Proceedings

First virtual Bilateral Conference on Functional Materials (*BiC-FM*)

8-9 October, 2020

Welcome to First virtual Bilateral Conference on Functional Materials (BiC-FM)!!!

Dear BiC-FM 2020 participant,

We are pleased to welcome you to the First Bilateral Conference on Functional Materials organized between two neighboring countries with a long history of successful scientific collaboration: Finland and Russia!

The aim of this conference is to strengthen the existing mutual research and to establish new collaborations between scientific groups from Russia and Finland. We would like to motivate groups to share their recent advancements in both fundamental and applied science of functional materials. We wish that the Conference forms as a substantially important platform for students and young scientists to attend lectures and interact with the leading senior scientists at the forefront of their fields. Equally importantly, the Conference offers opportunities for the young scientist to introduce their state-of-the-art research work.

The BiC-FM 2020 Conference has attracted more than 130 participants registered not only from Finland and Russia, but also from various universities and institutions around the globe from such countries as India, Malaysia, Israel, Vietnam, USA, Great Britain and Brazil. Together we create new traditions, we support intensive idea exchange and virtual networking!

We thank our committed organizers, conscientious scientific committee and tireless administrative staff for their priceless help. We are grateful to the financial support by our generous sponsors and in particularly acknowledge Russian Science Foundation (Project identifier: 17-19-01787).

We wish that you will have enjoyable, enlightening and productive days during our Conference. We also look forward the pandemic situation in the World becoming better to organize face to face meetings in the forthcoming years!

Sincerely yours,

Conference chairs

Albert G. Nasibulin and Tanja Kallio

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Scope

The aim of the Conference is to provide a platform for discussion of the recent advances in both fundamental and applied science of novel functional materials with a special attention to low dimensional materials to force birateral collaboration.

The Conference will be held October, 8-9, 2020.

Scientific program

1. Synthesis (of functional materials)
2. Modelling (of functional materials)
3. Electrochemical Applications (of functional materials)
4. Photonics (of functional materials)
5. Modification/functionalization (of functional materials)

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Program

	Thursday, October 8	**Friday, October 9**
9.45	**Opening Speech**	
	Session 1: Synthesis	***Session 4: Photonics. I***
10.00	Keynote Talk 1: Alexander Okotrub	Keynote Talk 9: Zhipei Sun
10.25	Keynote Talk 2: Esko Kauppinen	Keynote Talk 10: Yury Gladush
10.50	Oral Talk 1: Vladimir Kuznetsov	Oral Talk 9: Aleksei Emelianov
11.05	Oral Talk 2: Hasaan Butt	Oral Talk 10: Dmitry Mitin
11.20	**Break**	
	Session 2: Modelling	***Flash presentations***
11.45	Keynote Talk 3: Olga Glukhova	Please find the schedule below
12.10	Keynote Talk 4: Kari Laasonen	
12.35	Oral Talk 3: Stefan Shcherbinin	
12:50	Oral Talk 4: Alexander Kvashnin	
13:05	Sponsor talk (Swagelok)	
13.20	**Break/lunch time**	
	Session 3: Electrochemistry. I	***Session 4: Photonics. II***
14.40	Keynote Talk 5: Keith Stevenson	Keynote Talk 11: Elena Obraztsova
15.05	Keynote Talk 6: Carita Kvarnström	Keynote Talk 12: Sergey Makarov
15.30	Oral Talk 5: Bernardo Barbiellini	Oral Talk 11: Bakhysh Bairamov
15.45	Oral Talk 6: Stanislav Evlashin	Oral Talk 12: Dmitry Chermoshentsev
16.00	**Break**	
	Session 3: Electrochemistry. II	***Session 5: Modification/functionalization***
16.25	Keynote Talk 7: Cristina Flox	Keynote Talk 13: Polina Kuzhir
16.50	Keynote Talk 8: Jari Koskinen	Keynote Talk 14: Ayrat Dimiev
17.15	Oral Talk 7: Stanislav Fedotov	Oral Talk 13: Boris Gorshunov
17.30	Oral Talk 8: Muhammad Asghar	Oral Talk 14: Markus Ahlskog
17.45		**Closing remarks**

Time	*Flash session #1**: Synthesis of materials*** *Chairs: A. Nasibulin, D. Krasnikov*	*Flash session #2 **:Physics of materials*** *Chairs: D. Kopylova, Yu. Gladush*	*Flash session #3**: Chemistry of materials*** *Chairs: F. Fedorov, A. Goldt, E. Fedorovskaya*
11:45	**Alisa Shaikhulova** High-yield synthesis of single-walled carbon nanotube films for targeted applications	**Vasilii Vasilchenko** Polarons in Two-dimensional Pnictogens: DFT Study	**Anna Iurchenkova** Electrochemical behaviour of thermally reduced graphite oxide in Li-ion batteries
11:51	**Ilya Novikov** Residence time as a tool for optimization of aerosol CVD synthesis of single-walled carbon nanotubes	**Nikita Gudkov** Parametric modelling of electric percolation and conductivity of carbon nanotubes nanocomposite	**Vasily Artemov** Electrodynamic properties of low-dimensional water
11:57	**Alexey Zavorin** Topochemical transformations in MWCNTs-Si composites at high temperatures	**Aram Mckrtchyan** Pulse switchable fiber laser based on ionic liquid gated carbon nanotube saturable absorber	**Ahaliabadeh Zahra** Enhanced electrochemical performance of TiO_2 modified $LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$ cathode material via atomic layer deposition
12:03	**Elena Shlyakhova** Nitrogen –doped porous carbon obtained by precipitation of acetonitrile vapors on template C-CaO nanoparticles for electrochemical applications	**Denis Zhigunov** Enhanced imaging of single Si nanoparticles using non-reflective SWCNT membranes	**Andrey Shevtsov** Protective spinel coating for $Li_{1.17}Ni_{0.17}Mn_{0.50}Co_{0.17}O_2$ cathode for Li-ion batteries through single-source precursor approach
12:09	**Maksim Vladimirovich Lomakin** Preparation of carbon nanotube fibers by folding the randomly oriented SWCNT films	**Ivan Komarov** Low cost lasers as suitable instrument for graphene oxide thin film modification	**Natrah Shafiqah Rosli** Composites nano-titania graphite for photocatalytic and antibacterial activities
12:15	**Dharshini Perumal** Green synthesis of reduced graphene oxide for biomedical applications	**Tigran Prazyan** Optical Properties Of Carbon Nanodots Obtained From The Kuzbass Basin Coals	**Anna Vorfolomeeva** Phosphorus-filled single-walled carbon nanotubes: synthesis, characterization and electrochemical properties
12:21	**Svetlana Stolyarova** Thermal shock as a new approach for the synthesis of porous MoS_2	**Alexandr Parfenov** Influence of allotropy of carbon nanostructures on tribological and rheological processes in plastic lubricants	**Anna Kobets** Li-ion batteries with negative electrodes made of reduced graphite oxide
12:27	**Maria Vikulova** Preparation of functional carbon coatings on the surface of hollandite-like ceramics with composition of $K_{1.53}(Cu_{0.76}Ti_{7.24})O_{16}$	**Konstantin A Motovilov** Copper (2+) ions decrease conductivity of melanin in both bulk and film forms	**P. Murali Krishna / Gurdeep Rattu** Polyacrylic acid modified cerium oxide nanoparticles for non-enzymatic H_2O_2 Sensor
12:33	**Siti Nadiah Zulkifli** Synthesis, Characterization and Toxicity Studies Of Gold Nanoparticles For Biomedical Applications	**Nikita Nekrasov** Toxin detection through graphene Dirac point shift tracking	**Julia Bondareva** Naphthyl - functionalized dendrimers can regulate surface properties of materials
12:39	**Ashreen Norman** Green Synthesis Approach to Produce Luminescent Nanoparticles from Agricultural Waste and their potential biomedical application	**Vladislav Andryushkin** Investigation of structural and optical properties of three-dimensional InGaPAs islands	**Dmitrii Stolbov** N-doped graphene nanoflakes for catalysis and tribology
12:45	**Javier Antonio Ramirez Benavides** Synthesis of core shell Nano magnets with size tailoring by aerosol CVD	**Abinash Das** Visible light driven photocatalytic performance of Ag modified ZnO nanorod through effective charge carrier separation	**Anna Vershinina** The influence of chlorine and chloroauric acid treatment on electromechanical properties of SWCNT fibers

12:51	***Tatiana Abakumova*** *Prussian-blue lipid nanoparticles for effective siRNA delivery to liver*	***Asmaa Gamal Ahmed*** *Terahertz-infrared excitations in the Ba0.2Pb0.8Al1.2Fe10.8O19 single crystal*	***Daniil A. Ilatovskii*** *Stable doping of carbon nanotubes by V_2O_5 using fast sol-gel method*
12:57	**Emmellie Laura Albert** Toxicity evaluation of Herbs based Carbon Dots using Artemia Salina Cyst and its three larval stage	**Vladislav Nikolaevich Mironyuk** Dependence of frequency-capacitance curves for the «Air – Langmuir Monolayer – Water» system on the colloid solution amount spread out the water surface	**Yury Panasenko** Flexible supercapacitors based on free-standing films of polyaniline/single-walled carbon nanotube composites
13:03	**Che Azurahanim Che Abdullah** Fabrication of magnetic graphene oxide and its developmental toxicity to Artemia Salina Cyst and its three larval stage	**Dmitry Khudyakov** Nonlinear optical absorption in lead halide perovskite thin films	**Durga Sankar Vavilapalli** Multifunctional brownmillerites for efficient energy harvesting and storage applications
13:10	**Muhammad Azri Muhamad Yusop** Biogenic synthesis of titanium dioxide: its composite with iron oxide and their potential biomedical application	**Gee Een Lau** Eco-Friendly Photocatalysts for Degradation of Dyes	**Anton Vorobei** Deagglomeration of carbon nanotubes via rapid expansion of supercritical suspensions

Oral Sessions

Thursday,

October 8

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Structure of graphitized films formed on the diamond surface under high-temperature annealing

A.V. Okotrub[1], D.V. Gorodetskii[1], Y.N. Palyanov[2], A.L. Chuvilin[3], L.G. Bulusheva[1]
1 – Nikolaev Institute of Inorganic Chemistry, SB RAS, 630090 Novosibirsk, Russia

2 – Sobolev Institute of Geology and Mineralogy SB RAS, 630090 Novosibirsk, Russia

3 – CIC nanoGUNE Consolider, E-20018 San Sebastian, Spain

spectrum@niic.nsc.ru

Diamond crystals with a facet size exceeding the size of the focus of the X-ray beam incident on the sample were synthesized by the HPHT method were heated to a temperature of 850°C and 1250°C for 15 minutes. Annealing of samples of single crystals was carried out in a high-vacuum chamber of the Russian-German laboratory at the BESSY II synchrotron source. XPS spectroscopy was used to study the structure of carbon layers on diamond faces of different symmetries and with thin layers of iron and nickel deposited on a diamond. A higher rate of graphitization of the (111) face is shown. From the data of the angular dependence of NEXAFS, the directionality of the sp^2 carbon layers relative to the diamond surface is determined. The data obtained indicate a catalytic effect of the metal on the process of the formation of graphene structures. Transmission electron microscopy data demonstrate the characteristic size and misorientation of individual graphene layers for different symmetry of diamond faces.

Acknowledgement. This work was supported by the Russian Foundation for Basic Research, grant 19-03-00425.

Prof. Dr. Alexander Okotrub

Alexander Okotrub graduated from the Physics Department of Novosibirsk State University in 1980, specialized in the Chemical Physics. Since 1980, A. Okotrub worked as an intern-researcher at Nikolaev Institute of Inorganic Chemistry SB RAS (NIIC SB RAS) as post-graduate student, junior researcher, research associate, senior researcher, leading researcher and principal researcher. At present he is the head of the Laboratory of Physics Chemistry of Nanomaterials and the head of the Department of the Chemistry of Functional Materials of the NIIC SB RAS. He is professor in physical chemistry and leads the Laboratory of Carbon Nanomaterials at the Novosibirsk State University. In his work, an approach is used that combines methods for synthesizing carbon nanostructures (fullerenes, nanotubes, graphene, nanodiamonds, etc.), methods for their chemical modification and the creation of composite and hybrid structures, as well as methods for studying the structure and physicochemical properties of the produced materials. Considerable attention is paid to X-ray and photoelectron spectroscopy and quantum-chemical calculations for studying the electronic structure and properties of new materials. A. Okotrub published 360 scientific papers. He lectures on "Functional materials" for students of the Novosibirsk State University and "Materials and their properties" for post-graduate students of the NIIC SB RAS.

FC-CVD synthesis large diameter CNTs for transparent conductor applications

Qiang Zhang, Datta Sukanta, Hua Jiang, Esko I. Kauppinen
Department of Applied Physics, Aalto University School of Science, PO Box 15100, FI-00076 Aalto, Espoo, FINLAND

esko.kauppinen@aalto.fi

Many efforts have been devoted to increasing the conductivity of CNT TCFs made with the floating catalyst chemical vapor deposition (FC-CVD). However, intrinsic nanotube collisions in the aerosol process of FC-CVD lead to a tread-off between yield and performance, because bundling increases when increasing the yield i.e. production rate, with the bundling reducing the growth rate as well as increasing sheet resistance at the given film transmittance. Here, we report TCFs of large-diameter CNTs from methane-based FC-CVD overcoming the performance–yield tradeoff. Based on the Fe-C-S system, the double-wall CNTs (DWCNTs) with a mean diameter of 4.15 nm and a mean bundle length of 20 um have been synthesized via FC-CVD and directly deposited to form TCFs. After gold chloride solution doping, the TCFs have an excellent performance of 42 ohm/sq sheet resistance at 90% transmittance. Unexpectedly, these high-performance DWCNTs films have an ultra-high yield i.e. production rate, being two orders of magnitude higher than that of SWCNT based TCFs with similar performance. Especially, these high-yield DWCNTs films contain 'small' bundles with around 50% of CNTs being individual, which is completely different from other FC-CVD results for SWCNTs produced at much lower yield. Moreover, the large-diameter DWCNTs seem to flatten at the junctions, which may provide a larger contact area between the tubes and accordingly reduce the contact resistance. These unique features of large-diameter CNTs in 'small' bundles offer the route to obtain high-performance CNT TCFs with high yield. These results imply a new model with optimization windows for high-performance CNT TCFs with high yields and accordingly at reduced cost, and may accelerate the practical application of CNTs TCFs.

Professor Esko I. Kauppinen, PhD (Physics) is the Vice-Dean responsible for research, innovations and industry relationships at the Aalto University School of Science and Tenured Professor of Physics at the Department of Applied Physics. He has published more than 443 scientific journal papers e.g. in *Nature Nanotechnology*, *NanoLetters, ACS Nano, Angewandte Chemie, Carbon, Energy and Environmental Sciences* etc., having Hirsch-index over 52 and over 10 600 citations. He has given more than 120 keynote and invited conference talks and 220 talks at world leading companies and universities. He is considered one of the world leading authors in the area of single walled carbon nanotube synthesis, characterisation and thin film applications as well as in the gas phase synthesis of particles for inhalation drug delivery. He is the founding member of the companies Canatu Oy (http://www.canatu.com) and Teicos Pharma Oy (www.teicospharma.com).

Characterization of the distribution of multilayer carbon nanotubes in polymer composites using cyclic measurements of current-voltage characteristics

S. I. Moseenkov[1], A. V. Zavorin[1,2], and V. L. Kuznetsov[1,2]
[1] *Boreskov Institute of Catalysis SB RAS, Lavrentiev ave. 5, 630090 Novosibirsk, Russia*
[2] *Novosibirsk State University, Pirogova str. 2, 630090 Novosibirsk, Russia*
kuznet@catalysis.ru

In this paper we suggested a method for evaluating the uniformity of the nanotube distribution in the MWCNT-polymer composites based on sequential measurements of their current-voltage-conductivity (CVC) characteristics in a wide range of applied voltages (E, up to 10^3 V/mm). The MWCNTs in the composites form ohmic contacts (direct contacts between the nanotubes) and non-ohmic contacts (nanotubes in the contact are separated by several polymer chains). In our study we investigated composites with polyethylene and poly(methyl methacrylate) matrixes produced using MWCNTs with different aspect ratio (AR, 36 to 3000). In composites with uniform distribution of nanotubes (near the percolation threshold), large number of non-ohmic contacts results in high specific resistivity to 10^{13}–10^{14} Ω · cm. This makes it difficult to measure the resistance at low E and impairs reproducibility of the results because partial transformation of contacts due to the heat release under electrical current takes place during the measurements already at E = 0.3 V/mm and current density $4 \cdot 10^{-8}$ A/cm^2. Furthermore, in the case of a high applied voltage, the decrease in resistance can reach 10^5 due to the formation of new ohmic contacts between nanotubes. The number of ohmic contacts in the composites also increases when the conductivity and I–V characteristics are measured due to irreversible transformation of non-ohmic contacts into ohmic contacts under the action of electrical thermal breakdown. This effect increases together with the number of non-ohmic contacts in the composite, which was demonstrated for composites modified by MWCNTs with AR values ranging from 36 to 3000. Therefore, the MWCNT percolation threshold largely depends on measurement conditions and on the sample's "history". We demonstrated that cyclic I–V measurements can be used to characterize the nature of the contacts between the nanotubes in polymer composites, in particular, to determine the presence of non-ohmic and ohmic contacts, transformations of the former into the latter, and to control the conductivity of MWCNT based composites using electric fields with a strength higher than 1 V/mm.

The suggested method for activation of isolated contacts between nanotubes can be used for controlled modification of MWCNT based composites for production of functional materials or devices on their basis (e.g. pressure sensors or deformation sensors, etc.) [1,2].

Acknowledgments. The work was carried out within the framework of the RFBR project No. 20-33-70120.

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The electric resistivity and piezoresistive response of functional carbon nanocomposites

Hassaan A. Butt, Stepan V. Lomov, Iskander S. Akhatov, Sergey G. Abaimov
Centre for Design, Manufacturing and Materials
Skolkovo Institute of Science and Technology, Moscow, Russia
hassaan.butt@skoltech.ru

Functional nanocomposites are allowing fundamental changes to the way system and material monitoring and testing takes place, both during manufacturing as well as during composite usage lifecycle [1, 2]. One such application of these materials is the replacing of traditional sensors for deformation sensing, allowing the reduction in cost and weight of systems and potential usage has already been highlighted in fields such as the automotive, aerospace, renewable energy and sensor manufacturing sectors [3, 4].

In recent years, nano-carbon particles, in particular, carbon nanotubes and graphene/derivatives, have been under intense scientific scrutiny as additives for composite manufacturing, not only increasing the mechanical properties of composites but allowing the final composites to be electrically conductive and piezoresistive in nature [5, 6].

In this work, industrial masterbatches have been used to manufacture functional nanocomposites and evaluate their feasibility for large scale production of strain sensing thermoplastic nanocomposites. Masterbatches are high weight/volume fraction compounds premixed with nanoadditives in a selected matrix and provide a safe medium for implementing nanomaterials on an industrial scale. From a safety, production line modification and financial standpoint, masterbatches are the most feasible implementation medium for large scale production. However, very few publications deal masterbatch-based nanocomposites and of those available, even fewer deal with piezoresistivity or self-diagnostics.

Six types of carbon nanoparticle masterbatches were employed during this study, each type containing either single-wall carbon nanotubes (SWCNT), multi-wall carbon nanotubes (02 types, MWCNT), graphene (G), reduced graphene oxide (RGO) or nitrogen doped graphene (NDG). These particles were added to an epoxy matrix at three weight percentages of interest, 0.5%, 1.0% and 2%. The electrical and piezoresistive properties of the formulated nanocomposites were studied, with higher weight fractions yielding higher electrical conductivities whereas the same yielded lower piezoresistive response. Carbon nanotube (CNT) based nanocomposites outperformed graphene/derivative nanocomposites in terms of electrical conductance, showing resistivities between 2 - 10^{6} Ohm·cm as compared to G/RGO/NDG samples, with values between 10^{11}-10^{12} Ohm·cm. CNT based nanocomposites showed strain based gauge factors between ~2-7, while graphene/derivative nanocomposites showed extremely high resistivities infeasible for piezoresistive monitoring at the studied weight percentages. A clear relationship between the attained electrical conductance of CNT nanocomposites and their strain sensing ability (gauge factor) has also been established, with the dependency following a semi-logarithmic system; GF=A*log(R0)+B.

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Anisotropic electrical conductivity in graphene films with vertically aligned single-walled carbon nanotubes: new advances in mechanisms and applications

Glukhova O.E. [1,2] , Slepchenkov M.M. [1]

1 – Saratov State University, Saratov, Russia
2 – I.M. Sechenov First Moscow State Medical University, Moscow, Russia
glukhovaoe@info.sgu.ru

In this paper, we suggest an idea of a new approach to control the electrical conductivity and its anisotropy in graphene-nanotube films with vertically oriented single-walled carbon nanotubes (SWCNTs) seamlessly connected to graphene. The basis of this approach is the phenomenon of aromaticity occurred in the hexagons of armchair-type SWCNTs at a certain nanotube length, which induces the oscillations of electronic characteristics with increasing the SWCNT length [1]. The proposed idea was tested on the example of two graphene nanomesh (GNM) atomistic models with nanoholes for SWCNTs with the chirality (6,6) and (9,9) in the case of sequentially increasing the SWCNT length. These types of SWCNTs were revealed using original approach called “virtual growing”, which shown that among the armchair SWCNTs with a diameter of 0.6–1.2 nm, the energetically favorable SWCNT- graphene junction will be formed with the SWCNTs (6,6) and (9,9). The calculations of geometric parameters of graphene-nanotube atomistic models were obtained using the self-consistent charge density functional tight-binding (SCC-DFTB) method [2]. The calculations of the electron transmission function T(E) and electrical conductivity G were carried out at 300 K using the Landauer-Buttiker formalism [3]. It was found that the nanoholes in monolayer graphene form conducting pathways in one direction, inducing anisotropy of the conducting properties. The anisotropy of the G value reaches 5 times. The formation of SWCNTs in the nanoholes does not remove anisotropy, amplifying it up to 7 times. The value of electrical conductivity G is strongly influenced by the length of the formed nanotube. It was found that a sharp increase in the value of G occurs at a certain length of 0.615 nm, 0.984 nm, 1.353 nm, and so on with in steps of 0.369 nm. These values of the SWCNT length were determined by the number of atomic layers in the SWCNT framework that is a multiple of three. Especially noticeable jumps in electrical conductivity occur for the armchair direction of electron transport. Thus, by adjusting the SWCNT length, it is possible to enhance or weaken the anisotropy of the conductive properties of graphene-nanotube films.

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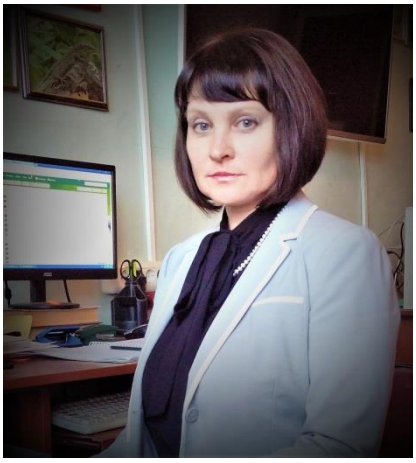
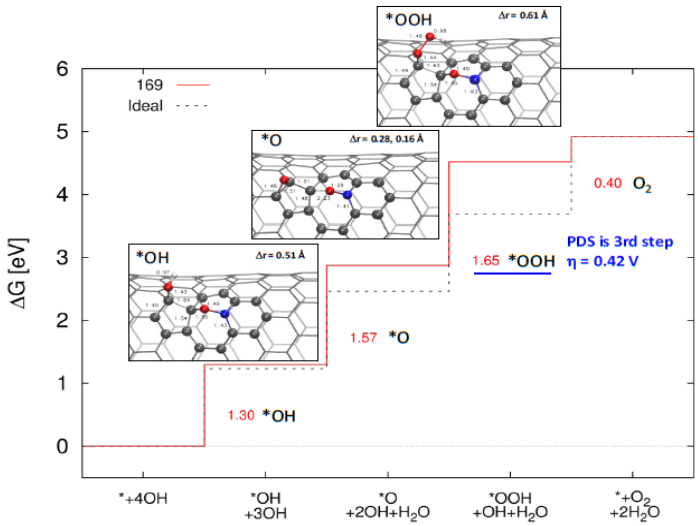


O.E. Glukhova received Ph.D. in Vacuum and Plasma Electronics (1997) and Dr. Sc. in Solid State Electronics and Nanoelectronics (2009) from the Saratov State University, Russia. She is a head of Department of Radiotechnique and electrodynamics at Saratov State University and leads the Division of Mathematical modeling in Educational and scientific institution of nanostructures and biosystems at Saratov State University. Her main fields of investigation are: nanoelectronics, molecular modeling of biomaterials and nanostructures, molecular electronics, mechanics of nanostructures, quantum chemistry and molecular dynamics, carbon nanostructures (fullerenes, nanotubes, graphene, graphane). She has published more 200 peer-reviewed journal papers and five monographs.

