes: Theoretical Analysis of Electrokinetic Data

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Theoretical approach is suggested to analyse electophoretic mobility of liposomes mesured at varied ratio of negatively charged (cardiolipine, CL) and neutral phospholipids (PC) in the membrane composition and at different polycation content in the suspension. Experimental data is usually presented by Smoluchovsky relation as zeta-potential values. The quantitative analysis is supposed to find principal characteristics of adsorbed polymer layer — lateral distribution and geometry of lipid-polymer clusters and their effect on the position of slipping plane and electric potential distribution close to membrane surface. Previously, we developed a theoretical model in assumption of irreversible adsorption of polylysines at the membranes composed from CL. This model allowed us to approximate data by two parameters — thickness h of polymer layer at the membrane surface and fraction,  $\beta$ , of the occupied area. In this report, we present an improved model that takes into account a number of features of the system previously unaccounted for. In particular, experimental data demonstrate the shift the point of zero zeta potential on the liposome composition and polymer chain length, which can not be explained in the framework of the previous model. In the present work we assume that during adsorption of polylysine molecules the slipping plane may shift relative to the surface of the membrane. In order to find the zeta potential, we determine the effective position of this plane by solving analytically the problem of electric potential distribution inside the polymer layer at the membrane surface. In addition, we take into account that counterions may penetrate to polymer layer and adsorb at the membrane. It allows us to explain the shift of the point of the zero potential as a result of the slipping plane shifted by adsorbed polymer. Furthermore, theoretical and experimental curves show the same dependence on the ratio CL/PC in the membranes. Increased amount of the charged lipid in the liposome composition results in the nonlinear increase of the polymer coverage  $\beta$ . Liposome becomes completely covered with the polymer at a relatively small fraction of the charged lipid in the liposome, which is in a good agreement with atomic force microscopy data. The longer macromolecules create the thicker layer at the membrane surface. Numerical characteristics and geometry of lipid-polymer clusters predicted by the model are in a good agreement with simulations of polylysine-CL systems by methods of molecular dynamics.

## Phase Transition of DMPS Monolayers studied by Molecular Dynamics and X-ray Reflectometry

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Monolayers of dimyristoylphosphatidylserine (DMPS) at the surface of electrolyte (~100 mM KCL) were constructed and analyzed by methods of molecular dynamics (MD) to compare with experimental data of X-ray reflectometry (XR). The MD method is actively used for the modeling of lipid monolayers. including research devoted to the study of the pressure-area isotherms of lipids (1-2). Constructing simulation boxes in the same way, we performed simulations in precise all-atom CHARMM36 (2) force field using GROMACS software under different area per lipid.

Analysis of the reflection curves was carried out on the assumption that the monolayer contains two sub-layers, which allowed us to reconstruct the electron density profile of the monolayer. This profile is in good agreement with the profile obtained in the MD. Moreover, the MD demonstrates that one sub-layer corresponds to the lipid tails region, and the second corresponds to the polar region that contain bound and free water molecules. According to the MD data, in the region of low surface pressure in the monolayer, a transition occurs from the state of drifting individual lipid aggregates to a two-dimensional liquid. The same phenomenon was observed in DPPC monolayers in coarse-grain MD (1). Lateral compression of DMPS monolayers reveals phase transition between liquid expanded and crystalline states with intermediate region of two states coexistence. MD visualization of the system demonstrates lipid phase transition to a crystal state as a result of hydrocarbon tails ordering, while the thickness of the polar region of DMPS remains practically unchanged. The total thickness of the monolayer increased from  $20 \pm 3$ Å to  $28 \pm 2$  Å in liquid and solid states, respectively. At the same process, hydration state of polar groups decreases at least twice. When analyzing the MD data, it turned out that the thickness of the monolayer in the liquid phase is about 25 A, in the solid 30 A. The dependence of the total potential of the system on the area on the lipid obtained from MD also qualitatively coincided with the analogous dependence obtained by the Langmuir monolayer method. The good agreement between the MD, XR and Langmuir monolayer method data allows us to correlate the Volta potential changes with certain molecular structures.

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# *In vitro* study of Porphyrins as candidate photosensitizers in Photodynamic Therapy against Cancer

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Photosensitizers (PS) are light-sensitive molecules used in Photodynamic Therapy (PDT), which is commonly applied in cancer therapeutics. These compounds generate singlet oxygen (SO) under excitation by visible light which leads to cell damage. PDT can be studied in vitro on bilayer lipid membranes (BLM) by the Intramembrane Field Compensation Method (IFC). Recently, we have studied with the help of this method, the binding and photodynamic efficiency of negatively charged Aluminum sulfonated phthalocyanines and sulfonated tetraphenyl porphyrines. In present studied 3 positively charged porphyrins: β-imidazolyl substituted study we have tetraphenylporphyrine ( $\beta$ -ImTPP) and corresponding Zn(II) ( $\beta$ -ImTPPZn) and In(III) ( $\beta$ -ImTPPIn) complexes. The adsorption of these PS on BLM was observed as a change of the boundary potential, which is proportional to the logarithm of their concentrations in water solution. Similarly to [2], the photodynamic efficiency of these porphyrins was assessed by determining the rate of damage of di-4-ANEPPS (target molecule of SO) adsorbed on BLM either on the same (cis) side with PS molecules or at opposite (trans) side. This rate was evaluated from the kinetics of change of dipole potential created by these molecules adsorbed on the surface of BLM under illumination and following restoration in the dark. The value of R was proportional to the amount of the PS molecules adsorbed on BLM. The rate of oxidation of ANEPPS molecules adsorbed at cis side  $(R_{cis})$  was almost the same than that for these molecules adsorbed on opposite (trans) side  $(R_{trans})$ . It can be explained by almost equal distribution of SO between two sides of the membrane despite it was generated by PS only on the one side. This result is in contrast with our earlier study of other PS -phthalocyanine, where R<sub>cis</sub> was less than R<sub>trans</sub> where quenching of SO by ANEPPS was more effective when they were at cis side.

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# Surface photovoltage study of GaInAsNSb layers for photovoltaic applications

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Dilute nitrides form a novel class of semiconductor alloys, which has emerged 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 [1,2], heterojunction bipolar transistors [3] and high-speed photodetectors [4].

The surface photovoltage (SPV) phenomenon is explained followed by a description of the advantages offered by the SPV amplitude and phase spectroscopy. Further, the study of the optical properties of GaInAsNSb layers carried out by SPV and photoluminescence (PL) spectroscopy is presented. The layers are nominally undoped, grown by molecular beam epitaxy on n-GaAs substrates. SPV spectra measured at room temperature clearly show a red shift of the absorption edge with respect to the absorption of the GaAs substrate. The band-gap energy determined from the SPV amplitude spectra is slightly lower than that found from the PL peak position. This may be explained by electronic transitions from the valence band to localized states near the conduction band minimum followed by thermal excitation of electrons to the continuum to contribute to the SPV. The combined analysis of the SPV amplitude and phase spectra has provided information about the photocarrier transport and the alignment of the energy bands across the structures. This way the type of the residual doping in the layers is determined and the results correspond to those obtained by Hall-effect measurements. The minority carrier diffusion length was assessed by means of the method called "constant SPV" [5]. The obtained value is in agreement with the values estimated from the Hall-effect measurements and time-resolved PL.

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### Preparation and characterization of TiO<sub>2</sub> thin films for harvesting applications and optoelectronic devices

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The present work aims to develop new and improved materials with high efficiency in solar energy harvesting and energy storage. The envisaged solar energy harvester will include a thin solar cell (< 300  $\mu$ m thick) and a dedicated storage and power stabilizing device.

Thin films of pure and V-doped  $TiO_2$  were fabricated by various techniques (sol-gel, hydrothermal synthesis and spray pyrolysis), according to the requirements of the final product. Appropriate substrates as glass, Si, Au and Pt, were used for the deposition of  $TiO_2$  thin films.

A systematic investigation of the relationship between the preparation techniques and the structural, optical and electrical properties of the thin films is presented. The crystalline structure of the samples was thoroughly characterized by XRD measurements and it was determined the anatase phase, which is more suited for applications as TCO due to a higher carrier mobility than that for rutile phase.

The morphology was studied using AFM and SEM analysis. According to these studies, the surface consists of small and compact particles, with low roughness. To confirm the presence of the V-dopant in the thin films, EDX analysis was performed.

The optical properties were studied by spectroscopic ellipsometry analysis. The results showed a nanometric dimension of thin films of tens of nanometers. The values of the refractive index at  $\lambda$ =630 nm are situated around 2.08 - 2.12 for all samples.

A MIS structure with an active layer of V-doped  $TiO_2$  was used for electrical measurements of C-V and G-V characteristics. From these measurements, electrical parameters such as doping concentration, density and energy density of deep levels, effective electron mobility, etc were estimated.

The next research directions are the development of new materials for the same function and the optimization of the deposition techniques for the integration of materials in solar cells active areas.

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# Mesoporous Ta<sub>2</sub>O<sub>5</sub> thin films as an active medium for pollution monitoring of air and water

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Ta<sub>2</sub>O<sub>5</sub> is multifunctional material that is interesting for optical applications due to its high refractive index value. The present study aims at investigation of possibility to use mesoporous Ta<sub>2</sub>O<sub>5</sub> in form of thin films as an active medium for detection of organic vapors in air and toxic ionic presence in water with optical read-out. Commercially available surfactants PE6800, PE6200 and PE6400 are used as porosity-forming agents within the thin films by utilization of soft-template preparation method. The addition of copolymer solution to tantalum sol provokes phase separation and after high temperature annealing a system of pores is generated in the spin-on thin film due to polymer decomposition and evaporation. Optical properties of the so-prepared films have been estimated using UV-VIS spectroscopy and spectral ellipsometry. The morphology of the films has been studied by Transmission Electron Microscopy (TEM) and the amorphous status of the films has been confirmed by Selected Area Electron Diffraction (SAED). By applying the Bruggeman effective medium approximation the porosity within the films have been calculated. The films have been then introduced in ambient of different organic vapors - acetone, methanol, and ethanol, etc. The condensed vapors in the films' pores modify their optical response that has been recorded. The presence of the toxic chromium and arsenic ions have been demonstrated by ellipsometrical measurements of the change of the effective refractive index of the film with raising of ionic concentration. The possibility of implementation of these films in optical structures such as Bragg reflectors to be used for sensing purposes is discussed.

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# Influence of deposition temperature on the structural and optical properties of electrochemically nanostructured ZnO films

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These works present the electrochemical deposition of ZnO nanostructured thin films on covered by SnO<sub>2</sub> glass substrates. The deposition of ZnO films at different temperatures in the range from 50°C to 80°C is performed by an electrochemical process using a three-electrode system with a saturated calomel electrode as reference electrode, in aqueous solution containing ZnCl<sub>2</sub> and KCl. The influence of the temperature on the properties of the obtained ZnO layers is investigated by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), spectrofluorometry and optical profilometry. The XRD spectra shown the polycrystalline nature of the films at all studied deposition temperatures with the presence of (100), (002), (101), (102), (110) and (103) characteristic reflexes of the ZnO. The SEM micrographs show that the ZnO films deposited at lower temperature. With a further increase in temperature to 80°C the deposited layers, consist mainly of nanorods. The influence of temperature on the transmittance and reflectance spectra and haze ratio of ZnO thin films is presented and discussed. The ZnO nanostructured layers exhibit high values of the diffuse transmission and reflection in the 400 – 900 nm spectral range; they can be applied as rear contacts of thin films solar cells thus increasing the light trapping.

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# Magnetic properties and magnetocaloric effect in low temperature ordered Tb<sub>1-x</sub>Dy<sub>x</sub>Ni<sub>2</sub> intermetallic compounds

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Unique physical properties of RNi<sub>2</sub> compounds result from the high localized magnetic moments, which are derived from the incompletely filled 4f-electron shell of lanthanide atoms. The non-magnetic state of Ni atoms in these compounds results in low magnetic ordering temperatures because the wave functions derived from the lanthanides have a small range as compared to interatomic distances, and 4f-4f interactions are weak. Due to these features, some of the RNi<sub>2</sub> compounds exhibit high magnetocaloric effect (MCE) and, therefore, show promise as ideal materials-refrigerants at low temperatures. The majority of reports on this subject are concentrated in the experimental investigations that are usually performed by heat capacity measurements with and without an applied magnetic field or by magnetic methods. In this work, the behaviour of magnetocaloric effect at both low and high magnetic-field changes has been studied experimentally of polycrystalline  $Tb_{1-x}Dy_xNi_2$  solid solutions with x = 0.25, 0.5 and 0.75. The application of direct measurements over a wide field range along with indirect methods allowed us to find high-field regularities of magnetocaloric effect in these compounds, which was estimated as the adiabatic temperature and isothermal magnetic entropy changes. Temperature dependencies of isothermal magnetic entropy change were obtained using magnetization and heat capacity measurements, while the adiabatic temperature changes were determined directly using a measuring device designed and constructed by the authors and were derived from the experimental data on the heat capacity as well. The magnetocaloric parameters obtained for the phase-transition temperature range are discussed in the framework of Landau theory for the second-order phase transitions. Precise experimental characterization of the structure and magnetic properties of the Tb<sub>1-x</sub>Dy<sub>x</sub>Ni<sub>2</sub> solid solutions was also preformed.

