Proceedings

# III International Workshop on Electromagnetic Properties of Novel Materials

Skolkovo Institute of Science and Technology

Moscow, Russia

18-20 December, 2018

# Welcome to EMPNM 2018!!!

**Dear EMPNM 2018 participant,**

we are pleased to welcome you to the III International Workshop on Electromagnetic Properties of Novel Materials!

This event follows two previous workshops organized first by Research Institute for Nuclear Problems of Belarusian State University in Minsk (2016) and Nikolaev Institute of Inorganic Chemistry SB RAS in Novosibirsk (2017). This year the Workshop is held in the heart of the Russian Silicon Valley, in the Skolkovo Innovation Center. We are happy to welcome you in a new campus of Skolkovo Institute of Science and Technology and wish you inspiring and groundbreaking ideas to flash your mind during the meeting!

The aim of the Workshop is to provide a floor for the recent advances in both fundamental and applied science of novel materials and their electromagnetic characteristics with special attention on carbon nanomaterials. The Workshop is of a substantial importance for students and young researchers to attend lectures by senior scientists and to interact with the leaders in their frontier fields and to learn from them the state-of-the-art research.

Being in the beginning only Russian speaking, this year the Workshop has become International, which allowed us to invite our foreign colleagues to support the meeting and widen the topic of the research areas within the Workshop program. The EMPNM 2018 Workshop has attracted 130 participants registered from 14 countries from 45 universities and institutions around the globe. We create new traditions, we support intensive idea exchange and 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. We have been able to offer free participation in the conference and support our invited speakers by travel funds and accommodation due to the support from the administration of Skolkovo Institute of Science and Technology. This Workshop was supported by SBI project “Magnetic nanoparticles and carbon nanotubes as enhancers for targeted RNA delivery in vivo” and Skoltech NGP Program. We acknowledge Russian Science Foundation (Project identifier: 17-19-01787) for the financial support. We hope that you will have enjoyable, enlightening and productive days during our Workshop!

Sincerely yours,
Albert G. Nasibulin
Conference chair

## Scientific committee

prof. Vladimir Kuznetsov
*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

prof. Polina Kuzhir
*Institute for Nuclear Problems, Belarusian State University, Minsk, Belarus*

prof. Sergei Maksimenko
*Institute for Nuclear Problems, Belarusian State University, Minsk, Belarus*

prof. Albert Nasibulin
*Skolkovo Institute of Science and Technology, Moscow, Russia*

prof. Alexander Okotrub
*Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia*

prof. Valentin Suslyaev
*National Research Tomsk State University, Tomsk, Russia*

prof. Georgy Fedorov
*Moscow Institute of Physics and Technology, Dolgoprudny, Russia*

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## Scope

III International Workshop on Electromagnetic Properties of Novel Materials follows two Workshops (Minsk 2016, Novosibirsk 2017). The aim of the Workshop is to provide a floor for the recent advances in both fundamental and applied science of novel materials and their electromagnetic characteristics with special attention on nanocarbons.

The workshop is held at Skolkovo Institute of Science and Technology (Moscow, Russia) on December, 18-20, 2018.

## Scientific program

1. Synthesis and characterisation of carbon nanomaterials
2. Hybrid materials
3. Electronic properties of nanocarbons
4. Application of THz and GHz radiation for the characterization of nanomaterials
5. Graphene Electronics
6. Magnetic Nanomaterials
7. Theoretical methods and approaches in nanoelectromagnetism
8. Biomedical application of carbon nanomaterials

## Sponsors

Workshop is supported by Russian Science Foundation project (№17-19-01787), Skoltech Biomedical Initiative project № 2017-7/SBI and Skoltech NGP Program.

# Venue


SHEREMETIEVO
BELORUSSKY RAILWAY STATION
CENTRAL MOSCOW
KIEVSKY RAILWAY STATION
SKOLKOVO
VNUKOVO
DOMODEDOVO
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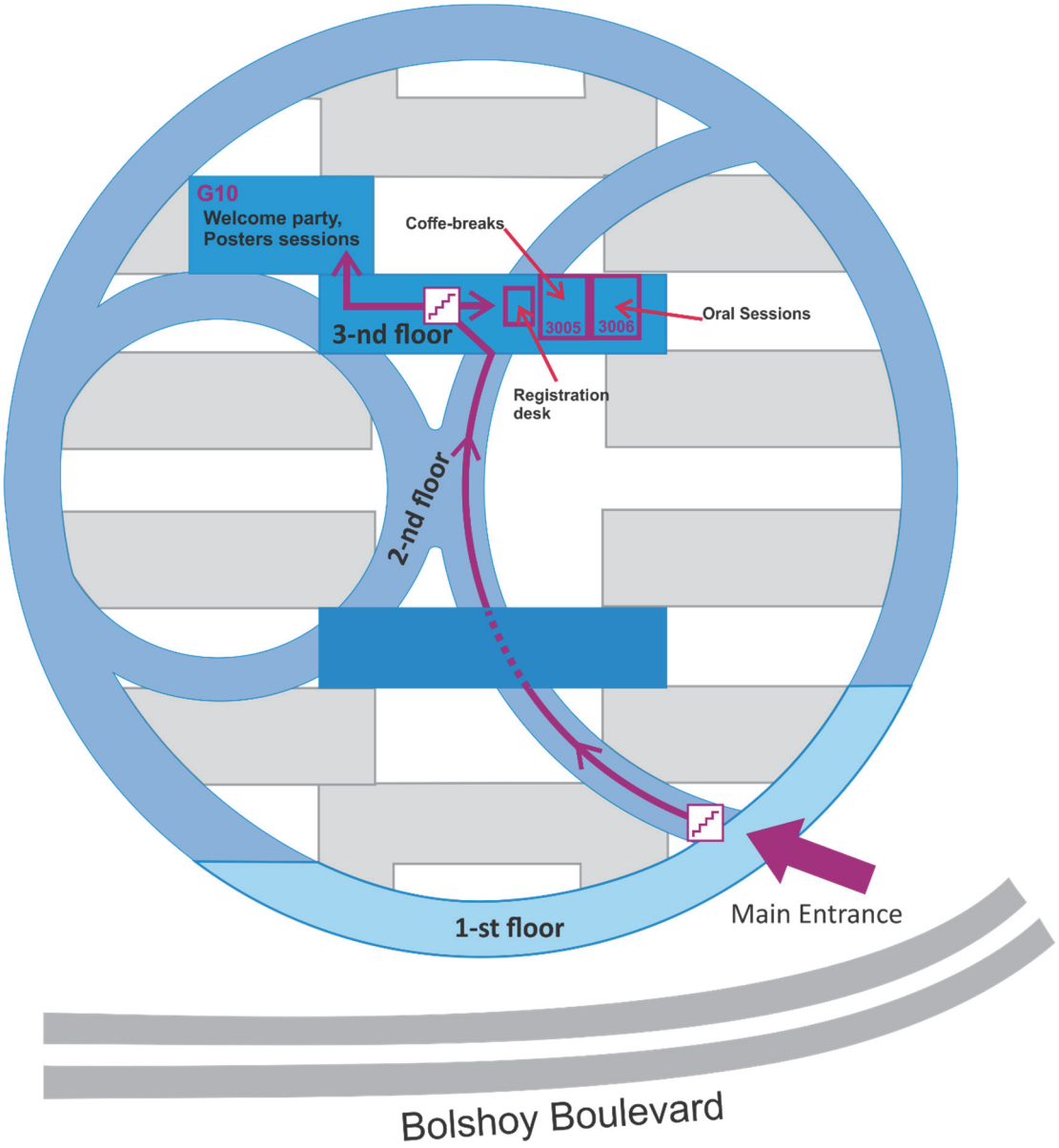
ИННОВАЦИОННЫЙ ЦЕНТР СКОЛКОВО
Skoltech New Campus
Big boulevard 30 bld. 1
Matreshka
Blaise Pascal str. 2
Skoltech Old Campus
Nobel str. 3
To Hotel Pamir & Tien-Shan
Novaya str. 100
D1
D2
D3
D4
Z1

## Plan of Skoltech New Campus



## Program

| | **Tuesday December 18** | **Wednesday December 19** | **Thursday December 20** |
|---|---|---|---|
| **9.00** | **Registration opens** | | |
| **9.45** | **Opening Ceremony** | | |
| | ***Session 1: Synthesis of novel materials*** | ***Session 3: Interaction with electromagnetic field*** | ***Session 5: THz/Optical properties of novel materials*** |
| 10.00 | Keynote Talk 1<br>Prof. Esko Kauppinen | Keynote Talk 11<br>Prof. Sergey Maksimenko | Keynote Talk 19<br>Prof. Michail Portnoi |
| 10.30 | Keynote Talk 2<br>Prof. Vladimir Mordkovich | Keynote Talk 12<br>Prof. Polina Kuzhir | Keynote Talk 20<br>Prof. Boris Gorshunov |
| 11.00 | Oral Talk 1<br>Dr. Nadezhda Nebogatikova | Oral Talk 5<br>Dr. Sergey Dyakov | Oral Talk 13<br>Dr. Irina Snigireva |
| **11.15** | **Coffee-Break** | | |
| 11.35 | Keynote Talk 3<br>Dr. Simas Rackauskas | Keynote Talk 13<br>Prof. Olga Glukhova | Keynote Talk 21<br>Prof. Georgy Fedorov |
| 12.05 | Keynote Talk 4<br>Prof. Krizstian Kordas | Keynote Talk 14<br>Prof. Mikhail Shuba | Keynote Talk 22<br>Prof. Anatoliy Snigirev |
| 12.35 | Keynote Talk 5<br>Prof. Artem Oganov | Oral Talk 6<br>Prof. Ayrat Dimiev | Keynote Talk 23<br>Prof. Pavlos Lagoudakis |
| 12.50 | | Oral Talk 7<br>Dr. Konstantin Batrakov | |
| **13.05** | **Lunch** | | |
| | ***Session 2: Electronic properties of novel materials*** | ***Session 4: Electrochemical properties of novel materials*** | ***Session 6: Biomedical impact of novel materials*** |
| 14.05 | Keynote Talk 6<br>Prof. Alexander Okotrub | Keynote Talk 15<br>Prof. Anvar Zakhidov | Keynote Talk 24<br>Prof. Dmitry Gorin |
| 14.35 | Keynote Talk 7<br>Prof. Lyubov Bulusheva | Keynote Talk 16<br>Prof. Tanja Kallio | Keynote Talk 25<br>Prof. Hye Jin Lee |
| 15.05 | Keynote Talk 8<br>Prof. Elena Obraztsova | Oral Talk 8<br>Dr. Stanislav Fedotov | Oral Talk 14<br>Sang Hyuk Lee |
| 15.20 | | Oral Talk 9<br>Dr. Ekaterina Fedorovskaya | Keynote Talk 26<br>Prof. Vladimir Drachev |
| 15.35 | Oral Talk 2<br>Dr. Olga Sedelnikova | Oral Talk 10<br>Dr. Anatoly Pushkarev | |
| **15.50** | **Coffee-Break** | | **Coffee-Break** |
| 16.10 | Keynote Talk 9<br>Dr. Kimmo Mustonen | Keynote Talk 17<br>Prof. Sergey Makarov | Keynote Talk 27<br>Prof. Albert Nasibulin &<br>Prof. Timofei Zatsepin |
| 16.40 | Keynote Talk 10<br>Prof. Ivan Bobrinetskiy | Keynote Talk 18<br>Prof. Harri Lipsanen | |
| 16.55 | | | **Excursions** |
| 17.10 | Oral Talk 3<br>Prof. Irina Antonova | Oral Talk 11<br>Dr. Ivan Mukhin | |
| 17.25 | Oral talk 4<br>Prof. Pavel Sorokin | Oral Talk 12<br>Prof. Marsil Kadirov | |
| 17.40 | Sponsor talk 1 Oxford Instruments/TechnoInfo<br>Dr. Francesco Reale | Sponsor talk 2 IMC Systems<br>Mikhail Trusov | |
| | | Sponsor talk 3 IMC Systems<br>Dr. Natalia Kuzmina | |
| **17.55** | **Photo** | | **Closing Ceremony** |
| **18.00** | **Poster session/ Welcome Party** | **Banquet** | |
| **18.15** | | | **Informal Discussions** |

## Location

**Registration** *@ New Skoltech Campus* on December 18 from 09.00 to 18.00

**Session 1:** Synthesis of novel materials *@ New Skoltech Campus (3005)*

**Session 2:** Electronic properties of novel materials @ New Skoltech Campus *(3005)*

**Session 3:** Interaction with electromagnetic field @ New Skoltech Campus *(3005)*

**Session 4:** Electrochemical properties of novel materials @ New Skoltech Campus *(3005)*

**Session 5:** Thz/Optical properties of novel materials @ Old Skoltech Campus *(301)*

**Session 6:** Biomedical impact of novel materials @ Old Skoltech Campus *(301)*

**Poster session/ Welcome Party** *@ New Skoltech Campus*

**Banquet** @Matreshka Restaurant

**Excursions** @ Old Skoltech Campus

**Closing Ceremony/ Informal Discussions** @ Old Skoltech Campus

# Oral Sessions

## Tuesday,
## December 18

| **Day 1, December 18** | | |
|---|---|---|
| 9.00 | Registration opens | |
| 9.45 | Opening Ceremony | |
| ***Session 1: Synthesis of novel materials*** **Chairman: Nasibulin** | | **Page** |
| 10.00 – 10.30 | Keynote Talk 1 Prof. Esko Kauppinen<br>*FC-CVD Synthesis and Direct Deposition of Colorful SWNT Thin Films* | **14** |
| 10.30 – 11.00 | Keynote Talk 2 Prof. Vladimir Mordkovich<br>*Extra-long carbon nanotubes from bench-scale to scaled-up carbon cotton and carbon thread* | **16** |
| 11.00 – 11.15 | Oral Talk 1 Dr. Nadezhda Nebogatikova<br>*$Bi_2Se_3$ thin films for van der Waals heterostructures* | **18** |
| **11.15-11.35** | **Coffee-Break** | |
| ***Session 1: Synthesis of novel materials*** **Chairman: Kallio** | | |
| 11.35 – 12.05 | Keynote Talk 3 Dr. Simas Rackauskas<br>*Direct observation of non-catalytic nanowire growth: mechanism investigation and application perspectives* | **22** |
| 12.05 – 12.35 | Keynote Talk 4 Prof. Krizstian Kordas<br>*$WS_2$ nanowire and nanoflake hybrid structure* | **22** |
| 12.35 –13.05 | Keynote Talk 5 Prof. Artem Oganov<br>*Computational Materials Discovery* | **24** |
| **13.05 – 14.05** | **Lunch** | |
| ***Session 2: Electronic properties of novel materials*** **Chairmen: Kauppinen & Maksimenko** | | |
| 14.05 –14.35 | Keynote Talk 6 Prof. Alexander Okotrub<br>*Magnetic and electromagnetic properties of aligned carbon nanotubes* | **26** |
| 14.35 – 15.05 | Keynote Talk 7 Prof. Lyubov Bulusheva<br>*Electronic structure of N- and P-containing graphenes grown by CVD method* | **28** |
| 15.05 – 15.35 | Keynote Talk 8 Prof. Elena Obraztsova<br>*Electronic and optical properties of non-covalently doped single-wall carbon nanotube or graphene films* | **30** |
| 15.35 – 15.50 | Oral Talk 2 Dr. Olga Sedelnikova<br>*Controlling of morphology and charge transport properties of arc-produced carbon by doping* | **32** |
| **15.50 – 16.10** | **Coffee-Break** | |
| ***Session 2: Electronic properties of novel materials*** **Chairmen: Fedorov & Lee** | | |
| 16.10 – 16.40 | Keynote Talk 9 Dr. Kimmo Mustonen<br>*Low-Dimensional Carbon Heterostructures for Electronic Applications* | **34** |
| 16.40 – 17.10 | Keynote Talk 10 Prof. Ivan Bobrinetskiy<br>*Direct laser writing of graphene-based photosensitive junctions* | **36** |
| 17.10 – 17.25 | Oral Talk 3 Prof. Irina Antonova<br>*Flexibility of graphene-based materials in 2D printed heterostructures* | **38** |
| 17.25 – 17.40 | Oral talk 4 Prof. Pavel Sorokin<br>*Flexoelectricity in 2D world: graphene and h-BN cases* | **39** |
| 17.40 – 17.55 | Sponsor talk 1 Dr. Francesco Reale<br>*Scaled-up fabrication of 2D materials and heterostructures: Technology and processes* | **40** |
| **17.55** | **Photo** | |
| **18.00** | **Poster session/ Welcome Party** | |

# FC-CVD Synthesis and Direct Deposition of Colorful SWNT Thin Films

Kauppinen E. I.

*Department of Applied Physics, Aalto University School of Science, Espoo, Finland*

We have explored floating catalyst chemical vapor deposition (FC-CVD) synthesis of SWNTs for tuning chirality distribution and obtaining narrower chirality distributions. By introducing various amount of $CO_2$ in FC-CVD using CO as a carbon source and in-situ ferrocene decomposition generated Fe catalyst nanoparticles, we have succeeded in directly synthesizing SWCNT films with tunable (n,m) i.e. helicity distribution as well as tunable colors (Liao et al. 2018). In particular, when operating the FC-CVD reactor at the ambient pressure and at 850°C temperature with 0.25 and 0.37 volume percent of added $CO_2$, the directly deposited SWCNT films display green and brown colors, respectively (Fig. 1). We ascribed various colors to suitable diameter and narrow (n,m) distributions of SWCNTs, which were determined in detail using the electron diffraction. Additionally, by increasing the reactor temperature to 880°C, we achieved much narrower (n,m) distribution clustered around (11,9) with extremely narrow diameter range (>98% between 1.2 and 1.5 nm). In addition, we present SWNTs in novel 3D electronics applications and also recent results on SWNT (n,m) distributions when using ethylene, ethanol and toluene as the carbon sources and discuss the effect S and water used as the growth promoters.

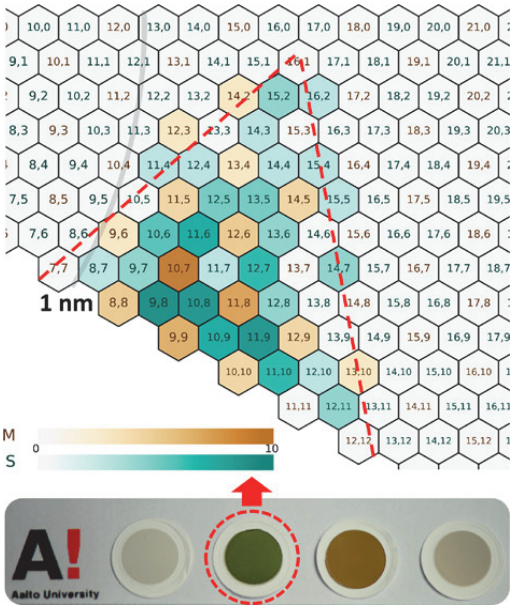



**Figure 1.** (n,m) distribution of the green SWNTs and photos of the SWNT thin films synthesized at 850 oC. with 0 %, 0.25 %(green), 0.37 % (brown) and 0.5 % of added CO2.

**References:**

Liao, Y., Jiang, H., Wei, N., Laiho, P., Zhang, Q., Khan, S.A. and Kauppinen, E.I. (2018) J. Am. Chem. Soc. 140, 31, 9797-9800.

**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).

# Extra-long carbon nanotubes from bench-scale to scaled-up carbon cotton and carbon thread

Mordkovich V. Z. [1,2]

[1]*Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Moscow 108840, Russia*

[2]*INFRA Technology, Moscow 108840, Russia*

The outstanding properties of carbon nanotubes can be translated into macro-material if two important requirements are met: firstly, the nanotubes must be aligned; secondly, the nanotube length must be comparable with dimensions of a macro-sample or device.

This work presents the results of the applied research comprising synthesis way for such centimeter-long aligned nanotubes; scale-up of the production process through growth, pulling of the nanotubes into big carbon cotton spools or pulling-and-spinning into threads. Although there are several methods discovered for synthesizing centimeter-long nanotubes, the macroscopic material requires the nanotubes in quantities, which are difficult or impossible to produce in laboratory bench scale. So, it is necessary to scale up, which is a difficult chemical engineering problem.