Oxygen evolution reaction on pristine and defective nitrogen-doped carbon nanotubes and graphene

Murdachaew G.[1], and Laasonen K.[1]
1) Aalto University, Department of Chemistry and Materials Science, Finland
kari.laasonen@aalto.fi

Hydrogen obtained by electrochemical water splitting on a suitable catalyst has raised a lot of interest. The ideal catalyst should be efficient, stable under operating conditions, and composed of earth-abundant elements. Density functional theory simulations within a simple thermodynamic model of the more difficult half-reaction, the anodic oxygen evolution reaction (OER), with a single-walled carbon nanotube as a catalyst, showed that the presence of < 1% nitrogen reduces the required OER overpotential significantly. We performed an extensive exploration of systems and active sites with various nitrogen functionalities [1] (graphitic, pyridinic, or pyrrolic) obtained by introducing nitrogen and simple lattice defects (atomic substitutions, vacancies, or Stone-Wales rotations). The lowest predicted overpotentials were about 0.4 V, close to what has been measured experimentally for the best-performing nitrogen-doped nanocarbon catalysts. The lowest predicted overpotential of 0.39 V was obtained for a model system with a Stone-Wales defect in combination with pyrrolic nitrogen doping. The most OER-active sites/systems were carbon atoms in the vicinity of Stone-Wales pyrrolic nitrogen, followed by graphitic nitrogen. For the majority of the nanotube-based systems, the third step of the four-step OER mechanism, the formation of attached OOH, is the potential-determining step of the reaction. The nanotube radius and chirality effects were examined by considering OER in the limit of large radius by studying graphene as a model system. They exhibited trends similar to those of the nanotube-based systems but often with reduced reactivity due to weaker attachment of the OER intermediate molecules.



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Kari Laasonen is a professor of physical chemistry in Aalto University (from 2010). He did his M.Sc. in University of Helsinki 1988, PhD. in 1991 in TKK (physics). Before Aalto he worked in EPFL (Lausanne), IBM Research Laboratory (Zurich), University of Pennsylvania (Philadelphia) and University of Oulu. He has specialized to computational chemistry and especially on modelling surfaces and electrochemical reactions. He has also long expertise of modelling reaction in solutions. He has published more 150 papers and these papers have been cited more than 10.000 times.

Starfish-like phosphorus carbide nanotubes

Kistanov A. A.[1], Shcherbinin S. A.[2], Huttula M.[1], Cao W.[1]
1 – Nano and Molecular Systems Research Unit, University of Oulu, Oulu, Finland

2 – Southern Federal University, Rostov-on-Don, Russia

stefanshcherbinin@gmail.com

Recently several allotropes of a novel two-dimensional material, phosphorus carbide (PC), have been predicted theoretically and some of them have already been successfully fabricated [1]. For one of these PC allotropes, α-PC, the possibility of its rolling to a PC nanotube (PCNT) at room temperature under compressive strain has been found [2]. These PCNTs of different sizes exhibit high thermal stability and possess well tunable band gap. In this work, PCNT obtained by the rippling of β_0-PC and β_1-PC monolayers along their armchair (APCNT) and zigzag (ZPCNT) directions are investigated in the framework of density functional theory.

It has been found that most of created β-PCNTs possess starfish-like structure (see Figure 1a). The dynamical stability of these β-PCNTs has been verified using *ab initio* molecular dynamics calculations conducted at 300 K. It is also found that β-PCNTs of the smallest/biggest size consist of 12/44 atoms. According to electronic band structure calculations, β-PCNTs can be semiconductors, semimetals or metals depending on their size and form (see Figure 1b). Therefore, due to their extraordinary form and highly tunable band structure, β-PCNTs may find the application in straintronic, optical and photovoltaic devices.

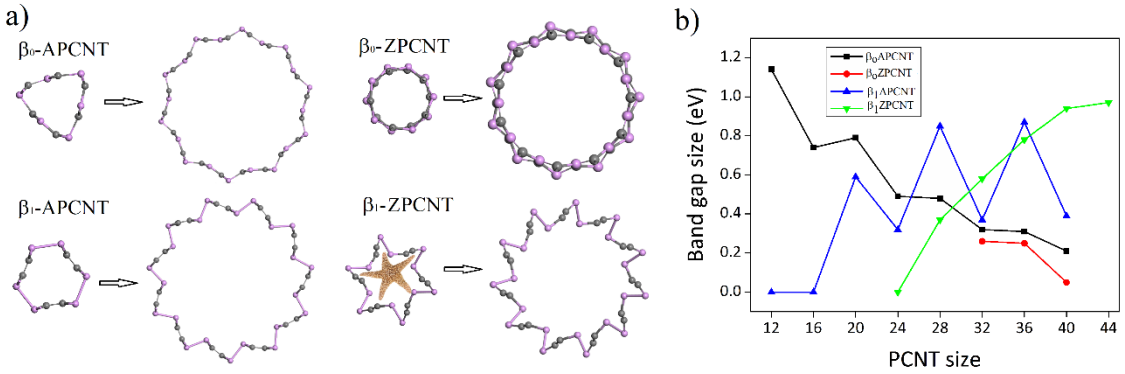

Figure 1. (a) Atomic structure and (b) band gap size as a function of size of β_0- and β_1-APCNT and β_0- and β_1-ZPCNT.

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Computational search for new high-T_C superconductors with subsequent synthesis

A.G. Kvashnin[1], I.A. Kruglov[2,3], D.V. Semenok[1], A.R. Oganov[1],
1 – Skolkovo Institute of Science and Technology, Moscow, Russia
2 – Moscow Institute of Physics and Technology, Dolgoprudny, Russia
3 – Dukhov Research Institute of Automatics (VNIIA), Moscow, Russia
A.Kvashnin@skoltech.ru

Hydrogen-rich hydrides attract great attention due to recent theoretical [1] and then experimental discovery of record high-temperature superconductivity in H_3S (T_C = 203 K at 155 GPa [2]).

Here we perform a systematic evolutionary search for new phases in the Fe-H [3], Th-H [4], U-H [5] and other numerous systems under pressure [6] in order to predict new materials which are unique high-temperature superconductors.

We predict new hydride phases at various pressures using the variable-composition search as implemented in evolutionary algorithm USPEX [7-9]. Among the Fe-H system two potentially high-T_C FeH_5 and FeH_6 phases in the pressure range from 150 to 300 GPa were predicted and were found to be superconducting within Bardeen-Cooper-Schrieffer theory, with T_C values of up to 46 K. Several new thorium hydrides were predicted to be stable under pressure using evolutionary algorithm USPEX, including ThH_3, Th_3H_{10}, ThH_4, ThH_6, ThH_7 and ThH_{10}. *Fcc*-ThH_{10} was found to be the highest-temperature superconductor with T_C in the range 221-305 K at 100 GPa. Actinide hydrides show, i.e. AcH_{16} was predicted to be stable at 110 GPa with T_C of 241 K.

To continue this theoretical study, we performed an experimental synthesis of Th-H phases at high-pressures including ThH_{10}. Obteined results can be found in Ref. [10].

Acknowledgement. This work was supported by RFBR foundation № 19-03-00100 and facie foundation, grant UMNIK №13408GU/2018.

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Enhanced Electrocatalytic Activities by Substitutional Tuning of Nickel-based Ruddlesden-Popper Catalysts for the Oxidation of Urea and Small Alcohols

Stevenson, K. J.[1]

1 – Skolkovo Institute of Science and Technology, Moscow, Russia

k.stevenson@skoltech.ru

The electrooxidation of urea continues to attract considerable interest as an alternative to the oxygen evolution reaction (OER) as the anodic reaction in the electrochemical generation of hydrogen due to the lower potential required to drive the reaction and the abundance of urea available in waste streams. In this talk the effect of Sr substitution in a series of $La_{2-x}SrxNiO_{4+\delta}$ Ruddlesden-Popper catalysts on the electrooxidations of urea, methanol, and ethanol are presented. We demonstrate that activities toward the urea oxidation reaction increase with increasing Ni oxidation state. The 75% Sr-substituted $La_{0.5}Sr_{1.5}NiO_{4+\delta}$ catalyst exhibits a mass activity of 588 mA $\mathrm{mg_{ox}^{-1}}$ $\mathrm{mg_{ox}^{-1}}$ and 7.85 A $\mathrm{mg^{-1}\ cm_{ox}^{-2}}$ $\mathrm{mg^{-1}\ cm_{ox}^{-2}}$ for the electrooxidation of urea in 1 M KOH containing 0.33 M urea, demonstrating the potential applications of Ni-based Ruddlesden-Popper materials for direct urea fuel cells and low-cost hydrogen production.[1] Additionally, we find the same correlations between Ni oxidation state and activities for the electrooxidations of methanol and ethanol, as well as identify processes that result in catalyst deactivation for all three oxidations. This demonstration of how systematically increasing Ni – O bond covalency by raising the formal oxidation state of Ni above +3 serves to increase catalyst activity for these reactions acts as a governing principle for the rational design of catalysts for the electrooxidation of urea and other small molecules going forward [2]

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Professor Stevenson is Full Professor and Provost at the Skolkovo Institute for Science and Technology in Moscow, Russia. His interests are aimed at elucidating and controlling chemistry at interfaces vital to many energy storage and energy conversion technologies. He has published over 280 papers, six patents, and six book chapters. He is the founding director of Skoltech's Center for Energy Science and Technology. In 2019, Skoltech became the youngest university in the world and only university in the Russian Federation to be ranked in top 100 Nature Index of Top Young Universities.

Electrochemical synthesis of copolymers containing porphyrine derivatives and their activity towards CO_2

Sachin Kochrekar,[1,2] Ajit Kalekar,[2] Shweta Mehta,[3,4] Pia Damlin,[2] Mikko Salomäki,[2] Sari Granroth,[5] Niko Meltola,[6] Kavita Joshi,[3,4] Carita Kvarnström[2]

[1]*Turku University Graduate School (UTUGS) Doctoral Programme in Physical and Chemical Sciences, FI-20014 Turku, Finland*

[2]*Turku University Centre for Materials and Surfaces (MatSurf), Department of Chemistry, University of Turku, Vatselankatu 2, FI-20014 Turku, Finland.*

[3]*Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune 411008 India.*

[4]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-200112, UP, India.*

[5]*Laboratory of Materials Science, University of Turku, FI-20014, Turku, Finland.*

[6]*ArcDia International Oy Ltd, Lemminkäisenkatu 32, FI-20521-Turku, Finland.*

carkva@utu.fi

This study reports the electropolymerization of novel keto functionalized octaethyl metal porphyrins (Zn^{+2} and Ni^{+2}) in presence of 4,4 bipyridine (4,4´ BPy) as bridging nucleophile on FTO surface. The polymer films were characterized by electrochemical, spectroscopic (UV-Vis, XPS, FT-IR and Raman spectroscopy) and microscopic (AFM and SEM) techniques. The absorption and electronic spectra establish the binding of monomer units in the polymer film, retaining most of the spectroscopic properties of the monomer with slight shift and peak broadening. The surface morphology reveals heterogeneous polymerization. Through computational studies, we aim to get insight into the effect of metal center (Zn^{+2} and Ni^{+2}) and presence of the keto group on the porphyrin unit. The first 4,4´ BPy prefers meso position next to β-keto group in ZnOEPK whereas it prefers opposite meso position in NiOEPK further leading to linear and branched orientation with the introduction of second 4,4´ BPy, respectively. The interaction between the polymer films in the absence and presence of CO_2 suggests a similar mechanism for both the polymers. The role of the 4,4´ BPy in the polymer unit in association with the activity with CO_2 is emphasized.

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Carita Kvarnström

Professor of Materials Chemistry

Department of Chemistry

University of Turku

Finland

1996 PhD, Åbo Akademi University, Åbo-Turku Finland

1996-2008 Assistant and Associate Professor, Åbo Akademi University, Åbo-Turku Finland

2009- Full Professor in Materials Chemistry University of Turku, Finland

2010-2014 Director for Turku University Centre for Materials and Surfaces

2017-2016 Head of Laboratory of Materials and Chemical Analysis

2017- 2019 Head of Department

Honors or Awards

1996 The Alftan prize for meritorious thesis published awarded by The Finnish Chemists Society

1996 The Elvings prize for the best thesis published at the Åbo Akademi University

1997 Representative for Finland at Scientia Europea 2. Organized by Académie des Sciences (French Academy of Sciences) France.

2006 The Pehr Brahe prize for meritorious research work awarded by the Foundation of Åbo Akademi University.

2020 Member of Finnish Academy of Science and Letters

Research Interests

Conjugated polymers, composite materials, graphene and graphene oxide, ionic liquids, CO_2 conversion, in situ spectroelectrochemistry, electrochemistry

Publications; 137 peer reviewed international scientific journals, 3 patent applications

Positronium emission from materials for Li-ion batteries

Bernardo Barbiellini[1,2*], Jan Kuriplach[3]

[1]*School of Engineering Science, LUT university, Lappeenranta 53851, Finland*

[2]*Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA*

[3]*Department of Low Temperature Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, CZ-180 00 Prague, Czech Republic*

bernardo.barbiellini@lut.fi

A positron and an electron annihilate into gamma-ray photons but before this annihilation, the positron and an electron can bind together to form a positronium (Ps). Mono-energetic positron beams can be used to bombard materials and to probe their atomistic properties. In particular, the implanted positron can diffuse back to the surface of a solid and be emitted as Ps with a range of kinetic energies that provides key information regarding the energy levels of the electrons in the material. These energies can be measured by time of flight (TOF) experiments, but the Ps lifetime before annihilation has been too short for precise measurements. Recently, Jones et al. [1], by exciting the emitted Ps with a laser to greatly increase its lifetime, obtained TOF measurements with an ultimate precision of the order of 5 meV that will allow materials simulations in systems pertinent for Li-ion batteries cathodes [2,3].

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The role of nitrogen and oxygen in the formation capacity of carbon materials

Evlashin S.A.[1,*], Fedorov F.S.[1], Dyakonov P.V. [1,2], Maksimov Yu.M.[2], Pilevsky A.A.[2], Maslakov K.I.[2], Akhatov I.Sh.[1]

1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Lomonosov Moscow State University, Moscow, Russia

s.evlashin@skoltech.ru

Carbon materials are attracting increasing attention as a material for supercapcitor fabrication due to availability and high specific surface area. However, the initial capacitance of raw carbon is quite low, so the N and O heteroatoms are introduced in order to increase their specific capacitance. Despite the vast amount of studies on carbon materials, a lot of grey areas in mechanisms that lead to the increase in the specific capacitance remain. We demonstrate an effective method for modification of the surface of Carbon NanoWalls (CNWs) using DC plasma in atmospheres of O_2, N_2, and their mixture. Processing in the plasma leads to the incorporation of ~4 atom % nitrogen and ~10 atom % oxygen atoms. Electrochemical measurements reveal that CNWs functionalized with oxygen groups are characterized by higher capacitance. The specific capacitance for samples with oxygen reaches 8.9 F cm^{-3} at a scan rate of 20 mV s^{-1}. In contrast, the nitrogen-doped samples demonstrate a specific capacitance of 4.4 F cm^{-3} at the same scan rate. The mechanism of heteroatom incorporation into the carbon lattice is explained using density functional theory calculations.

Acknowledgement. This work was supported by the Russian Science Foundation, grant 17-19-01787.

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Nickel-Nitrogen active sites towards selective High-rate CO_2-to-formate electroreduction

Cristina Flox[1], Fatemeh Davodi[1], Davide Pavesi[2,3] and Tanja Kallio[1]

1 - Department of Chemistry and Materials Science, School of Chemical Engineering, Aalto University, FI-00076, Espoo, Finland

2 -Avantium Chemicals BV, Zekeringstraat 29 1014 BV Amsterdam, The Netherlands

3 -Leiden Institute of Chemistry, Leiden University, PO Box 9502, 2300 RA, Leiden, The Netherlands

cristina.flox@aalto.fi

Electrochemical CO_2 reduction reaction is a key technology for the mitigation of the climate change. However, CO_2 reduction is highly energetic and unfavourable electrochemical reaction, requiring catalyst to achieve economically appealing performance. In this scenario, Nickel-Nitrogen (Ni-N)-active sites within porous carbon are attracting increasing interest as inexpensive and efficient electrocatalyst of CO_2 reduction. In fact, the Ni-N- active sites anchored to the carbon structures have been proposed as excellent solution for the conversion CO_2-to-CO, exceeding selectivity and partial current density values of the commercial electrocatalyst. Herein, the *in-situ* creation of Ni-N-active sites using Nickel Carbide nanoparticles-wrapped in a graphene shell (Ni_3C@graphene NPs) and Emeraldine as precursors in combination with the thermal treatments is evaluated. As a result, the Ni-N- active sites in combination with Ni_3C@graphene NPs provide a new paradigm, where the formate production is dominated leading a complete deactivation of CO route. Surprisingly, the unprecedent key performance indicators of the CO_2 reduction showed a Faradaic Efficiency up to 90% at 0.55V vs. RHE at 25ºC. Additionally, the CO_2-to-formate conversion showed a temperature sensitive- dependence, increasing the selectivity (up to 96%) in the voltage range tested (0.45 to 0.7V vs. RHE), when the electrolysis was performed at 40ºC. The apparent Energy Activation values were calculated, attaining values up to 45 kJ mol^{-1} at -0.55 V vs. RHE@40ºC, which agrees well with previous reports. Therefore, the creation of Ni-N- active sites in the Ni_3C@graphene NPs can effectively reduce the energy barrier towards the CO_2-to formate conversion, providing new mechanism insight for the CO_2 reduction.

Cristina Flox received her PhD in Electrochemistry applied to flow reactors from Universitat de Barcelona in 2008, followed by postdoctoral fellowships in LEITAT and Catalonia Institute for Energy Research, Spain (2008-2017). Subsequently, she joined Aalto University in 2017, working on the design of innovative nanomaterials for energy applications. Particularly, she is focused on the development of electrodes for CO_2 reduction and solid-electrolytes for lithium-ion batteries. Additionally, her research interest are fundamental aspects on energy storage systems, especially redox/semi-solid flow batteries, supercapacitors and Na-ion batteries. She published more than 47 refereed articles (h index 23, 2025 citations), 3 book chapters and 1 patent application.

Development of materials for electrochemical bio-sensing

Koskinen J[1]., Wester N[1]., Etula J[1]., Mynttinen E[2]., Laurila T[2].
[1]*Aalto University, School of Chemical Engineering, Espoo, Finland*

[2]*Aalto University, School of Electrical Engineering, Espoo, Finland*

Jari.Koskinen@aalto.fi

Bio-sensing by applying electrochemical measurements offers several benefits in development of fast and simple devices. They have been investigated for detection of neural transmitters (e.g. dopamine) and recently for detection of drug molecules in blood samples. In this presentation the development of electrode materials made of thin amorphous carbon films and single wall carbon nanotube networks are reported. Layered structures prototype thin film sensors applying perm selective nafion top coatings are also demonstrated. Sensitivity and selectivity for bio-molecules detection in physiologically relevant concentrations has been demonstrated for analytes such as opioids and other analgesics together with most relevant interfering molecules.

Acknowledgement. This work was supported by Business Finland (FEDOC 211637 and FEPOD 2117731 projects), Aalto CHEM Doctoral School and Orion Research Foundation Sr for funding. The authors acknowledge the provision of facilities by Aalto University OtaNano−Micronova Nanofabrication Center and Aalto University Raw materials Infrastructure.

Prof. **Jari Koskinen** is professor of Materials Science at Aalto University, School Chemical Engineering. He has an experience of over 35 years in the field of surface engineering and in particular on development of carbon nanomaterials and coatings. He has over 180 international publications of the topic. He is leading a research group: “Physical properties surfaces and interfaces”. The main impact of his research in material science are in the field of tribology and currently in electrochemical bio-sensing. Currently he is head of the Department of Chemistry and Materials Science. His H-index is 28.

Defects in olivine-type cathode materials for Li-ion batteries

Trussov I. A.[1], Nazarov E. E.[1], Aksyonov D. A.[1], Fedotov S. S.[1]
1 – Skolkovo Institute of Science and Technology, Moscow, Russia
s.fedotov@skoltech.ru

$LiFePO_4$ is a commercialized cathode material ensuring wide applications of Li-ion battery technology for stationary energy storage and renewable energy sources. Regardless of the obvious simplicity of its crystal structure and chemical composition, $LiFePO_4$ holds astonishing defects chemistry arising from the rearrangement of cations and vacancies within tetrahedral and octahedral sites, variations in their occupancies and iron oxidation state. It was demonstrated that so-called "Li-rich" phases might form with the Li excess being located at the Fe sites reaching up to 10%. At the same time the polyanion sublattice was rarely considered defective. It was taken for granted that the PO_4 group is highly durable, with no defects being possible at the P site.

In this talk, we will concentrate upon various old and new defect peculiarities in $LiFePO_4$ and its Li-rich counterpart studied by combined X-ray and neutron diffraction methods coupled with high-throughput DFT and MD calculations. The recently discovered cations arrangements and off-stoichiometry in $LiFePO_4$ due to a partial replacement of Fe with Li atoms or PO_4 with hydroxyl groups for hydrothermally prepared samples at different synthesis conditions will be discussed. Such off-stoichiometries can reach over 10% yielding $Li_{1+x}Fe_{1-x}PO_4$ ($x \leq 0.1$) and $Li_{1-x}Fe_{1+x}(PO_4)_{1-y}(OH)_{4y}$ ($x \leq 0.05$, $y \leq 0.1$) solid solutions respectively. Both Li and OH-substitutions trigger essential changes in the crystal structure and properties, increasing the migration barriers for Li ions and affect the electrochemical performance. We demonstrated that the off-stoichiometry significantly depends on the precursors and reducing agent concentrations and the order of mixing thereof, rendering them critical parameters that control the defects formation of the hydrothermally synthesized $LiFePO_4$-based cathode materials.

More data on the crystal structure and properties of Li-rich $LiFePO_4$ and OH-substituted $LiFePO_4$ as well as the interrelation between "new" and "old" defects in synthetic phosphates and natural olivine-type minerals will be presented and analyzed.

Acknowledgement. This work was supported by the Russian Foundation for Basic Research, grant 18-29-12097.

Ceramic fuel cell fabrication trend from conventional methods to digital printing

Muhammad Imran Asghar[1,2], Peter D. Lund[1]

1. *New Energy Technologies Group, Department of Applied Physics, Aalto University School of Science, P. O. Box 15100, FI-00076 Aalto, Espoo, Finland.*
2. *Faculty of Physics and Electronic Science, Hubei University, Wuhan, Hubei, 430062, China.*

imran.asghar@aalto.fi

Ceramic fuel cell, a.k.a. solid oxide fuel cell, has been emerging as a clean energy technology [1-3]. Researchers of the fuel cell community have been reporting promising electrode and electrolyte materials for the fuel cell since many decades. Many researchers reported fabrication of their cells using power-press methods [4,5]. Although this method is good for the small-scale research studies, this method is not suitable for large-scale upscaling of the technology. The current state-of-the-art ceramic fuel cells are manufactured using tape-casting and screen-printing techniques. Other techniques such as pulse laser deposition, spraying techniques, atomic layer deposition, physical and chemical vapor deposition methods, have been reported as well. Recently, the fabrication of ceramic fuel cell fabrication have been reported using ink-jet and 3D printing techniques. These low-cost printing techniques could solve many issues faced by the promising fuel cell technology. In this study, an overview on the trend of the ceramic fuel cell fabrication and their effects on the cell performance and stability will be presented. The key challenges related to the conventional and 3D fabrication will be highlighted in the work.

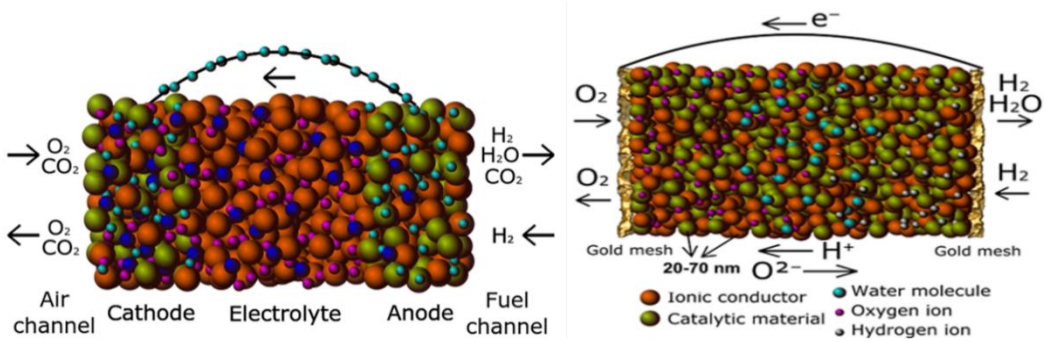

Figure 1: left) Traditional 3-layer ceramic nanocomposite fuel cell, right) so called “single-layer” ceramic fuel cell.