Keywords: A. Rare earth intermetallics; D. Magnetic properties; D. Magnetic application

#### High field pinning centers in NbTi wires and MgB<sub>2</sub> wires

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The results of a study that indicate the existence of pinning centers inside grains and between grains in NbTi wires. The transport measurements show the ranges of magnetic fields in which the individual pinning centers operate [1]. The pinning centers inside grains are activated in high magnetic fields above 6 T. Our research show the range of magnetic fields in which individual defects, dislocations, precipitates inside grains and substitutions in the crystal lattice can operate [1]. We show that dislocations form pinning centers, which most effectively anchor the vortex lattice in the range of magnetic fields from 6 to 8 T. In addition, our measurements suggest that the peak effect (increased critical current density ( $J_c$ ) near the upper critical field ( $B_{c2}$ )) could be attributed to martensitic (needle-shaped)  $\alpha'$ -Ti inclusions inside grains. We also indicate that the  $\alpha$ - Ti precipitates (between grains) with a thickness similar to the coherence length form pinning centers which work very effectively in magnetic fields from 3 to 6 T. In magnetic fields below 3 T, they act very efficiently in grain boundaries [1].

Our results show that high hot isostatic pressure (HHIP) process allows to significantly improve the structure and the critical parameters of the undoped MgB<sub>2</sub> wires. HHIP process allows to obtain small grains, more high fields pinning centers, increased homogeneity of the material and melting point of magnesium. We as first to indicate that HHIP process reduces the diameter of MgB<sub>2</sub> wire and diameter of filaments [2]. Additionally, this reduction does not change the circle shape of the wires. The HHIP process significantly reduces number and size voids allows to significantly increase the number of connections between the grains and MgB<sub>2</sub> material density. This is very important, because major problem MgB<sub>2</sub> wires are voids. It allow to obtain the highest high critical current density in the undoped MgB<sub>2</sub> wire in high magnetic fields (e.g - 4.2 K-1000 A/mm<sup>2</sup> in 8.1 T, 100 A/mm<sup>2</sup> in 13 T and at 20 K– 100 A/mm<sup>2</sup> in 5.2 T) [2]. Our research shows that reduction of the MgB<sub>2</sub> wires diameter during the annealing process is the only way allows to significantly enhancements of the structure, mechanical properties and critical parameters in undoped MgB<sub>2</sub> wires.

Our research show influence of isostatic pressure (from 0.1 MPa to 1.1 GPa), low annealing temperature of 570°C and the annealing time for the formation of high-field pinning centers in doped MgB<sub>2</sub> wires. Measurement results indicate that 1.1 GPa pressure significantly increases the density of high-field pinning centers below 20 K. In addition, research show that isostatic pressure of 0.6 GPa slightly increases the density of high-field pinning centers. Increasing the annealing time from 120 min to 210 min leads to a reduction of critical temperature ( $T_c$ ), irreversibility field ( $B_{irr}$ ), critical current density ( $J_c$ ) and upper critical field ( $B_{c2}$ ) suggesting that a long annealing time leads to a reduction of high-field pinning centers between the grains. The high pressures and low annealing temperature leads to high critical current density of 1000 A/mm<sup>2</sup> in 7.2 T and 100 A/mm<sup>2</sup> in 12.5 T at 4.2 K in MgB<sub>2</sub> wires.

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# Inter-granular effects at high magnetic fields of cuprate and iron chalcogenide superconducting materials

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The weak links effects are one of the main challenges for effective power applications of high temperature superconducting materials. Studies of these effects help for their better understanding and subsequent improvement. A comparative analysis of the inter-granular properties of cuprate (YCaBCO) and iron-based chalcogenide (FeSeTe) polycrystalline samples was carried out, by means of series of electro-transport experiments at different magnetic fields. The magnetic phase diagram of the Josephson coupling effects for the both systems was constructed. The FeSeTe compound shows very stable and superior behavior compared to YCaBCO up to the highest magnetic fields (14T) used.

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#### **Semiconducting Graphene**

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Here we consider a simple way for modification of graphene in order to open a band gap. The structural model is based on the so called buffer layer graphene that consists of a mix of sp<sup>2</sup> and sp<sup>3</sup> hybridized carbon atoms forming a corrugated layer. The buffer layer is derived for the C-Si interface in different polytypes of SiC- graphene systems. However, the formation of such buffer layer on 4H-SiC determines some lattice deformation in buffer layer graphene due to the 8 % mismatch between the (0001)Si SiC and graphene lattices. A replacement of the (0001)Si SiC by hydrogen atoms is suggested in our model thus eliminating the lattice deformation. With the help of ab initio simulations we established that the energy gap of the graphene in BLG is  $\Delta E = 1.94$  eV at a corrugation height of h =  $35.0 \pm 5.0$  pm. The numerically obtained band gap is consistent with the experimental results  $\Delta E > 0.5$  eV for a similar system. It should be noted that the energy gap opens as a result of the synergy between two effects: i) the first one being the corrugation caused by the covalently bonded carbon atoms, with a period of 250 - 260 pm; ii) the second one being the electronic effects caused by the change of hybridization of the covalently bonded carbon atoms (from sp<sup>2</sup> to sp<sup>3</sup>), and removal of p electron density from the delocalized system.



**Figure 1.** Top (upper panel) and side (lower panel) view of the periodically corrugated graphene supercell- the stick model. The bonded to  $sp^3$  hybridized carbon hydrogen atoms are colored in cyan.

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### Impact of substrate temperature on grain boundary reflection in chromium nanofilms

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The impact of substrate temperature on grain boundary reflection is studied as a function of thickness of chromium films in the range, 10-80 nm [1]. Substrate temperature happens to be one of the important and crucial deposition parameters, which regulates many physical properties of evaporated thin films. Hence, we have deposited the chromium films at four different substrate temperatures ( $T_s = 22$ , 100, 150 & 180  $^{\circ}$ C) in order to study and analyze its effect on grain boundary reflection coefficient and other electrical properties. The grain boundary reflection coefficients (R) have been calculated by estimating the resistivity data of the chromium nanofilms using Mayadas-Shatzkes model. The substrate temperature dependent resistivity of chromium films exhibits an unusual behavior.

**Keywords**: Thin chromium films, substrate temperature, grain boundary reflection coefficient, resistivity, electron mean free path.

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#### Frustated quantum magnetism: The flat-band scenario

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Frustration in magnetic and electronic systems may lead to novel quantum phases such as spin liquids or valence-bond crystals. A particularly interesting class of frustrated systems is the class of so-called flat-band systems (for a review see [1]). In such systems the frustrated geometry leads to dispersionless (flat) one-particle bands which have a strong influence on the many-body physics of strongly correlated quantum systems at hand. Thus, flat-band systems are receiving a great deal of attention right now, in particular with view of realizing new many-body phases there. In my talk I will give an overview on the low-temperature physics of flat-band Heisenberg spin systems and Hubbard electrons. Interestingly for a large variety of such strongly correlated quantum systems a set of exact many-body eigenstates can be constructed. Examples are the 1D sawtooth and kagome chains, the 2D kagome and checkerboard lattices, and the 3D pyrochlore lattice. The exact many-particle eigenstates consist of independent magnons (electrons) localized on finite areas of the lattice and become ground states for certain values of total magnetization (electron concentrations). The correlated quantum systems having localized eigenstates exhibit a highly degenerate ground-state manifold at the saturation field h<sub>sat</sub> (at a characteristic value of the chemical potential  $\mu_0$ ) for magnons (electrons). The degeneracy grows exponentially with the system size and leads to a finite residual entropy. By mapping the localized magnon (electron) degrees of freedom onto a classical hard-core lattice gas one may find explicit analytical expressions for the lowtemperature thermodynamics in the vicinity of  $h_{sat}(\mu_0)$ . Though the scenario of localized eigenstates is similar for spin and electron systems, the different statistics of spins and electrons leads to different construction rules for the localized eigenstates and, as a result, to a different hard-core lattice gas description. For electrons the scenario of localized eigenstates is related to the so-called flat-band ferromagnetism. For spin systems the localized many-body states lead to some spectacular features in strong magnetic fields, such as zero-temperature magnetization plateaus and jumps, magnetic-field driven spin-Peierls lattice instabilities, an extra peak in the specific heat at low temperatures as well as to an enhanced magnetocaloric effect. In real systems typically the ideal flat-band geometry is distorted and the above illustrate features are modified. However, for small distortions the basic low-temperature features are still present which is relevant for the experimental access to the physical properties related to the flat band.

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### A study on nucleation, growth and grain boundary reflection in thin tin nanofilms

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The present work incorporates a study on nucleation, and growth due to the changes in the nano-structural properties as a function of thickness and grain boundary reflection in tin thin nanofilms Thickness happens to be one of the important and crucial nanofilm preparative parameters which dictates majority of properties like, nano-structure, electrical, optical and morphological texture of evaporated tin nanofilms. Hence, we have selected tin nanofilms in the thickness range 20-160 nm, in order to study the thickness dependence of their nano structural and electrical properties, in the temperature range 77-450 K, in detail. All the nano films were grown in a conventional vacuum coating unit under a pressure of ~10<sup>-6</sup> Torr at room temperature of 22  $^{0}$ C, onto cleaned glass substrates. The tin film nano-structure was analyzed by Transmission Electron Microscope (TEM). The nano structural properties can be tuned to the desired level and application by the proper choice or proper combination of deposition parameters [1] and it is found to depend upon the nature of the substrate material, environment and the binding force between the substrate material and evaporated tin atoms.

Keywords: Thin tin nanofilms, structure, Microscope, grain boundary reflection.

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#### **D-D-A ternary organic solar cells**

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Because of the constant increase in electricity demand and the importance of protecting the natural environment, renewable energy sources, including photovoltaic cells, have become popular. Organic photovoltaic's (OPVis the promising technology for the low-cost energy production. One of the developed research trends is ternary mixture used as active layers, so-called ternary solar cells.

A typical active layer in bulk heterojunction (**Figure 1**) solar cell is most often made by mixing donor with an acceptor (molecules with a high-affinity electron). In the ternary organic solar cells, a typical mixture is enriched by an additional donor [1] or an additional acceptor [2].

The motivation to create ternary systems is primarily to extend the absorption spectrum and to facilitate the transport of loads.

The experimental results for three components active layer based on pyrazoloquinoline derivatives [3] and helicenes [4] will be presented as well as exordial absorption optimization model.



Figure 1: Bulk heterojunction solar cell architecture

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# Phthalimide derivative spun films for organic vapour sensing

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Thin film of the N-(3-Hydroxypropyl)phthalimide (N3HPP) molecule was deposited by spin coating [1] and studied for an application as sensing membrane for the detection of volatile organic compounds [2]. The optical properties of the N3HPP thin films were studied using UV-vis spectroscopy [3]. In addition, atomic force microscopy [4] and surface plasmon resonance [5] were also employed to characterize the deposition process of the N3HPP spun films. Sensing properties of the phthalimide derivative spun films [6] were examined using SPR measurements. The measured SPR curves were analyzed by applying a least square fitting procedure using Fresnel's reflection theory. Sensing measurement results showed a fast response and recovery times for all studied analytes. Our results can be concluded that thin films fabricated N3HPP molecules are demonstrating a good candidate material for room temperature vapor application.

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## Langmuir-Blodgett Films from Fluorescently Labelled Phospholipids Deposited on Surface Acoustic Wave Devices and Surface Plasmon Resonance Substrates

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Over the years several new effects in fluorescently labelled Langmuir monolayers or Langmuir-Blodgett (LB) monolayers deposited on solid support were discovered by us. Mostly layers from Dipalmytoyl Phosphatidyl Ethanolamine head labelled with Nitrbenzoxadiazole (DPPE-NBD) were studied. This molecule behaves exactly as the DPPE molecule which is part of the biological membranes. So it is expected that DPPE-NBD molecules can serve as an excellent matrix for incorporation of selectively reacting proteins or enzymes preserving their function. This combination can act as an active layer in a biosensor application for work in either gas or liquid environment. The newly discovered effects for this molecule can further increase the sensitivity in a possible biosensor application. The addition of the chromophore NBD head group also stabilizes the film and allows for multilayer deposition which is not possible for phospholipids.

In view of possible biosensor applications multilayer LB films were deposited on substrates which can be used to transduce the biosensor signal from the active layer. These were both Surface Acoustic Wave (SAW) devices or substrates for Surface Plasmon Resonance (SPR). Monolayers were deposited at surface pressure of 10 mN/m. Their structure was studied with Atomic Force Microscopy which reveals the phase coexistence of liquid and solid phases as well as higher bilayer height nanosized cylinders. The clear SPR response, provoked by detectable agent, is an eloquent proof of the efficiency of deposited layers. Fluorescence lifetime spectroscopy at the fluorescence maximum of 530 nm reveals complex 3-exponent decay.