A floating catalyst bed synthesis rig is reported capable of producing at 1200°C carbon nanotubes, which are aligned due to in-process pulling.

The aligned carbon nanotubes were investigated by electron microscopy (SEM/TEM), Raman spectroscopy and thermal analysis. It was shown that the material is dominated by aligned double-walled nanotubes. The direct measurement of the nanotube length by confocal profilometry method confirmed unprecedented length of individual nanotubes.

Investigation of electrochemical properties showed an unprecedented robustness to voltammetry cycling in alkali solutions. The capacity exceeded 27 F/g. The rolled carbon nanotubes and nanotube-reinforced polymers in the form of thin tapes or fiber or bulky composites demonstrate dramatic and anisotropic boost of mechanical and electrical properties such as jump of strength of a polyurethane tape from 18 MPa up to 500 MPa.

**Vladimir Zalmanovich Mordkovich, Ph.D., Dr.Sci.**

**Biography**

Vladimir Mordkovich earned his degrees from the Moscow State University (MS in chemistry 1981; Ph.D. 1984). The upper degree of Dr.Sci. was awarded in 1995.

Vladimir Mordkovich has dedicated his career to R&D in chemistry and technology of fuels and materials. He had spent 11 years in Japan working for R&D companies, before returning to Russia, where he joined the team of founders of YUKOS R&D Center focusing on carbon materials research and the development of the new generation of GTL technology.

Since 2009 he leads the New Chemical Technologies and Nanomaterials Research Department at the Technological Institute for Superhard and Novel Carbon Materials (TISNCM) in Moscow. Vladimir Mordkovich serves as a full professor in Moscow Physico-Technical Institute (since 2010) and Moscow State University (since 2018). He is a member of the Materials Research Society in the USA and the Russian Carbon Society in Russia, Elected Chairman of the Chemical Technology and Petrochemistry Advisory Board at The Russian National Agency of Research Institutes.

52 inventions in the field, 160 publications in peer-reviewed journals.

# $Bi_2Se_3$ thin films for van der Waals heterostructures

Nebogatikova N. A. [1,2], Antonova I. V. [1-3], Kustov D. A. [1], Golyashov V. A. [2], Koch K. A. [4], Tereshchenko O. E. [1,2]

[1]*Novosibirsk State University, Novosibirsk, Russia*

[2]*A.V. Rzhanov Institute of Semiconductor Physics SB RAR, Novosibirsk, Russia*

[3] *Novosibirsk State Technical University, Novosibirsk, Russia*

[4]*V.S. Sobolev Institute of Geology and Mineralogy SB RAS Novosibirsk, Russia*

*nadonebo@gmail.com, antonova@isp.nsc.ru*

Bismuth selenide (Bi2Se3) demonstrates the properties of a topological insulator, it has a small band gap (Eg ~ 0.25-0.35 eV). The huge interest in the topological materials resides not only in fundamental research but also in the promising properties of these materials for future applications. Possible applications are spintronics, quantum computing, magnetic memories, and thermoelectric materials. The most promising for applications are Bi2Se3 thin films with nanometer- sized thickness. To create thin films and heterostructures based on them, the same methods as for graphene can be used. These methods are (PVT) growth, electrochemical (ECS) and mechanical (MS) splitting.

The study was focus on exfoliation of thin films from Bi2Se3 monocrystalline and to investigate their electrical and structural properties. For the formation of films, PVT growth on the mica surface and electrochemically splitting of bulk bismuth selenide were used, followed by transfer to the substrates of SiO2 / Si. The structural properties of the films were studied using SEM and atomic force microscopy. A resistivity of the electrochemically exfoliated films as a function of its thickness is shown in Fig.1. The p-type of conductivity, the resistivity of ~ 4–20 kΩ and carrier mobility of ~ 10–50 cm2 / Vs was found for films with thickness lower 70 nm. PVT grown Bi2Se3 films with a thickness of 4 nm turned out to be non-conductive, in contrast to 4-nm ECS films. A vertical heterostructures of 4-8-nm ECS Bi2Se3 on graphene demonstrate carrier mobility enhanced up to 100 – 150 cm2 / Vs. Another advantage of used ECS method was relative large size of obtained flakes with size up to 0.3-0.5 mm and monoatomically flat surface.

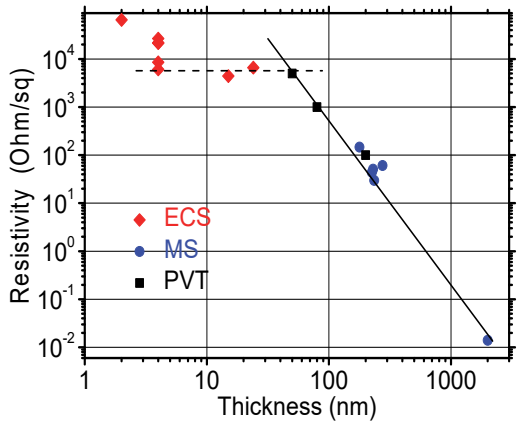



**Fig. 1.** The dependence of the $Bi_2Se_3$ films resistivity on their thickness.

**References:**

[1] Wang B. T., Zhang P. Phonon spectrum and bonding properties of $Bi_2Se_3$: Role of strong spin-orbit interaction //Applied Physics Letters, 2012, V. 100, №. 8, P. 082109.

[2] Zhang H. et al. Topological insulators in $Bi_2Se_3$, $Bi2Te_3$ and $Sb2Te_3$ with a single Dirac cone on the surface //Nature physics, 2009, V. 5 (6), P. 438.

# Direct observation of non-catalytic nanowire growth: mechanism investigation and application perspectives

Rackauskas S. [1,2]

[1]*Institute of Materials Science of Kaunas University of Technology, K. Barsausko Str. 59, LT-51423, Kaunas, Lithuania*

[2]*University of Turin, Department of Chemistry,Via P. Giuria 7, 10125, Torino, Italy*

The majority of the nanowire (NW) synthesis methods utilize catalyst particles to guide the nanowire geometry. In contrast, catalyst-free methods are attractive for facile fabrication of pure nanowires without the need for catalyst preparation. Nonetheless, how nanowire growth is guided without a catalyst is still widely disputed and unclear. Here, we show that the nanowire growth during metal oxidation is limited by a nucleation of a new layer. On the basis of in situ transmission electron microscope investigations, using CuO NWs as a model material, we found that the growth occurs layer by layer at the lowest specific surface. Atomic layers nucleate at the edge of twin boundary ridges and form a long-range ordering along the twin boundary. One can anticipate that it will be possible to use defects to drive and even control the process of growth and the geometry of nanowires in a similar manner to what can be done with the help of catalyst particles. Although we have investigated the formation of only CuO nanowires, similar growth mechanisms could be also extended to non-catalytic growth of other nanowires and ionic crystals grown by oxidation−reduction reactions [1,2]. Nanowire application perspectives for sensing will be also disscused.

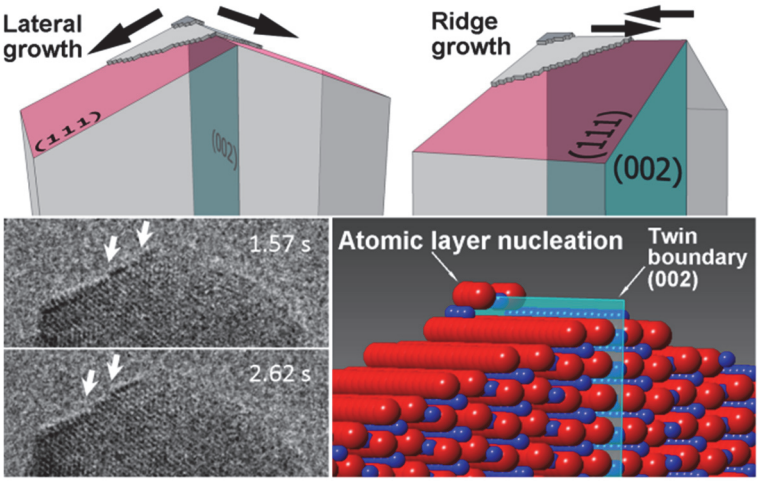



**Fig. 1.** *In situ* TEM observation of CuO nanowire growth [1].

**Keywords:** metal oxide nanowire; non catalytic growth; ETEM; sensing.

**References:**

S. Rackauskas et al., Nano letters **14**, 10 (2014)

S. Rackauskas et al., Scientific reports **7** (1), 12310 (2017).

**Simas Rackauskas** defended his PhD in Physics at Aalto University, Finland in 2011. He was a Marie Curie Fellow in University of Turin (Italy). He also held post-doctoral positions in Aalto University (Finland) and State University of Campinas (Brazil). He had fellowships in Swiss Federal Institute of Technology in Lausanne (EPFL, Switzerland), Technical University of Denmark (DTU) and University of Nagoya (Japan). His research interests are mainly focused on non-catalytic growth of metal oxide nanowires, application in sensing, carbon nanomaterials and flexible electronics.

## $WS_2$ nanowire and nanoflake hybrid structure

Kordas K.

*Microelectronics Research Unit, University of Oulu, Finland*

Our talk discusses on the structural, chemical, electrical and optoelectronic properties of $WS_2$ nanowire-nanoflake hybrid structures that we synthesized by a simple thermal sulfurization of hydrothermally grown $WO_3$ nanowires.[1] We show that the nanowire-nanoflake nanohybrids are semiconducting and have excellent gas sensing behavior. High sensitivity (0.043 $ppm^{-1}$) and selectivity towards $H_2S$ with a detection limit of 20 ppb is measured in air buffer.[2] We also demonstrate very good visible light response of photodetector devices based on the nanohybrids with photoresponsivity of up to 400 $mAW^{-1}$.[3,4]

**References**

Asres, G. A., Dombovari, A., Sipola, T., Puskás, R., Kukovecz, A., Kónya, Z.,Popov, A., Lin, J.F. Lorite, G.S. Mohl, M., Toth, G., Spetz, A.L., Kordas, K. (2016) A novel $WS_2$ nanowire-nanoflake hybrid material synthesized from $WO_3$ nanowires in sulfur vapor. Scientific Reports 6, 25610.

Asres, G.A., Baldovi, J.J., Dombovari, A., Järvinen, T., Lorite, G.S., Mohl, M., Shchukarev, A., Paz, A.P., Xian, L., Mikkola, J-P., Spetz, A.L., Jantunen, H., Rubio, A., Kordas, K. (2018) Ultra-sensitive $H_2S$ gas sensors based on p-type $WS_2$ hybrid materials. Nano Research 11, 4215

Asres, G.A., Järvinen, T., Lorite, G.S., Mohl, M., Pitkänen, O., Dombovari, A., Toth, G., Spetz, A.L., Vajtai, R., Ajayan, P.M., Lei, S., Talapatra, S., Kordas, K. (2018) High photoresponse of individual $WS_2$ nanowire-nanoflake hybrid materials. Applied Physics Letters 112, 233103.

Asres, G.A, (2018) Synthesis, characterization and application of $WS_2$ nanowire-nanoflake hybrid nanostructures. Doctoral thesis, Acta Universitatis Ouluensis. C 652, University of Oulu.

**Krisztian Kordas** earned his M.Sc. Physics and Chemistry (1998) and Dr. Tech. Microelectronics (2002) degrees at the University of Szeged (Hungary) and University of Oulu (Finland), respectively. He has become Docent of Nanotechnology in 2005 and full Professor in Micro- and Nanoelectronic Materials and Components for ICT Applications in 2016 at the University of Oulu. He spent several shorter periods abroad as visiting scholar at the University of Arkansas (2004), Rensselaer Polytechnic Institute (2004, 2005), University of Szeged (2017) and Rice University (2014, 2017), and was working as an assistant professor at the Umeå University (2012-2013). His research is focused on the synthesis, structural and electrical characterization, and implementation of nanostructured materials for electronics, sensors and catalyst applications. Prof. Kordas has supervised or participated in more than 20 national and international research projects, published 160+ papers in refereed scientific journals and co-authored 4 book chapters receiving ~4700 citations (Google Scholar). Under his supervision, 8 doctoral students graduated.

## Computational Materials Discovery

Oganov A.

*Skolkovo Institute of Science and Technology*

Since mid-2000s, when crystal structure prediction problem was solved, it has become possible to predict new materials with desired properties. A large role in this computational revolution has been played by my USPEX method/code (http://uspex-team.org), freely available to academic researchers. In this talk, I will discuss some of its applications to the discovery of novel compounds with unusual chemical bonding, and novel superhard, superconducting, and thermoelectric materials.

**Artem R. Oganov** is an expert in computational materials discovery and crystal structure prediction. He has edited 2 books and authored >220 papers, with total citation of >11000(>15000) and h-index 53(61) according to the Web of Science (Google Scholar). He was born in 1975, in 1997 graduated from Moscow State University (Russia) and got his PhD at University College London (UK) in 2002. In 2008-2014 he was an Associate Professor and then Full Professor at Stony Brook University (USA). In 2014 he moved back to Russia, where he is a Full Professor at Skoltech. In 2015 he was elected to Academia Europaea. Since 2017 he serves on Russian President's Council for Science and Education.

## Magnetic and electromagnetic properties of aligned carbon nanotubes

Okotrub A. V. [1], Sedel'nikova O. V. [1], Bulusheva L. G. [1]

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Composite materials based on polymers matrix with various nanocarbon inclusions are promising materials for electromagnetic shielding. Arrays of multiwall carbon nanotubes (MWNTs) oriented perpendicular to the surface exhibit anisotropy of mechanical, electrical and optical properties that allows producing new types of functional materials and devices. MWCNTs were synthesized on silicon substrates by CVD method in the reaction of catalytic thermolysis of ferrocene/toluene mixtures. Polystyrene/iron-filled MWNT composite films were prepared by solution processing, forge-rolling and stretching methods. Effect of fabrication on the structure of obtained carbon filler/polymer composite was discussed. The efficiency of stretching and forge-rolling for anisotropic composite production was demonstrated [1, 2]. Magnetic susceptibility measurements as well as records of isothermal hysteresis loops performed in three perpendicular directions of magnetic field confirmed that the nanotubes have a preferential alignment in the matrix. Strong diamagnetic anisotropy in the composites emerges not only from the MWCNTs but also from the polystyrene matrix [3]. The contribution of iron nanoparticles to overall magnetic response strongly depends on nanotube concentration in the composite as well as on matrix-filler non-covalent stacking, which influences magnetic interparticle interactions. We investigate the electromagnetic response of MWCNTs filled with iron-containing nanoparticles (ICNs) in the terahertz frequency range. The composites showed an enhanced permittivity and anisotropy in the transmittance spectra when iron content increased [4]. This behaviour was related to the mechanism based on electrical conductivity and polarization of ICNs and ICN/MWCNT interfaces. Since terahertz field penetrates inside MWCNTs, the filling of their cavities can be a way of varying the electromagnetic properties of MWCNT-containing composites.

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**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.

# Electronic structure of N- and P-containing graphenes grown by CVD method

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The films of graphene have been grown on copper foils using a low-pressure variant of chemical vapor deposition (CVD) method. Pure graphene was produced from methane at 1050 °C, for the graphene doping with phosphorous, phosphine was added to methane and the gaseous mixture was decomposed at 850 °C. N-doped graphene was synthesized from acetonitrile at 900 °C. The obtained graphene films were transferred to $SiO_2$/Si substrates using a copper etching by iron chloride. Morphology and electronic structure of the samples were studied by optical and atomic force microscopy and by methods of X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy at the Russian-German beamline at synchrotron radiation station BESSY II. We studied the as-transferred films and those after annealing in ultra-high vacuum conditions. Two main forms of nitrogen – graphitic (direct substitution of lattice carbon atom for nitrogen one) and pyridinic (two-fold coordinated nitrogen) were detected in N-doped graphene, while phosphorous was mainly in oxidized $PO_x$ form with small admixture of the P-C form. From the results of electrical measurements, such graphene modification causes decrease of the conductivity, which is especially large for N-doped graphene.

**Lyubov Bulusheva** is a graduate of the Novosibirsk State University, Russia. She has a Doctor of Science degree in Physical Chemistry awarded for work in the investigation of electronic structure of fullerene and carbon nanotube derivatives by the methods X-ray spectroscopy and quantum chemistry from the Nikolaev Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia. Currently, she is a principal researcher in the laboratory of physics-chemistry of nanomaterials at this Institute. The main research activity of Lyubov Bulusheva is related to the studies of electronic structure and properties of novel carbon nanomaterials and their derivatives. According to the Web of Science database, she has 260 papers, which have been cited more than 3600 times. Lyubov Bulusheva has managed several projects supported by the Russian Foundation for Basic Research and at present time, she is a leader of the Russian Science Foundation grant entitled “Metal-carbon nanohybrids for lithium-ion batteries and hydrogen generation”.

# Electronic and optical properties of non-covalently doped single-wall carbon nanotube or graphene films

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Last few years a great interest exists to thin single-walled carbon nanotube (SWNT) films non-covalently doped with electron-acceptor molecules [1-4]. They are a macroscopic object and have a transparency of about 90% and a surface resistance of 50 Ω / square [3]. These parameters make them a real candidate for replacing the most popular material for transparent electrodes today - ITO (indium tin oxide). Filling of nanotubes leads to p-type doping, confirmed by the shift of position of the tangential Raman mode (1592 cm-1) and the suppression of E11 and E22 transitions in the optical absorption spectra. The shift of the Fermi level to the valence band was estimated as 1 eV. After doping, the electrical resistance of the tubes decreases by almost an order of magnitude, and the optical transmission increases by 3-5% [2,3]. The effect is more pronounced in the fractions of the tubes, separated over the type of conductivity [4]. In photoluminescence (PL) spectra (in contrast to the case of pristine nanotubes), new peaks have been observed [5]. They were assigned to trions, quasiparticles consisting of two holes and one electron. The redistribution of PL intensity between the exciton and trion peaks is demonstrated with an increase in the doping degree. Pump-probe experiments have revealed the ways of energy transfer in doped SWNTs. Gas phase non-covalent doping also has been successively realized for graphene.

The prospective of application of non-covalently doped SWNT or graphene films as transparent conductive electrodes in solar cells and GaN diodes is discussed.

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Elena Obraztsova was graduated from the quantum radiophysics chair of the Physics Department of M.V. Lomonosov Moscow State University (MSU) in 1981. She got her PhD in optics at MSU in 1990. Since 1992, she worked at A.M. Prokhorov General Physics Institute of the Russian Academy of Sciences (GPI RAS), heading the Nanomaterials spectroscopy laboratory since 2001. Since 2018 she is also a Head of Nanocarbon materials laboratory in Moscow Institute of Physics and Technology (MIPT), formed as a joint laboratory of Russian Academy of Sciences and MIPTsHer scientific interests concern optical spectroscopy of low-dimensional materials. Last years, she was involved in studies of different forms of nanocarbon. An important cycle of works on laser applications of carbon nanotubes was performed. She is a coauthor of more than 270 papers in reviewed journals. Her Hirsh factor is 32. She was a supervisor of 12 PhD defended theses. She is a coordinator of several national and international research projects and a member of the editorial advisory board of 2 international scientific journals: Carbon, Laser Physics Letters.

# Controlling of morphology and charge transport properties of arc-produced carbon by doping

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Chemical doping is powerful rout to modify functional properties of carbon materials. Here we used arc discharge process for production of inhomogeneous composite containing a random distribution of carbon nanotubes, polyhedral nanoparticles and graphite plates. The morphology of nanoparticles was examined by scanning electron microscopy (SEM) and transmission electron microscopy (TEM), the defect density and chemical composition are investigated by Raman spectroscopy, X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure spectroscopy (NEXAFS).

Incorporation of foreign elements during growth affects both morphology and transport properties of deposit. Doping with nitrogen and boron was achieved by variation of synthesis conditions. Despites incorporation of nitrogen in both electron donor (graphitic) and electron acceptor (pyridine-like) configurations, the prevalence of n-type conduction in N-doped composite was observed. Structural analysis showed that N-doped sample contains big graphite plates ensuring ordinary Lorentz magnetoresistance effect. Acting as electron donor, boron atoms enhance hole concentration considerably ensuring p-type conduction in B- and BN-doped samples. Addition of boron produces disorders in the graphitic structure and negative magnetoresistance. The possible mechanism for the MR of arc-discharge composites can be partially understood using ordinary MR theory, weak localization theory and diffuse scattering theory.