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Oral Sessions

Friday,

October 9

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ул. Криворожская, д. 23, корп. 3

Тел.: +7 495 374 04 01
E-mail: sales@imc-systems.ru
www.imc-systems.ru

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Nonlinear Optics with Nanomaterials

Zhipei Sun[1,2]

1. *Department of Electronics and Nanoengineering, Aalto University, Finland*
2. *QTF Centre of Excellence, Department of Applied Physics, Aalto University, Finland*

zhipei.sun@aalto.fi

In this talk, I will discuss our recent results on nonlinear optics with one-dimensional (e.g., carbon nanotubes and nanowires [1]) and two-dimensional layered (e.g., graphene [2-3], transition metal dichalcogenides [3-5], and black phosphorus [6-7]) materials. These results show advantages of utilizing low-dimensional nanomaterials for various photonic and optoelectronic applications, such as high-purity quantum emitters [1], wavelength converters [2-5], and actively [8] and passively [2,6,7] mode-locked ultrafast lasers. Further, I will present our recent advances employing hybrid structures, such as two-dimensional heterostructures [2], plasmonic structures [8-10], and silicon/fibre waveguides integrated structures [8-10].

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Zhipei Sun is Professor of Photonics and the head of the Photonics Research Group at the Department of Electronics and Nanoengineering of Aalto University, Finland. He earned his PhD from Institute of Physics, Chinese Academy of Sciences, in 2005. Currently, he is actively involved with European quantum flagship, Academy of Finland Photonics Flagship and Academy of Finland Centre on quantum technology projects. Recently, he received a European Research Council Advanced Grant for his work on nanomaterials based photonics. His research interests include nonlinear optics, nanophotonics, and ultrafast photonics. In particular, he focuses on carbon nanotubes, graphene, and other two-dimensional layered materials for photonics and optoelectronics.

Aerosol synthesized carbon nanotube thin films for nonlinear optical applications

Yuriy Gladush, [1] Aram Mkrtchyan, [1] Diana Galiakhmetova, [1] Georgy Ermolaev, [2] Eldar Khabushev, [1] Dmitry Krasnikov, [1] Albert Nasibulin[1]

[1]*Skolkovo Institute of Science and Technology, Nobel St. 3, Moscow, Russia*

[2]*Center for Photonics and 2D Materials, Moscow Institute of Physics and Technology, Dolgoprudny 141700, Russia*

Y.Gladush@skoltech.ru

Single walled carbon nanotubes (SWCNTs) are known to demonstrate high third order optical nonlinearity. Applications in this field requires high power illumination which may cause damage of SWCNT thin film. In the presentation we discuss the application of aerosol synthesized SWCNTs for short pulse generation in the fiber lasers with emphasis on the stability of the SWCNT saturable absorber. We compare the PVA/SWCNT composites and polymer-free SWCNTs and demonstrate that different types of saturable absorber implementation result in different mechanisms of degradation. This investigation provides a root for a stable and efficient saturable absorber for a short pulse generation. In the second part of the talk we discuss the carbon nanotubes nonlinear properties in evanescent field interaction geometry when carbon nanotubes are deposited on top of the waveguide. We demonstrate that we can control the nonlinear response of the SWCNT saturable absorber by electrochemical gating and switch pulse generation regimes in the fiber laser. Finally, we discuss other nonlinear optical effects with carbon nanotubes.

Acknowledgement. This work was supported by a grant of Russian Science Foundation (No. 17-19-01787).

Yuriy Gladush is a senior research scientist in Laboratory of Nanomaterials of Skoltech. His research area is optics and laser physics. In Nanomaterials lab Yuriy is responsible for projects related to optical properties of carbon nanotubes and other nanomaterials and its application for fiber laser ultrashort pulse generation, photoresponce, etc. Prior to Skoltech Yuriy was working in Institute of spectroscopy where his research was dedicated to resonance energy transfer in organic/inorganic semiconductor hybrid structures. His PhD, obtained in the same institute, was related to theoretical investigation of nonlinear wave phenomena in Bose-Einstein condensates and optics.

Individual SWCNT Transistor with Photosensitive Planar Junction Induced by Two-Photon Oxidation

Emelianov A.V.[1], Nekrasov N.P.[1], Nevolin V.K.[1], Bobrinetskiy I.I.[2]
1 – National Research University of Electronic Technology, Zelenograd, Moscow, Russia

2 – BioSense Institute, University of Novi Sad, Novi Sad, Serbia

emmsowton@gmail.com

The fabrication of planar junctions in carbon nanomaterials is a promising way to increase the optical sensitivity of optoelectronic nanometer-scale devices in photonic connections, sensors, and photovoltaics [1]. Utilized a unique lithography approach based on direct femtosecond laser (fs-laser) processing [2], a fast and easy technique for modification of single-walled carbon nanotube (SWCNT) optoelectronic properties through localized two-photon oxidation is developed. It results in a novel approach of quasi-metallic to semiconducting nanotubes conversion so that metal/semiconductor planar junction is formed via local laser patterning.

In this study, we demonstrate the application of newly developed technology based on two-photon oxidation of carbon nanostructures upon ultrafast laser pulses for bandgap engineering of individual SWCNT [3]. The array of field-effect transistors (FETs) with individual SWCNT channels on a 4-inch substrate was fabricated through a versatile chemical vapor deposition technique and directly placed on the substrate with desired density. Fs-laser processing was used to form a local planar junction in individual SWCNT under standard conditions.

The fabricated planar junction in FETs based on individual SWCNT drastically increases the photoresponse of such devices. The broadband photoresponsivity of the two-photon oxidized structures reaches the value of $2 \cdot 10^7$ A W^{-1} per single SWCNT at 1 V bias voltage. The SWCNT-based transistors with induced metal/semiconductor planar junction can be applied to detect extremely small light intensities with high spatial resolution in photovoltaics, integrated circuits, and telecommunication applications.

Acknowledgement. This work was supported by the Russian Science Foundation, grant № 19-19-00401.

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Strategies to optimize the optoelectronic performance of patterned single-walled carbon nanotube layers

Mitin D.M.[1,2], Berdnikov Y.S.[3], Vorobyev A.A.[1], Mozharov A.M.[1], Raudik S.A.[1,4], Ilatovskii D.A.[4], Nasibulin A.G.[4,5], Mukhin I.S.[1,3]

1 – Saint Petersburg Academic University, St. Petersburg, Russia

2 – Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia

3 – ITMO University, St. Petersburg, Russia

4 – Skolkovo Institute of Science and Technology, Moscow, Russia

5 – Aalto University, Espoo, Finland

mitindm@mail.ru

We report on the theoretical and experimental study of patterned layers of single-walled carbon nanotubes and suggest strategies aimed at the relief the trade-off between high transmittance and high conductivity of the nanotube-based transparent electrodes. We present the model to predict the characteristics of patterned films and demonstrate its consistency with the experimental observations. We extend these results to show that the best characteristics of patterned layers of single-walled carbon nanotubes can be achieved using the combination of films with low initial transmittance and high conductivity. That is the opposite to earlier reported approaches to improve the performance of nanotube-based electrodes. The proposed strategy allows the patterned layers of single-walled carbon nanotubes to outperform the widely used indium-tin-oxide electrodes on both flexible and rigid substrates.

Acknowledgement. This work was funded by RFBR, project number 19-38-60008.

Graphene for laser applications

E. D. Obraztsova [1,2*], A.V. Tausenev[3], M.G. Rybin[1,2], Bykov A.Y. [4], Murzina T.V. [4], Sorochenko V. R.[1], P.A. Obraztsov[1]

[1]A.M. Prokhorov General Physics Institute, RAS, 38 Vavilov str., 119991, Moscow, Russia
elobr@kapella.gpi.ru
[2] Moscow Institute of Physics and Technology, 9 Institutskiy per., 141701 Dolgoprudny, Russia
[3] OOO "Avesta Proekt", 108840 Troitsk, Russia
[4] M.V. Lomonosov Moscow State University, Physics Department, Moscow, Russia
elobr@kapella.gpi.ru

Graphene is a two-dimensional hexagonal carbon network with unique physical and chemical properties. This material can be efficiently used in optics. The working spectral range of graphene is very wide: from 0.4 mkm up to 12 mkm (at least). The optical absorption is 2.3 % (per 1 layer). This property opens a possibility to form the saturable absorbers for mid -IR lasers [1]. Due to a high optical non-linearity graphene can be used for frequency multiplication in lasers [2]. Compactness of graphene saturable absorber providing realization of stable self-starting mode-locking operation in a diode-pumped waveguide Nd:YAG laser delivering picoseconds pulses at the repetition rates up to 11.5 GHz with an average power of 12 mW at a central wavelength of 1064 nm [3].

In this work we demonstrate the progress made for lasers of different wavelengths (from 1.5 to 10.5 mkm) with graphene saturable absorbers. The problems and possible further applications are discussed.

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Dr. Elena Obraztsova,
Head of Nanomaterials Spectroscopy Laboratory of
A.M. Prokhorov General Physics Institute of
Russian Academy of Sciences ,
38 Vavilov street,
119991, Moscow, Russia
Ph.: +7(906)097 3331
FAX: +7(499) 135 3002
elobr@kapella.gpi.ru

Obraztsova Elena Dmitrievna was graduated from the Faculty of Physics of M.V. Lomonosov Moscow State University (MSU) in 1975. She got her PhD degree in MSU in 1990 with specialty 01.04.05 "Optics". Since1992 she works in the Department of light-induced surface phenomena of A.M, Prokhorov General Physics Institute of RAS (GPI RAS). Since 2002 she is a head of the newly created Nanomaterials spectroscopy laboratoriy in GPI RAS.. Currently lab employs more than 20 people (10 full-time employees, 3 PhD students, 3 graduate students, the rest - students of the Physics department of MSU and Moscow Institute of Physics and Technology).

Scope of scientific interests of E.D. Obraztsova includes synthesis, optical spectroscopy (Raman scattering, optical absorption in a wide spectral range, photoluminescence spectroscopy, nonlinear optical spectroscopy) and applications of various low-dimensional materials (especially carbon materials: diamond, graphite, diamond-like amorphous materials, fullerenes, onion-like structures, one-, two- and multi-walled carbon nanotubes, carbon pods, carbon nanotubes, graphene and graphene nanoribbons). In recent years, a great progress has been made in the application of single-walled carbon nanotubes and graphene in vacuum electronics and nonlinear optics.

E.D. Obraztsova is a co-author of more than 300 articles in peer-reviewed scientific journals. In the past 5 years, she has participated in many (more than 30) Russian and international scientific conferences and seminars with the invited talks. Her citation factor for her scientific papers (Hirsch factor) is 34. Under her supervising 13 PhD theses has been defended.

In 2018 E. D.. Obraztsova won the grant for creation of a new Laboratory of nanocarbon materials in the Moscow Institute of Physics and Technology (MIPT) in frame of the program of creating joint laboratories of MIPT and Russian Academy of Sciences (project “5- 100"). Since August 2018 she is a Head of this laboratory with 15 scientist staff (in parallel to her work in GPI RAS).

Obraztsova E.D. is a member of the program committees of international conferences and seminars (Annual International Euroconference “Electronic Properties of New Materials (IWEPNM)” (http://www.iwepnm.org) and “International Scientific Workshop on Photonics and Optoelectronics of Nanocarbon”, held every 2 years in Finland (http://www.npo.fi). She is a member of Editoral Board of international scientific journals: “Carbon”, “Nanomaterials”, “Laser Physics Letters”.

Functional Halide Perovskite Nanostructures

Makarov S.V.
ITMO University, Saint Petersburg, Russia

s.makarov@metalab.ifmo.ru

Nanophotonics and meta-optics based on optically resonant all-dielectric structures is a rapidly developing research area driven by its potential applications for low-loss efficient metadevices. Recently, the study of halide perovskites has attracted enormous attention due to their exceptional optical and electrical properties. As a result, this family of materials can provide a prospective platform for modern nanophotonics [1] and meta-optics [2], allowing us to overcome many obstacles associated with the use of conventional semiconductor materials. Here, we review the recent progress in the field of halide perovskite nanophotonics starting from single-particle light-emitting nanoantennas [3,4] and nanolasers [5] to the large-scale designs working for surface coloration, anti-reflection, and optical information encoding [6,7,8].

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Sergey Makarov received a Ph.D. degree in 2014 at the Lebedev Physical Institute of the Russian Academy of Sciences (Moscow, Russia), and Habilitated at the ITMO University (St. Petersburg, Russia). The topics of his research activity include nanophotonics, halide perovskites, laser-matter interaction, and nanotechnology.

Currently, he is Professor, Head of Laboratory of Hybrid Nanophotonics and Optoelectronics, as well as Director of Shared Research Facilities on Nanotechnology at the ITMO University. He was a long-term visiting research fellow at Australian National University, City University of New York, and Vienna Technological University. He was awarded by Presidential Award for Young Researchers, Medal of Russian Academy of Sciences for Young Researchers, Gold Medal of Alferov's Foundation, Saint-Petersburg Government Award in the field of technology, and many others.

Referee in journals: Advanced Materials, Materials Today, ACS Nano, Nature Communications, Advanced Functional Materials, Nano Letters, Angewandte Chemie, etc. Referee for grant agencies Russian Science Foundation, Czech Science Foundation. Chair of Program Committee of International Conference "METANANO 2017", permanent chair of School on Advanced Light-Emitting and Optical Materials (SLALOM), and co-organizer of special sessions in many conferences.

Nanophotonic molecular engineering of functional quantum dots and biomedical structures

B.H. Bairamov[1,2], V.V. Toporov[1], F. B. Bayramov[2], E.D. Poloskin, and H. Lipsanen[3]

[1]*Ioffe Institute of the Russian Academy of Sciences, 194021 Saint-Petersburg, Russia*

[2]*Alferov Federal State Budgetary Institution of Higher Education and Science Saint Petersburg National Research Academic University of the Russian Academy of Sciences, 194021 Saint-Petersburg, Russia*

[3]*Aalto University, Department of Micro- and Nanosciencies, Micronova, P.O.Box 13500, FI-00076, Aalto, Finland*

bairamov@mail.ioffe.ru

Exploiting strong-light matter interactions at the nanometer scale are increasingly important for modern emerging fields of nanophotonics and nanophononics. Fundamental research issues in a topical area of engneered nanostructure materials science having technological relevance will be addressed.

We present several novel phenomena observed in an all-optical non-destructive and ultra-sensitive study of a high spectral resolution inelastic light scattering measurements in doped semiconductors, a wide range of nanostructures (NSs) – quantum dots (QDs) and nanowires (NWs), biomedical structures (proteins, DNAs) as well as semiconductor QDs functionalized by DNAs. Biomedical researches have become one of the most promising applications of the NSs.

It is shown that for the most effective study of the novel fundamental crystalline and electronic properties of the NSs with multiple electronic and vibrational states created in the NSs with the well controllable and dynamically selected radiative and non-radiative transitions using different energy transfer pathways can be tailored by manipulating the geometry and size of the NSs for the suitable excitation laser light parameters selected.

The developed approaches combined with the strong quantum confinement effects observed by us in the semiconductor NSs allowed to find unprecedented multiple resonance energy transfer pathways in the study of the artificial complex mixtures of the QDs dots functionalized by the DNAs. In this case, a selective light scattering enhancement by the single molecule of the DNA is discovered. Semiconductor QDs functionalized by the biomedical structures with unique light-matter interaction properties have turn out to be are one of a particularly important class of novel materials for molecular engineering. It is established that the QDs iself can be used at the nanoscale as a flexible quantum interface allowing to improve sufficiently bimolecular recognition. Based on these results, the obtained new knowledge of organic-inorganic nanostructures can help for to develop practical approaches to tailor many interesting innovative nano-optoelectronic capabilities in a broader perspective for future applications.

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Dimensional confinement and waveguide effect of Dyakonov surface waves in twisted confined media

D. A. Chermoshentsev [1,2,3], E. V. Anikin[1], S. A. Dyakov[1], N. A. Gippius[1]

1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Moscow Institute of Physics and Technology (SU), Moscow Region, Dolgoprudny, Russia

3 – Russian Quantum Center, Moscow, Russia

dmitry.chermoshentsev@skoltech.ru

We theoretically study Dyakonov surface waveguide modes that propagate along the planar strip interfacial waveguide between two uniaxial dielectrics. We demonstrate that due to the one-dimensional electromagnetic confinement, Dyakonov surface waveguide modes can propagate in the directions that are forbidden for the classical Dyakonov surface waves at the infinite interface. We show that this situation is similar to a waveguide effect and formulate the resonance conditions at which Dyakonov surface waveguide modes exist. We demonstrate that the propagation of such modes without losses is possible. We also consider a case of two-dimensional confinement, where the interface between two anisotropic dielectrics is bounded in both orthogonal directions. We show that such a structure supports Dyakonov surface cavity modes. Analytical results are confirmed by comparing with full-wave solutions of Maxwell's equations. We believe that our work paves the way towards new insights in the field of surface waves in anisotropic media.

Acknowledgement. This work was supported by the Russian Foundation for Basic Research (Grant № 18-29-20032)

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Macro-, Micro- and Nano-Roughness of Carbon-Based Interface with the Living Cells: Towards a Versatile Bio-Sensing Platform

Lena Golubewa [1,2], Hamza Rehman [3], Tatsiana Kulahava [2,4], Renata Karpicz [1], Marian Baah [3], Tommy Kaplas [3], Ali Shah [5], Sergei Malykhin [3,6,7], Alexander Obraztsov [3,7], Danielis Rutkauskas [1], Marija Jankunec [8], Ieva Matulaitienė [1], Algirdas Selskis [1], Andrei Denisov [4,9], Yuri Svirko [3] and Polina Kuzhir [2,3,*]

[1] *Center for Physical Sciences and Technology, Sauletekio Ave. 3, LT-10257 Vilnius, Lithuania; lena.golubewa@ftmc.lt (L.G.); renata.karpicz@ftmc.lt (R.K.); danielis@ar.fi.lt (D.R.); ieva.matulaitiene@ftmc.lt (I.M.); algirdas.selskis@ftmc.lt (A.S.)*

[2] *Institute for Nuclear Problems, Belarusian State University, Bobruiskaya 11, 220030 Minsk, Belarus; tatyana_kulagova@tut.by*

[3] *Institute of Photonics, University of Eastern Finland, Yliopistokatu 2, FI-80100 Joensuu, Finland; hamzarehman241@gmail.com (H.R.); marian.baah@uef.fi (M.B.), tommi.kaplas@gmail.com (T.K.); sermal92@mail.ru (S.M.); alexander.obraztsov@uef.fi (A.O.); yuri.svirko@uef.fi (Y.S.)*

[4] *Department of Biophysics, Belarusian State University, Nezavisimosti ave. 4, 220030 Minsk, Belarus; an.denisov@gmail.com*

[5] *Department of Micro and Nanosciences, Aalto University, Espoo, P.O. Box 13500, FI-00076, Finland; ali.shah07@outlook.com*

[6] *Division of Solid State Physics, Lebedev Physical Institute of the Russian Academy of Sciences, Leninskiy Prospekt 53, 119991 Moscow, Russia*

[7] *Department of Physics, Lomonosov Moscow State University, Leninskie gory 12–, 119991 Moscow, Russia*

[8] *Institute of Biochemistry, Life Sciences Center, Vilnius University, Sauletekio av. 7, LT-10257, Vilnius, Lithuania; marija.jankunec@gmc.vu.lt*

[9] *Institute of Physiology of the National Academy of Sciences of Belarus, Minsk, Belarus, 28 Akademichnaya Str., Minsk BY-220072, Belarus*

** polina.kuzhir@uef.fi*

Integration of living cells with nonbiological surfaces (substrates) of sensors, scaffolds, and implants implies severe restrictions on the interface quality and properties, which broadly cover all elements of the interaction between the living and artificial systems (materials, surface modifications, drug-eluting coatings, etc). Substrate materials must support cellular viability, preserve sterility, and at the same time allow real-time analysis and control of cellular activity. We have compared new substrates based on graphene and pyrolytic carbon (PyC) for the cultivation of living cells. These are PyC films of nanometer thickness deposited on SiO_2 and black silicon and graphene nanowall films composed of graphene flakes oriented perpendicular to the Si substrate. The structure, morphology, and interface properties of these substrates are analyzed in terms of their biocompatibility. The PyC demonstrates interface biocompatibility, promising for controlling cell proliferation and directional intercellular contact formation while as-grown graphene walls possess high hydrophobicity and poor biocompatibility. By performing experiments with C6 glioma cells we discovered that PyC is a cell-friendly coating that can be used without poly-L-lysine or other biopolymers for controlling cell adhesion. Thus, the opportunity to easily control the physical/chemical properties and nanotopography makes the PyC films a perfect candidate for the development of biosensors and 3D bioscaffolds.

Polina Kuzhir, PhD, senior researcher and a Marie Skłodowska-Curie fellow (H2020-MSCA-IF-2018, TURANDOT, 836816) in the Institute of Photonics, University of eastern Finland. She got her PhD in Theoretical physics in 1996 from the Inst. of Physics, Belarus Academy of Science, Minsk, Belarus. She is internationally recognized expert in the field of graphene/2D materials, theoretical and experimental photonics. Her research focuses on theory and experimental validation of 2D materials-based passive and active devices, including detectors, filters, shields, polarizers, collimators and emitters. She has published 288 peer-reviewed papers with 11535 citations and h-factor of 50 (Scopus 08/06/2020). Dr. Kuzhir is Associate Editor at Microelectronics Reliability, Elsevier, member of International Editorial Boards of IOP and MDPI journals.

Polymer composites, comprising single-atomic-layer graphenic inclusions. Preparation, structure and properties.

Ayrat M. Dimiev

Laboratory for Advanced Carbon Nanomaterials,

Kazan Federal University, Kazan, Russian Federation

dimiev.labs@gmail.com

Doping with conductive inclusions is the most straightforward approach to alter conductivity of dielectric materials. Carbon nanostructures have several advantages as inclusions for their high aspect ratio. However, it is very difficult to uniformly disperse 2D graphenic materials in the polymer matrix. In a series of studies, we have developed the homogeneous liquid phase transfer method, allowing uniform distribution and nearly fully exfoliated condition of GO in the matrix.

Viscosity of the uncured liquid resin increases by 390% after introducing 0.4% GO, and by 4700% after its subsequent in-situ reduction. The latter is explained by the reorganization of the original liquid crystalline structure of the GO-Epoxy formulations with GO reduction. At the filling fractions >0.1%, the single-atomic-layer RGO flakes are assembled into the clusters, where they alternate with a thin resin layer. This structure is also responsible for very unusual dielectric behavior of the cured solid composites. From one side, the real part of the complex permittivity reaches relatively high values at extremely low filling fractions: 14 at 0.1%, and 60 at 0.4% RGO content. At the same time, the permittivity dispersion is accompanied with the well-pronounced symmetrical loss peaks on the imaginary part functions, which is typical for low permittivity materials. Such dielectric behavior is difficult to interpret in the frames of any single existing model. The relaxation time and activation energy, calculated from the temperature dependence experiments, suggest that the RGO clusters, but not individual RGO flakes, serve as conductive inclusions. The extremely long relaxation times are due to the charge transfer between the individual RGO flakes within the clusters. The striking difference between the newly prepared composites and control samples, comprising multi-layer RGO particles, exemplifies the unique structure of our materials.

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Ayrat Dimiev, received his PhD degree in physical chemistry from Kazan State University, Russian Federation. In 2008 he joined the group of Prof. James Tour at Rice University, USA, where he started his works with carbon nanomaterials. In 2013, he accepted a personal invitation to join AZ Electronic Materials (presently EMD Performance Materials Corp., USA, a business of Merck KGaA, Darmstadt, Germany) to help in developing their newly started carbon program. In 2016 Dr. Dimiev returned to his Alma Mater in Kazan as research professor and head of the Laboratory for Advanced Carbon Nanomaterials. Ayrat Dimiev is the first and/or corresponding authors of the well-known publications in the field of graphene oxide.