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# On measuring the characteristic length of the cooperativ molecular dynamic in glass-forming liquids

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The cooperative molecular dynamics is commonly accepted to govern the physical properties of the glass-forming liquids. In the most widely accepted Adam and Gibbs theory, the cooperative scale is measured by the size of the cooperatively rearranging region, defined as the number of the molecules rearranging into anode configuration by surmounting simultaneously the individual potential barriers, independently of its environment. The length of this size forms the characteristic length of the cooperative molecular dynamics. In post Adam-Gibbs theories and methods: random first order transition (RFOT) theory, Takahara et al. method, "four-point" dynamic susceptibility theory and generalized entropy theory different methods for the measuring the characteristic length (the cooperative length, the correlation length or the dynamic heterogeneity length) has been suggested. An analysis of this methods is presented, and it is concluding that post Adam-Gibbs methods practically are equivalent and can be obtained by an extension of Adam-Gibbs theory at its molecular level, assuming the rearrangements in the cooperatively rearranging region are realize during the relaxation time, from specific dynamic units known as "beads". The molecular origin of the "fragility" of the glass-forming liquids or forming the size of the cooperatively rearranging region is discussed from the point of view of the number of configurations into the cooperatively rearranging regions.

# **ABSTRACTS OF FIRST POSTER SESSION**

# 1.1 Electrogenic transport of Na<sup>+</sup>, K<sup>+</sup> and H<sup>+</sup> ions in the cytoplasmic access channel of Na, K, ATP-ase studied by admittance measurements in model system

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The electrogenic transport of Na<sup>+</sup>, K<sup>+</sup> and H<sup>+</sup> ions by Na,K,ATPase has been studied in the model system consisting of the membrane fragments with the enzyme adsorbed on the one side of the bilayer lipid membrane. The movements of ions in the ion access channel of the Na,K,ATPase was detected by measurements of the fast change of the membrane admittance (capacitance and conductance) initiated by stepwise shift of pH. These shifts were achieved by the photoactivated release of protons from so-called "Caged-H+" - 2-methoxi-5-nitrosulphate (MNPS) bound on the surface of the membrane. The pH shift leads to change of the capacitance of membrane with Na, K, ATP-ase, but similar changes of the capacitance were observed also on BLM without Na,K,ATPase. To discriminate the electrical signals caused by Na,K,ATPase, the influence of K<sup>+</sup> and Na<sup>+</sup> ions on the capacitance changes was studied. The effects of these ions were observed only with native Na,K,ATPase and they disappeared after inhibition of Na,K,ATPase by vanadate. The effects of K<sup>+</sup> and Na<sup>+</sup> ions were explained by the model of movement and competitive binding of these ions with protons in the ion access channel at cytoplasmic side of the Na,K,ATPase. The fitting of experimental data by theoretical curves allows to determine the binding constants of Na<sup>+</sup> and K<sup>+</sup> ions and influencing on these constants of ATP and Mg<sup>2+</sup> ions. In the presence of 0.5 mM of ATP the effects of K ions on the  $\otimes$ pH-driven change of the capacitance were attenuated, which can be explained by a shift of the protein conformation to a state with low K ion affinity caused by binding of ATP to the low affinity site. The Mg ions depressed the binding of Na ions. In the case of potassium ions the Mg ions transformed the kinetics of changes of capacitance into more complex: it consisted of a fast step followed by a slow relaxation into a new steady state value within 1-2 s. These kinetics depended on pH and the concentration of K ions. The effect of Mg ions can be explained by an influence of these ions bound to the Na,K,ATPase on the binding of K ions due to modifying either the protein conformation or electrostatic fields in the ion access channel on the cytoplasmic side. Another possible explanation of Mg ions effect is modifying of electrical double layer at lipid membrane with the Na, K, ATP-ase.

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# 1.2 Dose-dependent genotoxicity of ammonia-modified graphene oxide particles in lung cancer cells

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Graphene oxide (GO), the water-soluble form of newly discovered two-dimensional (2D) graphene, have received much attention because of its attractive properties for a wide range of applications and products [1-3]. Surface modification with different functional groups can improve GO toxicity and biocompatibility for further biomedical applications [4, 5]. Here, we have evaluated genotoxicity of pure and ammonia-modified graphene oxide (GO-NH<sub>2</sub>) nanoparticles (NPs) in a human A549 lung epithelial cell line, exposed to different concentrations of the NPs (0,1, 1-, 10-, 20- and 50  $\mu$ g/ml) for 24 h. Quantification of reactive oxygen species (ROS) indicated that exposure to higher concentrations of both types of NPs resulted in enhanced ROS generation, leading to cell injury and death. Tail migration in single cell gel electrophoresis in the cells treated with 20- and 50  $\mu$ g/ml GO and GO-NH<sub>2</sub> indicated damage in the DNA strand. Cell cycle analysis showed that after treatment of A549 cells with NPs for 24h the percentage of viable cells decreased compared to the control cells. In general, ammonia modification of GO slightly increase genotoxicity in A549 cells compared to pure GO and can cause an adverse biological effect that should be taken into account for future biomedical applications.

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# **1.3 A study of room temperature vapor sensing properties** using perylenediimide thin film

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Organic thin film materials have been extensively studied in recent years, with high technological potential for application as an active layer of organic devices. In this context, perylenediimide derivatives have attracted attention due to properties as stability, easy processability, physical and chemical properties. In here, perylenediimide molecule was selected to study in the form of thin film fabricated by the Langmuir-Blodgett thin deposition technique. This LB film was characterized by Surface Plasmon Resonance technique allowing the evaluation of the material concerning the technological potential to the manufacture of organic vapor sensors. Perylenediimide LB film was exposed to acetone, benzene, dichloromethane, ethanol, chloroform, carbon tetrachloride, methanol, and toluene vapors to determine the response and recovery time, selectivity, response rate and reproducibility performance. It suggested that perylenediimide material has high sensitivity towards dichloromethane, benzene and chloroform vapors with a short response and recovery times than others.

# 1.4 Electrical measurements of a Calix[4]acid/amine alternate layer Langmuir-Blodgett thin film

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The Langmuir-Blodgett (LB) thin film deposition technique provides one of the best method to fabricate organic thin films in the nanoscale and the structure of these thin films can be controlled at the molecular level by transferring monolayers from the air-water interface onto a solid substrate. They can be utilized within optical, electrical and biological applications in many different fields. In this work, calix[4]acid and amine molecules are selected to prepare alternate layer LB film and to study the electrical characteristic of these films using I-V, C-f, tan $\delta$ -f measurements. Calix[4]acid/amine LB film demonstrates a highly non-linear I-V behaviour which obeys a Schottky conduction mechanism.

# 1.5 α-naphtol Based Monomer Langmuir-Blodgett Thin Films for Vapor Sensing Applications

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In this study, the Langmuir-Blodgett (LB) thin film fabrication and vapor sensing properties of the  $\alpha$ -naphtol based monomer is reported. In order to investigate the monolayer behaviour at the air-water interface, the isotherm ( $\pi$ -A) graph was taken with the compression speed of 30 cm<sup>2</sup> min<sup>-1</sup> at the room temperature. This graph was repeated several times to check the stability of monolayer and to determine the deposition pressure value. The monomer LB thin films were deposited onto a quartz crystal for an application of chemical sensing element as an organic vapor sensor. Quartz Crystal Microbalance (QCM) and UV-vis Spectroscopy were used to control the deposition of LB film monolayer onto a suitable substrate. Our results indicated an increasing on absorbance value (for UV-vis measurements) or on the resonance frequency shift (for QCM measurement) when the number of deposited layers increased. A study of vapor sensing properties of these LB films against volatile organic compounds (VOCs) is also studied using the time dependent kinetic measurements taken by the QCM technique.

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#### 1.6 Surface plasmon resonance assisted with bilayer phospholipid membrane

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Phospholipids (PLs) are structural units forming biological, respectively model cell membranes. They exhibit liquid crystal phase, allowing their hydrophilic polar "head" and hydrophobic "tail" to be approximated as rodlike conformations. This PL unit structure gave us reason to study their optical, in particular their plasmonic properties, using a liquid crystal approach. PL bi-layers possess very small birefringent and molecular length, thus needing very sensitive tool. An ideal candidate for that purpose is surface plasmon resonance (SPR), because it is a non-invasive method, very sensitive to changes of metal – PL interface.

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# 1.7 Influence of the Stretching Elasticity Modulus on the Thermal Shape Fluctuations of Nearly Spherical Vesicles

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The influence of the bending elasticity of a vesicle's membrane on the thermal shape fluctuations was determined by Milner and Safran [1]. Within the present work, improved model [2], including stretching elasticity of the membrane, was applied. For this aim, the study of the relation of the stretching elasticity modulus with the thermal fluctuations was done using Monte Carlo computer simulations. Stretching elasticity was introduced in the coarse grained triangulated surface model of vesicle membrane [3]. According to the above mentioned model, an ensemble of non-correlated nearly spherical vesicle membrane shapes was acquired (see Figure 1). From the simulated data, the bending and stretching elasticity moduli were determined to verify the validity of the model.



Figure 1: A shape of the vesicle's membrane, obtained via Monte Carlo coarse grain computer simulation.

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# 1.8 Influence of Gold Nanoparticles on the Elastic Properties and Phase Behaviour of Model Lipid Systems

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Despite the variety of their functions all biological membranes have similar structure. They comprise of a lipid bilayer, giving fluidity and elasticity to the membrane and embedded in it protein molecules responsible for the various cell functionality. SOPC (1-stearoyl-2-oleoyl-sn-glycero-3-phosphocholine) is a synthetic phospholipid widely used for experiments with model lipid systems.

Gold nanoparticles are non-toxic and have unique optical properties. They are known to be attractive for targeted drug- and gene delivery applications. Besides their inert nature gold nanoparticles are easily synthesised, ranging from 1 nm up to 150 nm, depending on the certain requirements. And talking further about their advantages, gold nanoparticles could be triggered to release the substances through their photophysical properties. In the current work we aimed to investigate the elastic properties and phase behaviour of SOPC membranes incorporated with small (about 3nm) hydrophobic gold nanoparticles. The influence of the nanoparticles on the mechanical properties of lipid membranes is studied by the analysing the thermal shape fluctuations of giant quasispherical vesicles. Detailed differential scanning calorimetry studies of pure SOPC and decorated with gold nanoparticles systems are performed to trace the influence of nanoparticles on the phase behaviour of the bilayer. The results obtained by examining the properties of liposomes with incorporated nanoparticles are necessary for the subsequent creation of modern devices for the diagnosis and delivery of drugs in the human body and for predicting the possible negative effects of the nanoparticles inclusion on the integrity of the cell membranes.

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# 1.9 Bending elasticity of phosphatidylcholine membranes containing archaeal lipids

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The elastic properties of biomembranes are relevant to many cellular processes [1,2]. The lipid molecules composing biological membranes are characterized by various molecular geometry and electrostatics. Therefore, variations in the lipid composition of biomembranes may result in alterations of their bending rigidity. We report here on the bending elasticity of model lipid membranes [3] containing archaeal lipids (bolalipids) [4]. Archaeal lipids denotes a class of molecules constituting the membranes of archaeal microorganisms. In some Archaea, the lipid bilayer is replaced by a monolayer. This particularity is a result of the tail fusion of two independent lipid molecules into a single molecule with two polar heads, thus producing a more rigid membrane with increased resistance to extreme environmental conditions (temperature, acidity, etc.) [5]. The bending elasticity modulus of palmitoyl-oleoyl phosphatidylcholine (POPC) bilayers containing up to 20 wt% of bolalipids was determined by analysis of the thermal shape fluctuations of nearly spherical giant unilamellar vesicles (GUVs) [6] in double distilled water. In the presence of 20 wt% of bolalipids in the bilayer we measured approximately 20 % decrease of the bending modulus of the two component bilayer compared to pure POPC bilayer in double distilled water. This finding supports the hypothesis for a probable U-shape conformation of bolalipid molecules in the membrane in the studied range of bolalipid concentration. Laurdan spectroscopy measurements of large unilamellar vesicles (LUVs, nanometers in size) provided evidences for increased lipid ordering at the glycerol level induced by the presence of 20 wt% of bolalipids in the bilayer. Further experiments will be conducted in order to probe the contribution of the vesicular membrane curvature (GUVs versus LUVs) to the conformation of bolalipids within the lipid bilayer.

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# **1.10 Structural parameters of DMPS lipid monolayer during liquid/gel phase transition: X-ray reflectometry analysis**

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Phospholipid molecules deposited on a water surface form two-dimensional film (also known as Langmuir monolayer) oriented normally to the water substrate. Under normal conditions, increase in surface pressure  $\Pi$  leads to the phase transition of monolayer from two-dimensional liquid to gel (liquid crystal) structure [1]. Theoretical models of such phase transition, including molecular dymanics (MD) calculations, still holds a number of ambiguous problems, which makes it necessary to apply methods of direct probing the structure of a monolayer.

Here we present the analysis of the structural state of dimyristoyl phosphatidylserine (DMPS) monolayer on a water substrate by means of X-ray reflectometry (XRR). The samples have been prepared by standard droplet method [2], the quantity of lipid has been varied in accordance with area-per-lipid parameter from 134 Å<sup>2</sup> to 41 Å<sup>2</sup>. Experimental measurements of XRR curves have been performed on a customized butterfly-type laboratory diffractometer [3] at radiation energy E = 8048.05 eV. Analysis of experimental data has been conducted by simultaneous use of the classical model-based approach [4] and of model-independent (free-form) approach based on the extrapolation of reflectivity asymptotic [5].