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## Low-Dimensional Carbon Heterostructures for Electronic Applications

Mustonen K. [1], Hussain A. [2], Hofer C. [1], Inani H. [1], Tripathi M. [1], Liao Y. [2], Monazam M. [1], Susi T. [1], Kauppinen E. I.[2], Meyer J. C. [1] and Kotakoski J. [1]

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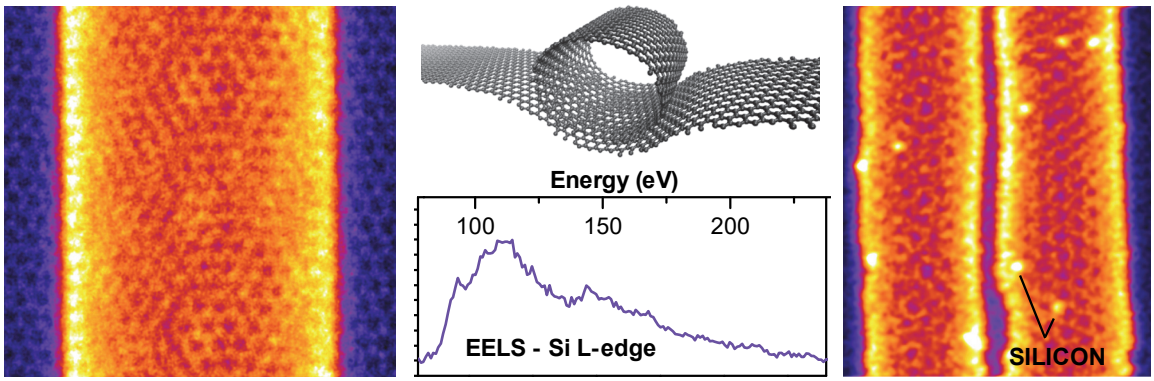
Graphene and single-walled carbon nanotubes (SWCNTs) have been among the most studied structures in materials science during the past decades. Building on enormous advances in graphene research, interest has recently shifted towards the creation of so-called van der Waals heterostructures [1-3]. Such materials typically combine graphene or other two- or lower dimensional molecules into vertical stacks [2-3]. The leading idea of the concept has been to preserve the covalent bonding structure of the constituent molecules binding mainly through van der Waals interactions (vdW). My talk will cover our recent work in fabrication and atomic-level characterization of single-walled carbon nanotube/graphene heterostructures [4] followed by a short discussion of their transport properties [5]. I will very shortly cover their band-structure modifications by substitutional doping [6] and conclude my talk by showing that, similar to graphene [7], silicon heteroatoms in SWCNTs can be moved in the lattice by a sub-Å scanning transmission electron microscope probe [8].

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**Kimmo Mustonen** is a Post Doctoral Research Associate in the oldest German speaking university in the world, the University of Vienna in Austria. He received his PhD in the field of synthesis and electronic applications of single-walled carbon nanotubes from Aalto University, Finland in 2015. Since his graduation he's been developing electron microscopic techniques for in situ covalent modifications in nanocarbon and related materials as a part of Professor Jannik C. Meyers and professor Jani Kotakoskis research groups. His current research revolve around ultra-microscopy and spectroscopy of low-dimensional heterostructures and in situ electronic measurements, with the emphasis on single-molecule experiments.

## Direct laser writing of graphene-based photosensitive junctions

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Single and few-layer graphene photodetectors have attracted much attention in the past few years. Pristine graphene shows a very weak response to visible light; hence, fabrication of complex graphene-based detectors is a challenging task. In this work, we utilize the ultrafast laser oxidation of single-layer CVD graphene for highly desirable maskless fabrication of micro- and nanoscale devices. This technique can be applied to process carbon nanomaterials at large scale with relatively high speed. In perspective, fs-laser treatment with submicrometer resolution can fully replace the lithography and plasma etching processes. We investigate the optoelectronic response of pristine and functionalized devices under femtosecond and continuous wave lasers irradiation [1]. The laser processed graphene photodetectors show a high photoresponsivity and photocurrent generation.

**Acknowledgement.** This work was partly supported by the Russian Science Foundation, grant 14-19-01308.

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## Flexibility of graphene-based materials in 2D printed heterostructures

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Currently, 2D electronics is becoming established, namely, the rapid development of technologies for producing 2D materials, technological methods of working with these materials, the development of heterostructures with a new design, and the search for prospects for monolayer materials and devices applications. The advantages of 2D materials include basic compatibility with traditional materials and technologies (after adapting some technological processes), a breakthrough in miniaturization, including 3D design, the ability to control the electronic properties of materials, create new types of heterostructures that are not achievable by other methods, and so on. The development of flexible (stretchable, wearable) electronics using materials based on graphene, as an integral part of the electronics of monolayer materials, is currently showing tremendous progress. Short review recent advances in the development of flexible electronics using graphene-based materials in combination with our results will be presented in the report. In particular, heterostructures created with the use of printed technologies from graphene, fluorinated graphene (FG), and FG-based composites for flexible applications will be discussed.

## Flexoelectricity in 2D world: graphene and *h*-BN cases

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The presented talk I will devote to the considering in details the appearance of polarization in 2D materials in particular in graphene and *h*-BN. It is known that a homogenous mechanical distortion of graphene cannot induce electrical dipole due to graphene lattice central symmetry center (no piezoelectric effect). This rule however does not apply to the second order electronic flexoelectric effect induced by the strain gradient, especially by the bending of graphene sheet, which is one of the most intriguing properties of graphene. Moreover, all graphene based nanostructures will succeed such property. We show a correlation between atomic scale characteristic (pyramidalization angle) and macroscopic characteristic (curvature) of material and substantiate that slight variations in atomic structure will lead to significant changes of macroscopic characteristics of material by the example of dipole moment. We established the linear dependence of flexoelectric dipole moments on the local curvature for different carbon networks with various atomic arrangements by combining direct *ab initio* calculations with, wherever possible, analytical phenomenological equations. Using the obtained universal flexoelectric coefficient, the large dipole moment values of various carbon nanocones are predicted and their scaling with cone dimensions is elucidated. Our analysis suggests the possibility of predicting the electric dipole moments of complicated low-dimensional graphene-based systems using only their atomic geometry [1].

We applied the developed theory to the naturally polar counterpart of graphene, h-BN. We showed that it is necessary to distinguish the polarity in h-BN based nanostructures to polar bonds and flexoelectric effects associated with a curved *h*-BN lattice. The latter phenomenon is also described through establishing universality of the linear dependence of flexoelectric dipole moments on local curvature in various nano-*h*-BN networks (nanotubes and fullerenes). Finally, we applied the theory to the description of various h-BN nanocones with different apex angles and showed the advantageous properties of such nanostructures.

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# Scaled-up fabrication of 2D materials and heterostructures: Technology and processes

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Traditional vapour-phase synthesis methods of bulk semiconductors have undergone a resurgence of research interest over the last decade for the growth of low-dimensional materials and heterostructures [1-3]. In particular, the chemical vapour deposition (CVD) has been extensively rediscovered to achieve large-area atomic planes of Van der Waals solids such as graphene and transition metal dichalcogenides [4, 5]. Heterostructures created by stacking atomic planes with complementary characteristics have also been demonstrated to achieve novel functionality [6]. These hybrid nanomaterials revealed unforeseen electrical, optical and mechanical properties which make them unique candidates for next-generation nanotechnologies, ranging from large scale consumer electronics to quantum electronics.

Nevertheless, for the successful scaling up of prototypical applications demonstrated to date, technologies and processes for the wafer-sized deposition of these materials need to be developed. In this talk I will give an overview of the progress we have made at Oxford Instruments Plasma Technology towards the high-performance synthesis of low-dimensional structures (e.g. graphene, $MoS_2$, h-BN, CNTs) by CVD and plasma-enhanced CVD. Further, we compare the relative merits of CVD and atomic layer deposition (ALD) to grow 2D materials, and introduce results on atomic layer etching (ALE). Finally, I will discuss our developments in technology for the fabrication of 2D materials-based devices such as dielectric deposition and device pattern etching.

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| 17.25 – 17.40 | Oral Talk 12 Dr. Marsil Kadirov<br>*Multifunctional Materials from Carbonized Organometallic Coordination Pectin Biopolymers* | **69** |
| 17.40 – 17.50 | Sponsor talk 2 Mikhail Trusov (IMC systems)<br>*Nanomaterials high-end research with ScientaOmicron equipment* | |
| 17.50 – 18.00 | Sponsor talk 3 Dr. Natalia Kuzmina (IMC systems)<br>*Imaging Spectroscopic Ellipsometry in Graphene and 2D Materials research by Accurion* | **70** |
| **18.00** | **Banquet** | |

## Electromagnetic waves in carbon nanostructures

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A research discipline – nanoelectromagnetics – is introduced as a synthesis of macroscopic electrodynamics and microscopic theory of electronic properties of different nanostructures. The approach is exemplified by graphene, carbon nanotubes (CNTs) and briefly touches upon other nanocarbon forms. Electromagnetic scattering theory is applied to calculate polarizabilities of finite-length single- and multi -walled carbon nanotubes (SW- and MWCNTs) in terahertz and IR ranges. Antenna properties of CNTs and CNT bundles are described. We demonstrate theoretically the dominant role of finite size effect in the non-Drude conductivity of CNT films due to the strong slowing down of surface plasmon-polariton in CNT [1,2]. The experimental evidence of the CNT length dependence of the THz spectra of SWCNT films [3] is presented.

We demonstrate that surface plasmon-polariton waves with low phase velocity in carbon nanostructures can be utilized for the generation of coherent terahertz radiation through the Chrenkov mechanism [4], the effect being especially pronounced in spatially expanded double- and and multi-layer graphene structures [5,6]. In addition to a strong slowing down, other two basic properties of graphene and carbon nanotubes, anomalously large electron free pass length, and extremely high electron current density reachable in structures, are considered, allowing proposing them as candidates for the development of nanoscale Cherenkov-type emitters, analogous to traveling-wave tube and free electron laser. In graphene/polymer multi-layered structures exposed to external electron beam, the generation is possible on macroscopic scale, and generation frequency tuning appears to be possible by varying the graphene doping, the number of graphene sheets, the distance between sheets, etc. Theoretical and experimental results on absorption in and reflection from graphene/polymer sandwiches are analysed as evidence of a strong electromagnetic field/graphene structure coupling [7-9].

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## 3D printing: two routes toward perfect electromagnetic absorbers

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The modern 3D-printing technology with high spatial resolution offers many promising opportunities for creating the 3D periodic structures of sofisticated geometries.

In this communication we will discuss the electromagnetic properties of lossy periodic crystals composed of fully carbon [1] or carbon-containing polymer [2] skeleton of finite conductivity.

We will concentrate on two different routes toward highly absorptive carbon based structure:

Fully carbon cubic / Kelvin cell: its template could be made by laser spattering of the photo-curable resin, and then converted into glassy carbon form, which possesses high dc conductivity, i.e. a few thousands S/m.

3D printed crystals of the same geometry as produced via the first route, but made by FDM printing directly from the carbon containing polymer filament, having relatively low conductivity, i.e. 1-50 S/m.

The advantages and disadvantages of using both methods as well as the peculiarities of the electromagnetic response of each type of lossy structure will be highlighted. The possibilities to achieve perfect resonant or high broadband absorption will be estimated. The tuning ability of the both type of crystals vs the conductivity of the skeleton, its thickness, the structure lattice parameters as well as impregnation with the dielectric media will be discussed. Innovation potential of both types of lossy photonic crystals for producing passive electromagnetic components such as compact and light waveguides, energy concentrators, and electromagnetic memories/logic components will be examined.

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Specialization: •

- main field: electromagnetic waves interaction with condensed matter
- other fields: quantum field theory, high energy and particle physics
- current research interest:

Electromagnetic materials for microwave and THz: The theoretical and experimental research of electromagnetic response of graphene, graphene/polymer sandwich structures, ultrathin carbonateous films, carbon nanotubes, nanocarbon based composites, carbon porous structures (foams, periodic cellular architectures, aero- and herogels) in wide frequency range (from radio frequency to THz). Materials and structure for high current electronics (explosive lectron emission cathodes on th basis of carbon nanotubes arrays, graphene-like materials, etc) Nanocarbon and graphene based nanoelectronic devices.

# Transverse magneto-optical Kerr effect in magnetite covered by array of gold nanostripes

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Transverse magneto-optical Kerr effect (TMOKE) attracted attention of researchers in past decade due to its potential in data storage, optical isolation systems, biosensing, optical filtering and other applications. In the case of planar samples consisting of conventional magnetic materials, the TMOKE has values less 10-3, which substantially limits its applicability. It has been shown that the TMOKE could be enhanced by using of surface plasmon polaritons in magnetoplasmonic crystals [1] and magneto-plasmonic nanoantennas [2]. Yttrium Iron Garnet (YIG) is the most often used as magnetic material for theoretical and experimental studied of TMOKE.

In this work we use the concept of the magnetoplasmonic crystal [1] and study theoretically and experimentally the TMOKE in Fe3O4 (magnetite) film covered by gold nanostripes array which support surface plasmon polaritons. Our rigorous coupled wave analysis (RCWA) simulations of optical reflection and transmission coefficients of the structure under study predict a multiple enhancement of TMOKE response in transmission as compared with a plain magnetite film without gold nanostripes. We demonstrate that due to the high absorption losses in magnetite film, the quality factors of the optical resonances in our sample are low which results in wide areas on the dispersion diagram where the TMOKE enhancement can be observed. Our experimental data are in agreement with RCWA theoretical calculations.

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# Interaction of CNT-films and CNT-graphene composite films with electromagnetic waves of IR-visible-UV Range

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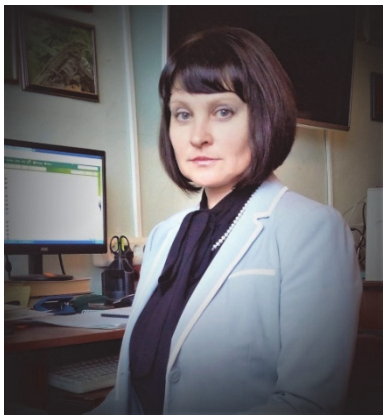
Research on the interaction of carbon nanotube (CNT) films and CNT-graphene composite films with electromagnetic waves of IR-visible-UV - range is very relevant today. One of the most correct ways to theoretically predict patterns of interaction of such films with electromagnetic waves is the quasi-classical approach that uses the Kubo approach developed in the framework of the quantum theory of irreversible processes and the classical Maxwell electromagnetic field theory. The calculations of the dynamic conductivity tensor and permittivity tensor, transparency coefficients of the films depending on their topology are carried out using the quasi-classical approach. CNT films with various ways of stacking nanotubes and with various methods of their joining (sutural and seamless junctions) have been studied. CNT-graphene composites in the form of pillared graphene, when the nanotubes are vertically oriented with respect to graphene monolayers,were also investigated. The s-and p-polarized electromagnetic waves incident at different angles to the surface of the films are considered. Comparison of transparency and electrical conductivity of the films of various types allows us to identify the most effective topological models for use in electronics.



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## Electromagnetic characterization of carbon nanotube based composite

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The frequency and concentration dependencies of the effective conductivity of carbon nanotube (CNT) based composites are analysed in the microwave and terahertz range. The ratio of the microwave to terahertz effective conductivities was proposed as a parameter to estimate how effectively carbon nanotube inclusions contribute to the effective conductivity of composite materials in the microwave range [1]. Carbon nanotube thin film is proposed to consider as a "perfect" composite. Hybrid composites comprising CNTs and $WS_2$ nanotube was shown to have strong interaction with microwave field [2]. Electron relaxation time in the terahertz range has been measured at different temperatures [2].

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# The Dielectric Behavior of the Polymer Composites Comprising Truly 2D Graphenic Inclusions

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The physics behind the dielectric properties of polymer composites comprising conductive inclusions remains elusive. This is especially true for materials containing the 2D inclusions such as graphene nanoplatelets, graphene oxide and reduced graphene oxide, on which very different data have been reported. In this work, for the first time we experimentally demonstrate the dielectric properties of composite materials comprising truly 2D structures. In particular, the composites of epoxy resin with graphene oxide (GO) as conductive filler were prepared via the homogeneous liquid phase transfer method, allowing uniform distribution and nearly fully exfoliated condition of GO in the matrix. The ~0.6% GO content is the absolute maximum that can be inserted into the epoxy matrix (at the flakes' size 5-20 μm) without sacrificing the exfoliation level of the 2D filler and the uniformity of the composition. Curing at 180 ºC causes the in-situ disproportionation, or so-called "thermal reduction" of GO in the matrix. The resulted composites exhibit relatively low permittivity values and the ultra-low percolation threshold at ~0.2% filling fraction. The imaginary part of the complex permittivity demonstrates highly lossy behavior at the 0.3-0.4% GO content. The presented experimental data strongly suggests that the Maxwell-Wagner polarization is suppressed in composites comprising truly 2D structures with the atomic level thickness despite their relatively large lateral size. And contrary, the strong Maxwell-Wagner polarization along with the high loading fractions (>0.6% at the flakes' size 5-20 μm) are indicative of the non-single-layer character, and/or the aggregation of the 2D inclusion particles in the polymer matrix.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 16-13-10291.

## Cherenkov-type Terahertz Emission in Graphene Structures

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Collective emission in graphene like structures due to slowing down of wave phase velocity up to velocity of moving electrons is considered. Graphene materials and nanotubes support eigen plasmon-polariton modes with small phase velocity i.e. with high slowing down coefficient ($c/v_{ph} \gg 1$, where $v_{ph}$ is wave phase velocity and $c$ is speed of light) [1 - 2]. Some advanced graphene structures, such as sandwich graphene, which consist of spatially separated graphene monolayers, provide additional possibilities for frequency tuning of terahertz emission. Sandwich supports symmetric, asymmetric and hybrid electromagnetic modes that have different physical properties. Symmetric mode corresponds to in-phase oscillation of electrons in all graphene layers. Effective chemical potential that defines emission frequency of such mode is the sum of all single layers chemical potentials, therefore frequency tuning can be provided by changing of graphene layers number (discrete tuning) or by electrostatic tuning of any single layer in sandwich (flexible tuning). Electrons oscillation corresponding to asymmetric modes is in antiphase condition for nearest graphene layers. Slowing down coefficient $c / v_{ph}$ of these modes depends on interlayer distance. This dependence gives additional possibility for tuning. Frequency tuning by variation of electron beam energy, temperature and other physical parameters are also considered.

**Acknowledgement.** This work was supported by Project ID 644076 Call H2020-MSCA-RISE-2014 Programme H2020 (CoExAN).

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# Recent Advances in Carbon Nanotube Sheets and Fibers Multifunctional Applications

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Carbon nanotubes, both multiwall and single wall keep attracting great interest, despite the recent progress in graphene and related 2D materials. The exceptional mechanical strength of CNT is still very attractive for multiple applications, while development of semi-industrial methods to process CNTs into strong fibers, yarns and transparent sheets, allowed to achieve progress in some novel multifunctional applications. In this talk, I will describe several new phenomena, that can be achieved by creating nanoscale composites of strong MWCNT sheets with functional materials.

Particularly combining CNT with superconductors, biological tissues (such as cancer cells) thermoelectrics, nanoenergetic solids, Ag nanowires, etc.; and then processing them into twist fibers and laminated aerogels brings to life new possibilities. Several applications will be described, including dual function selective solar coatings for evacuated solar collectors [1], nanoenergetic composite yarns for high power actuation [2], thermoelectric composites with increased figure of merit ZT [3], stable electrodes for perovskite photovoltaic and optoelectronic devices, and biological scaffolds for cancer cells [4].

By adjusting parameters and catalysts in CVD synthesis, it is possible to create very tall MWCNT forests on transparent quartz substrates, that have twisted and even coiled bundles of MWCNT, that are highly dry-spinnable and allow to create highly stretchable and low transparency CNT sheets.

High power and large-stroke actuators based on twisted and coiled multi-wall carbon nanotube (CNT) composite yarns were created by integrating high-density nanoenergetic gas generators (NGG) into carbon nanotube sheets. Such powerful yarn actuators can also be operated in vacuum, enabling their potential use for deploying heavy loads in outer space, such as to unfold solar panels and solar sails [2].