H_2O molecule in nano-space

M.Belyanchikov[1], M.Savinov[2], Z.Bedran[1], V.Abalmasov[3], E.Zhukova[1], V.Thomas[4], A.Dudka[5], A.Zhugayevych[6], R.K.Kremer[7], P.Lunkenheimer[8], M.Dressel[1,9], B.Gorshunov[1]

1- Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Moscow Region, Russia

2- Institute of Physics, Czech Academy of Sciences, Praha 8, Czech Republic

3- Institute of Automation and Electrometry SB RAS, Novosibirsk, Russia

4- Institute of Geology and Mineralogy, RAS, Novosibirsk, Russia

5- Shubnikov Institute of Crystallography, RAS, Moscow, Russia

6- Skolkovo Institute of Science and Technology, Moscow, Russia

7- Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

8- Experimental Physics V, University of Augsburg, Augsburg, Germany

9- 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

bpgorshunov@gmail.com

The ever-increasing requirements for the characteristics of electronic devices dictate the need for a transition to nanoscales in the production of electronic components. However, the smaller these components are, the harder they are to manufacture. A way to avoid such problems is to manipulate charge/spin states of separate ions or molecules placed in certain frameworks, natural or artificial. Corresponding activities are presently very intensive and include, e.g., studies of single molecular magnets as candidates for quantum computing [1], using extraordinary properties of graphene for building field-effect transistors [2], terahertz detectors [3] or spintronic devices [4], using molecular nanoflakes as gas sensors [5], making use of carbon-based architectures with 0D (fullerenes [6]) or 1D (nanotubes [7]) spaces, empty or filled with ions or molecules. In this talk, we consider the properties of separate water molecules located within sub-nanosized spaces. Recently, we introduced [8] to the community a family of water-containing beryl crystals that allow for the studies of single-particle and collective states of polar (dipole moment 1.85 Debye) H_2O molecules that reside in ≈5 Å diameter voids within crystal lattice. Separated by a distance of 5-10 Å, these molecules only weakly interact with crystal lattice, do not experience H-bonding and strongly interact via electric dipole-dipole coupling thus representing a kind of “new state of water” [9]. Studies of such network not only are of fundamental importance [10,11], they also contribute to deeper understanding of natural phenomena and may even find practical applications in ferroelectric electronics, artificial quantum systems, and biocompatible nanoelectronics.

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Surface characteristics control the attachment and functionality of (chimeric) avidin

Shao D.[1], Tapio K.[1], Auer S.[2], Toppari J.J.[1], Hytönen V.[2], Ahlskog M.[1]
1 – Nanoscience Center and Department of Physics, University of Jyväskylä, Finland

2 – BioMediTech, University of Tampere, Tampere, Finland

ahlskog@jyu.fi

The physical adsorption (physisorption) of proteins to surfaces is an important but uncomplet ely understood factor in many biological processes, and of increasing significance in bionanotechnolo gy as well [1]. Avidin is a most important protein due to the strong avidin-biotin binding which has n umerous applications [2]. We have undertaken thorough experimentation on the physisorption of av idin, to chemically different flat surfaces, Si and graphite, and also to the curved version of the latter, on multiwalled carbon nanotubes (MWNT) of different diameter.

The difference between the behavior of avidin on Si and graphite is drastic, in that on Si avidi n deposits as single globular tetrameric units, while on graphite it forms irregular networks of two la yers thick filaments. On MWNTs avidin also deposits as one dimensional formations, or stripes, but a s opposed to the irregular network appearance on graphite, the cylindrical nanometer sized curvatur e orders the stripes in a perpendicular and quasiperiodical arrangement to the MWNT axis. We also demonstrated the preserved functionality of the deposited avidin with respect to biotin binding.

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Flash Oral

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ScientaOmicron образована слиянием двух ведущих компаний в области производства научного оборудования для анализа поверхности — VG Scienta (Швеция) и Omicron Nanotechnology (Германия). На сегодняшний день, ScientaOmicron является уникальной компанией с наибольшим количеством аккумулированных компетенций в области анализа поверхности и материаловедения.

ООО «Группа Ай-Эм-Си»
Россия, г. Москва,
ул. Криворожская, д. 23, корп. 3

Тел.: +7 495 374 04 01
E-mail: sales@imc-systems.ru
www.imc-systems.ru

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Prussian-blue lipid nanoparticles for effective siRNA delivery to liver

Abakumova T.O.[1], Prikazchikova T.A.[1], Komkova M.A[2], Karyakin A.A.[2], Zatsepin T.S.[1,2]
1-Skolkovo Institute of Science and Technology, Moscow, Russia

2-Lomonosov Moscow State University

t.abakumova@skoltech.ru

Reactive oxygen species (ROS) play an essential role in liver cell damage and the progression of diseases. Therefore, the development of therapeutic strategy that will combine antioxidant and anti-inflammatory activity is an urgent task. For this purpose, we synthesized lipid nanoparticles loaded with Prussian blue nanoparticles (PBNP) and small interfering RNA (siRNA) that will neutralize ROS and effectively deliver siRNA to the hepatocytes. First, we synthesized PBNP with an average diameter 53±10 nm. These nanoparticles demonstrated high catalytic activity (k_{cat} 550-560 s^{-1}) and low cytotoxicity values (AML12, RAW264.7 cell lines). Encapsulation of PBNP and siRNA into lipid nanoparticles led to increase of average diameter up to 90±10 nm and almost no affect catalytic activity (k_{cat} 540 s^{-1}). We also demonstrated that obtained nanoparticles could successfully accumulate in cells (AML12) and neutralize ROS (DCFDA assay, HyPer probe). Taken together, we developed novel hybrid PBNP-lipid nanoparticles that could effectively deliver siRNA to the cells, neutralize ROS and potentially reduce inflammation and the toxicity of lipid particles.

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Fabrication of magnetic graphene oxide and its developmental toxicity to Artemia Salina Cyst and its three larval stage

Che Azurahanim Che Abdullah[1,2], Emmellie Laura Albert [1,2] and Nurul Anis Athirah Ab Aziz[3]

[1]*Materials Synthesis and Characterization Laboratory, Institute of Advance Technology, University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.*

[2]*Department of Physics, Faculty of Science, University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.*

[3]*Department of Physics, Faculty of Science, University Teknologi Malaysia, 80990 0 Skudai, Johor, Malaysia*

azurahanim@upm.edu.my

Current research focusing on the fabrication of magnetic graphene oxide (GO-IO) using graphene oxide (GO) and Iron (III) oxide (IO) via simple emulsion method. GO specialty such as big surface to volume ratio combined with IO superparamagnetic properties produce interesting nanocomposite material for removing pollutant from water [1]. After decontamination, the GO-IO residues can be collected and removed from the water using a magnetic field. Initially, the nanocomposites crystallinity, chemical interaction, structure, surface morphology and magnetic behavior were investigated using X-ray diffraction, Fourier transform infrared spectroscopy, Raman spectroscopy, and Vibrating Sample Magnetization correspondingly. Afterward, the potential effects of GO-IO on marine ecosystems were explored using Artemia salina cysts and larvae (instar I, II and III) as experimental models, hatchability, and mortality were selected as endpoints to define the toxic responses. GO-IO attached onto the gills and body surface, resulting in irreversible damages. The combined results so far indicate that GO-IO have the potential to affect aquatic organisms when released into the marine ecosystems.

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Toxicity evaluation of Herbs based Carbon Dots using Artemia Salina Cyst and its three larval stage

Che Azurahanim Che Abdullah[1,2], Emmellie Laura Albert [1,2] and Muhd Afiq Aizzat Abd Kadir[3]

[1]*Materials Synthesis and Characterization Laboratory, Institute of Advance Technology, University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.*

[2]*Department of Physics, Faculty of Science, University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.*

[3]*Department of Physics, Faculty of Science, University Malaysia Terengganu, 21030 Kuala Terengganu, Terengganu, Malaysia*

emmellielaura@gmail.com

Current research focusing on the fabrication of green synthesis of carbon materials, carbon dots. Nanosized materials may generate harmful physiological effects or potential health risks due to their unique physical and chemical properties. Herein, the toxicity of carbon dots (CDs) from commercial herbs was confirmed through a systematic study. The potential effects of various types of carbon dots on marine ecosystems were explored using Artemia salina cysts and larvae (instar I, II and III) as experimental models, hatchability, and mortality were selected as endpoints to define the toxic responses. Carbon dots expected to attach onto the gills and body surface, resulting in irreversible damages. The combined results so far indicate that there is lower potential to affect aquatic organisms when released into the marine ecosystems.

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Investigation of structural and optical properties of three-dimensional InGaPAs islands

Andryushkin V.V.[1], Gladyshev A.G.[1,2], Dragunova A.S.[3,5], Babichev A.V.[1,2], Nadtochiy A.M.[3,5], Kolodeznyi E.S.[1], Nevedomskii V.N.[4],Novikov I.I.[1,2], Karachinsky L.Ya.[1,2], Kryzhanovskaya N.V.[5] and Egorov A.Yu.[1]

1 – ITMO University, St. Petersburg, Russia

2 – Connector Optics LLC, St. Petersburg, Russia

3 – Saint Petersburg National Research Academic University of the Russian Academy of Sciences, St. Petersburg, Russia

4 – Ioffe Institute, St. Petersburg, Russia

5 – National Research University Higher School of Economics, St. Petersburg, Russia

vvandriushkin@itmo.ru

At present, the creation of single photons sources and micro-emitter arrays has great interest. The best candidates for the role of active region for such emitters are quantum dots (QDs). However, in contrast to typical laser applications where QDs arrays must have a high density, the opposite requirement is imposed on QD arrays in the above applications — low QDs density (less than $1 * 10^{10}$ cm^{-2}) [1]. In this work, we propose a new method to obtain the three-dimensional quantum-sized objects (QD) arrays with reduced surface density formed by elastic transformation of the InGaP layer grown on the GaAs surface.

During the epi-growth QDs were formed by replacement of phosphorus in the InGaP epitaxial layer by As, upon exposure of InGaP layer in the As flow at temperatures of 520-535°C. Using this procedure, a several heterostructures were grown on GaAs (100) substrates by molecular beam epitaxy (MBE). The influence of the InGaP layer thickness, growth temperature, and exposure time in the As flow on optical and structural properties of the formed QDs was studied.

Photoluminescence spectra were measured in the temperature range 77 – 300 K at different optical pump power densities. It was found that when P is replaced with As in a thin InGaP layer, three-dimensional islands are formed with estimated density of $1.3 \cdot 10^{10}$ cm^{-2} and demonstrated the photoluminescence in the spectral range ~1 μm at 300 K. Obtained results are very promising for possible use of proposed QDs in single photon sources and micro-emitter arrays.

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Electrodynamic properties of low-dimensional water

Artemov V.G.
Center for Energy Science and Technology, Skolkovo Institute of Science and Technology, Moscow, Russia

v.artemov@skoltech.ru

Interfacial (low-dimensional) water is ubiquitous in nature. It is a media where catalytic reactions, ion exchange, and phase transformations take place. Although these processes are key to understanding the most challenging questions of physical chemistry, our knowledge of the low-dimensional water is quite limited.

We discuss the electrodynamic properties of interfacial water confined in nano-pores of various sizes, ranging from 5 nm to 5 μm in diameter [1], and compare them with those for bulk water [2]. We show that the short-order nanoscale molecular dynamics in water governs the electrodynamic properties of interfacial and confined water. Using the infrared spectroscopy, we find that short-living ions, with concentrations of 2%, coexist in water with long-living pH-active ions [3]. We assume that short-living ionic species govern the electrodynamics of low-dimensional water, resulting, for example in anomalous high DC conductivity, five orders of magnitude higher than that of the bulk water [2].

Our results shed light on the physical and chemical properties of both interfacial and bulk water, as well as pave the way to the development of new type of highly-efficient proton conductors for applications in electrochemical energy systems, membrane separations devices and nano-fluidics.

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Terahertz-infrared excitations in the $Ba_{0.2}Pb_{0.8}Al_{1.2}Fe_{10.8}O_{19}$ single crystal

Asmaa Ahmed[1], Anatoly S. Prokhorov [1,2], Vladimir Anzin [1,2], Denis Vinnik[3], Alexander Bush[4], Boris Gorshunov[1], Liudmila Alyabyeva[1]

1-Laboratory of Terahertz Spectroscopy, Center for Photonics and 2D Materials, Moscow Institute of Physics and Technology (State University), 9 Institutskiy per., Dolgoprudny, Russia

2-Prokhorov General Physics Institute of the Russian Academy of Sciences, 38 Vavilov Str, Moscow, Russia

3-South Ural State University, 76 Lenin prospect, Chelyabinsk, Russia

4-Research Institute of Solid State Electronics Materials, MIREA – Russian Technological University (RTU MIREA), 78 Vernadsky prospect, Moscow, Russia

a.gamal@phystech.edu

The single-crystalline M-type hexaferrite with double-cation substitution $Ba_{0.2}Pb_{0.8}Al_{1.2}Fe_{10.8}O_{19}$ [1] was investigated using methods of terahertz and infrared spectroscopy. The spectra of reflectivity $R(\nu)$, transmissivity $T(\nu)$ and complex dielectric permittivity $\varepsilon^*(\nu) = \varepsilon'(\nu) + i\varepsilon''(\nu)$ were studied over a wide range of frequencies, 8-8000 cm^{-1} (0.24-240 THz), at temperatures 4-300 K. To interpret the absorption bands discovered in the terahertz region, at 8-80 cm^{-1}, a model of the electronic transitions within the fine-structured ground state of four-fold coordinated Fe^{2+} is developed [2]. It is shown that the trigonal distortions of the crystal field lead to lowering of the symmetry of $4f_1$ and 4e tetrahedral site-positions of Fe^{2+} and, as a result, to further splitting of the ground state spin-orbital sub-levels. It is electro-dipole transitions between the corresponding sub-levels that are considered to be at the origin of the observed absorption bands [3]. Absorption resonances at 80-1000 cm^{-1} are assigned to lattice vibrations (phonons) basing on the factor group analysis. The study paves the way for the development of low-cost materials with high dielectric permittivity (about 30) at terahertz frequencies that are promising for the manufacture of electronic devices with enhanced characteristics.

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Direct measurement of THz plasmon propagation length in graphene

Belosevich V.V.[1,2], Fedorov G.E.[1]

1 – Moscow Institute of Physics and Technology, Dolgoprudny, Russia

2 – Moscow State Pedagogical University, Moscow, Russia

vsevolod.belosevich@phystech.edu

Despite years of research, the concept of a terahertz (THz) gap cannot be considered completely obsolete. THz technologies are evolving but sources and detectors are still in need. In 1996 M.Dyakonov and M.Shur proposed [1] a method of rectifying THz radiation with High Electron Mobility Transistor (HEMT). In this configuration THz radiation is coupled between source and top-gate and DC signal occurs between source and drain. They have also proved this geometry of a device to be efficient for detecting terahertz radiation.

At the same time graphene appears to be one of the most promising materials in this field. Various graphene based THz detectors have been demonstrated [2,3]. Among all the ways to obtain graphene, chemical vapor deposition (CVD) is the simplest and cheapest one. There is a possibility for automatization of device fabrication based on this method that is not less important.

In this work we fabricated series of devices in Dyakonov-Shur configuration with different top-gate electrode position. We used CVD-grown graphene as a transport channel. In this configuration source and gate act as sleeves of bowtie antenna.

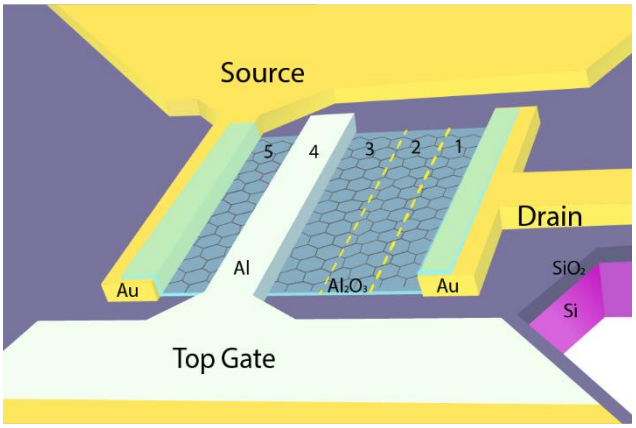

Figure 1: Schematic representation of the detector

The mechanism of THz radiation rectification and resulting DC voltage signal across the channel involves in particular nonlinearities and excitation of plasmons in graphene. Different top-gate positions allow us to estimate the length of plasmon propagation.

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Naphthyl - functionalized dendrimers can regulate surface properties of materials

Bondareva J.V.[1]
1 – Skolkovo Institute of Science and Technology, Moscow, Russia

julia.bondareva@skolkovotech.ru

Control over synthetic macromolecules' peripheral functionalization constitutes a considerable perspective on future applications and challenging task for chemists. One of such exciting and promising macromolecules is a dendrimer. Dendrimers are a class of polybranched synthetic macromolecules characterized by high monodispersity, good biocompatibility, and multivalent surfaces. [1] Selective peripheral functionalization of dendritic macromolecules having a well-defined constitution and a perfect shape is of high importance. Dendrimer research is currently associated with numerous technological and biomedical applications such as coatings, films, and in vivo contrast agents in magnetic resonance imaging. [2]

Our approach is based on functionalized sulfonimide dendrimers capable of forming stable monomolecular films at the air-water interface (so-called Langmuir films [3]) with subsequent polymerization the compressed state. The principle of covalent stabilization of monolayers is the dimerization of beta-naphthyl groups, which make up the outer shell of dendrimers, under the influence of UV radiation. The main advantages of the selected approach are (i) simplicity of experimental setup for the monolayer production and characterization, (ii) obtained films can easily be transferred onto a variety of solid substrates (e.g., silicon wafers, copper grids, HOPG, etc.), (iii) the latter expands the number of analytical tools to characterize the dendrimer films (e.g., optical and DIC microscopy on metal grids, ellipsometry analysis on silicon wafers, AFM and STM studies on HOPG, etc.)

The scientific project assumes the collaboration with physics-oriented experimental teams for performing conformational analysis of dendrimer molecules in the liquid phase. In practice, these films are interesting for changing the properties of polar hydrophilic surfaces to the opposite - hydrophobic ones using minimal amounts of a substance.

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Visible light driven photocatalytic performance of Ag modified ZnO nanorod through effective charge carrier separation

Abinash Das[a], Mathan Kumar P[b], Muthuraaman Bhagavathiachari[b], Ranjith G. Nair[a1]

a. Solar Energy Materials Research & Testing Laboratory (SMaRT lab), Department of Physics, National Institute of Technology Silchar, Silchar, Assam-788010 (India)

b. Department of Energy, School of Chemical Sciences, University of Madras, Guindy Campus, Chennai-600025 (India)

rgnair2007@gmail.com

Over the past few decades, a lot of interest has been generated among the researchers to use ZnO based photocatalyst for energy and environmental applications. However, most of the work suggests that the effectiveness of implementing bare ZnO is limited due to several inherent shortcomings of the photocatalyst. Considering the same, current study has shown that the modification of ZnO with silver (Ag) can significantly improve the visible light driven photocatalytic activity through suitable modification in physicochemical properties. Highly active silver modified ZnO has been prepared using modified hydrothermal method. The structural, morphological, elemental and optical properties were characterised using XRD, TEM, FESEM, EDS, FTIR, UV-Vis and photoluminescence (PL) spectroscopy. The visible light driven photocatalytic performance of Ag doped ZnO was studied for the degradation of methylene blue (MB), and it is found that silver modified ZnO shows approximately seven times higher performance in terms of rate constant than the pristine ZnO. The improved performance of Ag modified ZnO was further supported by the photoelectrochemical (PEC) study, indicating the reduced charge transfer resistance of Ag doped ZnO. The PEC study emphasizes on the role of Ag in obstructing the recombination pathway of photogenerated charge carriers.

Parametric modelling of electric percolation and conductivity of carbon nanotubes nanocomposite

N.A. Gudkov[1], S.V. Lomov[1], I.S. Akhatov[1], S.G. Abaimov[1]

1. CREI Centre for Design Manufacturing and Materials, Skolkovo Institute of Science and Technology, Bolshoy blvd., 30, bld.1 Skolkovo, 121205 Moscow, Russian Federation

Nikita.Gudkov@skoltech.ru

Conductive polymers are widely used in different industry branches. Adding carbon nanotubes (CNT) is one of the most efficient ways to make a polymer conductive, because of high intrinsic conductivity of CNTs and their 1D nature, which provides nanocomposites with relatively low electric percolation thresholds. All these properties lead to low weight fraction of filler and therefore low weight of a nanocomposite. The present work aims at developing of a digital twin of a CNT nanocomposite, representing its electric conductivity.

To obtain conductivity of an infinite medium, a representative volume element (RVE) approach was utilized. The digital twin creation can be divided into three parts: geometry generator, connection finder, and conductivity calculator. Geometry generator builds a set of uniformly and isotropically distributed CNTs inside the RVE. The distribution of CNT lengths is assumed to be Weibull. The maximal curvature of the CNTs is controlled. The periodicity of the geometry is ensured: a CNT crossing one face returns back to the RVE at the opposite face. The new approach was implemented here to consider geometrical torsion of CNTs. This made the digital twin independent from the size of segments, by which CNT curves are approximated. Connection finder is based on the sub-region division to make algorithm check less possible pairs of segments, which speeds up the searching process. Periodic boundary conditions are used for current calculations; they are compared with uniform potential conditions commonly used in the literature, and it is shown that the latter significantly overestimate the RVE conductivity.

Sensitivity of the model to input geometry generation parameters is investigated. It is found that 5 µm size is the optimal RVE size for reasonable volume fractions of CNTs. All results are obtained for multi-walled CNTs with diameter 50 nm. Segment size 0.3 µm was chosen based on the calculation accuracy. For a CNT volume fraction of 2%: changing mean length of CNTs from 2.5 µm to 5 µm increases conductivity more than 4 times; changing curvature from 0 to 3.46 µm-1 decreases conductivity 5 times; changing torsion from 0 to 3 µm-1 increases conductivity 6 times.

Influence of non-zero ballistic resistivity of CNTs is investigated. The results show that neglecting intrinsic resistivity causes error of 0.5 decimal order of magnitude.

Due to enormous difference in electrical conductivity between matrix and CNTs, nanocomposite percolation behavior can be described with Kolmogorov's zero-one law. It means that an infinite medium has a jump in conductivity when volume fraction increases and goes through the percolation threshold. However, there is a finite-size effect, which depends on size of the RVE and smooths this jump. Conductivity of the nanocomposite near the percolation threshold is investigated and its scaling

is found to follow the power-law and finite-size dependencies. We obtained percolation threshold equals 0.61% volume fraction for our default configuration (see above). For 10 μm mean CNT length percolation threshold moves to 0.32% Vf. For 2 times decreased curvature it moves to 0.54% Vf, and for 2 times decreased torsion it moves to 0.7% Vf. However, critical index seems to be nearly invariant with regard to geometric parameters. Its value changes in the range between 1.184 and 1.747.

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TiO_2 nanotubes and black TiO_2 nanotubes: application to solar electricity and hydrogen production

Hou X.L.[1], Lund P.D.[1]

[1] *New Energy Technologies Group, Department of Applied Physics, School of Science, Aalto University, FI-00076 Aalto, Espoo Finland*

Xuelan.hou@aalto.fi

TiO_2 nanomaterials have attracted much scientific and technological in recent years. TiO_2 nanomaterials can be used for direct splitting of water into H_2 and O_2 to generate hydrogen fuel [1] and also in Grätzel type solar cells for electricity.[2]

In order to create a high surface area of TiO_2 to achieve a maximum turn-over rate, various 1D and highly defined TiO_2 morphologies have been explored for the replacement of nanoparticle networks. Nanotubes can be grown by hydro/solvothermal or template methods, or even more large area fabricated application, by self-organizing anodic oxidation. The latter is not limited to TiO_2 nanotubes (TNTs) but to a full range of other functional oxide structures on various metals and binary and ternary alloys can be formed. [3] In order to absorb and utilize solar light as much as possible, excellent black TiO_2 are emerging, which have not only a suitable bandgap of 1.8 eV- 2.8 eV, but also has enhanced light absorption ability. [4, 5] The light absorption of black TiO_2 was broadened to NIR light (2 um)).

The presentation will focus on these highly ordered TNTs and discuss the most recent progress in synthesis and modification of black TNTs for solar cells and hydrogen production.

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Stable Doping of Carbon Nanotubes by V_2O_5 Using Fast Sol-Gel Method

Ilatovskii D.A.[1], Krasnikov D.V.[1], Goldt A.E.[1], Nasibulin A.G.[1,2]
1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Aalto University, Espoo, Finland

Daniil.Ilatovskii@skoltech.ru

The promising tendency of the use of single-walled carbon nanotube (SWCNT) thin films is to apply them as a transparent conductor of new generation [1]. Despite the fact, that many materials have been tested for this purpose: metal oxide ceramics, conducting polymers, thin-film metals, metal microgrids, and nanowires, neither has replaced the only one industrial product – indium tin oxide (ITO). Nevertheless, ITO does not satisfy requirements for modern transparent conducting films (TCFs): mechanical flexibility for flexible electronics and high refractive index [2]. Moreover, availability of indium is limited [3], so its price continuously increases (near 300 USD per kg) and it is necessary to develop indium-free electrodes.

Vanadium pentoxide has a great potential as a doping agent for SWCNTs due to its nature: high work function (WF) of 7.0 eV giving doping effect and high stability to humidity, sun irradiation and inert gases [4].

In this work, we show for the first time fast, simple and cheap method for treatment of thin films based on SWCNTs by V_2O_5 using sol-gel method for synthesis, which provides effective and highly stable adsorption doping. We used optical and Raman spectroscopy, contact 4-probe measurement of conductivity, XPS, and TEM in order to characterize the obtained materials and to check their stability in time. According to this method, we obtained films with equivalent resistance less than R_{90} = 100 Ohm/sq; which increased less than by 5% after one month of ageing.