According to the model-independent electron density distributions and structural parameters of two-layer fitting model, relative thickness  $L_T$  of  $-C_{14}H_{27}$  tails sub-layer changes from  $\approx 6$  Å to  $\approx 15$  Å while keeping relative electron density  $\rho_T \approx 0.9\rho_{H2O}$ , indicating the transition from liquid to crystallic state, which corresponds with estimated area-per-lipid values. Inclination angle for  $-C_{14}H_{27}$  tails in ordered phase found to be  $\theta = 26\pm7^{\circ}$ . Meanwhile, electron density of polar heads  $\rho_{PH}$  increases from  $1.1\rho_{H2O}$  to  $1.4\rho_{H2O}$  with increase in surface pressure, indicating the reduction in hydration state (from  $\approx 20$  to  $\approx 8$  H<sub>2</sub>O molecules per each lipid molecule). Comparison of experimental electron density profiles against MD simulated profiles shows a good agreement between them, with estimated surface rms roughness  $\sigma = 3.2\pm0.5$  Å, which corresponds with predictions of capillary wave theory [6].

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# **1.11** Monomer density profiles for phantom ideal ring polymer chains in confined geometries

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Taking into consideration the well known polymer – magnet analogy developed by de Gennes [1] the calculations of the monomer density profiles for a dilute solution of phantom ideal ring polymer chains in a  $\Theta$ -solvent confined in a slit geometry of two parallel repulsive walls and for the mixed case of one repulsive and the other one inert wall were performed. Furthermore, taking into account the Derjaguin approximation [2] the monomer density profiles for phantom ideal ring polymer chains confined in a solution of big colloidal particles with different adsorbing or repelling properties were calculated. The density-force relation for the above mentioned case was analyzed and the correspondent universal amplitude ratio B was calculated. The obtained results are in good qualitative agreement with previous numerical results obtained by Monte Carlo simulations [3].

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# **1.12 CBAMINE LB films and the vapour detection of those against volatile organic compounds**

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Thin films of calix[4]resorcinarene (CBAMINE) were deposited at air-water interface by the method of Langmuir-Blodgett (LB) technique [1] onto a suitable substrate. Atomic force microscopy technique [2] and UV-visible absorption spectroscopy [3] were used to characterize its thin film properties. The results indicated that a uniform LB film monolayer from the water surface onto glass or quartz crystal substrates deposited with a transfer ratio of over 95%. Gas sensing properties and thickness of the LB thin films of CBAMINE were investigated using surface plasmon resonance technique [4]. Its vapour sensing properties were investigated for different volatile organic compounds. Reversible changes in the optical behaviour were observed and thin films of this material were highly selective for chloroform vapour with fast response and recovery times.

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#### 1.13 Reconfigurable networks of nematic topological defects

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Topological defects (TDs) are an unavoidable consequence of continuous symmetry breaking phase transitions [1]. They can be observed at all scales of physical systems ranging from particle physics to cosmology. Due to their topological origin they display several universalities that are independent of the microscopic details in the system. They can also be used to support the theory of fields being the fundamental entity in nature [2]. Therefore, it proves valuable to find systems where TDs are relatively easily accessible and liquid crystals are the ideal choice [3], since they exhibit an ideal mix of optical anisotropy, fluidity, and softness. They also possess a rich variety of different phases and configurations which contain qualitatively different TDs from a symmetry perspective. Therefore, liquid crystals can be an ideal environment to study the behaviour of TDs.

In this presentation we present our studies of thermodynamically stable controllable assemblies of TDs in orientationally ordered nematic liquid crystal [4]. We show how one could manipulate their positions and behavior by geometry and appropriate external electric fields. We demonstrate how such configurations could be used in various nano-based devices.

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# 1.14 Electroanalytical Survey of Charge Trapping in NaIO<sub>4</sub>: (PEO/PVP) Ion-Conducting Polymer Electrolyte

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Currently, the solid (in sense of no-liquids, no solvents) polymer electrolytes (SPEs) are widely applied in the field of rechargeable solid-state batteries, in polymer electronics, electrochemical devices, sensorics, etc. Among the most promising and most studied hosts for efficient SPEs, is the ion-conducting organic polymer polyethylene oxide (PEO), as well as its polymeric blends with polyvinylpyrrolidone (PVP). They possess very suitable physical properties and characteri-stics such as efficient electrical conductivity and dielectric behaviours. Moreover, their biocompatibility and good mechanical properties make them extremely interesting for advanced electrochemical sensors, biosensors and biomedical diagnostics, environmental monitoring, as well as for organic molecular electronics and mechatronics. Recently, we have investigated microstructural, mechanical, thermal, electrical and dielectric characteristics of SPEs based on PEO/PVP blends complexed with ionic compound sodium metaperiodate (NaIO<sub>4</sub>) and their nanocomposites with GO [1,2]. It is of further interest any information about possible electric charge trapping (CT) in such ion-polymer coupled systems. That is why, we have inspected the NaIO<sub>4</sub>:(PEO/PVP) SPE for the presence of CT under static electric field. In view of above mentioned practical applicability, samples of this SPE at composition PEO:PVP=70:30 wt.% and 7.5 wt.% NaIO<sub>4</sub>, were produced as stable stand-alone flexible thin films with a thickness of 110 µm. They were studied at room temperature by means of pulsed chronoamperometric technique. Our electroanalytical measurements clearly indicated that the inclusion of the ionic NaIO<sub>4</sub> molecules into the PEO/PVP network does not lead to ion CT, they only enhance the ionic conductivity of the coupled ion-polymer ion-conducting system. The results obtained were interrelated with the microstructural and other physical properties of the SPE under study.

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# 1.15 Benzyne based aryl cycloaddition and indenoannelation from a common starter

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Halo derivatives 1 (pyrazoloquinolines) and 4 (bispyrazolopyridines) in the presence of boiling quinoline and KOH gives exclusively derivatives 3, 5 and 6 containing a hetero azulene moiety [1, 2]. In terms of the application of carbon materials to electronic devices and other nano-scale materials, the ability to incorporate seven-membered rings may become a key factor [3]. Indenoannelation can be achieved by a palladium assisted coupling when bromo analogues of 1 and 4 are used. The obtained compounds can be used as effective materials in organic light emitting diodes and solar cells devices [4, 5]. Properly substituted azulenes 3, 5 and 6 are chiral compounds and can be possibly employed in circularly polarized light emitting (CPL) devices.



X = Cl, Br;  $R_2$  = Ph, leads to a seven-membered ring annelation X = Br;  $R_2$  = alkyl, aryl, leads to indenoannelation



**Figure 1:** Cycloaddition of *in situ* generated benzyne and palladium assisted indenoannelation of neighboring aryl rings.

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## 1.16 Electret and Dielectric Properties of Lyophilized Polymer Films

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Polymer electrets are one of the most important types of electrets, which are widely used both in academic research and industrial applications. The effect of trapped charges on dielectric properties of the polymer electrets is crucial for more intelligent utilization of these materials. The aim of the present paper is to investigate the lyophilization effect on the electret and dielectric properties of polymer films. The properties of one synthetic polymer (polystyrene - PS) and two biopolymers (polylactic acid - PDLA and poly  $\varepsilon$ -caprolactone - P $\varepsilon$ C) were investigated and compared.

The samples were analysed by means of dielectric relaxation spectroscopy in the range of 20 Hz - 1 MHz using QuadTech 1910 Inductance Analyzer. The frequency dependencies of the impedance magnitude, the phase angle, the dielectric permittivity and the dielectric loss were investigated.

Regarding the electret properties, the samples were charged in a conventional three-electrode corona system. Positive and negative 5 kV voltage was applied to the corona electrode and 600 V voltage with the same polarity was applied to the grid as of the corona electrode. The results show that the lyophilization increases time relaxation of the trapped charges. It was established that the samples charged in a positive corona are more stable than those charged in a negative corona.



Figure 1: Time dependences of the normalized surface potential of lyophilized PLA electrets.

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# 1.17 Calorimetric studies on tensile stress-induced crystallization of amorphous poly (ethylene terephthalate) filaments

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There are present results from high temperature uniaxial extension of amorphous poly (ethylene terephthalate) yarns. The thermal deformation experiments were carried out under isothermal conditions. Obtained experimental data illustrates the role of the applied to the filaments tensile stress on the structural changes in the studied objects. The structural changes in the processed fibers have been analyzed using differential scanning calorimetry (DSC).

**KEYWORDS**: poly (ethylene terephthalate), amorphous filaments, tensile stress, differential scanning calorimetry.



**Figure 1:** DSC curves of untreated sample and heat mechanically modified under different strain stresses at temperature of 850C (the curves are shifted vertically for clarity).

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## 1.18 Ring polymer chains with Dirichlet-Neumann boundary conditions in confined geometries

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We have investigated a dilute solution of ring polymer chains with the excluded volume interaction in a good solvent immersed in a confined geometry of two parallel walls with Dirichlet-Neumann boundary conditions (D-N b.c.) and in the solution of big colloidal particles with different adsorbing or repelling properties in respect for polymers. Taking into account the Derjaguin approximation [1] we investigated two cases: a) mesoscopic spherical colloidal particle near the wall; b) two big spherical colloidal particles. We considered dilute polymer solution in equilibrium contact with the equivalent solution in the reservoir outside the slit which allows exchange of polymer coils between the slit and the reservoir. Besides, we follow the thermodynamic description of the problem as it was given in [2, 3]. Taking into account the polymer-magnet analogy developed by de Gennes [4] we performed calculations for the dimensionless depletion interaction potential and the depletion force in the framework of the massive field theory approach at fixed space dimensions d=3 up to one-loop order for the above mentioned cases. The obtained results for a dilute solution of ring polymer chains with the excluded volume interaction in a good solvent indicate that the depletion force in the case of D-N b.c. becomes repulsive in contrast to the case of linear polymer chains (see [3]) and gives some additional insight in comparison to Gaussian model of phantom ideal ring polymer chains (see [5]) and is in agreement with the scaling predictions proposed by de Gennes some time ago [6].

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# 1.19 Phase diagrams of Heisenberg chains with three-spin exchange couplings and different composite spins in the unit cell

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The Heisenberg spin models with additional frustrating three-spin exchange interactions-naturally arising, for example, in the strong-coupling expansion of the electron Hubbard model as well as in various effective spin Hamiltonians--can stabilize exotic spin phases [1-3] which are not typical for the Heisenberg models on frustrated lattices and/or with extra biquadratic exchange terms. The reason for this peculiarity is hidden in some special features of the isotropic three-spin exchange interaction such as the promotion of collinear classical spin configurations as well as the enhanced tendency towards clustering of the quantum spins on the shortest exchange bonds. Thus, in systems with integer and half-integer composite spins in the unit cell one might expect completely different quantum phase diagrams. In this work, we are studying this phenomenon by comparing the quantum phase diagrams of two Heisenberg chains with two different pairs of alternating site spins  $S_{1n}$  and  $S_{2n}$  [  $(S_{1n}, S_{2n}) = (1, 1/2)$  and (3/2, 1/2)] and an additional three-site interaction  $V_3 = (S_{1 2 n}, S_{2 2n-1})(S_{1 2 n}, S_{2 2n+1}) + h.c.$  Apart from various magnetic phases, in the system with a half-integer composite spin in the unit cell  $S_{1n}+S_2$  $_{n}$  =3/2 the interaction V<sub>3</sub> stabilizes two specific non-magnetic states, i.e., a critical spin-liquid phase with the central charge c=2 and a nematic-like phase with pronounced nematic short-range fluctuations. In the other case with integer composite spin in the unit cell  $S_{1 n} + S_{2 n} = 2$ , the above non-magnetic phases are replaced by a doubly-degenerate gapped spin-liquid phase. In the latter case the system describes a crossover between the spin-1 and spin-2 Haldane-type states.

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# 1.20 Model parameters and the spin trimer system A<sub>3</sub>Cu<sub>3</sub>(PO<sub>4</sub>)<sub>4</sub> (A = Ca, Sr, Pb)

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Molecular nanomagnets enjoy great interest on both theoretical and experimental sides [1,2]. They have unique magnetic properties suitable for practical purposes in addition to being promising candidates for studying the interplay of quantum and classical worlds. The antiferromagnetic linear trimers Ca<sub>3</sub>CuNi<sub>2</sub>(PO<sub>4</sub>)<sub>4</sub>, Ca<sub>3</sub>Cu<sub>2</sub>X(PO<sub>4</sub>)<sub>4</sub> with X = Ni, Mg and A<sub>3</sub>Cu<sub>3</sub>(PO<sub>4</sub>)<sub>4</sub> (A=Ca, Sr, Pb) [3–6] stand as ideal tools for testing and comparing different microscopic spin Hamiltonians involving distinct physical parameters.

In this work we discuss in details the relevant parameters [7] entering in the Hamiltonian for studying the magnetic properties of the trimer molecular magnets  $A_3Cu_3(PO_4)_4$ , with A = Ca, Sr, Pb. We focus on their relation to the conventional exchange and single-ion anisotropy parameters. A comparison between the calculated values for the linear copper trimers  $A_3Cu_3(PO_4)_4$  (A=Ca, Sr, Pb) and the Heisenberg nearest and next-nearest couplings reported in Ref. [6] are presented.

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# 1.21 Interaction of solitons with a qubit in an anisotropic Heisenberg spin chain

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The interaction between soliton, propagating in a magnetic chain, with a qubit is studied. The spin chain is described by the Heisenberg model in a nearest neighbour approximation with anisotropy and external magnetic field. The quantum bit (qubit) is modelled by a two level quantum system. The equation for the evolution of the qubit is obtained. The role of the parameters of the soliton for the quantum bit dynamics is investigated. The results are analysed using a geometrical representation for the qubit as a Bloch sphere.