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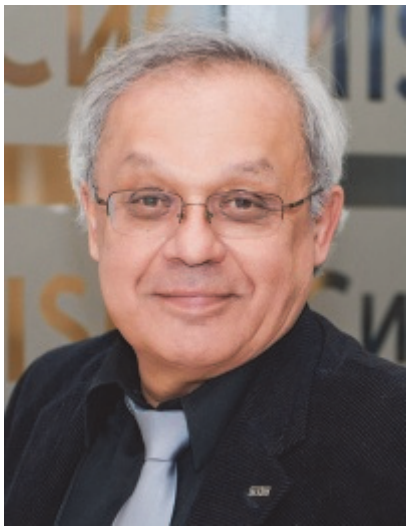

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2017 till present, Head of Laboratory for Hybrid Optoelectronics and Nanophotonics, ITMO University, St. Petersburg.

2015-till present, leader of Innovative project on "Flexible Perovskite photovoltaics.." NUST MISIS, Moscow

August 2001- Present: Professor of Physics, Adjunct Professor of Chemistry and Associate Director of NanoTech Institute, University of Texas at Dallas,

August 2010-Present: Affiliated Professor of Materials Science, University of Texas at Dallas

1996-August 2001: Started as Principal Scientist and from 2000, Senior Research Scientist at Honeywell Intl, (former AlliedSignal)

1988-); Head of Thermal Physics Laboratory, Department of Thermo-Physics, Uzbek Academy of Sciences (1988-);

1992-95, Visiting Professor in Department of Electronics, Osaka University,

1990-91, 94-95 Visiting Professor of Solid State Chemistry lab of the Institute of Molecular Science, Okazaki, Japan;

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International Scientific Leader Award, National University Sci&Technology, MISIS, 2014

Foreign member Kazakhstan National Academy of Natural Sciences (KazNAEN), 2011

APS Fellow, November 2009

Foreign Member, Russian Academy Natural Sciences (RAEN), 2006

MRS Award for Top 5 Cool Paper/Best Talk, Spring 2007

Kapitza Medal for Scientific Discovery (2007)

Nano 50 Award from Nanotech Briefs Magazine (2006)

NanoVic prise from Australia (2006)

Asian-American Engineer of the Year Award, 2003

Japanese Society for Promotion of Science Fellowship, 1994

Italian Consorcia "Phyzika Materiali" Fellowship, Genova (1992-1993)

Fellowship of Ministry of Science, Education and Culture, Japan (1990-1991, 1994)

# Pt lean and fee CNT electrocaltayst for hydrogen evolution

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Based on the recent IEA energy outlook [1], both solar and wind based energy supply will increase by more than one decade by the year 2040. Such drastic increase requires development of energy storage technologies, as their availability already now is considered forming the bottleneck for further adoption of renewables. Electrochemical water splitting in a membrane electrolysis cell is a promising technology for converting excess electrical energy into chemical bond energy, namely hydrogen bond energy. Hydrogen can serve as an energy carrier and connect energy sector to chemical industry and transportation sectors. In electrolysis cells, the water splitting proceeds via two half reactions: the hydrogen evolution reaction at the cathode (HER: $2H^+ + 2e^- \rightarrow H_2$) and the oxygen evolution reaction met in the anode (OER: $H_2O \rightarrow 2H^+ + 2e^- + ½O_2$). In acidic membrane cells, scarce platinum group metals (PGMs) are utilized at both the electrodes for electrocatalyzing the above-mentioned reactions.

The anode reaction is one of the major sources for energy losses in electrolyzers. However, the cathode processes contribute to degradation and consequently, affect the durability of the device. Moreover, it is well recognized that the known Pt reserves cannot cover the foreseen increasing need for energy conversion applicaions. Hence, developing durable altenative electrocatalyst for the HER is essential.

Carbon nanotubes (CNTs) have several beneficial properties needed for electrocatalyzing: In addition to high conductivity and good stability, they have appropriate properties for fabricating 3D electrodes. CNTs can be modified as earth-abundant element containing [2, 3] or ultra-low-Pt electrocatalysts [4]. These materials have inherently different activities towards the HER, but their activity can be also affected by selected synthesis method and starting materials resulting in end product with different morphology, surface properties or conductivity, for example. The most active hybrid materials show similar activity to the commercial Pt/C catalyst and excellent durability under the HER conditions. In this presentation, CNT based electrocatalysts promoting the HER are introduced and their properties are discussed.

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**Dr. Tanja Kallio**, D.Sc .(Eng.), has been appointed as an Associate Professor at the Aalto University Department of Chemistry and Materials Science (Finland) in the year 2015. She received a D.Sc.(Eng.) degree on Physical Chemistry and Electrochemistry from the Helsinki University of Technology in the year 2003. Since then she has been visiting scientists in groups with excellence in electrochemistry and material science including Univesidad de Alicante, Tartu University and Skolkova Institute of Science and Technology.

Tanja Kallio's research focuses on investigation and development of materials for electrochemical energy conversion and storage devices including polymer electrolyte fuel cells, electrolyzers, lithium ion batteries and supercapacitors. The core theme is reducing the utilization of non-earth-abundant-elements without sacrificing the performance. She is known, in particularly, on her applied and fundamental work on functionalized carbon nanomaterial based electroactive materials.

She has published some one hundred journal articles reflecting her interest in material development for electrochemical energy applications and understanding of activity and durability complexities. Her recent publications include development of platinum group metal free carbon encapsulated iron electrocatalyst for hydrogen evolution reaction in acidic electrolyzers whit similar performance to commercial platinum catalysts and ultra-low-platinum catalyst for hydrogen oxidation and reduction reactions with excellent activity and stability.

# $KTiOPO_4$-type $AVPO_4F$: a universal high-voltage host for reversible alkali-ion de/insertion

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Reversible de/insertion of many monovalent ions in a single framework is a rare property, which is deeply studied only for transition metal hexacyanoferrates capable of accommodating five alkali-ion cations from $Li^+$ to $Cs^+$ [1]. A similar feature was demonstrated for the $FeSO_4F$ fluoride sulfate framework maintaining de/insertion of $Li^+$, $Na^+$ and $K^+$ [2]. Such materials provide a new playground for designing new polyanion-based electrode materials for the next generation of rechargeable metal-ion batteries.

A novel series of vanadium-based $AVPO_4F$ (A = Li, K, Rb) fluoride phosphates adopting the $KTiOPO_4$ (KTP)-type structure was designed and synthesized by our group using hydrothermal and freeze-drying techniques [3,4]. The carbon-coated $AVPO_4F$ electrode materials offer a reversible de/insertion of $Li^+$, $Na^+$, $K^+$ and even $Rb^+$ ions. Electrochemical behavior and solid-state ion transport were found quite different for these alkali ions. The chemical diffusion coefficients were the lowest for $Li^+$ ($10^{-12}$ – $10^{-14}$ $cm^2/s$) and highest for $K^+$ ($10^{-10}$ – $10^{-12}$ $cm^2/s$). Energy barriers for alkali ion diffusion calculated by DFT-NEB do not exceed 0.21 eV, which correlates with experimentally observed rapid ion transport characteristics. Moreover, a full extraction of $K^+$ in $KVPO_4F$ occurs at the highest potentials comparing to $Li^+$, $Na^+$ and $Rb^+$ above 4.6 V vs $K/K^+$, which defines $KVPO_4F$ as the highest-voltage electrode material for K-ion batteries investigated so far.

In this talk, our recent activities on the KTP-type fluoride-phosphates considered as promising electrode materials for Li, Na and K-ion batteries will be highlighted with a special focus on the structure-property relationships.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 18-73-00313.

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## Electrochemical properties of functionalized reduced graphene oxide

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Carbon nanomaterials are promising for use in electronics, energy storage devices, sensors, catalytic systems, etc. due to high conductivity, large specific surface area, chemical inertness and physical stability. Functionalization of the surface of graphene materials with oxygen or nitrogen containing functional groups opens significant opportunities for their use. Surface modification allows to change the morphology, hydrophilicity and conductivity of material. Functional groups provide an increase in capacity due to the involvement of redox processes. In addition, selective modification by elementary functional groups opens up broad prospects for the addition of complex molecular fragments. One of the main applications of graphene materials is their use as electrode materials for supercapacitors and Li-ion batteries. The cyclic voltammetry method is used to study the redox processes in the electrode material. It clearly demonstrates the reactions on the graphene surface.

The purified graphite was oxidized to graphite oxide of approximate composition $C_2O$ by the modified Hammers method. The reduction of graphite oxide was carried out by thermal decarboxylation of $C_2O$ in concentrated sulfuric acid. The reduced graphite oxide had a large set of different oxygen-containing functional groups. The functional composition of the surface was modified by treating the reduced graphite oxide with chemical oxidizing agents or reducing agents, as well as heat treatment. Morphology of the graphene material surface was determined from the analysis of TEM and SEM images. FTIR, Raman and XPS spectroscopy, thermogravimetric analysis were used to study the functional composition and morphology of the synthesized samples. Electrochemical studies of functional materials were carried out at room temperature by cyclic voltammetry. The conductivity of the surface, electrolyte and the features of processes in the double layer was studied by electrochemical impedance spectroscopy. Studies of reduced graphite oxide as anode materials for Li-ion batteries were carried out in flat cells of type 2032. Li plates were used as a counter electrode. A 1M solution of LiPF6 in a mixture of 1:1 ethylene carbonate and dimethyl carbonate was used as an electrolyte. The cells were cyclized in the galvanostatic regime in the voltage range from 0.01 to 3.00 V at a current density of 0.1 A/g to 1 A/g.

It was shown that the functionalization of the surface leads to a change in the electrochemical properties of reducing graphene oxide due to the involvement of redox processes and changes in the morphology of the graphene surface.

# A rapid synthesis of $CsPbBr_3$ nanolasers with a high quality factor

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Since the breakthrough reports dedicated to utilization of MAPbI3 material for efficient photoconversion in solar cells, researchers working in the field of organic electronics and dielectric nanophotonics have been discovering new applications of lead halide perovskites. One of the recent cutting-edge applications is perovskite nanowires (NWs) generating laser emission in the broad spectral range 420-800 nm [1,2] that can be exploited for the development of photonic chips capable of super fast information processing. Although such nanowires have already demonstrated lasing with very low excitation threshold 0.22-40 μJ cm-2, high cavity quality factor (Q = 1500-3600) and short radiative decay (τ ≈ 20 ps), there are some problems with their fabrication. To the best of our knowledge they can be grown as a nanoforest onto PEDOT:PSS covered substrates immersed in an alcohol solution or by means of chemical vapor deposition. Further optical characterization and practical application of the individual nanolasers requires their separation and careful transfer to the auxiliary substrate. The reshaping caused to the nanowires (especially very long ones with lengths larger than 10 μm) during these procedures dramatically decreases their performance. Furthermore, the wet synthesis presented in previous works was conducted for 12-24 h.

Herein we report the rapid production of separated nanowires on glass substrate at ambient conditions. CsPbBr3 in DMSO was spray-casted onto the substrates and then treated with antisolvent vapor to give the wide dispersion of the NWs with lengths from 2 to 50 μm and different aspect ratio. SEM images of the samples revealed the formation of well-shaped objects with orthorhombic facets. Their XRD patters also confirmed the existence of the orthorhombic phase. The measured under pulsed laser excitation (λ = 400 nm, τ = 180 fs) 22.5 μm nanowire showed laser generation with a record high Q = 4480 and relatively low excitation threshold.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 18-73-00346.

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## Nanophotonics based on Halide Perovskites

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Halide perovskites have emerged recently as promising materials for many applications in photovoltaics and optoelectronics. Recent studies of optical properties of halide perovskites suggest many novel opportunities for a design of advanced nanophotonic devices due to their low-cost fabrication, relatively high values of the refractive index, existence of excitons at room temperatures, broadband bandgap tunability, high optical gain, and strong nonlinear response, as well as simplicity of their integration with other types of optical and electronic structures. This paper provides an overview of our recent results in the study of optical effects originating from nanostructured perovskites. Namely, we improved perovskite solar cells with silicon nanoparticles [1], showed tunable coupling of excitons with Mie resonances in perovskite nanoparticles [2, 3], as well as fabricated halide perovskite metasurfaces [4, 5] and nanolasers [6] by high throughput approaches. We also oversee a range of potential applications of resonant nanophotonics with halide perovskites.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 18-73-00346.

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## Advances in compound semiconductor nanowires

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Among the many families of nanostructures semiconductor nanowires have been shown to exhibit interesting properties for both scientific research and applications. The ability to create nanostructures and their assemblies with chosen atomic scale composition and structure on many length scales opens fascinating possibilities. The synthesis of semiconductor nanowires based on III-V compound semiconductors has progressed a great deal in recent years, and new device concepts have been proposed. In optical applications tailored nanowire arrays add another degree of freedom for tailoring the light-material interaction.

One of the critical issues concerning future applications is the cost of manufacturing. We have demonstrated synthesis of high-quality GaAs nanowires on very low-cost substrates such as regular window glass [1]. In addition, the processing of catalytic gold nanoparticles for nanowire arrays was demonstrated without expensive nanolithography steps [2]. Also, more complex structures such as InAs nanowires on black silicon have been demonstrated [3].

The presentation shows how the nanowires and their arrays are used to study fundamental properties such as phonon confinement [4] and mechanical properties [5]. The demonstrated nanowire applications include second-harmonic generation [6], THz generation [7], nano-LEDs [8] and all-optical logic gates [9].

**Acknowledgement.** This work was supported by the Academy of Finland, grants 12-34-56789.

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# Development of solar cell based on GaAs heterostructures and carbon nanotubes

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One of the most sufficient problems in development of high-efficiency semiconductor solar cells (SC) related to realization of the front electrical contact. Conventional approaches use conducting metallic bar's net which enhances reflection of the incident light leading to reduction of the energy conversion efficiency. Our goal is to realize efficient carrier collection through the contacts without losses in light absorption.

Carbon based nanomaterials have made significant contributions to the development of SCs due to their advantages as in flexibility, surface area, carrier mobility, thermal conductivity, chemical stability and optoelectronic properties. These are intriguing for many research groups in the present semiconductor technology to incorporate carbon nanotubes (CNTs) into CNT/III-V semiconductor hybrid devices [1-3]. GaAs on the other hand has superior electrical and optical properties owing to its diffusion length and better carrier mobility in comparison with Si. All the discussed properties together with proper bandgap of GaAs for single p-n junction SC, transparency and flexibility of the CNTs from an energy conversion view, make the CNT/GaAs hybrid devices very promising.

In our work we made numerical calculation of hybrid CNT/GaAs SC and optimized the photoactive and support layer's properties to achieve high efficiency of structure. GaAs/AlGaAs heterostructures and CNT layers were synthesized my means of molecular beam epitaxy and chemical vapour deposition, respectively. The developed transfer method was applied to integrate CNT layer and GaAs/AlGaAs structure in order to fabricate hybrid SC. The I(V) characteristics measurements showed that applying CNT layer helped to improve SC efficiency.

**Acknowledgement.** The work was supported by Skolkovo Institute of Science and Technology(General agreement no. 3663-MRA dd. 25.12.2017).

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# Multifunctional Materials from Carbonized Organometallic Coordination Pectin Biopolymers

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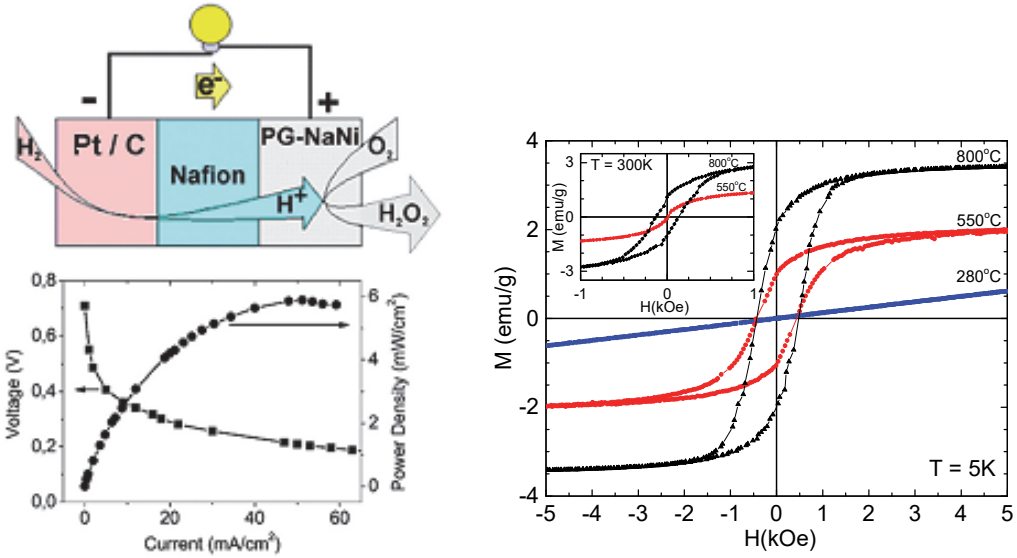


The representation (top left) of the $H_2/O_2$ Proton Exchange Membrane Fuel Cell and polarization and power density curves (bottom left) with the catalyst from complex of pectin polygalacturonates with sodium nickel (PG-NaNi) (annealed at 90 °C) at the cathode and commercial Pt/C catalyst at the anode.

The dependences (on right) of the specific magnetization on the magnitude of the magnetic field at a temperature of 5K and 300K (in the insert). PG-NaNi have been annealed at 280, 550 and 800 °C.

# Imaging Spectroscopic Ellipsometry in Graphene and 2D Materials research by Accurion

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The new generation of microscopic thin film, surface and materials metrology tool uses a combination of auto nulling ellipsometry and microscopy to enable surface characterization with lateral resolution as small as 1 micron. This enables resolving sample areas 1000 times smaller than most non-imaging ellipsometers, even if they use micro spot spectroscopic option.

The nanofilm_ep4 uses a variety of unique features that allow the visualization of your surface in real time. You will see the structure of your sample on a microscopic scale and measure parameters like thickness, refractive index and absorption. 3D profile maps of selected areas can be recorded. Instrument combinations with other technologies like AFM, QCM-D, reflectometry, Raman spectroscopy, etc. are possible to receive even more information from your samples.

Imaging spectroscopic ellipsometry is applied to characterize graphene and other 2D materials. CVD grown, exfoliated and epitaxically grown flakes of 2D materials are investigated with the imaging ellipsometer nanofilm_ep4. It allows:

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• Determination of the optical dispersion

• Distinction between mono-, bi- or n-layers

• Automatic flakesearch algorithm for identification of monolayers or well-defined thickness regions

• Exploration of hetero structures

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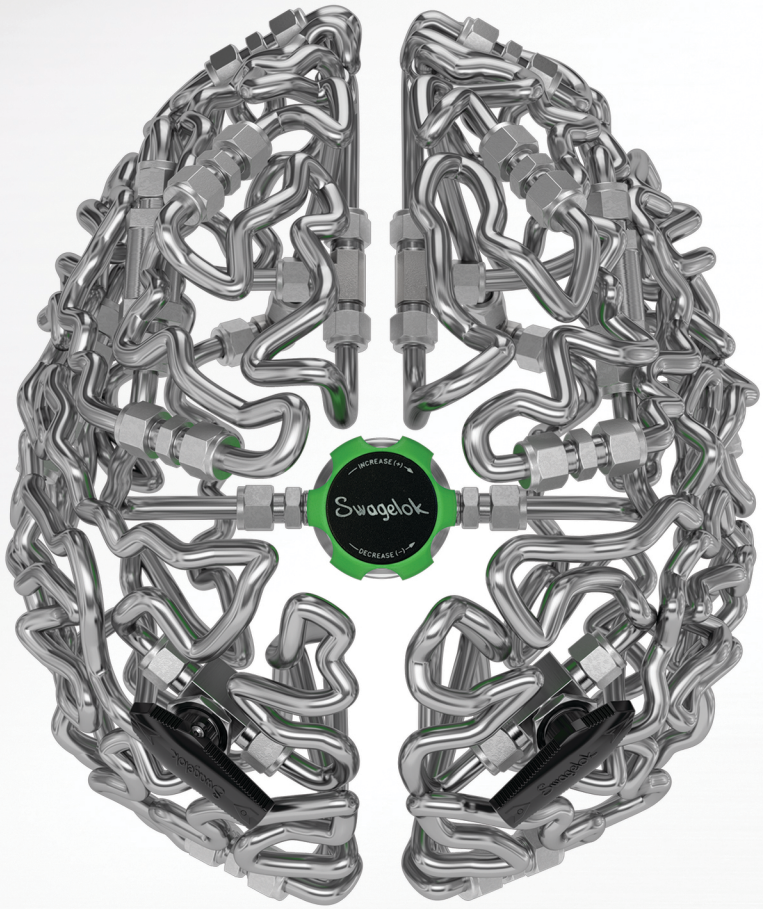


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# Oral Sessions

## Thursday,
## December 20

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# Terahertz transitions in carbon nanotubes and graphene nanoribbons

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Creating reliable, portable, tuneable sources and detectors of terahertz (THz) radiation is one of the most challenging tasks of contemporary applied physics. One of the recent trends in bridging the so-called THz gap is to use carbon-based nanostructures [1]. Several original schemes utilizing the unique electronic properties of carbon nanotubes (CNTs) and graphene for THz application were brought forward by our group [2-5]. These schemes include THz generation by hot electrons in quasi-metallic CNTs, frequency multiplication in chiral-nanotube-based superlattices controlled by a transverse electric field, tuneable THz radiation detection and optically-pumped emission in metallic CNTs in a strong magnetic field and using graphene p-n junctions for sub-wavelength polarization-sensitive THz detection. In the current presentation, we will focus on direct interband dipole transitions in narrow-gap CNTs and graphene nanoribbons.