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Electrochemical behaviour of thermally reduced graphite oxide in Li-ion batteries

Iurchenkova A.A.[1], Lobiak E.V.[2],Fedorovskaya E.O[1,2,3]

1 – Novosibirsk State University, Laboratory of hybrid nanomaterials for electrochemical storage devices, Pirogova st. 1, Novosibirsk, 630090, Russia.

2 – Nikolaev Institute of Inorganic Chemistry, SB RAS, 3 Acad. Lavrentiev ave., 3., 630090, Novosibirsk, Russia.

3 – Research Group of Electrochemical Energy Conversion and Storage, Department of Chemistry, School of Chemical Engineering, Aalto University, P.O. Box 16100, FI-00076, Finland.

a.iurchenkova@g.nsu.ru

The popularity of Li-ion batteries as storage devises rapidly grow in recent years. It relates to their high energy and power density, long cycling life. Despite a large amount of research in the field of creating and improving materials for Li-ion batteries, many questions remain.

Our work is devoted to study the influence of the functional composition and morphology of reduced graphite oxide (RGO) on its characteristics as an anode material for Li-ion batteries. Graphite oxide synthesized by Hammers method was chosen as precursor for RGO synthesis. Firstly, graphite oxide (GO) was ultrasonicated in concentrated sulphuric acid, washed by distillate water and freeze dried. After that grey-brown powder of GO was thermally expanded in Ar atmosphere and then thermally treated at different temperatures (500°C, 600°C, 700°C). Investigation of functional composition of obtained samples were carried out by Fourier-transformed infrared, X-ray photoelectron and Raman spectroscopic methods. Morphology of samples was investigated by scanning electron and high-resolution transmission electron microscopic methods. Electrochemical performance in Li-ion batteries was studied by charge-discharge method in two-electrode cell. RGO samples synthesized at different temperature were applied on copper foil and dried under the vacuum. The foil with active material was cut to electrodes and placed in a two-electrode coin-cell. Metallic Li and 1M LiPF6 in DMC/EC solution were used as counter electrode and electrolyte, respectively.

It is obtained that materials have epoxy, hydroxyl, carboxyl and carbonyl oxygen-containing groups (OCFG) on the surface. The amount of OCFG on the surface decreases and its defectiveness increases with an increase in the processing temperature of the material. Also, OCFG are removed from material's surface in order: epoxy (250ºC), carboxyl (250-600°C), hydroxyl (600-800 °C) and carbonyl (700-1000 °C). Maximal specific capacitance of samples reaches 400 $mAhg^{-1}$.

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Nonlinear optical absorption in lead halide perovskite thin films

Khudyakov D.V.[1], Ganin D.V.[1], Lyashedko A.D.[3], Frolova L.A.[4,2], Troshin P.A.[4,2], Lobach A.S.[2]

1 – Physics Instrumentation Center of Prokhorov General Physics Institute of the RAS, Troitsk, Moscow, Russia

2 – Institute of Problems of Chemical Physics of the RAS, Chernogolovka, Russia

3 – Optosystems Ltd., Troitsk, Moscow, Russia

4 – Skolkovo Institute of Science and Technology, Moscow, Russia

dimakh65@gmail.com

Metal halide perovskites have attracted intensive attention primarily because of their excellent optical and electronic properties. Beyond the well-known properties of the perovskite materials, they also have recently been investigated as a potential media for nonlinear optical modulators [1,2]. In the present report, we employed the Z-scan technique to investigate the nonlinear optical response of $CsPbI_2Br$, $MA_{0.15}FA_{0.75}Cs_{0.1}PbI_{2.85}Br_{0.15}$ and $MA_{0.15}FA_{0.75}Cs_{0.1}PbI_3$ perovskite films (PF) with 45-350 nm thickness under irradiation of pulsed Yb-doped fiber laser (τ_p=400 fs, λ=1.064 μm) as the pump source. It was found that thin PF (45-65 nm) have stronger nonlinear absorption with large coefficient β=261-928 cm/GW and lower saturation intensity (I_{sat}) compared with thick PF (250-350 nm) with smaller β=47-55 cm/GW and higher I_{sat}. It was shown that I_{sat} of the nonlinear absorption in PF depends on the pump pulse duration and increases for shorter pulses.

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Li-ion batteries with negative electrodes made of reduced graphite oxide

Kobets A.A.[1], Fedorovskaya E.O.[2]

1 – Novosibirsk State University, Novosibirsk, Russia

2 – Research Group of Electrochemical Energy Conversion and Storage, Department of Chemistry and Materials Science, School of Chemical Engineering, Aalto University, Aalto, Finland

a.a.kobets@mail.ru

Lithium ion batteries are the alternative energy sources with long life durability, high reversible power, long cyclic stability and high ecological safety. Carbon nanomaterials, transition metal oxides, electroactive polymers are the perspective electrode components of Li-ion batteries. This work is dedicated to investigation of nanostructure carbon materials with oxygen containing functional groups on the surface as negative electrodes in lithium-ion batteries.

Carbon materials are considered as suitable materials for negative electrode materials of Li-ion batteries due to their thermal and chemical properties, electrochemical stability, accessible surface, good reversibility of lithium ion intercalation/deintercalation. Functional groups on the surface of the carbon materials affect on the electrochemical behavior of the negative electrode, for example, increase the specific capacitance, stabilize the reversible capacitance, and improve the process of intercalation/deintercalation of lithium ions.

In this study, we used reduced graphite oxide (RGO), which has all the advantages of nanostructured carbon materials. RGO was obtained by heating graphite oxide in concentrated sulfuric acid. Graphite oxide was obtained by a modified Hammers method. Further, RGO was modified in a mixture of concentrated acids (1:1 HNO_3:H_2SO_4), in a 50% alkali solution, in oxalic acid, and annealed in an argon atmosphere. The idea of work was to find correlation between functional composition and electrochemical processes during charge and discharge process. The morphology of all samples was investigated by SEM and TEM methods. The functional composition of these materials was also studied using FTIR, Raman and XPS spectroscopy. In addition, charge-discharge characteristics of lithium-ion batteries with electrodes prepared from the obtained samples were studied. All methods of modification lead to changes in morphology and functional composition that influence on electrochemical properties.

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Low cost lasers as suitable instrument for graphene oxide thin film modification

Komarov I.A.[1], Struchkov N.S.[2], Danilova E.A.[1], Denisenko E.I.[1], Pretyagin V.G.[1]
1 – Bauman Moscow State Technical University, Moscow, Russia
2 – National Research University of Electronic Technology
ikomarov@emtc.ru

Our work is related to the processing of graphene oxide films for large variety of applications including formation of bio- and chemical sensor transducer, coatings with different drugs for faster healing, transparent conductive coatings etc. One of the most important goals for sensing and drug transfer is to control number and type of functional groups remaining on the graphene oxide surface. This goal can be achieved by different approaches including UV [1] and laser irradiation [2]. But in our opinion laser irradiation is more perspective due to the possibility of maskless direct patterning of the graphene oxide film.

In this work we used two types of low-cost lasers: near IR (1060 nm) and blue (445 nm) to modify graphene oxide film. We successfully showed possibility of graphene oxide reduction with both types of lasers, but blue laser showed better uniformity of reduced graphene oxide film parameters including film morphology, resistance (from 4 to 12 kOhm) and Raman intensity ratios. Usage of near IR laser leads to large nonuniformity of resistance with relatively high values (from tenth of kOhm to MOhm). We also showed presence of carboxyl functional groups in reduced graphene oxide areas that is suitable for biosensor, drug transfer and implants applications.

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Eco-Friendly Photocatalysts for Degradation of Dyes

Lau. G.E [1], Che Azurahanim, C.A. [1,2], *, Wan Amir N.W.A [3], Suvik. A[4] and Alvin. L.T.Z.[5]
1 –Universiti Putra Malaysia, Serdang 43400 UPM, Selangor, Malaysia.

2 – Institute of Advanced Technology (ITMA)

eenlau313@gmail.com

In the current era of globalization, synthetic dyes are one of the key factors of water pollution. Photocatalysis constitutes a promising technology for the treatment of wastewater, especially to those containing hard-to-remove organic compounds. Zinc oxide nanoparticles (ZnONPs) play a vital role as a photocatalyst material. This research highlights the synthesized ZnONPs with roselle flower and oil palm leaf extract. The extracts and sodium hydroxide (NaOH) act as reducing agents during the synthesis process. Synthesis without the addition of plant extract is used as blank control for the experiment. Structural and optical studies of the three variants of ZnONPs were performed. High purity of ZnONPs with element Zn and O was obtained. The size of the three variants of ZnONPs was from 10–15 nm and found in agglomerated spherical shape. Large band gap, 3.2 eV was obtained by UV-Vis and high thermal stability was proven by TGA. Oxygen vacancies that assist in the degradation phenomenon were found in ZnONPs. Five percent of ZnONPs with the presence of 10 W UV light could effectively degrade 10 ppm MO in 5 h and MB in 3 h. Besides, high antioxidant properties and low toxicity demonstrated the ability of ZnONPs to be used as photocatalysts. In conclusion, ZnONPs can be further developed for pharmaceutical and industrial use.

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Preparation of carbon nanotube fibers by folding the randomly oriented SWCNT films

Lomakin M.V.[1], Vershinina A.I.[1], Zhilyaeva M.A.[2], Rybakov M.S.[1], Kosobutsky A.V.[1], Shandakov S.D.[1]
1 – Kemerovo State University, Kemerovo, Russia

2 – Skolkovo Institute of Science and Technology, Moscow, Russia

maximius13@yandex.ru

The growing demand for wearable electronics requires flexible and stretchable conductive materials. Compared to ordinary conducting materials, single-walled carbon nanotubes (SWCNTs) are extremely lightweight and demonstrate a higher ability to prevent corrosion and oxidation. CNTs are usually used in the form of fibers, arrays or films [1]. In this work, we investigated the preparation of CNT fibers from the randomly oriented SWCNT films using a recently developed wet pulling technique [2]. Crucial phenomena in the wet pulling process are a folding of a solvent soaked SWCNT film due to the liquid surface tension and fiber densification during the solvent evaporation. It is shown that application of the wet pulling technique to randomly oriented SWCNT films results in low-density fibers with large number of the folds on their surface. Depending on the solvent nature (ethanol, acetone, dimethyl sulfoxide, and tetrahydrofuran), the fiber density varies in the range of 0.03–0.09 g/cm^3. By applying a twisting process, the density might be increased up to 0.19 g/cm^3. The specific strength is found to be only weakly dependent on the sample fabrication conditions. The obtained tenacity values of 0.60–0.78 N/tex are close to the published data for fibers directly spun from a CVD reactor using the bath-spinning or rotating-anchor spinning methods. The specific strength of the manufactured fibers is relatively high thus indicating a good interconnection of the CNT bundles. As a result of tensile tests conducted in this work, it is established that the fiber treated in the solutions of $HAuCl_4$ in ethanol had the highest value of a total absorbed energy up to fracture (127 J/g at 23% strain).

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Helicity sensitive plasmonic teraherts interferometer

Matyushkin Y.[1,2,3,4], Danilov S.[2], Moskotin M.[1,3], Belosevich V.[1,3], Kaurova N.[3], Rybin M.[1,5], Obraztsova E.D.[1,5], Fedorov G.[1,3], Gorbenko I.[6,7], Kachorovskii V.[6,8], Ganichev S.D.[2,8]

1 – Moscow Institute of Physics and Technology National Research University, Dolgoprudny, Russia

2 – Terahertz Center, University of Regensburg, Regensburg, Germany

3 – Physics Department, Moscow State Pedagogical University, Moscow, Russia

4 – National Research University Higher School of Economics, Moscow, Russia

5 – Prokhorov General Physics Institute, RAS, Moscow, Russia

6 – Ioffe Institute, St. Petersburg, Russia

7 – ITMO University, St. Petersburg, Russia

8 – CENTERA Laboratories, Institute of High Pressure Physics, PAS, Warsaw, Poland

ya.matyushkin@gmail.com

Plasmonic interferometry is a rapidly growing area of research with a huge potential for applications in the terahertz frequency range [1-3]. Here we present our recent work in which we explore a plasmonic interferometer based on a graphene field effect transistor connected to specially designed antennas. As a key result, we observe helicity- and phasesensitive conversion of circularly-polarized radiation into dc photovoltage caused by the plasmon-interference mechanism: two plasma waves, excited at the source and drain part of the transistor interfere inside the channel. The helicity sensitive phase shift between these waves is achieved by using an asymmetric antenna configuration. The dc signal changes sign with inversion of the helicity. A suggested plasmonic interferometer is capable of measuring the phase difference between two arbitrary phase-shifted optical signals. The observed effect opens a wide avenue for phasesensitive probing of plasma wave excitations in two-dimensional materials.

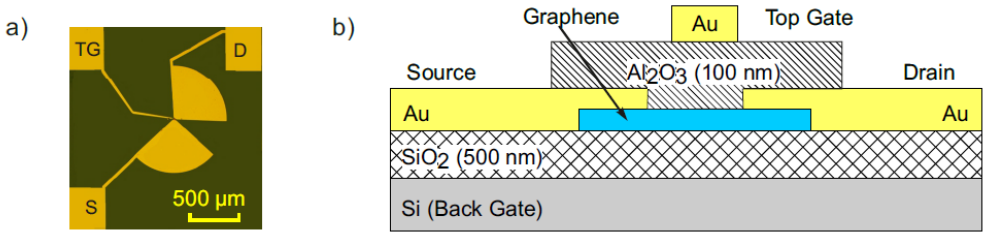

Fig.1. Device configuration. (a) Optical image. (b) Structure cross-section showing relative location of the source, drain and top gate electrodes.

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Dependence of frequency-capacitance curves for the «Air – Langmuir Monolayer – Water» system on the colloid solution amount spread out the water surface

Mironyuk V.N.[1], Begletsova N.N.[1], Chumakov A.S.[1],
Smirnova A.I.[2], Usol'tseva N.V.[2], Glukhovskoy E.G.[1]
1 – Saratov State University, Saratov, Russia

2 – Nanomaterials Research Institute, Ivanovo State University, Ivanovo, Russia

glukhovskoy@gmail.com

Obtaining additional information on frequency-dependent processes occurring in Langmuir monolayers is an urgent task, especially in cases where methods for measuring surface tension may not provide complete information. Such situation often arises when a monolayer of complex composition is formed on the water surface. For example, it can be a monolayer of nanoparticles in an organic matrix [1, 2], a mixture of amphiphilic and non-amphiphilic molecules [3], etc.

This work we present the frequency-capacitance characteristics of a flat capacitor, where the «Air – Langmuir Monolayer – Water» (A–LM–W) system was used as the dielectric. A monolayer was formed in a Langmuir bath KN 2002 from the solution of potassium polytitanate (PPT) nanoparticles with arachidic acid (ArA) in chloroform (C = 10^{-3} M). A highly sensitive Agilent B1500A analyzer was used to register the frequency-capacitive characteristics. C-f dependences were recorded in the frequency range of 1 kHz – 5 MHz. The condenser consisted of two 20x20 mm copper plates – one at the bottom of the bath and the other above the monolayer.

When 20, 30, 40 μl of colloid solutions of PPT and ArA were spread out the water surface, the frequency-capacitance curves for the A-LM-W system were obtained in semi-logarithmic coordinates. The maximal capacity level decrease of 20% compared with the initial values (pure water) was detected for 40 μl solution amount.

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Pulse switchable fiber laser based on ionic liquid gated carbon nanotube saturable absorber

Mkrtchyan A. A.[1], Gladush Yu. G.[1], Kopylova D. S.[1], Khabushev E.[1], Nasibulin A. G.[1]
1 – Skolkovo Institute of Science and Technology, Moscow, Russia

Aram.mkrtchyan@skoltech.ru

Saturable absorber (SA) based pulse generation in a fibre laser cavity is conditional on modulation characteristics determined by the nonlinear material and implementation geometry of the SA. Commonly, these parameters can be controlled during the satuable absorber fabrication. For instance, modulation depth of a single-wall carbon nanotube saturable absorber (SWCNT-SA) transferred on a D-shape fiber is governed by its thickness and length [1]. Here we demonstrate switching of pulse lasing regimes in an all-PM fibre laser using electrochemically gated in-line SWCNT-SA. SWCNT-based electrochemical cell prepared from high quality aerosol synthesized SWCNTs collected on the cellulose filter directly from the reactor zone. SWCNTs were dry-transferred on a polarization maintaining D-shape fiber, then covered by ionic liquid and implemented it into the fiber laser (Fig. 1a). By applying the voltage on the SWCNT-SA we were able to switch the laser operation between the ultrashort mode-lock and microsecond Q-switch regimes [2]. A transmittance-voltage dependent map with pulse lasing regime regions is shown in Fig. 1b. In Fig. 1c shown the optical spectra of these regimes. Thus, pulse regime switching in the fibre lasers with the ionic liquid gated SWCNT-SA was established.

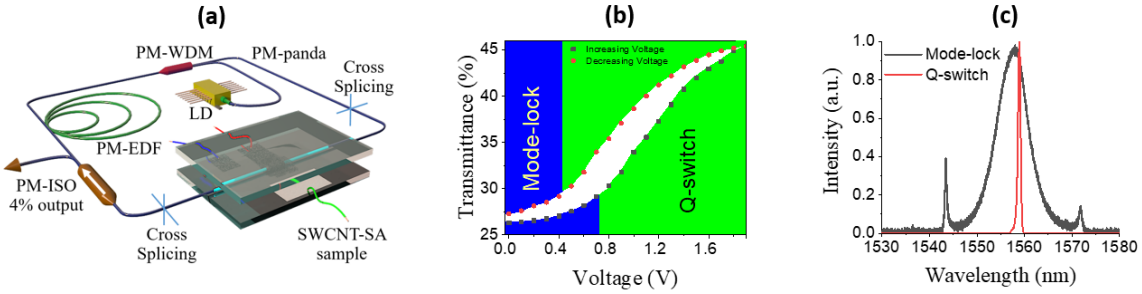

Figure 1. (a) Scheme of the fiber laser with a gated SWCNT-SA; (b) SWCNT-SA sample linear transmittance depending on the voltage. Colour corresponds to the generation regime depending on the voltage; (c) Optical spectra measured both in Mode-lock and Q-switch regimes

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Copper (2+) ions decrease conductivity of melanin in both bulk and film forms

Gerbenko A.K.[1,3], Savinov M.[2], Zhukov S.S.[3], Mostert A.B.[4], Motovilov K.A.[3]
1 – Skolkovo Institute of Science and Technology, Moscow, Russia
2 – Institute of Physics AC CR, Prague, Czech Republic
3 – Moscow Institute of Physics and Technology, Dolgoprudny, Russia
4 – Department of Chemistry, Swansea University, Wales, UK
k.a.motovilov@gmail.com

Melanin, the most widespread pigment among living systems [1], has emerged as promising material for bioelectronic devices and interfaces due to its ability to form device-grade thin films, sufficient conductivity and biocompatibility [2-4]. The nature of melanin conductivity is still a matter of controversies, however, in synthetic melanin the protonic origin of the hydration dependent contribution to conductivity obviously dominates.

Enhancement and linearization of melanin conductivity with respect to hydration level should assist in further development of melanin-based applications. One of the discussed approaches is doping of melanin with metal ions to substitute protons in corresponding protonogenic groups and to stabilize semiquinone-anion monomers which are thought to be responsible for hydration dependent increase of protonic conductivity.

In current study we demonstrated that doping of hydrated melanin with copper 2+ ions leads to complex dose-dependent response. Low concentrations of dopant (3.81 mg/g) slightly increase complex conductivity of bulk melanin. Growth of dopant concentration (29,14 mg/g) breaks the tendency and strongly decrease conductivity of melanin both in bulk and film forms. However, it was shown earlier that greater copper concentration also pushes melanin to change its organization towards formation of more ordered and prolonged structures [5], leading to the observed increase of the dispersionless frequency area for σ`.

Being a porous material melanin demonstrates colossal values of ε` up to $10^8$ and even higher at frequencies below 0.01 Hz. We show that higher concentration of copper 2+ ions leads to more smooth dependence of ε` on frequency.

In the framework of study we offer a model to explain the observed phenomena based on peculiarities of Cu^{2+} ion interactions with the functional groups of melanin monomers and water molecules in coordination sphere.

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Toxin detection through graphene Dirac point shift tracking

Nekrasov N.P.[1], Emelianov A.V.[1,2], Bobrinetskiy I.I.[1,3] (12 pt)

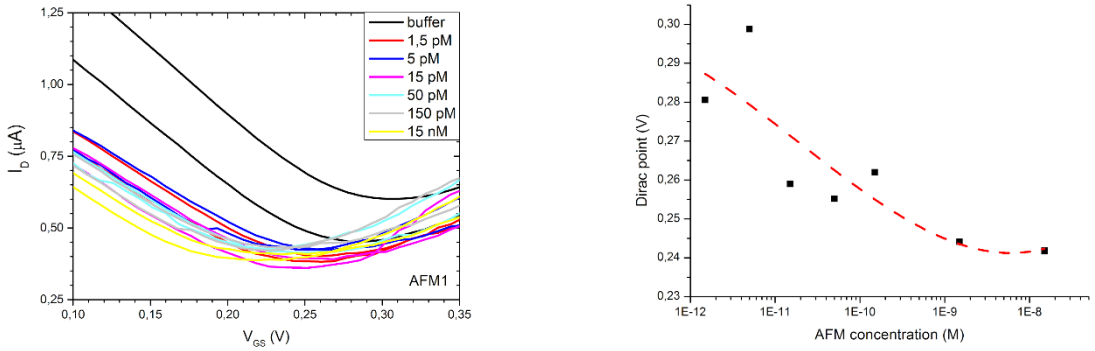
1 – National Research University of Electronic Technology, Moscow, Zelenograd, Russia

2 – P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia

3 –Biosenes Institute, Novi-Sad, Serbia

8141147@gmail.com

To accurately track the response of specific aptamer to the presence of the toxin, measuring the liquid transfer characteristics of graphene transistor can be performed. This method is possible using sensor development based on a solution-gated ions-sensitive field-effect transistor (ISFET) with a graphene channel [1]. Graphene is supremely sensitive to its surroundings, enabling to see chemically induced reaction between specific aptamer and toxin [2]. Owing to the ~1-nm-thick electric double layer, ionic liquids enable low-voltage operation of the ISFET. Specific aptamers, that reacts with specific micotoxin were assembled to graphene through 1-pyrenebutyric acid N-hydroxysuccinimide (PBASE) layer Sensor demonstrates high sensitivity for toxin concentration form 1 pM to 100 nM showing ~10 mV shift of Dirac point per one decade of concentration change.



a b

Figure 1. (a) transfer current-voltage characteristics for aflatoxin-M1 detection, (b) Dirac point change according to toxin concentration

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Green Synthesis Approach to Produce Luminescent Nanoparticles from Agricultural Waste and their potential biomedical application

Ashreen Norman [1,2] , Che Azurahanim Che Abdullah [1,2], Ahmad Kamil bin Hj Mohd Jaaffar[3]

1- Institute of Bioscience, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

2- Biophysics Lab, Department of Physics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

3- Lembaga Koko Malaysia, Tingkat 5-7, Wisma SEDCO, Lorong Plaza Wawasan, Off Coastal Highway, Beg Berkunci 211, 88999, Kota Kinabalu, Sabah, Malaysia

ashreeeen@gmail.com

Malaysia has a large agricultural potential that can support economic activity. Rubber, palm oil, and cocoa are major agricultural export in Malaysia. Polyphenols are naturally occurring antioxidants found in foods like fruits and vegetables. They have been linked to numerous health benefits. Luminescent nanoparticles (LNPs) has attracted a great attention of researchers in the current era due to their unique properties. Though, the top-down synthesis of LNPs has always been one of the most preferred method to obtain CDs in significant yields. The LNPs used in this process could be obtained by a green approach such as the one-step hydrothermal method. The top- down synthesis method of LNPs has side effects such as toxicity which are still a major concern before it can be used as pharmaceutical excipients or drug delivery transporter. Owing to that, herein we proposed green LNPs from agricultural waste for bio-applications. The synthesis, structural and optical properties, as well as photoluminescence mechanisms of prepared nanoparticles are reviewed. Green technology opens new windows as there are readily available, renewable, economic and environmental-friendly in nature.

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Residence time as a tool for optimization of aerosol CVD synthesis of single-walled carbon nanotubes

Novikov I.V.[1], Khabushev E.M.[1,2] Krasnikov D.V.[1], Bubis A.V.[1],
Goldt A.E.[1], Nasibulin A.G.[1,2]
1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Aalto University School of Chemical Engineering, Espoo, Finland

ilya.novikov@skoltech.ru

Aerosol chemical vapor deposition (CVD) is one of the most promising methods for synthesis of single-walled carbon nanotubes (SWCNTs) as it provides stabilization of the fine catalyst nanoparticles by extreme dilution solving the problem of non-reversible agglomeration of SWCNTs. Moreover, being a one-stage and a liquid-free process for SWCNT film production, this approach results in a number of advanced SWCNT-based optoelectronic applications [1]. Yet, unable to immobilize aerosol nanoparticles, aerosol CVD is limited towards conventional methods for catalyst evolution studies. In this investigation, we vary residence time via total flowrate control and consider its effect on SWCNT growth maintaining all the processes preceding nanotube growth: catalyst formation and nanotube nucleation (by means of fixing feeding rate and catalyst precursor concentration). The latter has been proved by unchanged SWCNT diameter distribution assessed via UV-vis-NIR spectroscopy. Furthermore, optoelectronic performance of the SWCNT films collected dependence on the residence time has been studied as well.