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### 1.22 Synchronization in fluctuating networks with delay interactions

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The presence of delay in the interaction systems is an important problem in many real-life systems such as communication networks, neural systems or social networks. Of special interest is the study of networks with changing topology that might elucidate some important behaviours in different systems such as continuous changing neural networks due to the synaptic plasticity or real social networks. In the present communication we study the generic properties of directed delay-coupled networks, which topology changes with time and make comments on the role of the hierarchical organization regarding synchronization properties.

In a previous publication [1] we numerically studied synchronization properties of delaycoupled networks with a time-varying topology. We considered an interaction network of coupled chaotic maps with a single coupling delay Td, with a topology fluctuating among an ensemble of Small-World networks, with a characteristic time-scale Tn. We found that random network switching may enhance the stability of synchronized states, depending on the interplay between the time-scale of the delayed interactions Td and that of the network fluctuations Tn.

In this communication we consider an interaction network of coupled chaotic Bernoulli maps in a fluctuating topology directed small-world network with delay, where the third timescale is the internal time scale of the nodes Tin. When the network fluctuations are faster than the coupling delay and the internal time scale, Tn<<Tin; Td, the synchronized state can be stabilized by the fluctuations. As the network time scale Tn increases, the synchronized state becomes unstable when Tn is similar to Td. Synchronization is more probable as the network time scale increases further. However, in the slow network regime, Tn>>Td>>Td>>Tin, the long-term dynamics is desynchronized whenever the probability of reaching a non-synchronizing network is finite. In the intermediate regime the system shows a sensitive dependence on the ratio of time scales, and specific topologies, reproduced as well by numerical simulations.

These results have been complemented with analytical results in the linearized limit, where by using the Master Stability Function [2] on a network of alternating topology [3], we expressed the effective adjacency matrix in terms of the three time scales. We showed that when the network fluctuations are much faster than the internal time scale and the coupling delay,  $Tn \ll Tin$ ; Td, the effective network topology is the arithmetic mean, while in the opposite case,  $Tin \ll Tn = Td$ , the effective topology is the geometric mean over the different topologies.

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# 1.23 Entropy and Specific Heat of a Critical Quantum System with Long-range Interaction

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A quantum spherical model [1] with a long-range interaction controlled by a parameter  $\sigma$ ,  $0 < \sigma \le 2$  [2], is considered at the upper critical dimension  $d = 3\sigma/2$  in the quantum critical region. The problem of finding the free energy involves the solution of a transcendental equation which can be solved using the Lambert W-function [3]. The free energy, the entropy and the specific heat are derived in terms of the Lambert W-function. For systems in real physical dimensions (chains, thin layers and three-dimensional systems) the exact results obtained in terms of the Lambert W-function ones, in terms of the natural logarithm, are compared. It can be concluded that for a class of quantum models in the upper critical dimension the Lambert W-function is a very effective tool for an exact computation of low-temperature critical properties, especially in a broader neighbourhood of the quantum critical point.

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## 1.24 Soliton-impurity interaction in two coupled ferromagnetic chains

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The propagation of soliton excitations in a system of two magnetic chains with impurities in the on-site anisotropy is studied. The inhomogenous chains coupled through ferromagnetic interaction between the opposite spins are described by a Heisenberg model in nearest neighbour approximation. The presence of the impurities leads to linear and nonlinear perturbing terms in the evolutionary equations. We investigated numerically the influence of the soliton parameters, the interchain coupling and the defect strength on the soliton dynamics. The conditions of perfect soliton switching are obtained.

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## **1.25 Quantum-optical analogies**

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In the past decade some of the very well-known techniques from coherent quantum control of atoms and molecules found analogues in the realm of optical physics. The quantum analogies provide a tool for simulations of quantum systems and give us possibility to investigate problems which are ordinary not so easy to be experimentally realized. Thanks to this transfer of ideas between quantum mechanics and optics, some optical devices can be improved and new effects can be considered as useful. Techniques for manipulation of light signals were theoretically investigated in the collaboration with Department of Physics at Sofia University, Laboratoire Interdisciplinaire Carnot de Bourgogne, and Laboratory LMOPS at Université de Lorraine and Centrale Supélec [1-3]. The evolution of the light in the proposed devices is considered to be adiabatic. An important feature of the adiabatic light transfer processes is their robustness with respect to the system design parameters. As a consequence, the spectral bandwidth is increased.

The development of a new method for manipulation of light polarization with optimal efficiency is a subject of investigation of high importance. In our work we will report the recent results on the experimental proof-of-principal of a quantum – optical analogy [4, 5] for development of robust methodology based on the usage of commercially available optical elements.

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## **1.26** Comparative statistical analysis of Bulgarian red wines on the base of optical and chemical characteristics

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Wine samples were studied – different in variety of grape, region, year of production and methods of production in accordance with 14 optical and chemical parameters as follows: color characteristics in SIE Lab colorimetric system and connected with them quality characteristics of wine – color intensity, brilliance of red, chroma, saturation, saturation and nuance of color, optical density at different wavelength in visible region and chemical parameters – antioxidant activity by using DPPH and ABTS methods, content of anthocyanins. The goals of this study were:

- Conducting a Correlation Analysis to find the inner relation between the studied parameters;
- Reducing their total number of parameters uniting the correlated ones in new factors on the base of Factor Analysis;
- Comparison of tested wine samples based on their difference and similarity using Cluster Analysis;
- Determining the parameters with the strongest influence on the distribution of wine in the clusters.

The number of studied indices were reduced to 3 factors by Factor Analysis using Principle Component Analysis (PCA), which explained 82,8% of the entire variation. The first factor contained chemical parameters and optical density coefficients, which were connected with the pointed chemical components and color parameters. The second one was connected with the quality characteristics of wine, which were important for consumers. The third factor was related with the optical density values for the red part of visible region.

The hierarchical cluster analysis divided the samples into three main clusters presented graphically by a dendrogram. The first one consisted of three subclasses: the first one - red wines with predominant content of Merlot mainly from the region in southern Bulgaria; the second one - red wines with a predominant content of Cabernet Sauvignon from Stara Zagora region; the third one - combined samples of different varieties of wine originating from the Thracian lowland. The third cluster combined wines of different varieties which were produced in a same year and from a same region (Harmanli, Svilengrad). There was a great heterogeneity in the samples of the second cluster, consisting of 12 samples - 6 of which are from the South region of Bulgaria, 2 samples of foreign wines and 4 samples - from different regions of the country.

It could be concluded that the optical parameters and related chemical indicators are more decisive for the division of wines based on the region of production than on the basis of the predominant grape variety.

# 1.27 Study of aged polymer bulk heterojunction solar cells by impedance spectroscopy

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Polymer bulk heterojunction solar cells have attracted great interest because of their potential to be realizable on flexible substrates by relatively low cost technology. However the poor device stability remains a key issue for this technology to become competitive on the market. In order to avoid fast degradation polymer solar cells are typically prepared in inert environment and encapsulated afterwards. In this work we investigate aged polymer solar cells by means of impedance spectroscopy in order to reveal the mechanisms of aging. The studied devices were prepared in ambient environment and are of the type glass/ITO/PEDOT:PSS/active layer/Al, where the active layer represents a bulk heterojunction formed either by polymer PCDTBT or by PTB7 in combination with fullerene derivative PCBM. The impedance measurements were performed in the dark and under one sun illumination at short-circuit conditions and as a function of applied bias.

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## 1.28 Al -doped ZnO for flexible polymer dispersed liquid crystal devices

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The era of flexible optoelectronics demands developing of variety of wearable and bendable structures, foldable touch screens, paper-like displays, and curved and flexible solid-state lighting devices [1]. In this paper we demonstrate the application of Al doped ZnO layers, as transparent conductive electrodes in flexible polymer dispersed liquid crystal (PDLC) devices. Al -doped ZnO films were fabricated by ALD technique, on a thin Al2O3 buffer layer covered PETand PEN by low temperature (100 °C) process as well as on mica substrates. Optical, electrical properties and bending ability were measured and discussed. The sheet resistance values remain unchanged over 1000 bending cycles. Based on obtained characteristics, flexible polymer dispersed liquid crystal (PDLC) devices are fabricated and characterized. The measured transmittance dependence on the driving voltage and response time shownthat the ZnO:Al possess great potential for the next generation ITO-free electrodes for flexible devices.



Figure 1:Optical transmittance of ALD ZnO and ZnO:Al films on flexible substrates

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# 1.29 Theoretical Study on Some Plasma Parameters and Thermophysical Properties of Gas-discharge Plasma in Various Gas Mixtures Using New Methods

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Nowadays, plasmas find applications in various fields of material science. Plasma sources and technologies are inseparable part of various devices for controllable synthesis (plasmaenhanced, -assisted, -enabled, -supported, -based), functionalization (in-situ and post-treatment methods) and characterisation (Laser Induced Plasma Spectroscopy) of matter at nano and atomic scale level for advanced applications. Plasma diagnostics, i. e. determination of basic plasma parameters, such as gas and electron temperatures, electron and ion densities, etc., as one of the main and relevant problems in plasma physics, is an emerging field of material synthesis, modification and characterization. Characteristic constants for heavy-particle interaction depend on gas temperature, while electron temperature and density determine characteristic constants for electron-heavy particle collisions. Theoretical determination of spatial distribution of gas temperature with analytically or numerically solving the steady-state heat conduction equation proves to be quite simple and effective method in comparison with the definitely imprecise experimental methods. Thermophysical properties of gases and gas mixtures are important parameters for solving the respective partial differential equations. Scientific and industrial plasma devices, gas-discharge lasers inclusive, often comprise multicomponent gas mixtures instead of pure gases. Due to the far-too complex character of the Wassiljewa's equation, a new simple method based on iterative application of the empirical method of Brokaw for binary gas systems is proposed and applied for the thermal conductivity determination for multicomponent gas mixtures of our interest. A comparison between thermal conductivity values obtained through Wassiljewa equation and the new method manifests the applicability of the latter one. Moreover, the new method could be used in the presence of molecules rendering also an account of their dissociation. Assuming that gas temperature varies only in the radial direction and using the calculated thermal conductivities, an analytical solution of the steady-state heat conduction equation is also found for uniform and nonuniform power input in various discharge tube constructions. Temporal and radial distribution of electron temperature  $T_e(r, t)$  is also determined for the first time through numerically solving the nonstationary heat conduction equation for electron gas for nanosecond pulsed longitudinal discharge used for excitation of two perspective high-power gas-discharge lasers. For that purpose the parameters of the nonstationary heat conduction equation for electrons, namely thermal conductivity and specific heat capacity of the electron gas, are determined for Maxwellian and Druyvesteyn electron energy distribution functions and 2D(r, t) numerical model is developed, in order to solve the equation.

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# **1.30 Polymer (PEO)-Liquid Crystal (LC E8) Composites:** The Effect from the LC Inclusion

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Polymer-based complexes composed of poly(ethylene oxide) (PEO) and liquid crystal (LC) E8, at weight percentage ranging from 10 to 50 %, were studied. Such flexible organic composites are of interest for practical applications in rechargeable mini-batteries, organic electronics and mechatronics [1]. Thin (100–150  $\mu$ m) films of these mixed soft-solid materials were structurally characterized by X-ray diffraction (XRD) and X-ray photo-electron spectroscopy (XPS), as well as by UV-Visible optical spectroscopy (electronic absorption spectra). The results obtained by our analyses indicate that a molecular polymer-LC coordination complex is formed by inclusion of E8 LC molecules at certain concentration level. By that, the structural rearrangement of PEO polymer network occurs through interactions between PEO oxygen atoms and LC molecules. By such conformation of PEO, the interfacial polymer-LC interaction plays a significant role. The results reported here will be of interest for engineering of multifunctional polymer-LC flexible composite systems. The produced PEO/E8 material could be a platform for advanced polymer-LC materials, for use in polymer solid-state ion-conducting electrical, electro-optic, optoelectronic, electrochromic and electrochemical devices.

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## **1.31 Exact results for the energy spectrum of the Jaynes-Cummings model** interacting with a spin chain

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We study the spectral properties of the XY spin chain when one of the spins is interacting with a quantized electromagnetic field. The total number of excitons (accounting for the number of photons and the sum of the projection of magnetic moments in the z direction) is a conserved quantity trough the evolution of the system, thus it commutates with the system's Hamiltonian. In the present work, we discuss the behaviour of the energy spectrum and the total number of excitons for different number of spins and photons.



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# **ABSTRACTS OF SECOND POSTER SESSION**

## 2.1 Investigation of Resistive Switching in SiO<sub>2</sub> Layers with Si Nanocrystals

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Among the technologies proposed to develop the next generation of nonvolatile memories resistive random access memories have attracted significant attention due to their simple structure, high switching speed, low operating voltage and potential scalability beyond 10 nm feature size. These memories are reversibly switched between a high and low resistance state by DC voltages or voltage pulses and the resistance changes are used to store information. Large number of metal-oxide-metal structures with metal oxides compatible with complementary metal-oxide-semiconductor (CMOS) technology have been studied for memory switching properties, in particular SiO<sub>2</sub> layers that are fully CMOS compatible. A switching mechanism based on competing field-driven formation and current-driven destruction of filamentary conductive pathways has been suggested in homogeneous SiO<sub>2</sub> films.