We show that the curvature effects in quasi-metallic single-walled CNTs and edge effects in gapless graphene nanoribbons not only open bang gaps, which are typically in the THz range, but also result in giant enhancement of the probability of optical transitions across these gaps with a sharp decrease in transition probability away from the band gap edge. A similar effect occurs in an armchair CNT with a band gap opened and controlled by a magnetic field applied along the nanotube axis [4,5]. There is a direct correspondence between armchair graphene nanoribbons and single-walled zigzag CNTs. The described sharp photon-energy dependence of the transition matrix element together with the van Hove singularity at the band gap edge of the considered quasi-one-dimensional systems make them promising candidates for active elements of coherent THz radiation emitters.

**Acknowledgement.** This work was supported by the EU H2020 RISE project CoExAN and FP7 ITN NOTEDEV and by ITMO University Fellowship and Professorship Program.

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# Terahertz-infrared electrodynamics of wafer-scale films made of single-wall carbon nanotubes

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We demonstrate that a broad-band optical spectroscopy is a unique contactless tool to study mechanisms governing physical properties of macro-scale films made of carbon nanotubes (CNTs) and that it is able to provide the effective recommendations for practical applications of such films. With terahertz and infrared spectrometers (frequencies ≈5 $cm^{-1}$ up to ≈20 000 $cm^{-1}$), we measure a temperature-dependent (5 – 300 K) electrodynamic response (complex permittivity, conductivity, surface impedance, etc.) of a series of films made of high-quality pristine and doped single-wall CNTs with different lengths and treated with plasma. While the high-energy (≥1 eV) response is determined by well-known interband transitions, the terahertz and far-infrared properties of the films are fully dominated by unbound charge carriers. Determination of single-particle and collective effects connected with the dynamics of carriers and their dependence on the films parameters allows to conclude about the universal mechanisms determining the low-frequency electrodynamics of CNT wafer-scale films. The results demonstrate a great potential of the material in the field of electromagnetic applications at frequencies up to few terahertz.

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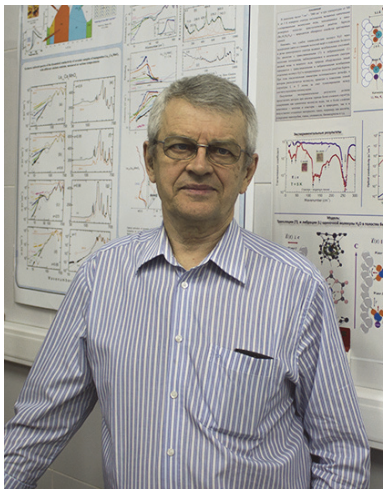

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# Hard X-ray in-situ full-field microscopy for material science applications

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Hard X-ray transmission microscopy based on refractive X-ray optics was employed as an instrument in material science to investigate buried-in microstructures in two or three dimensions with spatial resolution approaching 100 nm [1-6]. In this microscope, the incoming monochromatic beam goes through the condenser, and illuminates the sample. The objective lens magnifies the image of the sample on the high-resolution CCD camera (pixel size 0.65 m). The X-ray magnification typically lies in the 5-100 range but is not strictly limited at either bound. With the extra magnification from X-ray optics, the maximum spatial resolution is no longer limited by the detector pixel size, but by the X-ray optical components. The use of a condenser lens and a beam decoherer can greatly improve the image quality.

Switching from monochromatic to radiation with a broader bandwidth, frame rates down to a few milliseconds can be realized, opening new possibilities for in situ studies of microstructure evolution and response to external fields at spatiotemporal resolutions that go well beyond previous benchmarks, demonstrated by ~200 nm resolution tomograms of eutectic microstructures acquired in less than 2 s [5].

The Zernike phase contrast (ZPC) for X-ray microscopy based on compound refractive lenses was successfully realized at photon energies above 17 keV. Phase contrast was achieved by fitting a compound refractive lens with a circular phase plate. The sub-micrometer resolution has been demonstrated, and can be improved using already existing technology. The possibility of combining the technique with polychromatic radiation was considered, and a preliminary test experiment was performed with positive results. The implementation of ZPC expands the range of possible applications to cases which otherwise would produce only very faint contrast [6].

Potential application areas of fast 2D and 3D microscopy have been demonstrated with a few selected test cases, comprising regular and irregular eutectic solidification microstructure formation in different Al-based alloys, and self-assembly of colloidal crystal systems composed of different polymer particles with diameters in the micrometer range. The reconstructed tomogram slice of Al-Al2Cu eutectic microstructure recorded using 17 keVis shown in Fig. 1. Large dark pockets are -Al primary dendrites, while dark and bright areas inside the eutectic are the Al phase and the Al2Cu phase, respectively. The smallest lamellae half-period was 270 nm. The orange line in the zoomed view indicates where the lamellae were measured, averaging over 5 periods. The pixel size is 125 nm.

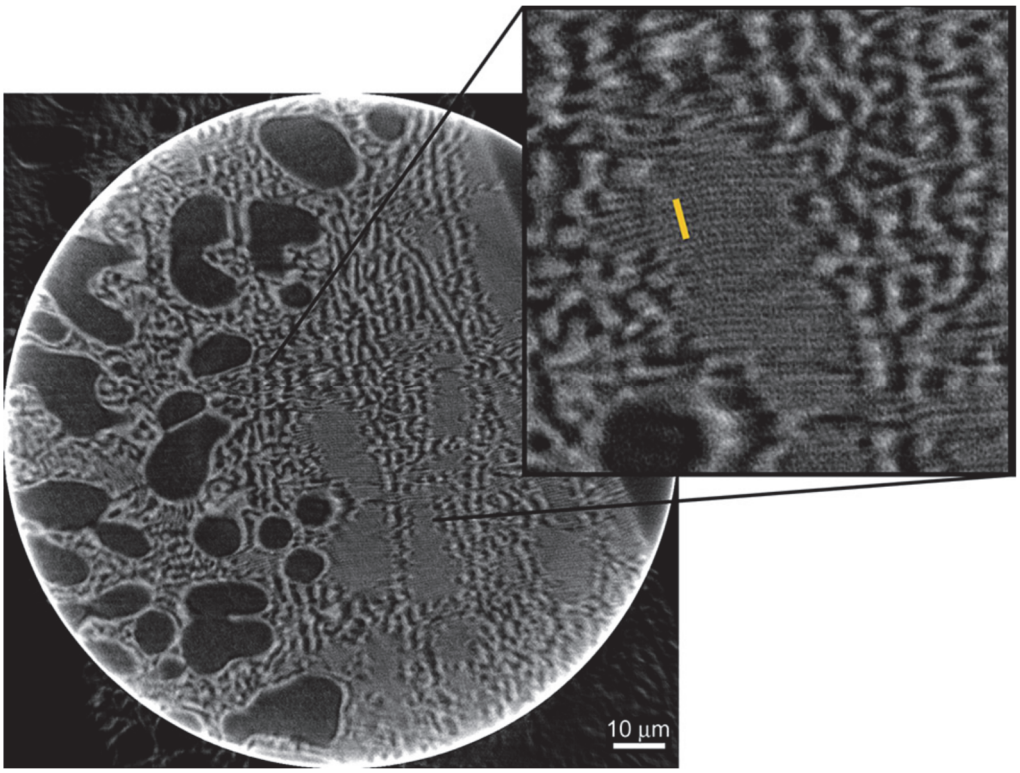


Fig. 1. Reconstructed tomogram slice of Al-Al2Cu eutectic microstructure.

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# Tunable graphene based plasmonic interferometer as a terahertz radiation detector

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Investigation of optical properties of a material brings valuable information about its electronic energy spectrum. Still use of traditional optical methods individual nanostructures with dimensions less than is challengeable. One of the possible approaches is to study modification of the transport properties of the nanostructure as it is exposed to the radiation. Here we employ this approach for graphene based nanostrucutres and prove that photoresponse is in most cases governed by collective phenomena in the electron system and shows signatures of plasmonic excitations and their spectrum.

First, we discuss response of graphene and graphene nanoribbons (GNRs) embedded into a THz range antenna with asymmetric metallization so that the sensitive element is p-doped at the contact with gold and n-doped at the contact with vanadium. We prove that such a structure operates as a Schottky diode [1]. Frequency dependence of the response is determined by excitation of the plasma ways in the channel between the antenna sleeves.

Next, we discuss photodetectors made of single (SLG) [2] and bilayer graphene (BLG) [3] encapsulated in hexagonal boron nitride (hBN) exploiting far-field coupling to incoming THz radiation. The photodetectors' architecture is a standard field effect transistor (FET) coupled to an antenna. We prove that the graphene channel hosts plasma waves with a long propagation length with dispersion law depending on the carrier concentration.

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# Coherent X-ray optics and microscopy for advanced material research applications

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New ultimate parameters of the beam provided by the diffraction-limited sources – new synchrotrons with the reduced horizontal emittance will open up unique opportunities to build up a new concept for the beam transport and conditioning systems based on in-line refractive optics [1]. In addition to traditional micro-focusing applications, the refractive optics can provide the various beam conditioning functions in the energy range from 3 to 200 keV: condensers, micro-radian collimators, low-band pass filters [2], high harmonics rejecters [3], beam-shaping elements [4] and Fourier transformers [5]. Taking an advantage of reduced horizontal source size, the refractive optics integrated into the front-end can transfer the photon beam almost without losses from the source directly to the end-stations. In this regard, development of diamond refractive optics is crucial [6-9]. The implementation of the lens-based beam transport concept will significantly simplify the layout of majority of new beamlines [10], opening novel opportunities for the material science research under extreme conditions [11-12].

The versatile beam conditioning properties of refractive optics enable to develop and implement new X-ray coherence-related techniques including Fourier optics [13,14], coherent diffraction [15-17], phase contrast imaging [18,19], and interferometry [20-22].

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In this period, he studied Xray diffraction by silicon-based microstructures leading to the invention of Bragg-Fresnel optics. In 1990, Anatoly Snigirev received a fellowship from the Alexander von Humboldt Foundation to work at the Dortmund University in Germany.

Between 1993 and 2015 he was staff scientist at the European Synchrotron Radiation Facility (ESRF) in Grenoble (France). He studied the coherence properties of thethird generation X-ray facilities for the application of imaging techniques, such as phase contrast imaging, holography and interferometry. Since the beginning of 1995, he put forward a new approach for X-ray focusing based on the idea of refractive optics. In December 2010, Anatoly Snigirev has received the Innovation Award on Synchrotron Radiation for "Pioneering work in the Development of Compound Refractive Lenses for Synchrotron Radiation and their Applications" from the Society of Friends of Helmholtz-Zentrum in Berlin.

In November 2011 AS has received the Gold Medal from the State Committee of Science of the Republic of Armenia for "valuable achievements in X-ray science and scientific collaboration within the French-Armenian partnership programme over the past 25 years.

In December 2013 AS was awarded the "Megagrant" (~2 M€) – "The World Leading Scientist Grant" from the Government of Russian Federation (Ministry of Education and Science) for period 2014-2018 for X-ray optics development in collaboration with the Baltic Federal University, Kaliningrad, Russia.

# Single-step polariton condensation via vibronic resonances in organic microcavities

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The regime of strong coupling between a Fabry-Perot cavity mode and an exciton of a semiconductor material embedded into the cavity results in the appearance of mixed light-matter quasi-particles known as exciton-polaritons [1]. Owning to integer spin, polaritons favor a phase transition into a Bose-condensed state, that was shown for the first time by Kasprzak et al. [2]. Emerging initially at cryogenic temperatures, polariton condensates can form even at room temperature by appropriate choice the crystalline semiconductor host [3,4]. However, the challenges of epitaxial growth has recently attracted great interest toward polariton condensates in soft-matter organic microcavities[polaritons going soft]. The broad range of organic materials with a considerable oscillator strength and high quantum yield covering the whole visible spectra is commonly-recognized as a valuable advantage over inorganic semiconductors. By now room-temperature polariton condensation from strongly coupled organic microcavities has been demonstrated across a broad spectral range from blue [5-7] to green [8] and yellow [9] spectral regions. Recent progress in the hydrodynamics of organic polaritons has led to macroscopic propagation lengths [10] and even superfluid phenomena feasible at room temperature [11].

Polariton physics have attracted a lot of interest from the early stages of the development of the field [12] and is still a subject of ongoing investigations [13,14]. Unlike inorganic systems, organic strongly coupled microcavities are still developing due to complexities arising from high disorder inherent to soft matter. Recently, a profound role of molecular vibrational modes in defining the overall population dynamics of polariton states was discovered experimentally in strongly coupled organic microcavities based on J-aggregates experimentally [15,16]. Analogous to high energy optical phonons in crystals, intramolecular vibrations in organic matter were observed mediating direct single-step energy relaxation. Single-step polariton relaxation is favorable for condensation as we have shown here for the first time. We report on vibron-mediated polariton condensation realized in the single-step relaxation from an exciton reservoir directly to the ground polariton state. To enable the relaxation scheme, large vibronic resonances are desirable that would compete with an internal conversion. Among the different organic semiconductors that have been used to realize polariton condensates, methyl-substituted

ladder-type poly [paraphenylene] (MeLPPP) offers a rigid molecular structure that carries high energy vibron modes [17]. Therefore, we utilise a strongly coupled microcavity consisting of 35 nm layer of ladder-type conjugated polymer (MeLPPP), sandwiched between $SiO_2/Ta_2O_5$ DBRs on a glass substrate. Resonantly exciting an exciton reservoir ($S_{0,0} \rightarrow S_{1,0}$) and varying the ground polariton state energy ($E_{LPB(k||=0)}$) we examine the photoluminescence (PL) intensity as a function of exciton to ground polariton state detuning ($E_{EXC}$-$E_{LPB(k||=0)}$).

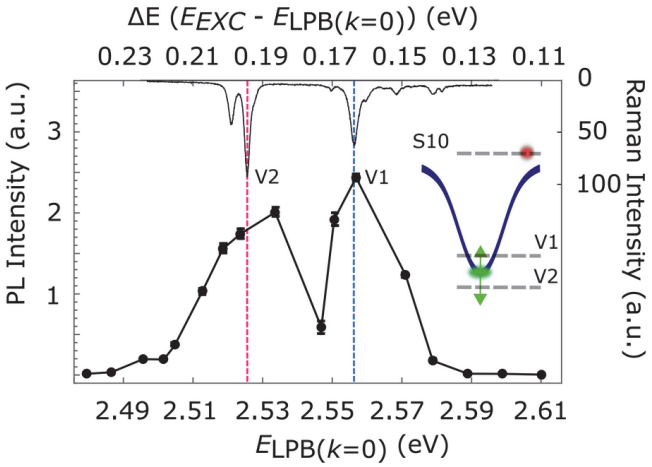


**Figure 1.** Vibrational modes govern polariton population. The dependence of non-linear PL on the energy of the ground polariton state ($E_{LPB(k||=0)}$) which is the variable parameter (inset - a schematic representation of the experiment). Raman measurements of MeLPPP (the upper graph) demonstrates two dominant vibrational modes (V1 and V2) with 165 and 200 meV characteristic energies respectively. The resonances match well with the PL maxima that indicates the primary role of vibron-mediated population in the build-up of the polariton condensed state.

Figure 1 shows the correlation between PL intensity maxima and the most intense Raman resonances of MeLPPP (top Raman spectrum) that relate to a single-step vibron-mediated polariton condensation. Here, we observe a sharp improvement in the energy relaxation yield that leads to polariton condensation through this channel. Notably, the threshold value of the absorbed excitation density required for polariton condensation is found to be less than 9.5 μJ/cm$^2$, which is the lowest value reported amongst any strongly coupled organic microcavity [18]. The vibron-mediated polariton condensation opens an opportunity to facilitate a range of nonlinear optical processes in a wide range of wavelength on a single strongly coupled organic microcavity that is crucial for room temperature applications.

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# Nanostructured particles as multimodal contrast agents and multifunctional drug delivery carriers: preparation, properties, biomedical applications

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New approach for loading of porous particles by proteins and nanoparticles was suggested [1]. Nanocomposite particles can combine ability to deploy drug in controllable manner with physical triggering [2] and sensing of important biological markers [3]. Physical targeting of carriers was realized by gradient of magnetic field [1], optical tweezers approach [4]. Acoustic field has a good perspectives for same purpose [5]. The carrier sensitivity to external influences as laser irradiation, ultrasound treatment [6] can be changed by variation of volume fraction and chemical composition of inorganic nanoparticles in the nanocomposite carrier shells [2-4, 6-8]. Same approach is applied for drug delivery carriers and biosensors imaging by MRI [7], OCT [8] and photoacoustics [9] using magnetite and gold nanoparticles as contrast agents, respectively. Combination of photonic and acoustic tools with multifunctional carriers has a good perspective for application in biomedicine for diagnostic and therapy.

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# Biofunctionalized Nanoparticle Colloids with Surface Sandwich Assays for Biomedical Applications

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Surface sandwich assay platforms have become an invaluable bioanalytical tool for the fast detection of biological and chemical molecules in real samples. In this talk, I will highlight our latest efforts on the development of highly sensitive and selective biosensing platforms in conjunction with different shapes and sizes of gold and carbon nanoparticles conjugated with biomolecules for biomedical applications. The first part of my talk will include the development of different sets of antibody-aptamer or aptamer-aptamer bioreceptor pair sandwich assays specific for disease biomarkers with surface plasmon resonance and electrochemical sensing methods. Target biomarker analytes for disease diagnosis include alpha-1-antitrypsin[1], tau 381[2], amyloid-beta(1-42)[3], hypoxanthine[4], and noro virus proteins[5] in biological fluids. The sensitivity of both sensing platforms can be greatly enhanced by the use of metallic and carbon nanoparticles. The second part of my talk presents our recent development on lateral flow based surface sandwich biosensing platforms in conjunction with biofunctionalized carbon and quantum dots in addition to hollow metallic nanoparticles for lung cancer diagnostics. Lastly, future aspects and challenging issues of our nanoparticle enhanced biosensing methodologies will be discussed.

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# A surface sandwich assay with biofunctionalized magnetic beads for proteins

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In this study, a microsized magnetic bead incorporated biosensor was developed for the detection of proteins which can be used for disease diagnosis. Two different ligands were used for the configuration of sandwich assay for the target protein. One of the ligand on a magnetic bead will be focused on the electrode surface via a simple magnetic force followed by interacting with the protein. The other ligand conjugated with alkaline-phosphatase (ALP) enzyme is then adsorbed onto the surface attracted protein. The final electrochemical signal was obtained by the reaction of the surface ALP with 4-aminophenyl phosphate (APP). The magnetic bead functionalized with the ligand here is to enrich the target protein for the signal enhancement. Some of preliminary results showing cyclic voltammetric responses as a function of the target protein concentration will be demonstrated. The same sandwich complex in the absence of ALP was further employed for an optical biosensing platforms of which preliminary data will also be presented.