We have demonstrated intuitive relation as the SWCNT bundles lengthen with residence time (by scanning electron microscopy (SEM) observations). SWCNT quality, bundling degree and yield dependence on the residence time have investigated as well (using Raman spectroscopy, transmission electron microscopy (TEM), differential mobility analysis (DMA)). Having revealed yield decrease with residence time, we then have found a drop in the aerosol phase concentration, which is attributed to crucial deposition losses. Nevertheless, such a tendency leads to even more pronounced increase in equivalent sheet resistance conductivity (compared to expected effect caused exclusively by SWCNT lengthening), which is likely caused by decrease in catalyst particles and shorter nanotubes.

Acknowledgement. This work was supported by Russian Science Foundation project No. 20-73-10256.

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Flexible supercapacitors based on free-standing films of polyaniline/single-walled carbon nanotube composites.

Y.V. Panasenko[1], A.A. Iurchenkova[1], M.O. Bulavsky[2], Y. Aguilar-Martinez[3], S.A. Romanov[2], F. Fedorov[3], E.O. Fedorovskaya[1,4], A.G. Nasibulin[2,4]

[1]*Laboratory of Hybrid Materials for Electrochemical Energy Storage Devises, Department of Natural Science, Novosibirsk State University, 1 Pirogova str., 630090 Novosibirsk, Russia*

[2] *Skolkovo Institute of Science and Technology, Laboratory of Nanomaterials, 100 Novaya str., Skolkovo, Moscow Region, 143025, Russia*

[3] *Escuela de Ciencia e Ingeniería de los Materiales, Instituto Tecnológico de Costa Rica, Cartago, 159-7050, Costa Rica*

[4.]*Research Group of Electrochemical Energy Conversion and Storage, Department of Chemistry, School of Chemical Engineering, Aalto University, P.O. Box 16100, FI-00076 Aalto, Finland*

i.panasenko@g.nsu.ru

Progress in the development of supercapacitors is usually associated with the improvement of its specific capacitance driven by the synthesis of new materials, and/or design of its architecture, also, at the nanoscale [1]. A recent focus on flexible energy storage devices draws greater attention to conducting polymers (CPs) and carbon nanomaterials, like carbon nanotubes due to appropriate mechanical properties. Polyaniline (PANI) is one of the most popular CPs possessing high electrochemical activity that contributes to pseudocapacitive properties; it is also characterized by simple synthesis protocols. One the other hand, single single-walled carbon nanotubes (SWCNTs) are rather promising material for the supercapacitor due to high conductivity, chemical stability in many media, and ability to work at high current density without degradation. Even though, a combination of these materials should lead to improved capacitive properties, the synthesis protocols which would provide the best performance are not yet well established. The use of free-standing SWNT films as an electrode to deposit the polymer on both sides of the film is a promising strategy to obtain fabricated flexible devices with improved capacitance without the influence of the “dead” weight of the substrate to which CNTs are usually attached.

In this study, we performed electrochemical polymerization of PANI just at SWCNT free-standing films to prepare SWNT/PANI composite materials. The properties of materials were studied as a function of the thickness of the SWCNT films and the polymer loading. It was shown that the composites based on the thinnest films have the highest specific capacities up to 541 F/g. The possible mechanism is proposed.

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Green synthesis of reduced graphene oxide for biomedical applications

Dharshini Perumal[2], Muhd Amir Faiz Muhd Shaifuddin.[2], Emmellie Laura Albert[2], Che Azurahanim Che Abdullah [1,2]* and Mas Jaffri Masaruddin[3]

1-Institute of Bioscience, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

2-Biophysics Lab, Department of Physics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

3-Department of Cell and Molecular Biology, Faculty of Biotechnology and Biomolecular Sciences, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

shinijessy@gmail.com

Graphene is the thinnest and lightest material with prominent properties. This offers an enormous potential for application in various sectors. The synthesis of high-quality graphene in an eco-friendly manner remains a major challenge. Reliable, economical, facile, and chemical reduction method is the option for the preparation of reduced graphene oxide (rGO). This method is considered to be eminent for mass production and offers safety to the environment and human health. Green technology opens new windows in the synthesis of green graphene oxide (GO) reduction using plant extracts[1]. Plant extracts are captivating alternative to the noxious chemical reducing agents. They are readily available, renewable, economical and environmentally friendly in nature. The present study focuses on the synthesis of rGO using extracts from leaves of *Elaeis guineensis*. Herein we present the preliminary data on structural and optical properties. Based on the characterization data by FTIR, XRD, UV and TEM revealed that we successfully synthesized green rGO [2,3,4]. The potential application of the prepared rGO will be on biomedical applications.

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Optical properties of carbon nanodots obtained from the Kuzbass basin coals

Prazyan T.L., Dyagilev D.V.
Kemerovo State University, Kemerovo, Russian Federation
Prazyan.tigran@yandex.ru

Carbon nanodots (C-dots) were first obtained in 2004 [1] in the process of electrophoretic purification of carbon nanotubes, and since then the methods of synthesis and control of the functional properties of such structures have been constantly improving. The search for facile and inexpensive methods of C-dots' producing has led researchers to the idea of using coal as a cheap and widely available raw material. One of the first successful attempts of C-dots' fabrication from anthracite and bituminous coal was reported in 2013 [2].

In this work, we employed the coal samples from the Kuznetsk Basin (Anthracite, Bituminous coals), which is the largest source of coal in Russia. In order to effectively extract the C-dots, we have developed a method consisting of the following stages: wet grinding of coal in a planetary ball mill, peroxidation with ultrasonic activation, stabilization and sedimentation of the suspension, evaporation and drying.

It is found that the yield of C-dots for various grades of coal ranges from 1 to 20%. The absorption spectra were used to estimate the band gap of the emitting particles, which was in the range of 2.3–3.8 eV. Upon excitation with light with a wavelength of 210 nm, the particles exhibited luminescent emission at the wavelengths of 280–500 nm with the strong peaks at 300 and 460 nm. The anthracite derived C-dots exhibited the most pronounced emission at 460 nm, which is possibly due to the presence of heavy metal impurities. Their presence in the form of the inner structural components or adsorbed species is known to strongly affect the optical properties of quantum-sized particles [3].

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Synthesis of core shell Nano magnets with size tailoring by aerosol CVD

Javier A. Ramirez B.[1], Dmitry V. Krasnikov[1] Alena A.Alekseeva[1], Anastasia E. Goldt[1], and Albert G. Nasibulin[1,2]

[1] Skolkovo institute of Science and technology, Centre for Photonics and Quantum Materials, Laboratory of nanomaterials, Moscow, 121205, Russian Federation.

[2] Aalto University, Kemistintie 1C, 00076 Aalto, Finland.

javier.ramirez@skoltech.ru

Interest in research of core shell nanoparticles is arising due to the unique, novel properties of these structures. Aerosol synthesis presents advantages compared with other methods, which involve many steps, post processing and are slow, and usually low yield. Scalability is very important for readily useful materials, where bulk amounts with restricted structural parameters are desired.

We propose and demonstrate the results of an innovative, single step, fast, continuous, environmentally friendly, industrially scalable Aerosol Chemical Vapour Deposition, inspired by [1] and based on the setup used in [2] to synthesize nanoparticles with mean size of 50 nm. by using organometallic compounds such as Metallocenes and hydrocarbons (C_2H_4) as precursors. Morphological properties were observed, size and crystal characteristics were altered by varying reactor conditions, achieving the production of carbon containing nanoparticles in a laminar flow vertical reactor.

Aerosol synthesis of particles was carried out successfully, at atmospheric pressure; concentration of reactants was changed by adjusting saturator temperature. Transmission electron micrographs (Fig. 2) of different particles were taken, XRD analysis of bulk samples was carried out, as well as Dynamic mobility analyser profiles (Fig. 1).

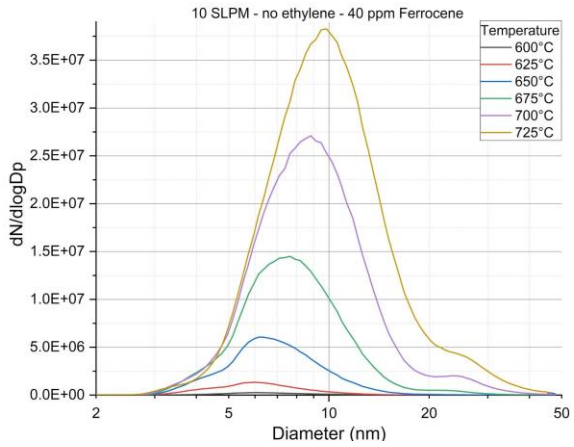

Figure 1. Dynamic mobility analyser profile for Different process temperatures.

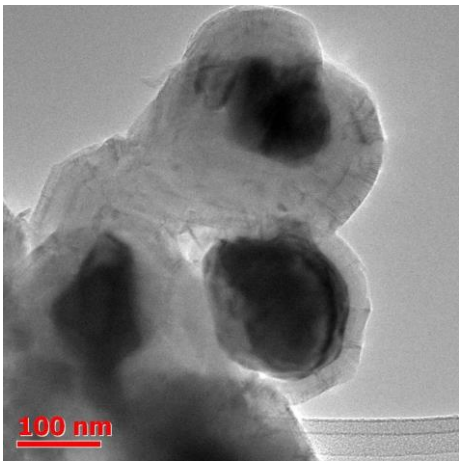

Figure 2. Micrograph of synthesized Nano magnets.

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Polyacrylic Acid Modified Cerium Oxide Nanoparticles for Non-Enzymatic H_2O_2 Sensor

Gurdeep Rattu[a] , Nishtha Khansili[a] and P.Murali Krishna[a] *;

[a] Department of Basic and Applied Science, National Institute of Food Technology Entrepreneurship and Management (NIFTEM) Kundli, Haryana 131028, India

mkprayaga@yahoo.co.in

Background: Cerium oxide nanoparticles (nanoceria) are efficient free-radical scavengers due to their dual valence state and thus exhibit optical and catalytic properties. This research revealed the development of fluorescence hydrogen peroxide nanosensor based on the peroxidase-like activity of polyacrylic acid stabilized nanoceria (PAA-CeO_2 Nps). Method: PAA-CeO_2 Nps were synthesized by simple cross-linking reaction at a low temperature and characterized by XRD, SEM, Zeta potential, TGA, FT-IR and UV-VIS spectroscopic analysis. H_2O_2 sensing was performed by a spectrophotometer.The XRD diffraction patterns confirmed the polycrystalline nature and SEM micrograph showed nanoparticles having hexagonal symmetry and crystallite size of 32 nm. UV-VIS measurements revealed a well defined absorbance peak around 315 nm and an optical band-gap of 3.17 eV by Tauc plots. As synthesized PAA-CeO_2 Nps effectively catalysed the decomposition of hydrogen peroxide (H_2O_2) into hydroxyl radicals. Then terephthalic acid was oxidized by hydroxyl radical to form a highly fluorescent product. Under optimized conditions, the linear range for determination of hydrogen peroxide was 0.01 – 0.2 mM with a limit of detection (LOD) of 1.2 µM. The proposed method is ideally suited for the sensing of H_2O_2 at a low cost and this detection system enabled the sensing of analytes (sugars), which can enzymatically generate hydrogen peroxide.

Composites Nano-Titania Graphite for Photocatalytic and Antibacterial Activities

Natrah Shafiqah Rosli[1,2,3] , Che Azurahanim Che Abdullah[1,2] , Roshasnorlyza Hazan[3]
[1]*Institute of Advance Technology (ITMA), University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.*
[2]*Department of Physics,Faculty of Science, University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.*
[3]*Malaysian Nuclear Agency, Bangi, 43000 Kajang, Selangor, Malaysia.*
natrahshafiqahrosli@gmail.com

Nano-Titania or Titanium dioxide (TiO_2) nanoparticles is a well-known photocatalyst that widely used for environmental cleanup due to its ability to decompose organic pollutant and kill bacteria [1]. Although TiO_2 nanoparticles have the advantages to be used in the environmental concern, their functionality depends mainly on both the precursor and the method used [2]. Typically, the synthesized TiO_2 nanoparticles involved expensive methods and the usage of hazardous chemical reagents. In this research, the low cost, easy to prepare, and environmental of synthesized TiO_2 nanoparticles were utilized. TiO_2 nanoparticles in anatase phase were successfully prepared via the alkaline fusion method using synthetic rutile as a precursor. The synthetic rutile used in this project was derived from natural Malaysian Ilmenite's waste to produce a low cost of TiO_2 nanoparticles via the environmentally friendly process and relative simplicity for a large scale. In attempts to improve the performance of the synthesized TiO_2 nanoparticles, some modifications were carried out to enhance their photocatalytic properties. The synthesized TiO_2 nanoparticles were incorporated with graphite as a non-metal material to produce TiO_2/G nanocomposites. The incorporation of non-metal material did not change the phase of TiO_2 nanoparticles but have a profound impact on the morphology and optical properties were affected as revealed from characterization by using XRF, XRD, TEM, PSA, FTIR, and UV-Vis analysis. The efficiency of synthesized samples as for potential photocatalytic application was examined by the capability in the degradation of methylene orange (MO) as a model of water pollutant under UV-irradiation. TiO_2/G nanocomposites showed the best performance where 10 ppm MO degrading up to 93% for 5 hours. Meanwhile, the modified samples were also tested by using Gram-negative bacterial strain *Escherichia coli* (*E-coli*) for the antibacterial activities test. The antibacterial activities were successfully evaluated based on the diameters of clear inhibition zone surrounding paper disk after 24 hours. From the results obtained, TiO_2/G nanocomposites have proven to be efficient antibacterial material to inhibit *E-coli*. The results obtained revealed and established that TiO_2/G nanocomposites have excellent performance for the

degradation of MO in photocatalytic tests as well as having the ability to inhibit *E-coli* in antibacterial activities.

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High-yield synthesis of single-walled carbon nanotube films for targeted applications

Shaikhulova A.R.[1], Khabushev E.M.[1,2], Krasnikov D.V.[1], Nasibulin A.G.[1,2]

1 – Skolkovo Institute of Science and Technology, Nobel 3, 121205, Moscow, Russia

2 – Aalto University School of Chemical Engineering, Kemistintie 1, 02015, Espoo, Finland

alisa.shaikhulova@skoltech.ru

Single-walled carbon nanotubes (SWCNTs) possess striking structural and electronic properties, which has drawn significant attention of scientists and researchers in the past 25 years [1]. This material can be used in a broad variety of applications like field emitters, supercapacitors, sensors, *etc.* [2]. One of the main challenges preventing common SWCNT implementation is cost-effective large-scale synthesis of high-quality nanotubes. Aerosol chemical vapor deposition (CVD) method is believed to be one of the most promising techniques for industrial nanotube production, which is easy to scale-up, however, lacks productivity [3].

We have tackled this problem by the development of cost-effective aerosol CVD method for SWCNT synthesis using ethylene as a carbon source, ferrocene as a catalyst precursor, and carbon dioxide as a promoter with a focus on transparent and conductive applications. The influence of various factors on SWCNT film production was examined by a complex set of methods (four-probe resistance measurements, Raman and UV-vis-nIR spectroscopy, SEM and TEM). Investigating synthesis conditions (temperature, catalyst precursor and reactant partial pressure), we found ethylene and carbon dioxide concentrations of 0.4 vol. % to correspond to the highest yield and to the lowest equivalent sheet resistance. At the same time, the variation ferrocene concentration from 0.05 Pa to 0.18 Pa revealed a trade-off between yield and conductivity. Obtained results will guide to further development of scalable and relatively low-cost process for SWCNT synthesis, with the most voluminously produced hydrocarbon and environmentally friendly growth process.

Acknowledgement. This work was supported by Russian Science Foundation project No. 20-73-10256.

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Protective spinel coating for $Li_{1.17}Ni_{0.17}Mn_{0.50}Co_{0.17}O_2$ cathode for Li-ion batteries through single-source precursor approach

A. Shevtsov [1], H. Han [2,3], E.V. Dikarev[3] and A.M. Abakumov[1]
1-Skolkovo Institute of Science and Technology, Moscow, 143026 Russia
2-Department of Materials Science and Engineering, Cornell University, New York 14850, USA
3-State University of New York at Albany, 1400 Washington Ave, Albany, NY 12222 USA
andrey.shevtsov@skolkovotech.ru

The layered oxide $Li_{1.16}Ni_{0.16}Mn_{0.5}Co_{0.16}O_2$ (Li-rich NMC) may exhibit a reversible capacity of 300mAh/g at C/20 rate for several cycles with further capacity fade. Its commercialization is impossible due to the degradation, which is attributed to the interaction of the material with the electrolyte at high voltages. The particle surface coating is an approach towards the physical separation of the cathode and electrolyte to diminish the capacity and voltage fade.

The employment of multi-source precursors to prepare specific functional materials may result in an inhomogeneous chemical distribution [1]. A surface-sensitive application, such as coatings, may result in the lack of the desired electrochemical properties. Thus, there is an interest in exploring new flexible synthetic pathways that yield “molecular pure” materials. Amongst the possible solutions: the single-source precursor approach - the usage of molecular precursors, which upon decomposition form the desired crystal phase [2].

The molecular precursor to the manganese spinel [3], $LiMn_2(thd)_5$ (thd = 2,2,6,6-tetramethyl-3,5-heptanedionate), was used as a parent molecule to further design the synthesis of the substituted manganese spinel, $LiMn_{1.5}M_{0.5}O_4$. Thereafter, the respective complex LiMnCo(thd) was successfully isolated and upon decomposition yielded the spinel oxide, $LiMn_{1.5}Co_{0.5}O_4$ [4]. These molecular precursors were then dispersed on the surface of the layered oxide $Li_{1.16}Ni_{0.16}Mn_{0.5}Co_{0.16}O_2$ (Li-rich NMC) and upon decomposition at 400ºC a core-shell cathode material was synthesized. The phase composition of the samples was characterized using powder X-ray diffraction coupled with a high-resolution TEM imagery. The HRTEM imagery of the Li-rich NMC particles shows an external layer 10-20 nm thick. The diffractions confirm the co-existence of the Li-rich NMC (*C*2/*m*) and spinel structures (*Fm*-3*m*). The sample of Li-rich NMC coated with ~12 wt.% of spinel and annealed at 400 ºC reveals much better capacity retention of 71% compared to 50% for the pristine material, as well as better structural stability over the first 25 cycles.

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Nitrogen –doped porous carbon obtained by precipitation of acetonitrile vapors on template C-CaO nanoparticles for electrochemical applications

Shlyakhova E.V.[1], Fedoseeva Y.V.[1], Nischakova A.D.[1], Vorfolomeeva A.A.[1], Bulusheva L.G.[1], Okotrub A.V.[1]

1 – Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia

shlyakhovaev@niic.sbras.ru

Porous nitrogen-containing carbon nanomaterials are promising electrode materials for new generation electrochemical current sources due to developed pore texture, high electronic conductivity and high thermal stability. The synthesis of nitrogen-containing carbon nanomaterials was carried out in several stages: thermal decomposition of organic calcium salts of tartaric, glutaric, and adipic acids at 750 °C, subsequent CVD carbon deposition using acetonitrile as a source, and removal of template particles by treatment with an HCl solution. It has been established that as a result of the thermolysis of calcium salts, composite template particles are mainly consisting of CaO and carbon. The deposition of acetonitrile vapor on their surface leads to the formation of nitrogen-containing graphite-like layers containing 3-5 at.% nitrogen. Removal of template particles from the material leads to the formation of nanopores in the carbon material. The pore size of carbon materials varies from 3 to 30 nm, the gravimetric surface area is from 188 to 832 m^2/g, and the specific pore volume is from - 0.4 to 1.6 cm^3/g. The influence of the nature of calcium salts of carboxylic acids, which were the sources of template particles, on the structure and electrochemical characteristics of nitrogen-containing carbon nanomaterials was investigated.

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N-doped graphene nanoflakes for catalysis and tribology

Stolbov D.N.[1,2], Chernyak S.A.[1], Usol'tseva N.V.[2], Savilov S.V.[1], Parfenov A.S.[3]
1 – Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

2 – Ivanovo State University, Nanomaterials Research Institute, Ivanovo, Russia

3 – Ivanovo State Academy of Medicine, Ivanovo, Russia

stolbovdn@gmail.com

High demand for carbon nanomaterials (CNM) can be explained by the variety of their chemical and physical properties, as well as high potential of structure modification and possibility of introduction into various matrices to obtain various composite materials [1]. Changes in electronic structure and the formation of different surface defects can be achieved by the partial replacement of carbon atoms by heteroatoms, in particular, nitrogen ones.

In this work, pristine and N-doped graphene nanoflakes (GNF and N-GNF) were synthesized by template pyrolysis and studied by set of physicochemical methods. To study the effect of doping, the samples were studied as cobalt catalyst supports for the Fischer-Tropsch process, as well as additives for industrially produced lubricants.

It was found that the introduction of nitrogen atoms increases the dispersion of the deposited metal, thereby increasing the activity of the catalyst. Also, in the model system, the largest decrease in the friction coefficient (up to 42%) was exhibited by N-GNF at a concentration of 1.5 wt% at high loads.

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Thermal shock as a new approach for the synthesis of porous MoS_2

Stolyarova.S.G.[1], Kotsun A.A.[2], A. V. Okotrub,[1] L. G. Bulusheva[1]
1 – Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

stolyarova@niic.nsc.ru

The development of technology and user needs requires more powerful devices, energy sources, and materials. Metal ion batteries are widely used now and they can be easily modified by changing electrode materials. MoS_2 is actively explored as a promising anode material. Theoretical specific capacity of MoS_2 provided by the intercalation and conversion reactions is 669 mAh g^{-1}, which is 2 times higher than the corresponding value for graphite. The main disadvantage of bulk MoS_2 as an anode material is the short battery life. The MoS_2-based material can be stabilized by using a carbon component, but an alternative approach is to obtain nanostructured MoS_2. In this case, decreased size and formation of defects and pores contribute to a high capacity and decreased resistance of the material and increased diffusion rate of lithium ions. Traditionally, nanostructured porous sulfides are synthesized by self-assembling in solution or with use of templates.

We offer a simple synthesis of porous nanostructured MoS_2 materials by decomposition of ammonium tetrathiomolybdate $(NH_4)_2MoS_4$ aerogel in thermal shock conditions in an inert atmosphere at different temperatures. The obtained MoS_2 materials possess a three-level architecture: thin carbon skin/expanded MoS_2 layers/internal intertwined MoS_2 nanosheets. The presence of pores was confirmed by the nitrogen adsorption-desorption method and their size was 2-35 nm. Increasing the temperature leads to the creation of the extended MoS_2 layers at the plate surfaces. The lateral size and the number of adjacent layers on the surface and inside were also grown. The resulting materials were tested in lithium-ion half-cells. The porous MoS_2 synthesized at 700 °C showed superior rate capability 817 mAh g^{-1} at a current density of 2 A g^{-1} and 1139 mAh g^{-1} during cycling at 0.1 A g^{-1}.

Acknowledgment. This work was supported by the Russian Science Foundation, grant 19-73-10068.