In this study, thin films from  $SiO_x$  (x = 1.3) with thickness of 25 nm were deposited on n-Si crystalline substrates and annealed for 60 min at 1000°C in a nitrogen atmosphere in order to grow silicon nanocrystals in a SiO<sub>2</sub> matrix. The samples were provided with top and bottom contacts from evaporated aluminum. Current-voltage (I-V) characteristics were measured by applying positive voltage to the top contact of more than 10 samples. Switching behavior was observed at voltages in the range 4.0-7.0 V and the current increased with up to four orders of magnitude. In a part of the samples unipolar I-V characteristics with the reset voltage larger than the set voltage has been observed. Filaments formation facilitated by the existence of Si nanocrystals is considered as responsible for the observed resistive switching.

# 2.2 Ethanol Adsorption in TiO<sub>2</sub> Nanotubes Anodically Grown on Ti<sub>6</sub>Al<sub>4</sub>V Alloy Substrates

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Titanium dioxide (TiO<sub>2</sub>) nanotubes have high specific surface area, ion-exchangeable ability, and photocatalytic properties. Therefore they are very actively investigated for application in the biomedical field but also for various other potential applications as catalysts, chemical sensors, hydrogen generators, corrosion resistant and electro chromic materials, in solar cells, etc. Normally the resistance changes are measured when investigating the nanotubes' sensing properties. On the other hand, research and development in the optical sensor field is also active being motivated by the expectation that optical sensors have significant advantages compared to conventional sensor types, such as greater sensitivity, electrical passiveness, freedom from electromagnetic interference etc.

In this study, the optical response to ethanol vapours of highly ordered, as-prepared and annealed at 450°C, TiO<sub>2</sub> nanotube arrays is investigated at room temperature. The anodic oxidation method is applied for the preparation of nanotube arrays of four different internal diameters and wall thicknesses on Ti<sub>6</sub>Al<sub>4</sub>V alloy substrates by adjusting the oxidation time. The morphology of the sample surfaces is characterized by field emission scanning electron microscopy. The micrographs of both as-prepared and annealed samples reveal presence of nanotube arrays with diameter of around 60, 65, 80 and 120 nm uniformly distributed over the alloy surface. It is found that the optical response of the as-prepared (amorphous) nanotube arrays increases with decreasing nanotube size while in the annealed sample an opposite size dependence is observed. The dependence in the as-prepared samples can be related to the higher surface-to-volume ratio in the films with the lower diameter. The X-ray diffraction measurements performed on the annealed samples show presence of both rutile and anatase crystalline phases. The size dependence of the optical response in those samples is discussed taking into account the obtained Raman scattering results which indicate that the amount of the anatase phase increases with the nanotube size.

# 2.3 Two dimensional transition metals nanosheet for nitric oxide: A DFT study

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Due to the tremendous application of transition metal group, we have calculated the catalytic oxidation of Nitric Oxide (NO) to Nitric Dioxide (NO<sub>2</sub>) to improve air quality of environment. In this case, density functional theory (DFT) calculation using PBE functional has been introduced to check the adsorption process. We have also done structure, vibrational and electronic proper-ties of adsorbed NO, NO<sub>2</sub> and NO<sub>3</sub> on the surface of Pt nanosheet. We also check the adsorption with and without implement of the Vander waals interaction. Our results show that the charge transfers from the gas indicate the strong electron acceptor and binding energy on the surface. These studies provide an excellent new catalyst for reducing air pollution.



**Figure 1:** Figure illustrating the geometric of structure with side and top view and dynamic stability of the nanosheet.

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# 2.4 Charge transport mechanism in Vanadium doped TiO<sub>2</sub> sol-gel films

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Titanium oxide thin films could be an interesting option for long-lasting gas sensors due to their high chemical stability at elevated temperatures. Another attractive application is as transparent conductive oxide (TCO) films in optoelectronic devices. However, pure  $TiO_2$  is known for its high resistivity which is a real disadvantage in electronic applications. Doping the titania matrix with different transition metals can represent a path to decrease the electrical resistivity.

Here we report results on the study of Vanadium doped (0.03 at.% and 1.2 at.%) multilayered  $TiO_2$  films deposited on p-type Si substrates by the sol-gel method. At the  $TiO_2$ :V-Si interface a heterojunction of (n) $TiO_2$ :V-(p)Si is formed. For the electrical measurements, Metal-Insulator-Silicon (MIS) structures with the doped  $TiO_2$  films were prepared by vacuum evaporation of Al contacts. The current–voltage (I-V) characteristics of these MIS structures, taken at different temperatures, were analyzed to draw some conclusions regarding the charge carriers transport mechanism.

It has been established that the current asymmetry in these (n)TiO<sub>2</sub>:V-(p)Si heterojunctions is in the range of  $10^4$ -  $10^5$ . Under the forward bias above 3 V, the current follows the  $I \sim V^n$  dependence, where *n* values are in the 3.6 – 5.7 range indicating that the forward current is space charge limited current via deep levels with different energies in the TiO<sub>2</sub> energy gap. The temperature dependence of I-V curves has revealed that the current in the (n)TiO<sub>2</sub>:V films is predominantly carried out by inter-trap tunneling via acceptor deep levels in the (n)TiO<sub>2</sub>:V energy gap with concentration in the range of  $10^{19}$ -  $10^{20}$  cm<sup>-3</sup>. These concentrations are close to the concentration of V atoms ( $3.52 \times 10^{20}$  cm<sup>-3</sup>) incorporated in sol-gel TiO<sub>2</sub> films. This observation points out to the existence of strong Vanadium donor compensation in these n-type TiO<sub>2</sub>:V sol-gel films.

## 2.5 Sol-gel grown bare, Ni- and Li/Ni-doped ZnO thin films for gas sensor applications

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The study presents the preparation and characterization of Ni- and Li/Ni-doped zinc oxide (ZnO) thin films with properties suitable for gas sensor applications. For preparing the samples the sol-gel method, combined with dip coating, was used. Hence, bare, Ni- and Li/Ni-doped ZnO layers were deposited on quartz resonators and their properties were investigated.

Characterization of the films was carried out by various techniques. The surface analysis was performed using scanning electron microscopy (SEM), coupled with energy dispersive X-ray (EDX) analysis. As the surface properties are the most important for the gas sensing of the films, X-ray photoelectron spectroscopy (XPS) was also applied. The structure of the films was studied by X-ray diffraction (XRD), Raman and FTIR spectroscopy, while their thickness was determined by ellipsometry.

The ZnO and doped ZnO films of various thicknesses were deposited on quartz resonators and the quartz crystal microbalance (QCM) method was used for gas sensing, which is a highly sensitive method and is able to detect changes in the molecular range. Prototype QCM sensors with pristine and doped ZnO gas-sensitive films were tested for sensing NO<sub>2</sub> in the range between 10 ppm and 5000 ppm. On the basis of registered frequency change, the adsorbed mass for each concentration was calculated.

The films showed good gas sensitivity and fast reaction at room temperature. According to the results, the described fast, simple and cost-effective technology could be implemented for producing ZnO-based gas sensors working at room temperature and capable to register low concentrations  $NO_2$  in the environment in real time. Such sensors are also suitable for application in energy-effective portable equipment for on-line monitoring.

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## 2.6 Room Temperature Sensitivity of ZnSe Nanolayers to Ethanol Vapours

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Zinc selenide is an important electronic and optoelectronic material and finds applications in light emitting diodes, infrared laser gain medium, X-ray, gamma ray and UV detectors, optical windows, lenses, mirrors, etc. However the reports on the gas sensing properties of ZnSe are rather limited, which could be due to the fact that the sensing performance of ZnSe at room temperature is not good while its decomposition starts at around 200 °C, some oxidation occurs and therefore ZnSe could not be applied for chemical detection at high temperatures.

Thin nanostructured semiconductors are actively studied for gas sensor applications since in such layers the sensing surface is significantly larger than the geometric one. In this study ZnSe nanolayers having thickness of 45 nm, 100 nm and 150 nm were prepared by thermal evaporation of ZnSe powder in high vacuum. The layers were deposited on Corning 7059 glass substrates maintained at room temperature. Previous complex investigations had revealed that the films are porous (volume fraction of voids  $\sim 0.17$  in all films), they consist of randomly oriented crystalline ZnSe grains and an amorphous phase had been detected in the layers with thickness  $\leq 100$  nm. Structural relaxation with the time had been observed accompanied by a surface roughness increase. These results gave us motivation to investigate the layer's response to ethanol and acetone vapors at room temperature by measuring the changes of the electrical current through the layers in darkness at room temperature; planar Ohmic-like indium contacts on the top surface were used. The measurements were carried out under a closed, full of atmospheric air glass test chamber with a volume of 1.5 L in which vapors ware produced by evaporating 100-500 µL of liquid ethanol/acetone and homogeneously distributed inside the chamber during the measurement. No appreciable sensitivity to acetone vapours has been detected. The experiments on exposure to ethanol vapours have shown that at a given ethanol vapor concentration the layer's sensitivity increases with decreasing thickness. The sensitivity of the 45 nm layer has displayed an exponential increase within 4 orders of magnitude with increasing concentration of ethanol vapors.

# 2.7 Zeolites from fly ash embedded in thin niobium oxide matrix for optical sensing applications

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Thermal Power Plants (TPP) supplied by coal generate solid residues the landfilling of which is of severe ecological risk because of the leaching and penetration of variety of harmful components into the soil and underground waters. Recently, coal ash is considered as an abundant resource of valuable raw materials instead of waste. Coal ash allows to be converted into zeolite-like materials by alkaline treatment due to its predominant aluminosilicate macro composition.

In this study, zeolite samples were prepared by long-term alkaline atmospheric conversion of coal ash collected from the electrostatic precipitators in TPP "AES Galabovo" supplied by lignite coal from the "Maritza East" basin. The fly ash zeolites (FAZ) were obtained at alkaline activator (NaOH) to fly ash ratios of 0.5 and 0.6. Using SEM and XRD both samples were characterized and identified as Na-X zeolite phase. The specific surface and porosity of the samples were studied by N<sub>2</sub> adsorption/desorption studies at cryogenic temperatures. FAZ obtained at stronger concentration of the alkaline activator were characterized with higher specific surface value (S<sub>BET</sub>=284 m<sup>2</sup>/g). Both samples posses a mixed micro-mesoporous structure as reveal by their experimental adsorption / desorption isotherms.

Thin films consisting of sol-gel Nb<sub>2</sub>O<sub>5</sub> matrix doped with fly ash zeolites in different volume fractions were deposited by the method of spin-coating. The surface morphology and structure of the films were studied by electron microscopy (SEM and TEM) and Selected Area Electron Diffraction, respectively, while the surface roughness was determined from 3D optical profiler measurements. Optical constants (refractive index and extinction coefficient) along with thickness of the films were calculated using previously developed procedure comprising two steps nonlinear minimization of the discrepancies between measured and calculated reflectance spectra of films deposited on silicon substrates. The calculated dispersion curves were further used for determination of free volume fraction in the samples as a function of doping level.

Vapor sensing ability of fly ash zeolites was tested by measuring reflectance spectra of the films prior to and after exposure to probe molecule (acetone vapors were selected in our case). An increase of sensitivity with doping level was obtained. Further, the possibility of using the samples for detecting heavy metal ions in water was explored by calculating optical constants and thickness of the films before and after exposure to metal ions (Cu(II), Cr(VI), Pb(II), etc) using ellipsometric measurements in water. The application of zeolites from fly ash for optical sensing was demonstrated and discussed.

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# **2.8** Leakage currents in Al<sub>2</sub>O<sub>3</sub>/HfO<sub>2</sub> multilayer high-*k* stacks and their modification by post-deposition annealing steps

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Leakage currents of  $Al_2O_3/HfO_2$  multilayer high-k stacks (19, 16.5 and 15 nm thick) on Si deposited by atomic layer deposition in dependence on Al<sub>2</sub>O<sub>3</sub> sublayers thickness and the post-deposition annealing (PDA) in different ambient (O<sub>2</sub>, N<sub>2</sub>,) have been investigated. The leakage characteristics of stacks at low voltages were found to be almost symmetrical with respect to zero applied bias (0 V), and the current under positive biases is slightly higher. The current follows power law dependence in the low voltage range (V<sup>n</sup>, with n varying in the interval of about 0.7 to ~1, i.e. sub linear behaviour). At higher biases the slope of the currentvoltage characteristics increase suggesting a change of conduction mechanisms. The transition point is found to vary with the Al<sub>2</sub>O<sub>3</sub> content and post-deposition treatment. Although, PDA in oxygen does not affect significantly the leakage current at the low voltages, it seems to shift the transition point of the I-V curves towards higher voltages. Annealing in nitrogen definitely increase the leakage of the stacks. The applying of voltage pulses shifts parallel the low-voltage I-V curves towards higher or lower current values depending on the polarity of the pulse. Both the power law dependence of current and the shift of the I-V curves upon voltage pulses are consistent with the collective transport in array of small metal dots model in which the current is limited by the available sites for charge carriers to move on.

# 2.9 Two-dimensional materials with focus on AlN-possibility of experimental growth and characterization by ellipsometry

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Graphene success has shown that it is possible to create stable, single and few-atom-thick layers of van der Waals materials, and also that these materials can exhibit fascinating and technologically useful properties.