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# Magnetic Nanoparticles with High Quality Plasmon Resonance in the Deep-UV

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Our results show that Co nanoparticles with a single-domain crystal structure support an excellent plasmon resonance at about 280 nm with the quality comparable to gold nanoparticles. This type of plasmons is unusual in a way that two plasmons coexist in a particle at the same frequency and polarizations of excitation, but for electrons of opposite spin. Inter-nanoparticle interactions completely demolish plasmon quality resonance, which is the probable reason why it was not observed previously and why the results for bulk films [1] cannot be used for single domain nanoparticles evaluations. It is known that the exchange interaction of electrons splits the energy bands between spin-up (majority) electrons and spin-down (minority) electrons. We suggest that minority electrons with a partially populated d-band increase the relaxation rate of the conduction electrons and consequently reduce the plasmon resonance quality, while majority electrons with a completely filled d-band does not affect the plasmon resonance of the conduction spin-up electrons within magnetic nanoparticles.

Understanding the effect of spin polarization on plasmon oscillations of the free electrons is, essentially, unexplored and crucial in many envisioned applications at the cross road of magnetism and plasmonics. It is a common belief that the quality of the plasmon resonance of magnetic nanoparticles such as Co is quite low, which follows, in particular, from the experimental data for permittivity of bulk cobalt by Johnson and Christy [1].

To address the mechanism of new type of plasmons specific for magnetic nanoparticles our work involves an advanced fabrication, structural microscopy, SQUID magnetometry, and spectroscopy of Co nanoparticles. The main goal of the work is to explain the physical origins of the high quality plasmon resonance observed in the experiments. Note that the plasmon resonance of Co is in the ultraviolet spectral range, which is the range for bio-molecule resonances and therefore attractive for bio-medical applications.

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# Magnetic nanoparticles and carbon nanotubes as enhancers for targeted RNA delivery in vivo

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Today RNA interference provides the powerful instrumentation for specific, safe and cost-effective gene silencing *in vivo*. Development of RNAi therapeutic approaches for major diseases has leaped forward over the last decade; however efficient delivery of nucleic acids is still a challenge. Several types of carriers have been developed for this purpose, based on viral and non-viral vectors. Unfortunately, most of vehicles appeared toxic or are effective only *in vitro*.

In this work a novel lipid nanoparticles (LNP) bearing magnetic nanoparticles and single wall carbon nanotubes (SWCNTs) for improved targeted delivery of synthetic siRNAs to spleen macrophages has been proposed. In this system magnetic resonance imaging (MRI) will be used to study distribution of magnetic LNP in the body and photoluminescence (PL) in infrared region to study distribution of LNP with SWCNTs.

Magnetic iron nanoparticles covered by graphitic shell to protect metal from oxidation and aggregation and short SWCNTs were prepared by aerosol CVD technique and introduced into the liquid phase containing lipids to avoid agglomeration/bundling followed by LNP formation. Previously, nanoparticles and carbon nanotubes were stabilized by RNA for their subsequent simpler introduction into lipid phase.

**Acknowledgement.** This work was supported by the Skoltech Biomedical Initiative, project Assignment No 2017-7/SBI.

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**Dr. Timofei Zatsepin** is a strong scholar and entrepreneur with a solid background in oligonucleotide and siRNA chemistry. He received the Candidate of Science degree in Bioorganic Chemistry from M.V. Lomonosov Moscow State University (MSU) in 2003. After a year of research assistantship at the Laboratory of Chemistry of Nucleic Acids, MSU Department of Chemistry, Timofei was promoted to the Lab's Research Associate. In year of 2004 Timofei became the Head of the oligonucleotide production unit at the Central Research Institute of Epidemiology (CRIE), Moscow, where he still maintains the position and is in charge of provision of synthetic oligonucleotides for a range of diagnostic and sequencing applications. Since 2012 Timofei is a Senior Research Associate at the MSU Laboratory of Chemistry of Nucleic Acids. He is also a cofounder of DNA-Synthesis – a company that provides oligonucleotide based services like synthesis of primers, probes and genes.

Timofei is a recipient of the Academia Europea Prize for the synthesis and evaluation of 2'-modified oligonucleotides, as well as awards and prizes from International Soros Science Educational Program, MSU and the Government of Russia among others. His publication record features such respected scientific journals in the field of organic chemistry as Nucleic Acids Research, RNA and PLoS One. Timofei is also an enthusiastic teacher with more than ten years of experience in preparing and reading lectures on biochemistry and molecular biology.

# Poster Session

## Redox-sensitive polycationic micelles for effective delivery of methothrexate to breast tumor

**B01**

Abakumova T. O., Voeikov R. V., Grinenko N. Ph., Chelushkin P. S., Nukolova N. V., Zatsepin T. S. and Chekhonin V. P.

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One of the most promising materials for drug delivery are polymeric micelles - nanoparticles formed by amphiphilic block copolymers. These micelles have a relatively high loading capacity, stability, and sensitivity to environmental changes (pH and ionic strength). The conjugation of micelles with tumor-specific molecules (e.g., antibodies to VEGF) can increase accumulation of the loaded drug at the tumor site and reduce its side effects. The aim of this work was to synthesize micelles using poly(amino acid) block copolymers with redox-sensitive cross-links for targeted delivery of methotrexate (MTX) to breast tumor. In order to form micelles, the polylysine chains of $mPEG_{110}$-b-$PLL_{30}$ block-copolymer were modified by phenylisothiocyanate (PITC). DLS measurements showed that obtained micelles have a diameter 45±6 nm and relatively high ζ-potential 32±4 mV. After that, ditiopropionic acid was used to create the redox-sensitive cross-links. The resulting particles, with or without cross-links, were loaded by anticancer drug MTX with efficiency up to 25% and conjugated with monoclonal antibodies to VEGF (anti-VEGF). Cross-linking of obtained micelles using ditiopropionic acid led to a significant decrease of ζ-potential (from 32 mV to -3 mV), slower drug release and decrease of cytotoxicity. Biodistribution and therapeutic efficacy studies demonstrated that conjugation of obtained micelles with anti-VEGF antibodies promoted their preferential accumulation in the 4T1 cells, lead to increased survival rate of 4T1-bearing mice and reduced tumor growth.

# C01 Plasma functionalized defected single-walled carbon nanotubes as promising material for gas sensing application.

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Mobile gas sensors operating at room temperatures with low power consumption, high sensitivity and selectivity are required in many industries as well as in everyday life namely for detecting explosive, combustible and toxic gases, food and air quality monitoring.

The main element of the gas sensor is its' sensitive material which determines sensors' sensitivity, selectivity, response time and signal recovery, operation temperature and stability. Single-walled carbon nanotubes (SWCNTs) is a unique material for gas sensors application. Coupled with chemical, thermal and mechanical stability, SWCNTs have large specific surface area with all carbon atoms located on their surface making them exceptionally sensitive for adsorption of gases at room temperatures. In this work we propose a simple approach of SWCNTs low frequency plasma treatment, which on the one hand introduce defects into the structure of nanotubes, which increases gas adsorption and thus increase sensitivity. On the other hand, it allows to obtain different functional groups on SWCNTs surface depending on the plasma atmosphere, and thus, to increase selectivity of the material.

In this study we investigate SWCNTs conductivity upon adsorption of inorganic gases such like carbon monoxide, nitrogen dioxide and ammonia, which allows us to assess the optimal operation temperature and gas concentration detection limits. Particularly, we present the study of oxygen plasma treated SWCNTs with induced defects and oxygen containing groups on its surface which increase SWCNTs sensitivity to such gases as carbon monoxide (respond is 0,5%), nitrogen dioxide (respond is 15%), ammonia (respond is 1.5%), hydrogen disulfide (respond is 0.8%) at room temperature.

The authors acknowledge the Russian Science Foundation (project № 17-19-01787).

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# THz visualization of inhomogeneities in composites based on carbon nanotubes

**E01**

Badin A. V. [1], Dorozhkin K. V. [1], Moseenkov S. I. [2], Kuznetsov V. L. [2], Suslyaev V. I. [1], Berdygin A. I. [1] Golubtsov G. V. [2]

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The results of visualization of inhomogeneities of a composite material based on polymethyl methacrylate and multiwall carbon (MWCNT) nanotubes at 309 GHz are presented. Three samples of composite material with concentration of MWCNT 1.5% and different processing time ultrasonic disperser were prepared for research: 5 min, 7.5 min and 30 min. As can be seen from the graph (Fig. 1) of the two-dimensional distribution of the transmitted power of the THz radiation, ultrasonic treatment for 7.5 min gives a relatively homogeneous material. Marked black areas of strong local absorption caused by the increased concentration of MWCNT.

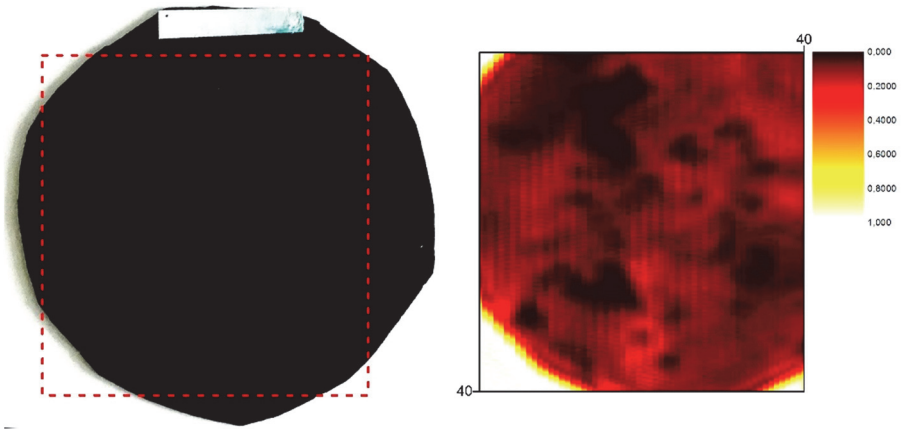


Figure 1 - Composite material based on polymethyl methacrylate and MWCNT (left) and THz image (right).

Investigations were carried out using the continuous wave measuring system based on the STD-21 THz spectrometer and the sample positioning system in the quasioptical beam [1].

Samples for research were obtained in the framework of the project of the Russian Science Fund No. 17-73-20293.

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E02

# Electrical properties of polystyrene composites based on arc-discharge carbon structures

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For efficient shielding of electromagnetic radiation, materials with carbon nanostructures, which have high conductivity, low weight, and high absorbing performance, are the most promising [1]. Changing geometry and concentration of carbon filler allows tuning the electromagnetic performance of polymer composite in a wide range.

To synthesize carbon fillers, we used the arc-discharge method described elsewhere [2, 3]. We found that morphology of synthesized nanostructure is strongly dependent on experimental conditions. In particular, introduction of melamine ($C_3H_6N_6$) into carbon arc results in formation of graphene layers and nanohorns. Polystyrene (PS) with high mechanical characteristics and dielectric constant was chosen as a base matrix. Composites with different types of carbon soot were fabricated using solution method in chloroform followed by homogenization of the samples by moulding. In the range of 1 kHz – 1 MHz, the dielectric constants and conductivities of the composites were calculated from the impedance of an electrochemical cell equivalent to a capacitor filled with a composite film [4]. The van der Pau method yielded direct current conductivity values.

The experimental study showed that introduction of melamine in electric arc could produce the soot with enhanced conductivity relatively the value of reference sample. Moreover, the composites containing this soot could exhibit lower percolation threshold.

**Acknowledgement.** This work was supported by the Russian Foundation for Basic Research, grant № 17-52-04077.

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# Response of carbon nanotube film transistor to the THz radiation

**E03**

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Despite years of research, the THz region of electromagnetic spectrum still have lack of sources and detectors. Almost all created high sensitive detectors require cooling to liquid nitrogen or even helium temperatures.

In 1996 M.Dyakonov and M.Shur have shown [1] that a short channel High Electron Mobility Transistor had a resonance response to electromagnetic radiation at the plasma oscillation frequencies of the two-dimensional electrons in the device. The described device implements Field-Effect-Transistor configuration and consists of transport channel framed by two contacts (source and drain) and a top-gate contact. As a consequence of the high plasma wave velocity and small FET dimensions, the plasma wave frequencies are in the terahertz range. The plasma waves are accompanied by a variation of a dipole moment created by charges in the FET channel and the mirror image charges in the gate.

In that view devices based on carbon nanostructures look promising because of operation with zero bias and their high electron drift mobility. In carbon nanonutubes (CNT) it reaches 100’000cm2/Vs. Besides, high mobility is not the only advantage of CNT. In comparison with graphene, used in a device CNT do not need to be so pure to get high responsivity. It means that it is possible to use cheap and simple CVD method for growing the tubes.

In this work we report on first studies of efficiency of such detectors. We grow our CNT films on oxidized silicon substrate that serves as a back gate of the transistor, while the radiation is coupled to a metallic top gate through a broadband antenna. Applying back gate voltage we control concentration and type of charge carriers in transport channel. We observed a strong photoresponse in a spectral range from 130 to 900GHz.

The main mechanism involved in rectifying the THz radiation was identified.

Thus, we showed that FET device with carbon nanotube film as a transport channel detect THz radiation in all temperature ranges.

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E04

## Raman spectroscopy analysis of onion-like carbon

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For characterization of various types of carbon nanostructures Raman scattering is widely used [1]. This method is also sensitive to changing the structure of onion-like carbon [2]. It was previously shown depending on the annealing temperature the shift of Raman D-mode towards high frequencies, and the shift of Raman G-mode towards low frequencies were observed [3]. However this study did not analyze the ratio of I2D/ID for estimation of defect-free graphene blocks. In this work we have performed study of carbon onions synthesized from nanodiamonds transformed into onion-like carbon by heating at 1000–1900 K with Raman spectroscopy. The data analysis is based on the point that the value of I2D/ID ratio correlates with the graphene fragment size. The fragments are considered as building blocks of onion-like carbon.

**Acknowledgement.** This work was supported by the the Russian Foundation for Basic Research, grant 18-02-01103_a.

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# GaP and its alloy nanowires for future hybrid materials for optoelectronics and photovoltaics

**E05**

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GaP is a semiconductor material of high interest due to several reasons. Low misorientation with Si allows to use it as a buffer layer material for integration of III-V direct band gap materials (e.g. GaAs) on Si platform. GaP plays an important role in modern nanophotonics as an efficient platform for second-harmonic-generation devices [1,2]. Dilution of GaP with other V materials such as N or As allows to obtain direct bandgap and vary its value in a wide range. Moreover, InGaP is a well-established material for record efficiency solar cells. Due to geometry III-V nanowires can be grown with high crystallinity on Si making this approach very promising in terms of future nanoelectronic devices development.

One of the main limitations on the way of III-V nanowires-based devices production is the lack of industrial methods for synthesis of the ordered arrays of these nanostructures having specified geometry and thus properties [3-5]. Typical methods of the ordered nanowires growth include fabrication of the patterned mask on the substrate surface with expensive and time-consuming lithographic methods that provide high resolution of the pattern.

In this work, we discuss novel methods for fabrication of the ordered nanostructures with a use of silica microsphere-enhanced lithography for synthesis of the ordered nanowire heterostructures on Si (111). We study growth and properties of the self-catalyzed nanowires by means of molecular beam epitaxy. We demonstrate method for incapsulation of the nanowires in a flexible matrix for development of hybrid materials for further device applications.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 18-72-00231.

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S01

## Growth of GaAs nanowires on graphite nanoflakes

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It is well known that graphene has many unique properties that allow to consider it as a very promising material with many potential applications. However, to get a uniform monolayer graphene films with quite a large area presents a real challenge. It is obvious that for a large number of applications the use of graphene is not required. Multilayer graphene (MLG) with number of layers more than 5 in their heat and electric properties are not strongly loses to a single layer. Therefore, it attracts more and more attention recently. Moreover, the technology of its extraction can be based on quite simple methods, e.g. based on liquid phase exfoliation of graphite and the modified method of Langmuir-Blodgett [1]. These methods, in principle, allow to obtain relatively cheap MLG flake film unlimited in size.

At the same time, semiconductor nanowires (NWs) attract also special attention due to variety of their properties and wide spectrum of their possible applications. They can be grown on different substrates, including graphene. Recently, the growth of InAs NWs has been demonstrated on graphite flakes by quasi-van-der-Waals epitaxy [2].

Here we report on Au nanoparticle assisted metalorganic vapour-phase epitaxy (MOVPE) synthesis of GaAs nanowires on MLG flake films deposited on $SiO_2$/Si substrates. It was found that different processes of nanowire growth can be observed depending on the position of Au nanoparticles in relation to the location and shape of flakes.

**Acknowledgement.** This work was supported by the Ministry of Science and Education of RF (grant 16.9789.2017/BCh) and Academy of Finland (grant 276376).

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## Nanostructured discrete monomers and their DNA-copolymerization

**B02**

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Fabrication of discrete DNA nanostructures containing covalent junctions requires simple and reproducible methods of branched oligonucleotide conjugates synthesis [1]. This study paves the way to V-shaped blocks which may be utilized in the synthesis of simple discrete nanostructures, dimers with a couple of double-stranded DNA sequences. These blocks are monomers in the DNA-copolymerization concept. Initially, we obtained complementary pairs of branched V-shaped oligonucleotides using the previously described pentaerythritol-based diazide via copper-catalyzed azide–alkyne cycloaddition. These complementary pairs of conjugates contained constant oligonucleotide fragments and variable parts comprising non-hybridizing (dT)-insertion at 5’-end. V-shaped blocks were used in further hybridization forming simple discrete DNA-nanostructures which were observed in native PAGE and AFM. Several conditions of hybridization reactions were tested, including different cooling rates, buffers and initial concentrations of complementary V-shaped blocks. Also, the role of non-hybridizing linker length was studied. The structure of the obtained “nanoethylene”-type structures was indirectly confirmed by comparison with model V-shaped double-stranded Cy3-labeled DNAs. The subsequent synthesis of the couple of “nanoethylene”-type nanostrucutures with two different strands, one of which has a sticky end, gives two “nanomonomers”. They can form a linear DNA-copolymer upon mixing.

**Acknowledgement.** This work was supported by the Russian Foundation for Basic Research, grants 18-33-01271, 17-54-04111 and 16-04-01170.

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E06

# The usage of conducting wire sphere models for the estimation of electrophysical properties of multiwalled carbon nanotube spherical aerogels

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Here we propose a method for estimating the effective parameters (effective conductivity) of spherical aerogels of multilayer carbon nanotubes using the measured values of their polarizability and the wire medium model. While aerogels have a structure formed with tangles of curved nanotubes with chaotic contact distribution we estimate the possibility to describe their electrophysical properties using the regular connected wire medium.

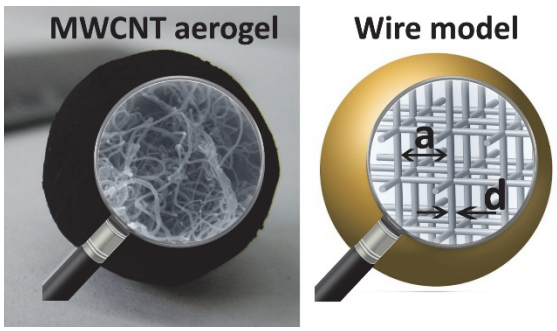


Figure 1. A spherical particle of MWCNT aerogel of 4.5 mm (left, the inserted in the form of lens presents scanning electron microscopy image of tangled nanotubes similar to those described in [1,2]) and an equivalent wire ball (right, where a is lattice parameter and d is nanowire diameter).

The calculations of the polarizability of regular structures consist of copper and CNT wires of identical diameters (not less than 50 nm) for different models were performed. It is suggested that by selecting the parameters of a regular medium, it is possible to achieve the closeness of the polarizability values of samples of the same shape consist of regular and irregular media. The calculated polarizability values of aerogels are consistent with the results of measurements of polarizability performed using the method of open resonators in the range 8-12 GHz. The possibility of estimating the electrophysical characteristics of carbon aerogels are considered for further modeling of the electromagnetic characteristics of composites based on them.