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Polarons In Two-dimensional Pnictogens: DFT Study

Vasilchenko V.[1], Gonze X.[1,2], Levchenko S.[1], Perebeinos V. [3], Zhugayevych A. [1]

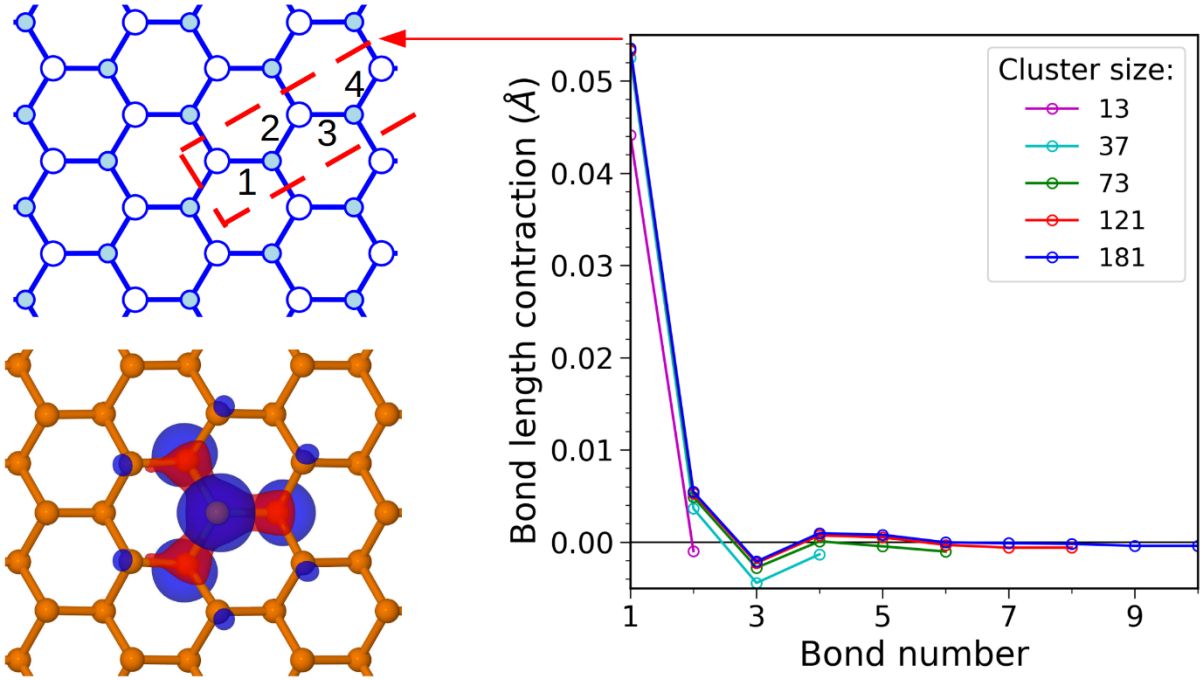
1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Université Catholique de Louvain, Louvain-la-Neuve, Belgium

3 – University at Buffalo, NY, United States

vasilii.vasilchenko@skoltech.ru

Present work is dedicated to the study of small polarons in emerging semiconductors: two-dimensional pnictogens. They are great candidates for application in electronics and the work done will allow for better understanding of the nature of charge carriers in these materials. Up to this point, no information on their polaronic character has been provided and generally they were considered as free electrons and holes. First-principles cluster calculations and finite-size scaling show stability of a small hole polaron in blue phosphorene and arsenene. It is localized on a phosphorus atom, leading to the contraction of the bonds around it. Commonly used hybrids including PBE0, HSE06, B3LYP show consistent results with the adiabatic polaron relaxation energy slightly below 0.1 eV for phosphorene and 0.15 eV for arsenene. The adiabatic barriers for motion of the polaron are small compared to the frequency of strongly coupled phonons implying barrierless motion of the polaron.



Multifunctional Brownmillerites for Efficient Energy Harvesting and Storage Applications

Durga Sankar Vavilapalli[1], M. S. Ramachandra Rao[2], Shubra Singh[1]
1-Crystal Growth Centre, Anna University, Chennai - 600025, Tamil Nadu, India.
2-Nano Functional Materials Technology Centre, Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India
v.durgasankar@yahoo.com

In search of new and advanced materials for energy harvesting and storage applications, we come across certain brownmillerite ($A_2B_2O_5$) multiferroic compounds, which are also called oxygen deficient perovskites (ABO_3). Oxygen vacancies and magnetic ordering in these compounds lead to possess smaller bandgap (less than 2eV) compared to regular perovskites. These materials are promising candidates for Ferroelectric photovoltaic (PV) applications, as it enhances the optical and electrical properties. A well-known multiferroic material, $BiFeO_3$, featuring relatively low solar cell efficiency (~ 7%) due to the relatively large band gap (2.6 eV), has attracted much attention. In the present case we have developed several multifunctional brownmillerite compounds and these are promising materials for PV, photocatalytic and energy storage application. The optical and catalytic properties of these compounds make them potential photocatalysts for waste water treatment[2]. Co-existence of transition metal-oxide active sites and oxygen vacancies in these brownmillerites is useful for efficient energy storage application. These studies point towards the role of multifunctional brownmillerites in the field of energy and environmental applications. The results will be presented in detail.

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The influence of chlorine and chloroauric acid treatment on electromechanical properties of SWCNT fibers

Vershinina A.I., Gordaya O.R., Lomakin M.V., Shandakov S.D.
Kemerovo State University, Kemerovo, Russia

annaver89@mail.ru

The effects of mechanical deformation on the electrical properties of carbon nanotubes are of interest in electromechanical devices. Single-walled carbon nanotubes (SWCNTs) doping with chloroauric acid ($HAuCl_4$) and treatment in gaseous chlorine (Cl_2) are effective methods for improving their electrical properties [1,2]. In this work, we study the electromechanical behavior of SWCNT fibers functionalized in chloroauric acid and chlorine.

The fibers have been fabricated from SWCNT films which were synthesized by floating catalyst (aerosol) CVD [3,4]. A part of the SWCNT films was treated in gaseous chlorine and then we prepared fibers using a recently developed wet pulling technique (WP) [5] with ethanol (C_2H_5OH), acetone (C_3H_6O), dimethyl sulfoxide (DMSO) (C_2H_6OS), and tetrahydrofuran (THF) (C_4H_8O) as solvents. We also obtained fibers from the pristine SWCNT films by WP technique using ethanol as solvent. These fibers were treated with a 0.1 M aqueous solution of $HAuCl_4$ diluted with ethanol to form 10 mM solution. The fibers' length were 10 mm. The electromechanical properties of the fibers were investigated using a tensile stage on the base of a microscrew and a stepper motor.

The study by a two-contact method employing the NI ELVIS II workstation showed the change of the SWCNT fibers' electrical resistance after the treatment in $HAuCl_4$ and Cl_2. The gauge factor (GF) of the fibers exhibited monotonic increase with deformation after the treatment by chloroauric acid, and the maximum GF value was found to be about 2. The GF of the samples treated in chlorine using ethanol, acetone, and THF as solvent had maximum value of about 3, while for the fibers prepared with DMSO, the value of GF reached ~4.

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Preparation of functional carbon coatings on the surface of hollandite-like ceramics with composition of $K_{1.53}(Cu_{0.76}Ti_{7.24})O_{16}$

Vikulova M.A.[1], Tsiganov A.R.[1], Artyukhov D.I.[1], Gorshkov N.V.[1,2]
1 – Yuri Gagarin State Technical University of Saratov, Saratov, Russia

2 – N.N. Semenov Federal Research Center for Chemical Physics RAS, Moscow, Russia

vikulovama@yandex.ru

Carbon-ceramic composite materials based on potassium titanate with hollandite structure are of great research interest due to the possibility of their application in potassium ion energy storage devices and as fillers in polymer matrices for elements of modern electronics producing. The advantages of using carbon are that it can be easily adapted to suit your needs. Carbon materials provide high surface area as well as good electronic and ionic conductivity. The use of carbon coatings makes it possible to compensate for the low electrical conductivity of potassium titanate with hollandite structure, which will increase the specific energy of electrode materials based on them.

However, obtaining carbon coatings on the surface of titanate ceramics is a difficult task. This may be partly due to the incompatibility of C with the TiO_2 lattice, along with the high temperature and pressure requirements for such materials production. Commonly used methods for preparing TiO_2-C composites include flame pyrolysis, high-temperature sintering, hydrothermal or sol-gel technology. In addition, it is usually required an external carbon source with little or no control over the degree or arrangement of the C atoms. Hence, another popular approach is to modify the TiO_2 surface with C nanostructures such as carbon nanotubes, graphene, reduced graphene oxide, and carbon nitride.

In this regard, the aim of this work is to study the possibility of obtaining hollandite-like ceramics $K_{1.53}(Cu_{0.76}Ti_{7.24})O_{16}$ with a carbon-modified surface by various methods.

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Phosphorus-filled single-walled carbon nanotubes: synthesis, characterization and electrochemical properties

Vorfolomeeva A.A.[1], Stolyarova S.G.[1], Bulusheva L.G.[1], Okotrub A.V.[1]
1 – Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

vorfolomeeva@niic.nsc.ru

Single-walled carbon nanotubes (SWCNTs) can fill with various inorganic compounds changing the electronic structure and chemical activity of the material [1]. Phosphorus can penetrate the cavity of a nanotube, forming various chain structures and nanoclusters, or be embedded in the graphene lattice with the formation of a phosphorus-carbon bond. SWCNTs have good conductivity and provide mechanical and chemical stability during electrochemical cycling. However, their theoretical capacity in the lithium-ion batteries (LIBs) does not exceed 600 mAh g^{-1}, which is not enough for use in new high-capacity devices. Phosphorus has a high theoretical specific capacity 2595 mAh g^{-1} [2]. Combination of SWCNTs as a conductive base and phosphorus in the internal cavity can allow the creating an effective electrode material for LIB LIBs.

One of the most effective and simple methods of synthesis of filled SWNTs is the ampoule method of synthesis. The filling was carried out in an H-shaped ampoule, in one part of which phosphorus was placed, and in another – SWCNTs. By varying such parameters as the ratio of reagents, synthesis time, and synthesis temperature, we achieve 8 at.% of phosphorus content according to XPS. To increase the degree of filling of nanotubes, the synthesis conditions were modified and ultrasonic treatment was introduced. Ultrasonic treatment was carried out at different stages of obtaining materials, due to which it was possible to increase the phosphorus content to 15 at.% according to XPS.

The resulting series of samples were studied as an anode material in LIBs. The best characteristics were demonstrated by a sample with a phosphorus content of 15 at.% and showed a specific capacity of 760 mAh g^{-1} at a current density of 0.1 A g^{-1}, which is three times higher than the capacity of the initial SWCNTs (245 mAh g^{-1} at a current density of 0.1 A g^{-1}). This effect is associated with the reversible reaction of the interaction of lithium with phosphorus with the formation of intermediates of various compositions Li_xP and with the reaction of lithium intercalation between bundles of nanotubes.

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Deagglomeration of carbon nanotubes via rapid expansion of supercritical suspensions

Zuev Ya. I.[1], Vorobei A. M. [1], Novikov I. V. [2], Fedorov F. S. [2], Goldt A. E. [2], Krasnikov D. V. [2], Parenago O.O. [1], Nasibulin A.G. [2]

1 – Kurnakov Institute of General and Inorganic Chemistry of Russian Academy of Sciences, Moscow, Russia

2 – Skolkovo Institute of Science and Technology, Moscow, Russia

vorobei@supercritical.ru

The main difficulty in the preparation of carbon nanotubes (CNTs) composites is the agglomeration of CNTs due to huge intermolecular attraction forces between them. The commonly used method for CNT de-aggregation is ultrasonication which sometimes can be harmful to CNT structure. In this work, we use a RESS (the Rapid Expansion of Supercritical Suspensions) method as an additional tool for CNTs de-bundling. In the RESS process, CNTs are suspended in a supercritical fluid (SCF) in a high-pressure vessel. After storing the suspension for the required amount of time at high pressure, it is rapidly sprayed into the precipitation chamber at atmospheric pressure. Following the spraying, the fluid rapidly expands behind the nozzle and undergoes a transition from supercritical to a gas phase. The microstructure of the dispersed material changes, mainly due to the rapid and non-uniform pressure drop.

It was shown that RESS treatment leads to a significant increase in CNT bulk volume (up to 11 times). Usage of supercritical nitrogen instead of carbon dioxide is more promising since due to a very low nitrogen critical temperature value there is no risk of the formation of a two-phase liquid-vapour system during fluid rapid expansion, which could bring up capillary effects detrimental to highly disperse materials. It is demonstrated that the dispersion of CNTs strongly depends on nanotubes type. For CNTs obtained from different manufacturers, the value of the increase in specific volume may differ in 10 times.

Moreover, RESS-processed CNTs were used preparation of polyurethane composites. The conductivity of such composites was several orders of magnitude higher than those synthesized without additional treatment. The use of RESS technology also gives a possibility to obtain composites with a percolation threshold of ca. 0.01 %-wt. which is 50 times lower when compared with unprocessed CNTs composites.

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Electrocatalytic Activities of Nitrogen Doped Carbon Nanostructures

Ram Manohar Yadav[#*]

[#]Department of Materials Science and Nano Engineering, Rice University, Houston -77005, USA
[*]Department of Physics, VSSD College Kanpur, INDIA-208002

rmanohar28@gmail.com

The conversion of CO_2 into fuels or commodity chemicals, incorporated with intermittent renewable energy sources like solar and wind, is an attractive venture that could offer an alternative solution to both the contemporary energy crisis and environmental issues. Elaborating highly active electrocatalysts for carbon dioxide reduction, oxygen reduction and oxygen evolution reactions are among the most promising areas of materials research. In this regards, chemically modified carbon nanostructures have emerged as a new metal-free electrocatalysts for these reactions due to their low cost, high activity and excellent durability. We have studied nitrogen doped carbon nanostructures (NCNTs, N Graphene etc) as electrocatalysts for oxygen reduction, carbon dioxide reduction and oxygen evolution reactions. The details about the work will be presented in the conference.

Biogenic synthesis of titanium dioxide: its composite with iron oxide and their potential biomedical application

Muhammad Azri Muhamad Yusop [1,2] , Che Azurahanim Che Abdullah [1], Roshasnolyza Hazan [2]

1-Department of Physics, Faculty of Science, University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia
2-Malaysian Nuclear Agency, Bangi, 43000 Kajang, Selangor, Malaysia

muhammadazri0909@gmail.com

In recent years, biogenic synthesis of nanoparticles has received substantial attention owing to the ability in develop clean and safe chemicals, low-cost methods, eco - friendly and renewable materials. In the current study, the biogenic synthesis of TiO2 nanoparticles (TiO2NPs) is attained by a chemical and biosynthesized method by using the aqueous plant extract of Malaysian based agricultural. Iron oxide been produced via co-precipitation and alkaline fusion. The product (iron oxide) been doped with biogenic synthesized of titanium dioxide. TiO2 NPs pure and doped with iron oxide (composite) are characterized by FTIR, UV, and XRD. The antimicrobial activities of biosynthesized nanoparticles are examined using disc diffusion method. The TiONPs expected to show significant antimicrobial activity against all the tested microorganisms.

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Topochemical transformations in MWCNTs-Si composites at high temperatures

Kuznetsov V.L.[1,2], Moseenkov S.I.[1], Zavorin A.V.[1,2], Tsendsuren Tsog-Ochir[2], Schmakov A.N.[1,2], Volodin V.A.[2,3].

1 - Boreskov Institute of Catalysis, Novosibirsk, Russia

2 - Novosibirsk State University, Novosibirsk, Russia

3 - Rzhanov Institute of Semiconductor Physics, Novosibirsk, Russia

zavorin@catalysis.ru

Multiwalled carbon nanotubes (MWCNTs) have unique physicochemical properties, allowing their use in a wide range of applications (composites, functional materials, electronics and others). One of the practical applications of carbon nanotubes is their use as part of an anode material in electrochemical power sources, where the addition of MWCNTs makes it possible to improve operational properties: maximum allowable charge-discharge currents, capacity and service life of lithium-ion power sources [1]. Another possible practical application of MWCNTs is their use as a reinforcing component of ceramic materials [2]. The introduction of MWCNTs in the composition of ceramics makes it possible to increase crack resistance, strength, improve tribological properties and achieve the appearance of electrical conductivity of such modified materials [3-4].

In this paper we study the high temperature initiated (700-1400°C) topological transformation of MWCNTs-Si [5] composites produced by gas-phase deposition of silicon on the surface of nanotubes (at 500°C). Si nanoparticles crystallization on MWCNTs surface and further topochemical reaction leading to SiC were studied using *in-situ* and *ex-situ* XRD and TEM, SEM, Raman spectroscopy. The data obtained were compared with results available after the study of macro Si-C systems. Industrial production of SiC regularly occurs at temperatures above 1500°C. In the case of using the processes of decomposition of silicon organic compounds, the formation of SiC proceeds above 1100-1200°C. In the case of MWCNTs-Si systems the formation of SiC began at temperatures of 700-800°C. It was found that the topology of SiC particles is influenced by the sizes of the initial silicon particles. The kinetic parameters of the formation of silicon carbide in the MWCNTs-Si systems were also estimated.

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Enhanced imaging of single Si nanoparticles using non-reflective SWCNT membranes

Zhigunov D.M.[1], Shilkin D.A.[2], Kokareva N.G.[2], Bessonov V.O.[2,3], Dyakov S.A.[1], Chermoshentsev D.A.[1,4], Mkrtchyan A.A.[1], Gladush Yu.G.[1], Fedyanin A.A.[2], Nasibulin A.G.[1,5]

1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Faculty of Physics, M. V. Lomonosov Moscow State University, Moscow, Russia

3 – Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Russia

4 – Moscow Institute of Physics and Technology, Russia

5 – Department of Chemistry and Materials Science, Aalto University, Finland

d.zhigunov@skoltech.ru

We demonstrate that single-walled carbon nanotube (SWCNT) membranes can be successfully utilized as nanometer-thick substrates for enhanced visualization and facilitated study of individual nanoparticles. As the model objects, optically resonant 200 nm silicon nanoparticles are transferred onto pristine and ethanol-densified SWCNT membranes by the femtosecond laser printing method. The nanoparticles are imaged by scanning electron and bright-field optical microscopy, and characterized by linear and Raman scattering spectroscopy. Using a pristine SWCNT membrane, an order-of-magnitude enhancement of the optical contrast of the nanoparticle bright-field image is achieved, as compared to the case of a glass substrate (Fig. 1). The observed optical contrast enhancement is in agreement with the spectrophotometric measurements showing an extremely low total reflectance of the pristine membrane (<1%). Owing to the high transparency, negligibly small reflectance and thickness, SWCNT membranes offer a variety of perspective applications in nanophotonics, bioimaging and synchrotron radiation studies.

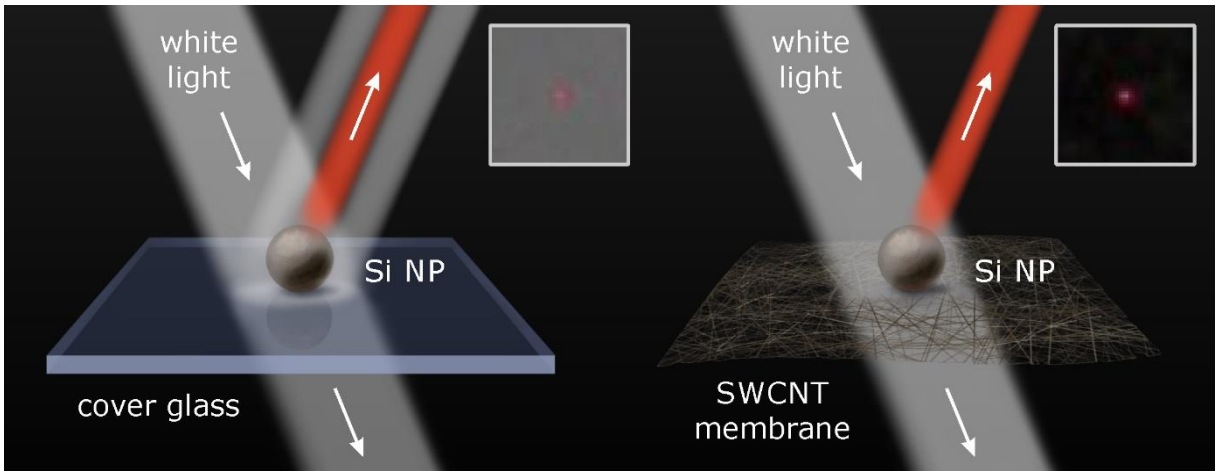

Fig. 1. Proof-of-concept demonstration of bright-field optical microscope image contrast enhancement using 200 nm Si nanoparticles (Si NP) transferred on a cover glass (left) and SWCNT membrane (right).

SYNTHESIS, CHARACTERIZATION AND TOXICITY STUDIES OF GOLD NANOPARTICLES FOR BIOMEDICAL APPLICATIONS

Siti Nadiah Zulkifli[1], Manali Haniti Zahid[2], Iskandar Zulkarnain Alias[2,] Che Azurahanim Che Abdullah[1]

[1]*Institute of Advanced Technology (ITMA), Universiti Putra Malaysia, 43400 Serdang, Selangor*

[2] *Department of Chemical Pathology, School of Medical Sciences, Health Campus, Universiti Sains Malaysia, 16150 Kubang Kerian, Kelantan*

sitinadiahzulkifli@gmail.com

Gold nanoparticles (AuNPs) is chosen for this project due to the fact that it is widely used in a variety of applications as well as straightforward synthesis methods that allow the fast and cheap production of AuNPs. Comparative analysis on characterization between two methods have been studied. One step synthesis method can reduce metal ions to nanoparticles. Both approaches chemical and green synthesis were successfully synthesized by using modified Turkevich method. The prepared samples were analyzed using ultraviolet and visible spectrophotometry (UV-Vis), Transmission Electron Microscopy (TEM) and Dynamic Light Scattering (DLS). X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy have been used to study their structural phase composition and their functional group. The toxicity of AuNPs was then tested on brine shrimp. The nanoparticles produced will offer a potential materials for biomedical application.

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Abstracts of Participants

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Enhanced Electrochemical Performance of TiO_2 Modified $LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$ Cathode Material via Atomic Layer Deposition

Zahra Ahaliabadeh[1], Tanja Kallio[1]

1 – Department of Chemistry and Materials Science (CMAT), Aalto University, School of Chemical Engineering, 02150, Espoo, Finland

Zahra.ahaliabadeh@aalto.fi

Developing high-energy and high-power lithium-ion batteries (LIBs) is a key challenge to meet the demands for practical applications in electric vehicles. These demands have driven the recent studies on positive electrode materials. Ni-rich layered lithium transition metal oxides are promising positive electrode material for the next generation high energy density LIBs because of their good electrochemical stability, comparatively low cost, low toxicity, and high capacity. However, high Ni content leads to severe side reactions at positive electrode/electrolyte interface and secondary particle cracking during cycling which significantly degrade the electrochemical performance of this material [1]. Improving the performance of positive electrode by using surface coatings has proven to be an effective method for developing LIBs, while a high-quality film satisfying all requirements of electrochemical issues, chemical stability, and lithium ion conductivity is yet to be implemented [2]. Recently, surface modification via atomic layer deposition (ALD) has gain attention as an effective strategy to enhance the electrochemical performance of high-specific-capacity electrode materials [3]. In this study, we reported a strategy that employed metal oxides (TiO_2) coating by ALD technique, in order to improve the bulk integrity, structure, and interfacial stability of the $LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$ (NMC622) and, hence, the long-term cycling capability. By varying the ALD parameters such as cycle number, mass of the substrate and precursor, an optimal ALD coating was achieved. The effects of TiO_2 coating on the surface states, crystal structure and electrochemical performances of NCM622 material are studied in detail. All characterizations results confirm the coating layer on the surface of NMC622 particles. The electrochemical characterization results indicated that the coating of TiO_2 ALD improved the cycling stability of NMC622 based electrodes by suppressing side reactions between the electrolyte and electrode. The improved electrochemical performance is ascribed to the high conformal and ultrathin TiO_2 coating, which enhances the kinetics of Li^+ diffusion and stabilizes the electrode/electrolyte interface.

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Development of ceramic composites based on hydroxyapatite and carbon nanomaterials

Ávila E.S. [1], Antônio L.M. [1], Ladeira L.O. [1], Barabás R.[2]
1 – Universidade Federal de Minas Gerais, Escola de Engenharia Química, Belo Horizonte – MG – Brasil.
2 – Universitatea Babeș-Bolyai, Facultatea de Chimie și Inginerie Chimică, Cluj-Napoca – Romania.

erickavila@gmail.com

Graphene oxide has been studied [1-4] as an alternative instead graphene because the presence of carboxylic and hydroxyl functional groups, it has excellent mechanical properties and biocompatibility.

Carbon nanotubes (CNT) were first synthesized by Iijima in 1991[5]. The great potential of applications of CNT are their physical and chemical properties and the possibility production of new biomaterials and composites [1,6,7].

Hydroxyapatite is one ceramic material produced using calcium phosphate and is good candidate already widely used as artificial bone in orthopedic or maxillofacial surgeries to repair bone defects, on the olther hand, present fragility and other imperfections [8,9]. The ideal bone substitute must be biocompatible and gradually replaced the new bone tissue, need to have osteoinductive or osteoconductive properties [2].

The production of ceramic nanocomposites based in hydroxyapatite and carbon nanomaterials can be the solution of join the better qualities of each separate materials.

This work is one study of the composites production based on graphene oxide, carbon nanotubes and hydroxyapatite with possibilities of application in engineering of bone tissues, mainly for the clinical treatments of bone defects caused by trauma, cancer, infection or congenital deformity also in dental restoration and implant processes field [10].

Acknowledgement. This work was supported by the Erasmus Mundus Program.

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About the intercalation of carbon dioxide molecule into the BC_5 nanotube

Zaporotskova I.V.[1], Boroznin S.V.[1], Zaporotskov P.A.[1], Boroznina N.P.[1]
1 – Volgograd State University, Volgograd, Russia

boroznin@volsu.ru

The article is devoted to the study of methods of catching CO_2 molecules using boroncarbon nanotubes of type BC_5. The paper considers the capillary method of filling nanotubes with a carbon dioxide molecule. The main method used in the work is the density functional theory (DFT) method within the B3LYP functional. As a result of the work, the most likely method of catching carbon dioxide molecules using boroncarbon nanotubes was established and the physicochemical characteristics of these phenomena were determined.