Here we present a review of the theoretical calculations focused on the stability of an infinite hexagonal AlN (h-AlN) sheet, differences that occur in the electronic structure between the bulk and single layer and discuss various method of tuning their electronic and magnetic properties by manipulating the surface and strain using DFT (density functional theory) computations.

As well on the basis of DFT we present a review for further application of 2D-AlN in spintronics, gas sensing and gas storage.

Additionally we will outline the various strategies to grow single-layer and few-layers AlN on arbitrary substrates and propose an experimental guide for their identification and characterization. AlN adopts a graphite-like hexagonal lattice with larger lattice constant compared with bulk wurtzite AlN, Fig.1



Fig.1 a) RHEED patterns of bare Ag(111) and AlN/Ag(111) structures along [1-10] azimuth of silver. The overall streaky pattern shows that AlN grows epitaxially on the Ag(111) substrate. b) RHEED and c) intensity structures along [11-2] azimuth of silver [1].

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# 2.10 In-depth evolution of Tellurium films deposited by Frequency Assisted Thermal Evaporation in Vacuum (FATEV)

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The frequency assisted thermal evaporation in vacuum (FATEV) is a new approach for physical vapour deposition of thin films with predictable topography. It is based on application of mechanical vibrations with audio frequencies on the substrate during condensation of an evaporated material. The method is still under evaluation and only the changes of the deposits' surface have been studied. In order to enlighten the in-depth organization of the films, as well as its evolution with the increase of the thickness - spectroscopic ellipsometry (SE) and crosssection scanning electron microscopy (SEM) were performed. Both methods showed change of the growth mechanism of the tellurium films when higher input frequencies of the vibrations were applied. The films, deposited by conventional thermal evaporation in vacuum with no vibrations applied, as well as these, deposited by FATEV with application of 50 Hz vibrations, were characterized by initial densification followed by 2D nanoparticles growth when a certain border thickness was reached. On the other hand, the high frequency vibrations of 4 and 10 kHz preconditioned growth of tellurium nanoribbons oriented towards the z-axis from the very beginning of the film formation. These tendencies were kept the same after increase of the films thickness. The surface topography changes, as well as the structural parameters of the samples were traced up by atomic force microscopy (AFM) and X-ray diffraction (XRD) analyses, respectively.



a)

b)

Figure 1: Cross-section SEM microphotographs of tellurium films with nominal thicknesses of 100 nm, deposited by FATEV at frequencies of the mechanical vibrations of a) 50 Hz, and b) 4000 Hz.

# 2.11 Influence of deposition parameters on opto-electronic properties of spin – coated SnO<sub>2</sub> thin films

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The functional characteristics of thin films planar solar cells are very sensitive to the presence of pores, voids or holes. Thus deposition of compact, dense and uniform layers is essential in that technology. In nano – sized structures the shorts are a common problem and reason for failures. These issues are especially important in organometalic perovskite solar cells where the active layers are in the nano metric scale. In this emerging technology reduction of cost to efficiency ratio is a serious barrier for commercialization therefore application of cheap and abundant materials as electron selective layer will be advantage.

In this work we have investigated different parameters of the process of deposition of  $SnO_2$  thin films by spin coatings which influence its compactness and impenetrability. The thermal behaviour of the precursor substances was investigated by Differential Scanning Calorimetry in order to estimate the points of the important chemical and phase transformations and in consequence to define an appropriate annealing regime. Influences of the thermal treatments on the properties of the films were investigated by UV – Vis measurements, Raman spectroscopy, X-ray diffractometry, Scanning Electron Microscopy and Photoluminescence. The final assessments of the coverage ability of the  $SnO_2$  films were performed by cyclic voltammetry in aqueous redox solution. Between the used solvents ethanol, methanol and isopropanol for precursor ( $Sn^{4+}$ ) solutions the last ones give uniform layers without pinholes at low temperatures. After annealing in the temperature interval 100 - 180 °C the layers crystallized in typical tetragonal Rutile configuration. The electrical leakage of the films depends on the concentration of the precursor solution, but at higher concentrations, over 0.5 M SnCl<sub>4</sub>.5H<sub>2</sub>O, the formed films are rugged and the root mean square (RMS) roughness increase sharply.

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## 2.12 Alternative WO<sub>3</sub> Hole Transport Layer for Organic Solar Cells

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Bulk heterojunction organic solar cells need selective hole transport and electron transport layers in order to function efficiently. These layers could be organic or inorganic. The most widely used organic hole transport layer is PEDOT:PSS. A widely applied inorganic layer is MoOx deposited by thermal evaporation or from solution. In this contribution we study another possible hole transport layer, WOx, deposited by magnetron sputtering in argon only atmosphere from a WO<sub>3</sub> sputtering target. The layer is characterized by optical transmission spectroscopy, FTIR and Raman spectroscopy, XPS and conductivity measurements. WOx layers of different thickness deposited in the described manner are applied in polymer solar cells with PCDTBT:PC<sub>71</sub>BM active layer. The solar cells are characterised by measuring their current-voltage characteristics, their quantum efficiency as well as their impedance spectra. Their stability in the dark and under illumination is also investigated. The results are compared to those for solar cells with the same active layer deposited in the same run but having PEDOT:PSS hole transport layer. The advantages and disadvantages of WOx films as hole transport layers are discussed.

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#### 2.13 In-vivo study on titanium-niobium orthodontic archwires

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The choice of a suitable orthodontic archwire is based primarily on its mechanical properties, as it depends largely on its effectiveness. Most of the archwires contain Ni which can cause an immunological reaction. As an alternative to the Ni-containing archwires, an innovative archwire of Ti-Nb alloy has been proposed for the composition of which there is very little data. Because of their mechanical properties the TiNb archwires are suitable for finishing stages of orthodontic treatment.

The aim of this study is to investigate the chemical composition, the structure, the morphology, mechanical properties and the thermal phase transitions of Ti-Nb orthodontic archwires used in in-vivo environment. Retrieved Ti-Nb archwires (used up to 5 and more than 8 weeks) with dimensions 0.43 x 0.64 mm (0.017"x0.025") were studied. The analyses were carried out using the following techniques: X-ray Powder Diffraction (XRD), Scanning Electron Microscope (SEM), Energy-Dispersive X-ray microanalysis (EDX), Differential Scanning Calorimeter (DSC) and NanoIndenter G200 with Berkovich XP head.

The registered diffractions picks demonstrate presence of Ti and Nb. The composition of the wires, after usage (up to 5 weeks) was the same as as-received: Ti- 57,62wt% and Nb-42,38wt%, Up to 8 weeks, the chemical composition has no change. From the SEM analyses it can be observed that there is a remarkable change on the surface on the used after clinical usage. DSC analyses show that there is no thermal transitions for all investigated TiNb archwires, made in the temperature range from -50°C to +50°C. Mechanical properties results showed that the indentation hardness of the as-received TiNb archwire is 2.18 GPa and it's indentation modulus is 52.7 GPa. There isn't change in the mechanical properties of the Ti-Nb archwires after their using for 5-8 weeks.

The investigation made on clinically retrieved TiNb archwires in *in-vivo* environment, shows that the archiwres kept their properties up to 5 weeks. Up to 8 weeks of treatment, the archwires changes their morphology and can reduce their application.

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## 2.14 Temperature-Dependent Thermal Conductivity and Viscosity of Synthesized α-Alumina Nanofluids

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In the present work, we focused on the thermal conductivity and viscosity of the synthesis as well as characterize metal oxide  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> nanoparticles suspended in distilled water (DW): ethylene glycol (EG) (60:40) ratio based stable colloidal nanofluid. The band gap of the  $\alpha$ - Al<sub>2</sub>O<sub>3</sub> with and without surfactant is 4.42 eV and 4.59 eV, respectively. The results show that polyvinyl alcohol (PVA) surfactant having smaller crystalline size (~23 nm) then without surfactant has large (~36 nm). The synthesized nanofluids have good stability after 15 days of synthesis which is characterized by zeta potential analyzer. Thermal conductivity and viscosity are measured for 0.1 wt. % and 0.5 wt. % concentration of alumina for with and without surfactant. The concentration of particles and added surfactant are responsible for stable fluid, increased thermal conductivity and viscosity of nanofluid with respect to temperature. Therefore, the novel combinations of characterized properties of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> nanofluid proven the best thermally stable heat transfer fluid compare to conventional cooling fluids.

# 2.15 Structure investigation of thin films from Zn-cobaltite prepared by pulsed laser deposition

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Transition metal oxides have recently received increasing attention due to unique properties and potential applications. Among advantages we mention structural stability, good electronic conductivity, and reversible capacity.

Spinel  $ZnCo_2O_4$  can be widely used in gas sensors, electro catalysis, super capacitors because of the high electrochemical activity, low cost and environment friendliness. The aim of this work is to study thin films from Zn-cobaltite prepared by pulsed laser deposition (PLD) with respect to their morphology and structure. The bulk material of zinc cobaltite is prepared via precipitation reaction. Thin films from the synthesised cobaltite powder are deposited by PLD under different experimental conditions. The structure was investigated by X-ray diffraction. We observed that the synthesized powder is a composite containing two crystalline phases:  $ZnCo_2O_4$ (cubic) and ZnO (hexagonal). The composition of the PLD target, Zn-cobaltite powder and deposited thin films has been assessed by energy dispersive X-ray spectroscopy (EDS). The films have the powder composition and structure, irrespective of the deposition conditions.

The morphology and topography have been studied by scanning electron microscopy. The film density decreases when temperature and pressure increase Crystallites are larger and film thickness is higher as revealed from SEM images in top-view and cross-section mode.

This study demonstrates that PLD method could be considered appropriate for deposition of Zn cobaltite material.

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## 2.16 Experimental investigations on ultrashort laser ablation for micro and nanomachining of materials

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With the advantage of ultrashort pulse width and ultrahigh peak power, subpicosecond lasers can provide extremely precise machining, and therefore has been widely applied in micro and nano scale manufacturing.

We present the results of the experimental parametric study on efficiency, accuracy and quality of subpicosecond laser micromachining of materials that have a potential for application in innovative devices and technologies.

The laser micromachining process was performed with a Yb:KYW subpicosecond laser and a Ti:S femtosecond laser. The study contains a comparison between the two methods, and results analysis using advanced metrology techniques, such as 3D microscopy.



**Figure 1:** 3D (pseudocolor) image and linear profile of a micromachining crater formed by femtosecond laser ablation of aluminum.

# 2.17 Femtosecond laser surface structuring of thin chitosan/hydroxyapatite layers for biomedical applications

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Tissue engineering is an important biomedical area to assist repairing of defective and/or damaged bones and tissues based on creation of scaffold fabrication from various biomaterials. Laser-induced surface texturing has an essential role in creation of proper cell surface environment for diverse biomedical purposes. Mineral based structures typically occur in the extracellular matrix (ECM) of bones, providing a high degree of bioactivity and biocompatibility. Hydroxyapatite (HAp) is widely used in the field of bone regeneration since it's a main component of bones and provides mineralization characteristics and it is responsible for the high mechanical stability of the ECM. Other substantial material groups are the biopolymers such as chitosan which is widely distributed in the nature and possesses high degree of porosity necessary for cellular proliferation in depth, nutrient diffusion and resorbability respectively. Despite its advantages, chitosan has weak mechanical properties, which limits its application in bone tissue engineering as a stand-alone unit. The combination of HAp with chitosan for preparation of matrix substitutes attracts attention in the field of tissue engineering. Laser surface processing of biomaterials does not require special pre-treatment and chemical agents and gives opportunity for high functionalization of the substrate with greater roughness for improved cell adhesion.

The main goal of this paper is focused towards femtosecond laser treatment of thin film biopolymer/ceramic composites (chitosan and HAp) and estimating the influence of (laser fluence and number of applied laser pulses) over material surface structuring for tissue engineering applications.

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### 2.18 Crosslinked chitosan/casein polyelectrolyte multilayers for drug delivery

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Polyelectrolyte multilayers (PEMs) are widely used as drug delivery systems, but still remain challenging for their small drug immobilizing capacity. One way to increase the immobilized drug amount may be crosslinking of the PEMs, which stabilize them and increase their porosity.

The aim of the present study is fabrication and characterization of chitosan/casein PEMs, which are crosslinked with different crosslinking agents – glutaraldehyde, sodium tripolyphosphate,  $CaCl_2$  and combinations of two of them. SEM was used to observe film morphology and its variation due to cross-linking. Swelling behavior of PEMs in artificial saline was investigated. Release of model drug Benzydamine Hydrochloride was monitored spectrophotometrically at 306 nm. The crosslinking improves the PEMs stability when they were immersed in saline, and causes formation of porous surface. After crosslinking the amount of the immobilized drug increased several times.

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### 2.19 Light induced nonselective effects in the negative glow

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Two interfering effects in optogalvanic (OG) spectroscopy were identified in a hollow cathode discharge (HCD) - OG detector. The laser beam was found to induce photoelectron emission (PE) from the cathode surface with a sub-breakdown bias applied and non-resonant space ionization (SP). The convolution of the PE and SP signals was obtained experimentally as an instrumental function. In order to determine the actual OG signal, a deconvolution procedure was developed.