**Acknowledgement.** This work was supported by the Russian Science Foundation (grant 17-73-20293).

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## Electromagnetic properties of carbon nanofoam

**E07**

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Nowadays there is a need to fabricating of the lightweight absorbing materials. In this research the closed-cell polyurethane foam and open-pore polyurethane foam were used as a base for fabricating the absorbing carbon nanofoam. The carbon nanofoam were prepare from carbon nanotubes, latex paint and polyurethane foam.

The experimental samples with 0, 0.25, 0.5, 0.75, 1.0 and 2.0 wt.% of carbon nanotubes were fabricated. The experimental samples are first soaked in latex paint with carbon nanotubes and then the polymerization of it during 24 hours.

Firstly, the experimental samples permittivity was measured by rectangular cavity technique. Secondly, the reflection coefficient was calculated. It is show that the absorbing carbon nanofoam with 1.0 wt.% carbon nanotubes has a better absorbing properties. It is show that the particularly suitable for the construction of the lightweight absorbing materials is the open-pore polyurethane foam.

**Acknowledgement.** This Research is supported by Tomsk State University Competitiveness Improvement Program.

C02

## All-in-one graphene oxide/reduced graphene oxide gas sensor for environmental monitoring

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Graphene oxide (GO) and reduced graphene oxide (rGO) are known to be sensitive to temperature, humidity changes, and demonstrate chemiresitive response to pollutants and other gases [1]. Moreover, sensors based on these materials are characterized by low power consumption and do not require activation, e.g. by heating of UV illumination. Such broad cross-sensitivity makes these materials promising to be applied in gas analytical systems where selectivity is approached by combining several sensors in an array whose vector signal is processed by pattern recognition algorithms [2].

In this study we show system for environmental monitoring based on GO/rGO sensor array fabricated by laser irradiation of GO to transform it to rGO. Fabrication conditions favor tuning the ratio between GO/rGO areas what allows us finally to get different response for each sensor element in the array [3]. The reconstruction of the environment changes from property variations is realized by modern machine-learning algorithms. Thus, we could realize recognition of $H_2S$, $CO_2$ and $NH_3$ vapors in air as well as humidity and temperature changes.

The authors acknowledge MIT Skoltech Next Generation Project.

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## Light scattering by resonant nanoparticles in a 2D lattice

**E08**

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Photonic crystals are wide-spread optical materials that are actively applied for manipulating light in various cases. However, it is still a challenge to calculate optical properties of photonic crystals, which include small deep-subwavelength resonant inclusions, in a fast way with acceptable precision. Here, we present a method for calculation of scattering matrix of a 2D lattice of resonant nanoparticles embedded into a homogeneous layer far from any interfaces. The proposed approach combines both specialized techniques for a description of high-gradient nanoparticles' near-field and theory, which accounts for the interactions between the nanoparticles. Our method makes it possible to increase the computational speed by several orders of magnitude in comparison with FEM and paves the way to a solution of several types of problems.

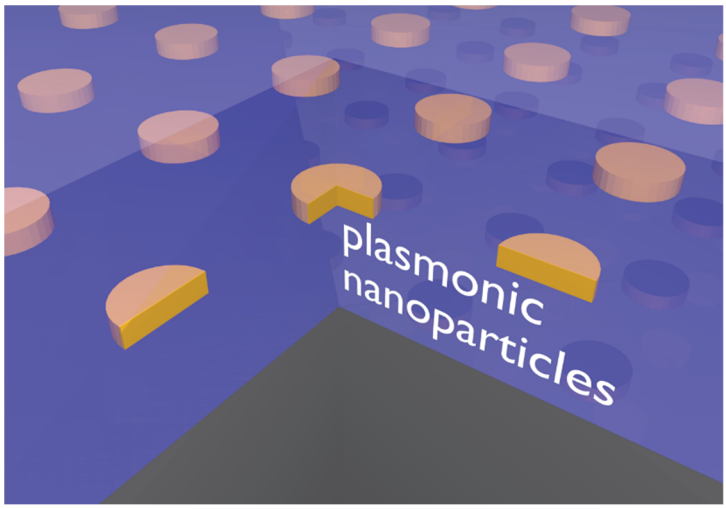


**Figure 1.** Schematic of a typical structure that might be calculated by the proposed theory. Plasmonic nanoparticles of a certain shape are embedded into a homogeneous layer far from interfaces.

# Sensitive bilayer graphene THz detector

**E09**

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Detection of THz radiation is an important task in modern optoelectronics offering a wide range of applications: from security and medical inspection to radio astronomy and wireless communications. Recently, it has been shown that graphene field-effect transistors (FETs) can act as THz detectors exhibiting a dc photoresponse to impinging radiation. A broadband photodetection in the sub-THz range with the responsivity reaching tens of V/W and noise equivalent power (NEP) of hundreds of $pW/Hz^{0.5}$ has been demonstrated [1].

Here, we demonstrate sensitive bilayer graphene (BLG) THz detector [2]. Our FET detector was made of bilayer graphene encapsulated between two slabs of hexagonal boron nitride (hBN). The FET was made in a dual-gated configuration such that the carrier density n in the channel was controlled by the graphite back gate electrode, whereas the top-gate as well as the source terminals were extended to a millimeter scale and served as sleeves of bow-tie antenna. Simultaneous action of two gates results in band gap opening and a steep resistance (gate voltage) dependence that, in turn, causes a drastic enhancement of responsivity. The latter exceeded 3 kV/W already for a weak displacement field D of 0.1 V/nm. This translates to the noise equivalent power (NEP) of about 0.2 $pW/Hz^{0.5}$ estimated using the Johnson-Nyquist noise spectral density obtained for the same D. The observed performance of our detectors makes them competitive not only with other graphene-based THz detectors operating in the broadband regime but also with some commercial superconducting and semiconductor bolometers operating at the same frequency and temperature.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 17-72-30036.

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## Light emitting mixed halide perovskite solar cells

**E10**

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Nowadays, the development of light emitting solar cells (LESCs) is one of the interesting research topics. LESC is a bi-functional device capable of working in two reciprocal regimes as a light emitting diode (LED) and as a solar cell (SC). Conventional LED and SC have device designs that maximize the efficiency of the primary function and suppress reciprocal function, however, theoretical investigations demonstrated that a good SC also should be a good LED [1]. Therefore, the development of efficient LESC is still a challenge.

This challenge could be solved with recently emerged organic-inorganic metal halide perovskites. Perovskites are very promising materials for the development of SCs and LEDs. Today, the efficiencies of perovskite-based SCs and LEDs are among the best. Also, perovskites have several advantages over conventional materials like smooth band gap tuning via simple solution processing, ease of use, smaller line FWHM of photoluminescence and electroluminescence. Several attempts to create such perovskite bi-functional devices were already made. But, in these cases special types of transport materials with polyelectrolyte properties or low work function cathode material was used [2, 3].

Another approach to achieve bi-functionality is the use of mixed halide perovskites with its intrinsic properties in conventional device design. Mixed halide perovskites suffer from halide ion segregation that manifests in the development of halide rich regions under external illumination or high current injection. As a result, device performance degrades but segregation has temporal character and after removal of external excitation device attains back its characteristics [4]. Although segregation is considered as a negative effect but it can aid for device bi-functionality.

**Acknowledgement.** This work was supported by the Russian Foundation for Basic Researches (Project 18-33-00669).

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# B03 Synthesis of metallic and Non-metallic Nanomaterials and Their Biological Application as an Optical Signalling Label

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In this work, some of metallic including CdSe, ZnS, Au and Ag in addition to non-metallic such as carbon materials were synthesized and functionalized with biomolecules as an optical signal labelling tool for the sensing of model target proteins on a paper chip platform. The first example is the synthesis of CdSe and ZnS quantum dots as a core and shell, respectively which were prepared in an organic phase and then transferred into a water phase using ligand exchanging mechanism [1]. The optimal functionalization conditions of QDs including variation of aqueous pH values, ionic strength, storage buffering solution were established and applied for the detection of model proteins on a paper chip. In addition, gold [2], silver [3] and also carbon nanomaterials [4] were synthesized and conjugated with biomolecules and further used for the protein sensing on a paper chip. Interesting preliminary biosensing results with different nanomaterials will be presented.

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# Comparing RNA binding to SWCNTs and carbon-encapsulated iron nanoparticles

**B04**

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Chemical vapor deposition (CVD) method is one of widely used for synthesis of single walled carbon nanotubes (SWCNTs) via the thermal decomposition of iron source in CO or hydrocarbon media and the high-pressure CO (HiPco) process where carbon encapsulated iron nanoparticles are byproduct. Thus, by varying synthesis conditions, both SWCNTs and core/shell nanoparticles can be obtained [1].

Single-walled carbon nanotubes (SWNTs) are promising candidates for imaging of biological systems due to their intrinsic photolumincescence (PL) in the second near-infrared window (NIR-II, 1.0−1.4μm). PL in this region provides an ideal probe for biological imaging deep inside the body due to much reduced photon scattering compared to in the visible (400−750 nm) and traditional NIR (NIR-I, 750−900 nm) regions [2]. Parallel, superparamagnetic metal nanoparticles are good candidate for medical diagnostics. Besides, magnetic iron nanoparticles in comparison with the most common use magnetic iron oxides (magnetite and maghemite) have more high saturation magnetization and lower coercivity, which allow to speak about iron nanoparticles as a more promising material as contrast agent for MRI (T2 contrast) [3].

For biomedical application both SWCNTs and core/shell metallic nanoparticles stabilization in biocompatible media is required. RNA are used for stabilization of nanotubes and their exfoliation into thin bundles. Despite the fact that RNA are used to exfoliate SWCNTs in aqueous solution, the problem of nanotubes stabilization remains open.

In this work, RNA was used to disperse SWCNTs and Fe@C nanoparticles in PBS solution. The optimal weight ratio between CNTs/Fe@C and RNA was investigated. All suspensions after sonication were centrifuged at 20 000 g for 2 hours and characterized by transmission electron microscopy and dynamic light scattering measurements. UV vis and PL spectra for SWCNT suspensions showed exfoliation of SWCNT bundles into thin ones, while for Fe@C nanoparticles stabilization by RNA molecules does not occur.

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E11

# Single-walled carbon nanotube membranes for optical applications in extreme ultraviolet range

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Constant demand of increasing optical resolution motivates technologies like photolithography and microscopy to master the short-wavelength range with λ ~ 1-10 nm. High natural radiation absorptance of various materials in this range generates challenges for designing high-performance optical systems. Under these conditions, optical elements composed of freestanding ultra-thin films become crucially important. This paper examines the feasibility of application of single-walled carbon nanotube (SWCNT) thin films as constructing elements for the short-wavelength optics. Test samples were fabricated using an aerosol chemical vapor deposition method. Synchrotron radiation was used to record transmission spectra of the samples in the spectral range of interest. The measured transmission exceeds 75% for wavelengths below 20 nm for a 40-nm-thick film, at the operational wavelength of the extreme ultraviolet lithography the transmission coefficient is 88%. The measured stress-strain curve for the test samples shows that the SWCNT-based films have rather high ductility unlike fragile films made of conventional condensed-matter materials. The combination of high radiation transmittance and unique mechanical properties makes the SWCNT-films very promising for applications in the short-wavelength optics.

# Functional composition and electrochemical propertiesof reduced graphite oxide

**C03**

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Graphene and other carbon materials can be used in a broad range of application due to physical strength, chemical inertness and good electrical conductivity. Possible applications reach from catalysis to energy storage in supercapacitors (electrochemical capacitor) or lithium batteries. This work focuses on the energy storage using carbon-material based electrodes. Compared to state of art graphite or activated carbon electrodes, electrodes made from graphene, mesoporous carbon or carbon nanotubes have superior properties as for example for application in supercapacitors or Li-ion batteries. Since the surface of these materials is larger than in graphite, the capacitance, which is proportional to the surface area, is increased. The presented work will focus on the composition, synthesis, characterization and electrochemical properties of reduced graphite oxide (rGO).

For the synthesis of graphite oxide (GO), graphite is oxidated by using a modification of Hummer's method. [1] For obtaining rGO the GO is treated with hydrothermal method in hydrazine solution. For this method water and hydrazinium sulphate (1.6 g for sample 1 and 0.5 g for sample 2) is added to the GO. After 15 minutes of ultrasonication, the black suspension is filled in an autoclave for 12 hours at 110°C. There the GO is reduced to rGO. After washing for removal of remaining salts, the product is freeze dried. Figure 1 displays the corresponding measurements of sample 1 and 2. The lower FTIR (a) and Raman (b) curve correspond to the SEM image of sample 1 (c). The upper FTIR (a) and Raman (b) curve correspond to sample 2, whose SEM image is shown in (d).

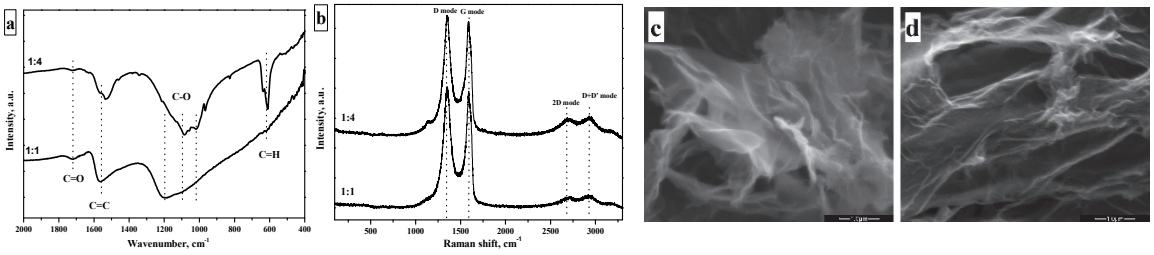


Figure 1: FTIR (a), Raman (b) and SEM images of rGO obtained using 1.6 g (c) and 0.5 g (d) of hydrazinium sulphate.

The electrochemical properties were measured by cyclic voltammetry, impedance spectroscopy and charge discharge cycling measurements. For these experiments coin cells were assembled in an argon-filled glove box with a lithium cathode and an anode prepared from Sn/C composite as active material. Graphene materials with microporous structure are synthesized as a result of our work. The FTIR and Raman spectra demonstrate significant functionalization of the graphene surface. rGO shows promising electrochemical properties. Its capacities reach 500 mAh/g in Li-ion batteries and about 100 F/g in supercapacitors.

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E12

# New Self-regulating Electric Heaters from Carbon-filled Composites

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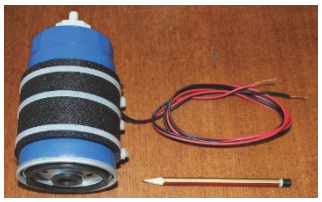
Currently, there is a steady transition from electric heaters with resistive material on a metal base to the heaters based on conducting polymer composite materials. The main advantage of polymeric materials concerning metal used as electrical heaters is a surface distribution of heat, which in itself reduces the temperature difference between the heated body and the heater at a specific site, causing greater reliability and lower power losses.

The carbon-containing composites based on polysulfide oligomers on their electro-physical properties are semiconductors, their resistivity is in the range of 100-1000 Om m. The combined mechanical, thermal and electrical interaction between the filler particles via the electrical contacts and the polymer environment determines the properties of such materials. The elastic properties of the polymer matrix has a strong influence on the electrical conductivity during a change in external mechanical and thermal loads. A nano-and microstructure of the carbon filler particles - their size, hardness, shape, and electrical and thermal conductivity - also affect the final properties of the compositions.



Fine Filter Heater

# New functional composite materials based on polyethylene and multi-walled carbon nanotubes modified by Co nanoparticles for electromagnetic applications

**C04**

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Multi-walled carbon nanotubes (MWCNTs) have been widely regarded as an attractive candidate to be used as fillers in composite materials due to their unique mechanical properties, high electrical and thermal conductivity, and chemical stability. The addition of a small amount of the MWCNT to the composite materials based on polyolefins provides significant improvement of their mechanical and electrical properties. The addition of the third component such as metal nanoparticles to the composite material at the preparation stage potentially allows the adjustment of the electromagnetic properties of the material by varying not only the dielectric properties of MWCNT, but also magnetic properties of metals. Moreover, the resulting "triple" composite materials are able to acquire completely new properties, for instance, electromagnetic shielding. In this work, a new approach for the synthesis of these materials based on *in situ* polymerization of ethylene using Ti-containing catalysts previously adsorbed on the surface of Co/MWCNTs has been developed and utilized. Co/MWCNT-PE composite materials with different ratios of the components Co:MWCNT:PE have been obtained. The study of electromagnetic response has shown that the Co/MWCNT-PE composites can be used as a promising material for the development of broadband shielding to be used for effective reflecting the electromagnetic radiation (10-16 GHz).

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S02

# Stabilization and growth of oriented nanoparticles of the face-centered iron phase

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Stabilizing nanoparticles on surfaces, such as graphene is a growing field of research. Thereby, iron particle stabilization on carbon materials is very attractive and finds applications in charge-storage devices, catalysis, and other applications. In this work, we describe the discovery of iron nanoparticles with the face-centered cubic structure that was believed not to exist at ambient conditions.

The solubility and solution phase processability of GO makes it possible to uniformly cover its surface with nucleation centers made from metal ions present in bulk salt solution. Thermal processing of GO induces its decomposition, which is accompanied by CO and CO2 formation, generating a distorted carbon lattice. This disproportionation is exploited to reduce metal-ions to form NPs on the carbon surface. Iron allotropes possess either the body-centered cubic (bcc) or the face-centered cubic (fcc) structure. At 917 °C, β-Fe transforms into the fcc lattice, and this allotrope is termed as γ-iron (γ-Fe) (austenite) with diamagnetic properties. According to the iron-carbon phase diagram, γ-Fe can incorporate up to 2.03% carbon. Lowering the temperature below 917 °C, carbon atoms diffuse out of the structure, and γ-Fe turns back to α-Fe. Up to now, γ-Fe could not be stabilized at room temperature, although kinetic hindrance of carbon atoms diffusion should stabilize γ-Fe.

Here, we show the stabilization of the γ-Fe allotrope NPs at room temperature on thermally processed GO (tpGO). In our two-step procedure, first $Fe^{3+}$ is complexed with oxo-functional groups present on the surface of GO, and second γ-Fe NPs are formed upon thermal annealing. They are clearly identified as the γ-form of iron, stable at room temperature, using Mössbauer spectroscopy and X-Ray diffraction (XRD) [1].

In addition to stabilization, the reduced graphene oxide can orient the nanoparticles growing on it. Obtaining nanoparticles with a controlled arrangement of atomic planes in a crystal is an interesting fundamental question. In this paper, we show the possible production of oriented nanoparticles of gamma iron on the surface of graphene oxide.

**Acknowledgement.** This work was supported by the Russian Science Foundation, Grant # 16-13-10291

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# Functionalization and study of the structure, kinetic and electrochemical properties of reduced graphite oxide

**C05**

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Various forms of carbon structures are studied and used as active materials for electrodes of electrochemical capacitors because they have high specific conductivity, electrochemical stability and large surface area. The ability for functionalization of carbon nanostructures allows improving electrochemical features of materials. Reduced graphite oxide is an excellent material for functionalization, due to its high conductivity, developed surface and simplicity to synthesize.

In this work graphite oxide was synthesized from purified graphite using modified Hummers method. The reduced graphite oxide was obtained by heating of graphite oxide in sulfuric acid. The carboxylation of reduced graphite oxide was carried out by treatment with oxalic acid, different combination of strong acids or alkaline. The structure and functional composition of the obtained graphite materials have been analyzed by scanning electron microscope, XPS, FTIR and Raman spectroscopy. The electrochemical measurements were carried out by cyclic voltammetry (CV). The processes occurring on the electrode with applying the potential shows the redox processes which as associated with oxidation and reduction of the oxygen–containing groups. The kinetic parameters of the obtained materials were calculated from the peak values on the CV curves. It was shown that the functionalization leads to increase of specific capacity and changes in mesoporous structure of the material. The calculated kinetic parameters can be used to obtain the electron transfer rate constant. This constant allows to predict the displacement of the peaks on the CV.

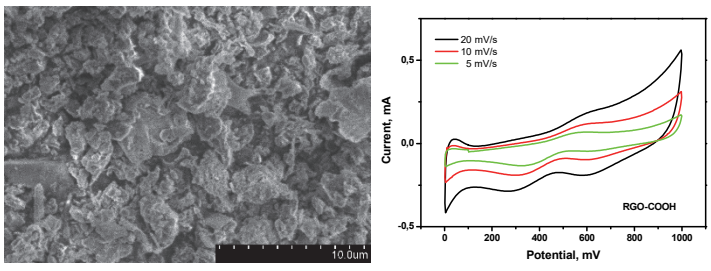


**Figure1**. SEM image of RGO-COOH and CV curves of carboxilated graphite oxide, measured at the scan rates of 5, 10 and 20 mV/s in 1M $H_2SO_4$ in the three-electrode cell.