It was found that upon penetration into the cavity of the nanotube, the molecule is forced to overcome the potential energy barrier. This barrier was identified with the activation energy of this process. The calculated activation energy turned out to be less than 1 eV. This value indicates that the implementation of this mechanism has a high degree of probability. Accordingly, these nanostructures can be used as filters to trap harmful molecules from the atmosphere.

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On the possibility of creating a highly efficient sensor based on carbon nanotubes for determining air quality

Boroznina N.P.[1], Zaporotskova I.V.[1], Boroznin S.V.[1], Zaporotskov P.A.[1], Ivanov I.I.[1], Petrov P.P.[2]

1 – Volgograd State University, Volgograd, Russia

boroznin.natalya@volsu.ru

The presented article conducts a theoretical study of the possibility of interaction of substances that affect the quality of inhaled air - carbon dioxide and sulfur dioxide - with carbon nanotubes modified by the functional amine group. The article analyzed the results of addition and carried out a comparative analysis of sorption interaction of the nanosystem with molecules of carbon dioxide (CO2) and sulfur dioxide (SO2). Recommendations are given for further use of the results as a basis for creating a new generation of highly sensitive sensor device for detecting micro-quantities of substances. The calculations were carried out by the DFT method.

Our research will allow us to create instruments that can conduct a more efficient and more subtle study of air quality. They will allow detecting micro amounts of harmful substances to prevent pollution in a timely manner. A sensor based on modified carbon nanotubes will respond to the presence of ultra-small amounts of substances. This allows us to judge the prospects of its use in the field of chemistry, biology, medicine, etc.

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Doping of inner and outer surface of single-walled carbon nanotubes

Anastasia E. Goldt[1], Orysia Zaremba[1], Mikhail O. Bulavskiy[1], Fedor S. Fedorov[1], Konstantin V. Larionov[2,3], Alexey P. Tsapenko[1], Zakhar I. Popov[2,4], Pavel Sorokin[2], Anton S. Anisimov[5], Albert G. Nasibulin[1,6]

1 – Skolkovo Institute of Science and Technology, Nobel str. 3, 121205 Moscow, Russian Federation

2 – National University of Science and Technology "MISiS", Leninsky prospect 4, Moscow 119049, Russian Federation

3 – Moscow Institute of Physics and Technology, Institutskiy lane 9, Dolgoprudny, Moscow region 141700, Russian Federation

4 – Emanuel Institute of Biochemical Physics RAS, Moscow 119334, Russian Federation

5 – Canatu Ltd., Konalankuja 5, 00390 Helsinki, Finland

6 – Aalto University, 00076 Espoo, Finland

mikhail.bulavskiy@skoltech.ru

An increasing growth of flexible electronics market facilitates the development of new generation of materials that to be employed as flexible transparent conducting films (TCF) [1]. Even though, single-walled carbon nanotube (SWCNT) films are considered the most promising candidates for flexible TCFs, they still cannot meet the demanded characteristics [2]. Thus, the existing approaches to doping need a revision or improvement to allow SWCNTs achieve optoelectrical properties required for application as new generation TCFs.

In this work, we have utilized and investigated the new approach, which comprises the thermal treatment of SWCNTS in ambient air atmosphere with subsequent doping in ethanol solution of $HAuCl_4$. We have shown that thermal treatment at temperatures higher than 300 °C leads to the SWCNT cap's removal. Consequently, such opening of nanotubes is responsible for the more efficient doping of the treated films due to providing an additional inner surface doping when compared to the untreated samples. Stronger level of *p*-doping effect of opened via thermal treatment SWCNT films in comparison to pristine ones were confirmed by DFT-calculations and open circuit potential (OCP) measurements during the doping procedure. The utilized approach has allowed us to achieve the record equivalent sheet resistance value of 31 ± 4 Ω/sq for the SWCNT films treated at 400 °C.

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Influence of boron atoms in surface-carboxylated boron-carbon BC_3 and BC_5 nanotubes in the creation of sensory devices

Zaporotskova I.V.[1], Dryuchkov E.S.[1], Vilkeeva D.E. [1], Elbakyan L.S. [1]

1 – Volgograd State University, Volgograd, Russia

dryuchkov@volsu.ru

In this article, discusses the possibility of the fabrication of a highly sensitive sensor based on single-walled boron-carbon BC_5 nanotubes surface modified with functional carboxyl groups (-COOH) and a comparative analysis of the sensory properties of BC_3 [1] and BC_5 single-walled boron-carbon nanotubes surface-modified with a functional carboxyl group (-COOH) was carried out. The potential of the sensor for detecting alkali (lithium, potassium and sodium) metals was investigated. Results of computer simulation of process of sensor interaction with arbitrary surface of modified tube containing atoms of analysed metals are presented. The effect of boron atoms on the sensory properties of the obtained systems is concluded. Calculations were carried out as part of the Density Functional Theory (DFT) method using a molecular cluster model. Surface-modified boron-carbon nanotubes according to the carboxyl group have been shown to exhibit high sensitivity to the metal atoms under study and can be used as a sensor device. However, modification of the surface of the nanotube BC_3 leads to a better result relative to BC_5: this system has the maximum energy of sensory interaction, which suggests that an increase in the number of boron atoms in the nanotubular system improves its sensory properties.

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Ultrashort optical Mathieu pulses in a carbon nanotube medium

Dvuzhilova Yu.V.[1], Belonenko A.M.[1], Dvuzhilov I.S.[1], Belonenko M.B.[1]

1 – Volgograd State University, Volgograd, Russia

dvuzhilov.ilya@volsu.ru

A theoretical study of three-dimensional ultrashort optical pulses, Mathieu cross-section, which propagate in the medium of semiconductor carbon nanotubes. Using numerical simulations, it is shown that such pulses propagate stably, while conserving their energy in a limited spatial region. The pulse undergoes reflection from the walls of the optical cavity and further interference. The calculations were carried out at times up to 140 ps, which is important for possible practical applications [1-4].

Thus, diffraction-free three-dimensional extremely short Mathieu pulses propagate stably in the medium of carbon nanotubes. The pulse energy remains localized in a limited spatial region. Evolving in time, the pulse moves from the axis of the resonator to its walls, reflecting from them, and then interference of counter propagating waves occurs, due to which the pulse retains its energy concentrated, with a slight change in shape.

As a result, it becomes possible to control pulse broadening along the cavity axis. It should be noted that the numerical simulation of the pulse dynamics was carried out at long times, which determines the importance of the results obtained for practical applications.

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The technology for producing new composite polymer materials based on polymethylmethacrylate doped with carbon nanotubes.

Elbakyan L.S.[1], Zaporotskova I.V.[1], Vilkeeva D.E.[1]
1 – Institute of Priority technologies, Volgograd State University, University Av 100, Volgograd 400062, Russia

lusniak-e@yandex.ru

Butylmethacrylate is used for the production of polybutylmethacrylates and related copolymers. BMA is used in the production of coatings and inks, plastics, paper, adhesives and sealants. In addition, BMA is a part of adhesives, photo-cured and other composites for dental use, various additives to lubricants, etc.[1]

To realize the possibility of obtaining composite polymer materials with improved strength properties, it is necessary to ensure the most uniform dispersion of carbon nanotubes into the polymer matrix. To create and test the technology of introducing CNT into polymer matrices, the method of ultrasonic action with simultaneous mechanical mixing under temperature influence was developed [2-4]. This method makes it possible to obtain stable polymer complexes, to increase the strength characteristics of the polymer. To study the strength properties of the obtained polymer materials, the breaking point of these samples with different percentages of CNT and the sample without them was determined.

Table 2. The breaking point composite polymer materials doped with CNT

CNT, %	0	0,01	0,03	0,05
Breaking point σ_{cp}, [MPa]	0,041	0,043	0,046	0,049

Experimental studies on the creation of stable polymer complexes make it possible to obtain new composite systems reinforced with carbon nanotubes. This makes it possible to predict a larger-scale use of polymer materials.

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Synthesis of Pt nano-microspheres at TiO_2 –decorated Ti wire

Fedorov F.S.[1], Vasilkov M.Yu.[2,3], A. Goldt[1], Shurygina L.I.[4], Nasibulin A.G.[1,5]

1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Saratov Branch of Kotelnikov Institute of Radioengineering and Electronics of RAS, Saratov, Russia

3 – Yuri Gagarin State Technical University of Saratov, Saratov, Russia

4 - Kemerovo State University, Kemerovo, Russia.

5 – Aalto University, Aalto, Finland

f.fedorov@skoltech.ru

Nowadays the development of new functional materials with improved characteristics for application in electrocatalysis [1], gas sensors, etc. [2] is directly related to their design at the nanoscale. However, one needs to consider appearing technological issues, i.e. the applicability of such nanostructured materials in the industry. For example, the use of arrays of titanium dioxide nanotubes at the Ti substrate may include potential applications when it is in the form of wires or meshes that enable flow-through design. But, anodization of the metal of such geometries is not trivial because the surface profile is characterized by a given curvature. Besides, modifying the surface of such structures with precious metals such as platinum, which helps to improve the catalytic activity, can be quite challenging. Here, we investigated the growth processes of titanium dioxide nanotube arrays obtained by anodizing titanium wire in aqueous organic solutions and the decoration of such arrays with platinum.

Electrochemical anodization of a titanium wire (d=250 µm, ω(Ti)=99.7%-wt.) was studied in an electrolyte containing glycerol, water, and ammonium fluoride with a mass ratio of 74.6 : 24.6 : 0.75 at a constant voltage of 30 V for 70 hours. Further, the obtained samples were modified with platinum in a solution of 400 µl 0.02 M H_2PtCl_6, 400 µl H_2O, and 400 µl 85%-wt. HCOH for 120 hours. The obtained samples were studied by scanning electron microscopy with a help of a focused ion beam and transmission electron microscopy.

The synthesized structures represent arrays of ordered nanotubes decorated with platinum. The platinum appears as polycrystalline spheres whose diameter ranges from 100 nm to 2-3 µm. The structure of the spheres is represented as a complex network of nanowires with voids made by titanium dioxide nanotubes. This material has a large surface area and is promising for application as a gas sensor and as a catalyst.

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New phosphates and fluoride-phosphates as promising electrode materials for rechargeable batteries

Luchinin N. D.[1], Samarin A. Sh.[1], Shraer S. D.[1], Fedotov S. S.[1]
1 – Skolkovo Institute of Science and Technology, Moscow, Russia
s.fedotov@skoltech.ru

The progress in grid applications of metal-ion batteries pushes forward the development of electrode materials for Na-ion and K-ion batteries (NIBs and KIBs) as cost-efficient alternatives to the conventional Li-ion technology. Analogous to the Li-ion systems, the Na and K-based mixed oxides and polyanion materials are being developed as potential cathodes with attractive specific energy, stability and rate performance. Contrary to layered oxides, the polyanion materials usually display better cycling and thermal stability, as well as higher C-rate capabilities due to covalently bonded structural frameworks. At the same time, the polyanion compounds reveal a much more diverse crystal chemistry, which significantly extends the playground for designing new materials with unique electrochemical properties. Further advancements come from the synergy of coupling different anion species (such as XO_4^{m-} and F^-) in the anion sublattice enabling higher redox potentials and richer structural diversity.

Recently we proposed a novel series of $AMPO_4F$ (A = Li, Na, K; M = Ti, V) cathode materials crystallizing in a unique $KTiOPO_4$ (KTP)-type structure [1-4]. The target materials were synthesized via different soft-chemistry routes including hydrothermal method and freeze-drying. The materials featured outstanding specific energy, rate capability, and capacity retention outperforming most of benchmarked NIBs and KIBs electrode materials.

A short overview of the recent research and activities of our group on novel transition metal phosphates and fluoride-phosphates adopting the unique KTP-type crystal structure as potential electrode materials for NIBs and KIBs will be presented with a special focus on the interrelation between chemical composition, synthesis conditions, crystal structure peculiarities, and electrochemical properties of the materials aimed at practical applications.

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Dip-coating as efficient technique for single-walled carbon nanotube doping

Anastasia E. Goldt[1], Orysia T. Zaremba[1], Eldar M. Khabushev[1,2], Stepan A. Romanov[1], Albert G. Nasibulin[1,2]

[1]*Skolkovo Institute of Science and Technology, 3 Nobel Street, Moscow, 121205, Russia*

[2]*Aalto University School of Chemical Engineering, Kemistintie 1, 02015, Espoo, Finland*

a.goldt@skoltech.ru

Single-walled carbon nanotube (SWCNT) based transparent and conductive films (TCFs) are one of the most prospective materials for novel flexible and stretchable electronic devices. Development of reproducible and scalable doping procedure is the key step towards the widespread implementation of SWCNT TCFs.

We propose and thoroughly investigate a novel approach for SWCNTs doping utilizing traditional dip-coating technique with gold (III) chloride solution as a dopant. Adjusting of the process conditions (dopant concentration and withdrawal speed) allows effectively govern SWCNT film doping degree and define the optimal conditions for fabrication of high-performance nanotube films. It leads to achievement of sheet resistance value of 36 Ohm/sq. at the 90% transmittance the middle of visible spectral range by increasing a work function value from 4.8 (for pristine SWCNTs) to 6.0 eV.

This method allows easy fine-tuning of SWCNT films optoelectronic parameters and achieve a sheet resistance value of 36 Ohm/sq. at the 90% transmittance in the middle of visible spectral range by increasing a work function value from 4.8 (for pristine SWCNTs) to 6.0 eV

In addition, the fabrication of uniform, highly conductive and transparent SWCNT films opens a space for the development of a robust continuous roll-to-roll process by immersing roller modules into a dopant solution.

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Dielectric properties of intercalated graphite fluoride compounds with bromine and acetonitrile

Grebenkina M.A.[1,2], Chekhova G.N.[1], Pinakov D.V.[1], Gusel'nikov A.V.[1], Bulusheva L.G.[1,2], Okotrub A.V.[1,2]

1 – Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

grmariya@mail.ru

Fluorinated graphite intercalated compounds (FGICs) consist of a layered matrix formed by graphene layers with attached fluorine atoms and guest molecules, which are embedded in the interlayer space [1]. The study of the dielectric properties of FGICs will provide information of the intercalated molecules' arrangement in the interlayer space and the effect of intercalated molecules and the matrix's composition on the dielectric permittivity of the material.

In this research we investigated the temperature and the frequency dependences of the dielectric permittivity of FGICs with matrixes' compositions $C_2F_{1,05}$, $C_2F_{0,85}$, $C_2F_{0,60}$ and inserted bromine (Br_2) or acetonitrile (CH_3CN). The temperature was varied from 180 to 25 °C, the frequency – from 1 Hz to 7 MHz. It was indicated that low-fluorinated graphite intercalated with bromine has extremely high dielectric permittivity. The effect is associated with the formation of Br_2^- and Br_3^- ions which lead to an increase in the dielectric response and the appearance of an ion-relaxation mechanism of polarization. In highly fluorinated samples, interaction between Br_2 molecules are similar to that of a liquid. Moreover, it was demonstrated that the freezing of the movement of acetonitrile CH_3CN molecules in the interplanar space of graphite fluorides occurs at temperatures below -100 °C what causes a decrease of the dielectric permittivity of FGIGs.

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Fine tuning of single-walled carbon nanotube properties for transparent and conductive applications

Khabushev E.M.[1,2], Krasnikov D.V.[1], Tsapenko A.P.[1,2], Zaremba O.T.[1], Kolodyaznaya Y.V.[1], Goldt A.E.[1], and Nasibulin A.G.[1,2]

1 – Skolkovo Institute of Science and Technology, Moscow, Russia

2 – Aalto University, Espoo, Finland

eldar.khabushev@skoltech.ru

Single-walled carbon nanotubes (SWCNTs) are still a material attracting a significant attention of the scientific community: current technological advances are focused on their implementation in novel optoelectronic devices [1]. Currently, aerosol CVD is a well-established technique to produce SWCNTs of high quality, possessing excellent scalability and material purity. Nevertheless, precise control over output parameters is still not achieved that hampers SWNCT widespread implementation.

In this work SWCNT synthesis by aerosol CVD based on the Boudouard reaction utilizing ferrocene as catalyst precursor. We inspected the influence of synthesis conditions (temperature, carbon dioxide and ferrocene partial pressure) on SWCNT parameters utilizing the four-probe technique, Raman and optical spectroscopy and electron microscopy. Finely tuning synthesis parameters, we obtained SWCNTs with a mean diameter varying in the range from 1 to 2 nm and Raman quality factor I_G/I_D up to 500. Analyzing the obtained results, we prove a high Raman peak ratio (I_G/I_D), length, and diameter of the nanotubes to decrease the equivalent sheet resistance of the nanotube-based film [2]. Temperature kinetic measurements revealed the change in the nanotube growth mechanism at the temperature coinciding with the phase transition between α-Fe and γ-Fe catalyst phases, which highlighted a significant difference in the conductive properties of films producing at different synthesis temperatures.

As a result of equivalent sheet resistance optimization, we obtained pristine films with R_{90}=250 Ω/□. Moreover, this value dropped down to 39 Ω/□ after $HAuCl_4$ doping providing

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Holey single-walled carbon nanotubes for ultra-fast bolometers

Daria S. Kopylova[1]*, Fedor S. Fedorov[1], Alena A. Alekseeva[1], Zakhar I. Popov[2], Pavel B. Sorokin[2], Anton S. Anisimov[3], and Albert G. Nasibulin[1,4]

[1]*Skolkovo Institute of Science and Technology, Nobel str. 3, Moscow, 121205,* Russia

[2]*National University of Science and Technology MISIS, Leninskiy prospect, 4, Moscow, 119049, Russia*

[3]*Canatu Ltd. Konalankuja 5, 00390, Helsinki, Finland*

[4]*Aalto University, Department of Applied Physics, 00076, Aalto, Finland*

D.Kopylova@skoltech.ru

The development of new materials for sensitive and fast broadband photodetectors remains actual problem in the fields of IR vision and spectroscopy. Carbon nanotubes have already been demonstrated as a promising material for bolometers [1]. However, the sensitivity enhancement of such bolometers while maintaining the speed of operation is still a great challenge. Here, we present a new material, holey carbon nanotube network, designed to improve the temperature coefficient of resistance (TCR), the key parameter that determine the sensitivity of bolometers [2]. Fine treatment with low frequency oxygen plasma allows to control the conductive properties of the material. The temperature coefficient of resistance of our films is much higher than reported values for pristine carbon nanotubes in wide temperature range up to 3 % K^{-1} in absolute value at liquid nitrogen temperature which is much higher than reported values for carbon nanotubes and comparable with vanadium oxides. The bolometer prototypes made of free-standing plasma treated SWCNT films possess high sensitivity in wide IR range (3-50 µm), smooth spectral characteristics of IR absorption, ultrafast (3 ms) response time and relatively low noise level comparing to similar devices made of carbon nanotubes.

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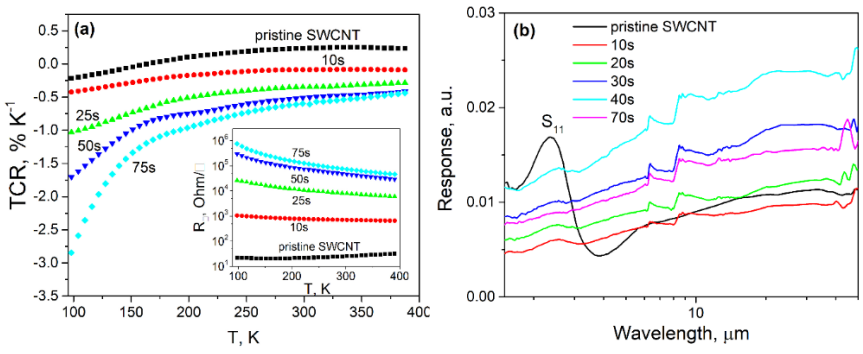

Fig.1 The plasma treatment effect on TCR of SWCNT films and bolometers response (a) TCR of pristine SWCNT films and the ones treated in oxygen plasma at different exposure time, inset: temperature dependence of film sheet resistance. (b) Spectral characteristics of bolometric samples made of 100 nm thick free-standing SWCNT film, pristine and oxygen plasma treated with different time of treatment.

A simple and reliable approach to fabricate arrays of single-walled carbon nanotube network field-effect transistor for advanced characterization.

Grigoriy B. Livshits[1], Alena A. Alekseeva[1], Anton V. Bubis[1], Dmitry V. Krasnikov[1], Albert G. Nasibulin[1,2]

[1]*Skolkovo University of Science and Technology, Moscow, Russia*

[2]*Aalto University School of Chemical Engineering, Espoo, Finland*

Grigoriy.Livshits@skoltech.ru

Nowadays, flexible electronics demands new materials for integrated circuits of high flexibility and stretchability[1]. Single-walled carbon nanotubes (SWCNTs) are one of the most promising materials for utilization in the flexible integrated circuits owing to the outstanding electrical and mechanical properties[2]. Field-effect transistors (FETs) with on/off ratio of 10^8 and 100 $cm^2/(V \cdot s)$ have already been reported on SWCNT films purified from metallic nanotubes[3] as well as on pristine films[4]. However, implementation of developed technologies in industry seeks advances in both the fabrication technology and deeper understanding of interplay between SWCNT film properties.

Here we present a technology for SWCNT film-based FETs that can be used as a versatile tool for examination of intrinsic properties of the films. The method relies on a simple capillary transfer technique of as-synthesized SWCNT film from a nitrocellulose filter. The method is simple, scalable, and does not require tedious and contaminating procedure of filter dissolution. We have fabricated a series of SWCNT FET arrays to demonstrate the advanced quality and uniformity of the transfer. The relation of FET parameters (such as opened and closed state resistance, on/off ratio *etc.*) can be easily brought to light via the procedure proposed. We have investigated the relations in the vast range of on/off ratio (10 - 10^6) and on-state resistance (10^4 – 10^8 Ω) on SWCNT film FETs with channel lengths in range of 60-350 μm. Moreover, this framework can provide access for more fundamental quantities such as SWCNT film density[5], metallic to semiconducting nanotube ratio, doping level *etc*[6].

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Investigation of sensory properties of CNT in relation to acetone vapors

Zaporotskova I.V.[1], Vilkeeva D.E.[1], Elbakyan L.S.[1], Dryuchkov E.S.[1].
1 – Volgograd State University, Volgograd, Russia

vidinara@mail.ru

Modern methods of diagnostics various diseases, despite their constant improvement, retain the need for fast and inexpensive screening technologies. One of the promising directions in this area is the analysis of exhaled air. Metabolic disorders typical of diabetes mellitus are due to increased acetone content in exhaled air, moreover, selective detection of acetone in breath is very important for diagnosing diseases in a non-invasive way. However, to date, inexpensive portable gas sensors for breath analysis have not been developed. This article provides a theoretical study of the possibility of reacting acetone, a common volatile organic compound (VOC) in human respiration, with carbon nanotubes modified with functional groups - carboxyl and amine. From studies conducted earlier [1,2], it is known, that carbon nanotubes, boundary-modified with carboxyl (COOH) and amine (NH_2) groups, form stable chemical complexes. In this paper, we used these sensor models to detect acetone vapor. Calculations of tubulens "zig-zag" (6.0) type were made within the framework of the molecular cluster model using the DFT calculation method. It was found that in both cases a stable chemical interaction is formed. Modified carbon nanotubes can be chemical and biological sensors that make it possible to fix micro amounts of substance. Specified functionalization will ensure high accuracy and selectivity of acetone detection in a complex mixture of gases, vapors and other volatile organic compounds present in exhaled air. Taking into account these features of functioning, it is worth noting the importance of creating a device with a sensor based on modified CNTs for contactless diagnosis of diabetes mellitus.

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New ultrathin medical coating of pvp-based medical biliary stents with addition of carbon nanotubes

Zvonareva D.A.[1], An E.E. [1], Zaporotskova I.V.[1]
1 – Volgograd State University, Volgograd, Russia

zvonareva@volsu.ru

We propose as a drug coating a coating based on a known polymer of polyvinylpyrrolidone (PVP) with an injected drug doxorubicin and carbon nanotubes (CNTs), known for their unique sorption and mechanical properties [1-3].

As a result of the experiment, it was found that the most stable is a 60% PVP solution. After the solution was infused, we divided it into three equal volumes, to which CNTs were added in quantities necessary to create concentrations of 0.1; 0.05; 0.01 wt% CNT. After application and complete drying, the thickness of the created coating averaged 0.02 mm. Then the drug-coated biliary stents were immersed in a saline solution - sodium chloride, which mimicked the internal environment of the human body. [4]

As a result of the study, it was found that the carbon nanotubes present in the coating have a positive effect on the durability and retention of the drug coating on the surface of the biliary stent. The optimal concentration is the concentration of 0.1 wt% nanotubes based on the solution weight.

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