## 2.20 Optical, Electro-Optical, Electrical and Dielectric Characterization of Nematic Liquid Crystal (E7) Layers Doped with Graphene and Graphene Oxide Nanoparticles for Electro-Optics

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Thin (7 µm) layers of nanocomposites from nematic liquid crystal (LC) E7 containing graphene and GO (both at concentrations of  $(10^{-3} \text{ wt.\%} \text{ and } 10^{-4} \text{ wt.\%})$  were characterized by various investigation techniques, such as micro-Raman spectroscopy, impedance measurements and dielectric spectroscopy, as well as by electro-optical measurements (optical transmittance of the films versus the voltage of the applied external AC electric field, Freedericksz transition). Conducting behaviour, dielectric permittivity and electric energy loss of our planar-aligned nematic samples were analysed as a function of frequency (0.1 Hz - 1 MHz) and temperature, the dielectric relaxation frequency  $(f_R)$  and the frequency corresponding to the minimum of their dielectric losses were determined from dielectric spectra using the Cole-Cole diagram (Figure 1). These frequencies are low (several Hz) and are due to a contribution of ion carriers to the observed dielectric relaxations.  $f_R$  for graphene-doped E7 LC (around 6 Hz) is lower than that for the undoped E7 (11 Hz). The lowering of  $f_R$  is due to the decrease of ion mobility. This effect can be explained by the ability of graphene to trap free ions. It was found that the presence of graphene reduces the electrical conductivity of E7 LC, while GO at the same concentration and temperature leads to its increase. As compared to pure LC E7, improved characteristics for the studied nanocomposites were observed, necessary in their practical applications in electro-optics.



**Figure 1:** Cole-Cole complex plot for the studied graphene-E7 nematic mixture and pure E7 at room temperature.

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## 2.21 Impedance and Dielectric Spectroscopy Study of Graphene-Doped Liquid Crystal E7

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The specifics of the electrical and dielectric response of graphene-doped liquid crystal (LC) E7 were studied. Graphene was included in the nematic LC E7 at concentration of  $10^{-3}$  wt.%. Thin planarly-oriented films with a thickness of 7 µm of the produced graphene-E7 nanocomposite (in its nematic phase) were investigated employing complex electrical impedance spectroscopy in the frequency range from 0.5 Hz to 1 MHz of the applied electric field. The change of ionic conductivity, the mobility of the free ion carriers and the dielectric function of graphene-E7 films were analyzed as depending on the temperature of the films, as well as on the field frequency. The corresponding values and characteristics were compared to those of films of undoped E7 measured under the same experimental conditions (**Figure 1**). As a result from the doping, a distinct reduction of the ionic conductivity of the films was present in wide frequency and temperature ranges. Thus, thin films made of the studied graphene-E7 LC nanocomposites exhibit improved electro-optic performance, compared to that of undoped LC E7. The observed important modification is useful for development of advanced and multifunctional nanocomposite nematic materials for electro-optic devices working at ambient temperatures.



**Figure 1:** Nyquist complex impedance plots for the studied graphene-E7 nanocomposite (b) and pure E7 (a) at various temperatures.

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### 2.22 Development of low-cost technology to obtain supercapacitors based on activated carbon

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A recent advance in supercapacitor technology reveals new opportunities for energy storage devices for many applications in electro-mobility and renewable energy sectors. In this paper results on device fabrication are reported. A low-cost screen-printing technology to obtain EDLC supercapacitors has been developed. The device structure is based on Cu plate/Activated carbon electrodes and gel electrolyte. Mesoporous activated carbon electrodes are prepared using local natural resources. The cyclic charge/discharge measurements and impedance spectroscopy confirm supercap behaviour and specific capacitance of more than 4.68 F/g at discharge current of 0.62 A/g. The flat configuration of the supercaps allows easy connection in series and adjustment to DC loads. A pack of four supercaps driving conventional LED has been thoroughly tested for more than 1000 cycles. The hybrid concept of PV module electricity generation to supercap energy storage mounted on the PV module back-side has been tested and evaluated.

# 2.23 Electrochemical behavior of BSCCO cuprate ceramics in alkaline solution

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Nickel-zinc alkaline batteries represent a potential cheaper alternative in the secondary battery market. Various metal oxide and hydroxide additives  $(Bi_2O_3, PbO, Ca(OH)_2)$  have been investigated as a solution to problems such as changes in the Zn electrode shape and formation of zinc dendrites, surface passivation and hydrogen evolution, and thus reducing the battery life. Other studies have shown that  $Bi_2O_3$  and CuO can be reduced to the metals under alkaline conditions similar to the Ni-Zn battery electrolyte creating a metal matrix which aids in nucleation and conductivity. The conductive cuprate ceramics  $Bi_{1,7}Pb_{0,3}Sr_2CuOx$  (BSCO 2201) and  $Bi_{1,7}Pb_{0,3}Sr_2CaCu_2O_x$  (BSCCO 2212) exhibiting superconductivity at low temperatures (80-100K) can also find an application as an additive to the zinc electrode in alkaline Ni-Zn batteries. Their positive effect on cycling stability has been demonstrated in recent investigations.

This study is focused on the electrochemical reduction behavior of BSCCO 2201 and BSCCO 2212 conductive ceramics produced by solid state synthesis. It is aimed to elucidate the positive role of these additives on the batteries' functions. Samples of BSCCO were investigated by Cyclic Voltammetry (CV) in a three-electrode cell in a 7M KOH electrolyte at 25°C by using Bio-logic SP-200 potentiostat/galvanostat. The ceramics were physicochemically characterized before and after electrochemical measurements using X-ray diffraction, scanning electron microscopy (SEM) and energy dispersion spectroscopy (EDX). The CV curves (Figure 1) reveal three cathodic peaks associated with the reduction of bismuth ions to bismuth metal and the two-step reduction of copper (II) to copper metal. The initial scan displayed no oxidation peaks until the oxygen evolution potential. Three oxidation peaks appear on subsequent scans. They are associated with the re-oxidation of bismuth and copper metals to their respective oxides.



Fig. 1. CV curves of BSCCO 2212 at room temperature ( $25 \pm 2$  °C) in 7 M KOH solution, scan rate of 5 mV s<sup>-1</sup>.

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### 2.24 Graphene/Polyaniline flexible supercapacitors using non-metallic electrodes

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Flexible supercaps are attractive devices for portable applications including those integrated in clothes. Highly conducting flexible electrodes can easily be fabricated by graphene powder and PE polymer foil but reliable fabrication of supercapacitor structure is still a challenge. A promising solution could be the incorporation of conducting polymer as polyaniline (PANI) intended to stabilize the mesoporous carbon and graphene plates, to form a conductive porous composite and to increase the capacitance. Low-cost aqueous electrolyte (1V) supercapacitor devices based on graphene/PANI composite were developed, tested in series configurations and compared in electrical performance. Preliminary applications in portable solar chargers are discussed.

## 2.25 Sol-gel synthesis and structural characterization of compositions in the system TiO<sub>2</sub>-TeO<sub>2</sub>-SeO<sub>2</sub>

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The sol-gel processing offers an attractive route for the fabrication of TeO<sub>2</sub>-based materials but most of the authors applied it mainly for obtaining of thin films. It was found that the addition of second or third component improve the thermal stability of TeO<sub>2</sub> thin films. Up to now, the investigations concerning bulk and powder materials are scarce. The aim of this paper is to study the gel formation tendency in the TiO<sub>2</sub>-TeO<sub>2</sub>-SeO<sub>2</sub> system. In order to overcome the problem with hydrolysis of tellurium alkoxides, the telluric (VI) acid (H<sub>6</sub>TeO<sub>6</sub>) along with selenium oxide  $(SeO_2)$  and titanium butoxide  $(Ti(OC_4H_9)_4)$  were used as a new combination of precursors during the synthesis. The structure and optical properties of several gel compositions with different TeO<sub>2</sub>:TiO<sub>2</sub>:SeO<sub>2</sub> ratios were studied. Transparent monolithic and bright yellow colored gels are located between 40-100 mol% TiO<sub>2</sub>, up to 20 mol% of SeO<sub>2</sub> and 65 mol% of TeO<sub>2</sub>. The phase transformations of the as-prepared gels heat-treated up to 700°C is investigated by XRD. Organic and OH groups participate in the amorphous organic-inorganic structure up to 250-300°C. The structure of the inorganic amorphous phases above 300°C consists of SeO<sub>3</sub>, TiO<sub>6</sub> and TeO<sub>n</sub> structural units. The UV-Vis spectra of the binary and three-component gels exhibited a redshift of the cutoff in comparison with those of Ti butoxide gel due to the presence of selenium and tellurium units.<sup>[1]</sup>.

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## 2.26 Surface plasmon for exploration the temperature dependence of hybrid cholesteric liquid crystal's pitch

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Knowledge of the molecular director profile near to the boundaries of a liquid crystal (LC) cell and its dynamic behavior under external influence is very useful for device design. For getting the need information the surface plasmon resonance (SPR) is used [1-3]

In this study we experimentally track the temperature dependence of the pitch of hybrid cholesterc LC by the SPR spectral shift.

The excitation of SPR is usually based on a prism coupling configuration. Metal gratings are also used for supporting surface plasmons and provide an alternative design of SPR excitation. For many applications gratings are more feasible. In our previous study [4] we optimized some parameters related to SPR excitation on grating for developing the structure for application.

Based on this experience, in present work we use a gold grating as bottom wall of liquid crystal (LC) cell. The top wall is a BK7 glass plate. The LC is induced hybrid cholesteric. The nematic matrix is commercially available E7, while the chiral supplement is S811. A prior work was done for finding an optimal concentration of S811, the corresponding pitch and its temperature dependence.

Two strips with thickness about 12  $\mu$ m are used as the cell gap spacers and the cell is capillary filled with induced hybrid cholesteric at optimal ratio nematic/cholesteric. Experimentally are provided indispensable condition for homogeneous alignment of LC's molecules. The temperature of LC cell is controlled in 30<sup>0</sup> – 60<sup>0</sup> C. The observation of SPR is provided by spectral read-off. The spectral shift vs. temperature is studied. The results are compared with the LC cell measurements provided by a polarization microscope. The conclusions about the director orientation and pitch are formulated. The possibility about the application of studied structure for a temperature sensor is discussed.

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### 2.27 Fabrication of thin films of phosphonated calix[4]arene bearing crown ether and their gas sensing properties

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Calix[4]arenes bearing phosphate and crown ether groups are used to as an active layer for volatile organic compound (VOC) vapor sensor. These organic architectures were successfully deposited by spin coating method on gold-coated glass surfaces. Surface Plasmon Resonance (SPR) technique was used for VOCs detection to evaluate the chemical-sensing properties of these calix[4]arene derivatives. Spun thin films of calix[4]arene derivatives were exposed to a variety of VOC vapors, and the resonance angles changes of these films were recorded for the specific analyte vapors such as chloroform, carbon tetrachloride, dichloromethane, ethanol, benzene, and toluene. Measurements were made at room temperature, and the responses were found to be fast and appeared to be completely reversible. The sensing results showed similar response patterns, and our data strongly indicate that response of used thin films of calix[4]arene derivatives to chloroform is much higher than those of any other VOCs used. It is also shown that the chemical sensing selectivity and sensitivity can be altered by different alkyl side chains.



**Figure 1:** Schematic illustration of the experimental process used to fabricate the spun thin films and the SPR gas cell used for the gas sensing measurements.

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## 2.28 Electronic transport in methylammonium lead halide perovskite single crystals studied by transient photoconductivity

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Methylammonium lead halide perovskites (hereafter termed 'perovskites' for simplicity) are of high research interest due to their remarkable performance as efficient PV absorber layers [1], and similarly remarkable instability on exposure to moisture, UV, moderate temperatures and bias-cycling [2]. Perovskites have been studied extensively, primarily in the form of spin-coated or vapour-deposited films targeted for application in single- and multi-junction solar cells and x-ray imagers. At Dundee, we have employed the *inverse temperature crystallization* technique [3] to grow lead bromide and lead iodide perovskite *single crystals*. Using the rudimentary facilities available in our prep lab, crystals of size (exceeding 1 cm<sup>2</sup> on a face) and quality (as measured by XRD, XRF, optical spectrophotometry) comparable to those reported in the literature [3] have been prepared. Here we report primarily on their electronic transport properties examined using steady-state, transient and modulated photoconductivity combined with dark-current measurements, conducted over a range of temperatures. We discuss our findings with reference to complementary work [4].

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### 2.29 LIBS analyses on glass materials doped with noble metal nanoparticles

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The current work is a case study of a project concerning investigation on noble metal doped glass materials radiated by laser pulses. Our motivation of the research is based on the specific properties of noble metal nanoparticles and their wide applications. The resonance frequency for noble metal nanostructures is in the near UV and visible spectral range, where most of the commercial lasers irradiate. This makes these materials attractive candidates for efficient study and application of their properties.

The laser ablation measurements are applied on glass samples with different ion concentrations 0.1, 0.5 and 1%. Two types laser processing are considered including application of nanosecond and femtosecond pulses. LIBS spectra are measured for each sample. Experiments with wide range of processing parameters including laser fluence, applied laser pulses, irradiation wavelengths are performed. The irradiation with different wavelengths applies for the femtosecond laser only, equipped with optical parametric amplifier.

The obtained results from this case study will provide a piece of information to our main project research on the properties of the noble metal doped glass materials radiated by laser pulses. Furthermore, this will be a basis of development of detailed theory of the interaction of laser radiation with transparent materials, mechanism of laser induced defects formation and their influence on the initial properties of the material and laser parameters.

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