B05

# Novel aminotriazide-based pathway to oligonucleotide dendrimers

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Previously, we obtained a set of branched azides based on pentaerythritol, which can be used to create branched oligonucleotide-oligonucleotide conjugates using copper (I)-catalyzed azide–alkyne cycloaddition reaction of alkyne-modified oligonucleotides and azido-containing branching reagents [1]. Such conjugates are of interest as blocks for self-assembly of discrete DNA nanostructures due to the formation of hydrogen bonds between the complementary oligonucleotide conjugates strands. Another type of supramolecular structures formed from DNA fragments is dendrimers, which are objects of interest in the field of high affinity labeling, bioimaging, and targeted delivery of biologically active compounds and antisense therapy [2]. To obtain such covalently bound pentaerythritol-based dendrimers, aminotriazide was synthesized. During the subsequent reaction of alkyne-modified oligonucleotides with a branching reagent, first-generation dendrimers containing an amino group were obtained.

The acylation of the amino group with the corresponding azide or alkyne-containing acid followed by a click reaction gives the second generation of dendrimers containing nine oligonucleotides of the same type or asymmetric dendrimers containing three oligonucleotides with two different sequences.

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# Holey single-walled carbon nanotubes for ultra-fast broadband bolometers

**E13**

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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.

This work was supported by the Russian Science Foundation (No. 17-19-01787)

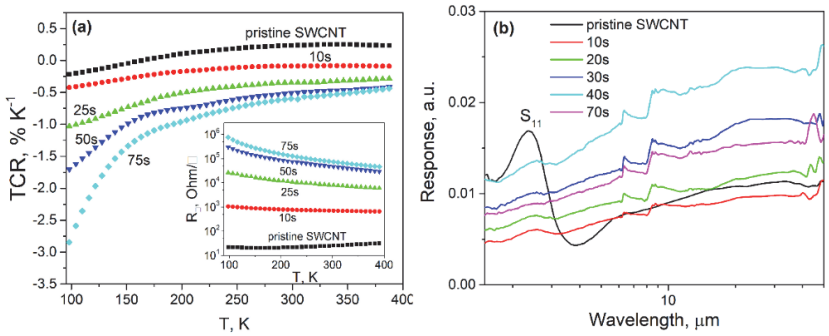


**Fig.1** The plasma treatment effect on TCR of SWCNT films and bolometers response (a) TCR of pristine SWCNT films and the ones treated in oxygen plasma at different exposure time, inset: temperature dependence of film sheet resistance. (b) Spectral characteristics of bolometric samples made of 100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

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E14

# Dynamic magnetic properties of hexaferrite nanopowders at microwave range

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This paper discusses the results of studying the temperature dependences of the spectra of complex magnetic permeability of hexaferrites with a Y, M, W crystallographic structure, which are most often used in the microwave region of electromagnetic radiation in the range of 0.4 - 14 GHz. The frequency dependences of the magnetic permeability of continuous hexaferrites, ultrafine powders and nanopowders, obtained by machining in high-energy mills with grinding 15 g and 65 g, were measured by the resonator method using the E8363B network analyzer.

The phase composition of the initial material and powders was monitored by X-ray diffraction. The static magnetic characteristics of the materials under study are given as follows: temperature dependences of the initial magnetic permeability and the field of magnetic crystallographic anisotropy.

In mechanically activated nanosized powders of hexaferrites, it was found that the position of natural ferromagnetic resonance is determined by the processing time in high-energy mills: at short times, the frequency of natural ferromagnetic resonance decreases, and then the frequency of natural ferromagnetic resonance begins to increase.

The frequency of natural ferromagnetic resonance for a powder (hexaferrite $Co_{1.2}Ti_{1.2}M$) activated for 30 seconds is about 4, 5 GHz. With further processing first (up to 90 seconds of processing), a shift in the high-frequency region of approximately 700 MHz is observed. The estimation of the location of natural ferromagnetic resonance from the results of measuring the anisotropy field and its shift during processing are almost coincide (Fres, 30 ~ 4 GHz, Δfres ~ 400 MHz).

Investigation of the temperature dependence of the spectra were carried out at a frequency of 750 MHz. It is shown that this material is relatively thermostable.

For the initial powder, the natural ferromagnetic resonance region coincides with the calculated value for $H_A$, but the shift is much further (not up to 5.6 GHz, but up to 10-11 GHz). The frequency shift of the natural ferromagnetic resonance can be caused by a decrease in the demagnetizing field when the powder is stuffed into a tube.

There is also a repetition of the results obtained on the material of similar composition, but manufactured three years ago.

# Oxygen-driven control of magnetism and stability of Co nanowires at Pt(111) steps

**E15**

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The best structures for nanoscale magnetic memory devices are the systems with large magnetic anisotropy energy (MAE), since they can conserve strong magnetisation under external magnetic fields, electric currents and temperature fluctuations. Strong spin-orbital interaction, large magnetic moment and structural anisotropy are required for obtaining the systems with high magnetic anisotropy energy. In this case the most promising structures for such kind of systems are atomic films, nanowires, chains and clusters of magnetic *3d* metals on different *noble-metal* substrates [1]. At the same time low-dimensional systems may be formed in the atmosphere of oxygen. The presence of such impurity on the surface and its close vicinity to magnetic atoms may lead to the significant changes of magnetic anisotropy energy [2].

In this work we present the theoretical study of magnetic properties and stability of oxidized *Co* nanowires as a prototype of *Co* 1D oxide on vicinal *Pt* substrates. Two different cleaves of Pt crystal have been considered to represent A- and B-types of step edges of Pt(111) surface. The structure of 1D *Co* oxide was based on the experimental evidence, reported before [3]. Our calculations revealed, that bonding with oxygen strongly effect the local magnetic moments, spin coupling and magnetic anisotropy of *Co* atoms inside the wire. Thus, we found, that the initial oxidation stage of *Co* nanowire at the step edge can lead to the degeneracy of the coupling states. It allows to precisely tailor the magnetic state by applying an external electric field, which can be useful for an industry of magnetic storage. The study of magnetic anisotropy revealed, that the presence of oxygen decreases the magnetic anisotropy energy of *Co* nanowires with respect to the pure ones. However, it remains large enough with regard to the single-atom magnetic units. Finally, we developed and applied the thermodynamic model in order to demonstrate, that 1D *Co* oxides are more stable, than the pure *Co* nanowires, adsorbed at the step edges of *Pt(111)* surface. That result is important for the synthesis of low-dimensional structures, since the intermixing of pure *Co* with *Pt* substrate may be avoided by the formation of low-dimensional *Co* oxides.

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# C06 Electric arc synthesis and study of mesoporous carbon with packing tin nanoparticles and their use as an anode material in Li-ion batteries

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Nowadays Li-ion batteries (LIBs) are the most usability for electrical energy storage devices in portable electronics, electro machines and one of the most perspective type of batteries for electrochemistry investigations in the nearest future. Graphite (volume capacity 273 mAh/g) is common anode material in conventional batteries. Due to graphite have low extensive volume expansion (10%), it is stable in the charge-discharge process. In the other hand tin have rather larger theoretical specific capacity (994 mAh/g), but it has huge volume expansion (254%), which leads to bulk tin pulverization and instability of solid electrolyte interface (SEI) film. Therefore, usage of tin nanoparticles is perspective for LIBs creation, because they have short diffusion distance for Li ions. In the same time nanoparticles don't distract under volume expiation during charge-discharge process, but they should be isolated to prevent contact and coagulation with each other. Arc discharge synthesis allows to produce uniform metal nanoparticles in the amorphous carbon matrix. [1] In this study mesoporous carbon materials packing tin nanoparticles were synthesized by the method of arc discharge with DC 150 A and voltage 25 V in helium atmosphere pressure 50 Torr with usage of composite anode consisting of a graphite rod and mixed graphite/tin powder (1:1 weight ratio). In the result the material was synthesized and TEM image is presented at Fig. 1A. The material contains tin nanoparticles with 2-30 nm in diameter (10 nm average size) inside amorphous carbon matrix.

The electrochemical properties were performed by cyclic voltammetry, impedance spectroscopy and charge-discharge cycling measurements. For the experiments coin cells were assembled in an argon-filled glove box with lithium cathode and anode prepared from synthesized Sn/C composite as the active material. It was shown tin nanoparticles are packed inside carbon matrix with 10 nm average diameter as a result of the synthesis. Specific capacity is 1800 mAh/g at the 1st cycle, 800 mAh/g at the 2nd cycle and nearly 600 mAh/g after 120 cycles as shown at Fig. 1B. That indicates high efficiently and stable rate of the synthesized material.

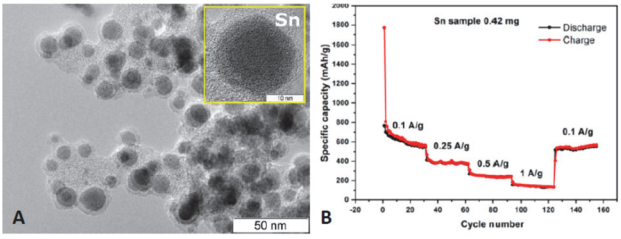


**Figure 1:** A –TEM image of the Sn/C composite; B – charge-discharge cycling performance of the Sn/C composite.

**Acknowledgement.** This work was supported by grant RSCF №18-79-00038

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# Aerosol CVD synthesis of single-walled carbon nanotubes for thin, conductive, and transparent films of exceptional characteristics

**S03**

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Carbon nanotubes are one of the most studied materials of the last decades, but still one of the most attracting for investigation. Indeed, efforts of the last two decades did not completely revealed the mechanism of the carbon nanotube growth or provided technique to produce single-walled ones with controlled and single chirality. However, when considering electronics, not the scalability but the material properties play as barrier for wide application requiring carbon nanotubes of specific morphology, defectiveness, structural characteristics. Aerosol CVD synthesis of the single-walled carbon nanotubes – a specific case of floating catalyst with low volume concentration of catalytic particles – is one of the best techniques to control the characteristics of individual carbon nanotubes (Figure 1) and the ratio and the morphology of the agglomerates providing the state-of-the-art devices – thin, transparent, and conductive electrodes, transistors etc.

In this work we examine the design of aerosol CVD reactor in terms of catalytic performance and carbon nanotube properties using a comprehensive set of the methods: the analysis of differential mobility of the aerosol particles, optical spectroscopy, scanning and transmission electron microscopy, Raman spectroscopy etc. Thorough kinetic analysis has revealed fundamental aspects of the catalyst activation.


**Figure 1:** The free-standing thin film of single-walled carbon nanotubes.

**Acknowledgement.** This work was supported by the Russian Science Foundation (No. 17-19-01787).

S04

# Synthesis of nanostructured carbon-carbon and carbon-mineral nanocomposites

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Carbon and mineral fibres are widely used as reinforcement additives to various materials. Yet their surface is too inert to provide appropriate adhesion level in composite. Possible way to solve such problem is to tailor carbon nanofilaments to microfibers' surface (MFs). This technique allows using advantages of nanostructures (developed surface area and pore structure) and macro objects (strength and ease in handling). Series of carbon-carbon and carbon-mineral nanocomposites (CNF/MF) with controllable properties have been synthesised. Materials have been tested within various polymer matrices and catalytic ethanol dehydrogenation. Modification of carbon fiber surface was carried out via catalytic chemical vapor deposition technique. Obtained materials are characterized with rather high surface area (up to 300 $m^2/g_{CNF}$). Carbon-carbon nanocomposites were found to have an improved physico-mechanical characteristics of polymer composite (both tensile strength and elastic modulus were increased up to 23 % and 34 %, respectively). In addition, catalytic behaviour of CNF/MF materials was demonstrated to be higher than that of conventional carbon-supported catalysts.

# Microwave electromagnetic properties of composite materials containing SWCNT and MWCNT

**E16**

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Recently, the rapid development of modern science and technology outstrips the theoretical work on obtaining new materials for the industry. Promising classes of materials for electronic devices are carbon nanotubes (CNT).

Composite materials consist of a binder (matrix) and a filler. Epoxy resin was used as the polymer base of the composite material. Powders of single-walled (SWCNT) and multi-walled carbon nanotubes (MWCNT) were used as fillers in concentrations from 0.5 to 4% by weight. Microwave measurements were carried on a vector network analyzer P4M-18 at frequencies up to 18 GHz. Complex dielectric and magnetic permeabilities were calculated.

The results show that values of the complex permittivity of composites with SWCNT is several times greater than ones of composites with MWCNT. Materials containing SWCNT can be used to create a thin, light absorbing coating at frequencies from 2 to 10 GHz. The tested MWCNT are more suitable for creating shielding coatings, since they have high values of the reflection coefficients.

**Acknowledgement.** This work was supported by RFBR grant №18-32-00810.

B06

# Electrochemical biosensing platforms for antibiotic drug species

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In this poster, we will show an electrochemical sensing platform featuring a polarized interface between two immiscible electrolytes solutions (ITIES) for ionized drug molecules. Here the ITIES can be referred as to an interface between the water and organic gelified phases. Charged drug species depending upon the pH of the aqueous solution can be transferred across a polarized ITIES and the current due to the transfer process is proportionally increased as a function of the concentration of charged drug species. We will show some sensing example for (levofloxacin) [1] and also other commonly used charged antibiotic drug species. Also the enhancement of the sensitivity for such drug molecules involving a differential pulse stripping voltammetry technique with a preconcentration step will be presented. Finally the electrochemical sensing data compared to those of using high-performance liquid chromatography will be demonstrated for validating our sensors performance.

**Acknowledgement.** This research was supported by the National Research Foundation (NRF) of Korea funded by the Ministry of Science, ICT and Future Planning (Grant number: NRF-2016R1A2B4012026).

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# Compact CVD system with embedded scanning tunnel microscope for graphene formation analysis

**S05**

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The chemical vapour deposition (CVD) setup with embedded scanning tunnel microscope (STM) was designed using principles described earlier [1, 2]. The exceptional feature of this setup is its ability to provide STM measurements at the same point on a substrate before and after heating (up to 1200°C) cycle. The principal scheme of the setup and sample holding system are represented in Fig.1.

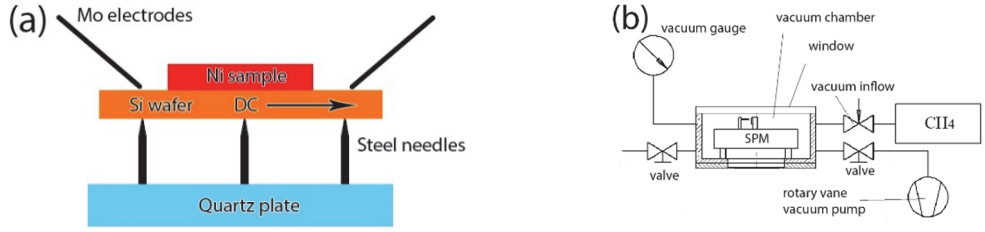


**Fig. 1.** (a) –scheme of the sample holder with embedded heating system; (b) – scheme of the CVD system with embedded STM

Herein we report on usage of the setup for in-situ monitoring graphene formation on Ni. 50 µm-thick Ni foil was heated up to 1000°C in 10mbar methane atmosphere for 15 seconds and then cooled down to room temperature with the rate of 100°C/s. Under such conditions the graphene growth was observed. Typical STM images of Ni surface before and after heating are shown in Fig.2. It was found that in some cases graphene forms nanobubbles, which might be easily forced to reorganize or even merge during STM scanning by varying potentials difference between the sample and the STM probe.

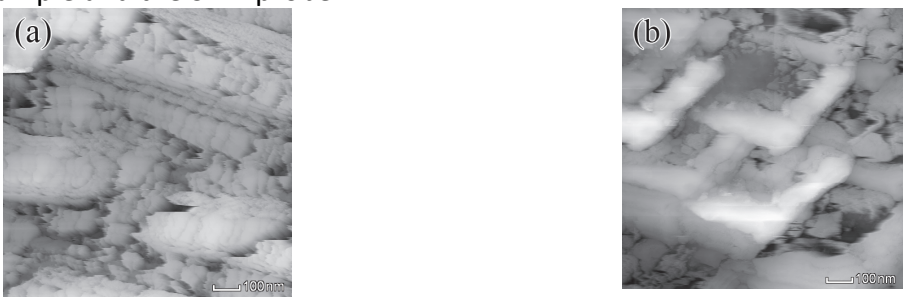


**Fig. 2.** (a) –STM image of Ni surface before heating (b) – STM image of graphene nanobubbles at the same place after heating

**Acknowledgement.**

The work was supported by RSF project 17-72-10173

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# S06 Effect of gaseous and condensate products of ethanol decomposition on aerosol CVD synthesis of single-walled carbon nanotubes

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In this study, the gaseous and condensate products of ethanol decomposition during the synthesis of single-walled carbon nanotubes (SWCNTs) by aerosol chemical vapor deposition (floating catalyst CVD) method were investigated. To determine the conditions for perfect and clean SWCNT formation the products synthesized at different temperatures and collected inside and outside the reactor were studied by transmission electron microscopy, Raman, Fourier transform infrared (FT-IR) and optical absorption spectroscopy. The individual and bundled SWCNTs of a predominantly small diameter (~1 nm) were revealed. The obtained tubes exhibit a stable distribution of chiral indices in a wide range of the set temperature (750-1000°C), which is promising for the development of controlled synthesis methods. The FT-IR analysis results show that the main gaseous products of thermal ethanol decomposition in our CVD system are methane and carbon monoxide. Acting as carbon source, the mixture of CO and CH4 makes possible to produce pure SWCNTs, as those obtained in the catalytic CO disproportionation method, with higher yield, taking into account twice the amount of carbon release during CH4 catalytic pyrolysis. The carbon deposit on the reactor wall is found to play important role in maintaining an optimal regime of CNT synthesis.

**Acknowledgement.** The reported study was funded by RFBR according to the research project №18-29-19169.

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# Giant Concentric Shell Carbon as a Valuable By-product of Homogeneous Partial Oxidation of Natural Gas

**C07**

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Carbon nanoparticles of almost ideal spherical morphology and perfect concentric onion-like structure were produced as a by-product of homogeneous partial oxidation of natural gas in the laboratory unit presented in the work [1]. The particles are unusually big for carbon onions and have an outer diameter of 10–50 nm while the inner cage is rather typical for onions and has a diameter below 1 nm. The concentric graphitic structure and spherical symmetry along with the absence of amorphous carbon are confirmed by transmission electron microscopy, electron diffraction, EDX spectroscopy, and Raman investigation. The spherical particles are deposited on a wall of a partial oxidation reactor as loose particles embedded in a beautiful low-density organic ovary, which can be detected by its luminescence or by cautious electron microscopy imaging. It is important that unlike literature reports on giant onions, the carbon deposit was dominated by these giant spheres, also it is interesting to note that our process allows producing regular giant onion-like particles from oxygen-containing feedstock despite claims in the work [2]. This process may be considered as a prototype for a production method for giant concentric shell carbon particle black.

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E17

# Bandstructure of individual carbon nanotubes probed using a tunnelling contact

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This paper is devoted to the study of the density of states of individual single-walled carbon nanotubes (CNTs) by means of a tunnel contact. The local density of electronic states of CNTs was first studied with the aid of a scanning tunneling microscope by tunneling spectroscopy [1] in which the I-V characteristics of the sample were measured locally via the microscope probe. The main disadvantage of STMs is that a conductive substrate (for example, gold) is needed to study the sample, which in the case of CNT screens electron-electron interaction, which in turn affects the energy spectrum of electrons in the tube [2].

Here we report on a technology for manufacturing devices in the configuration of field-effect transistors, where the channel of the transistor is an individual single-walled CNT, as a source, a tunnel contact is used, and as a drain, ohmic (Fig.1). We show that by measuring the current-voltage characteristics of our structures between the tunnel and ohmic contacts at a fixed value of the gate voltage at cryogenic temperatures, we actually realize the tunnel spectroscopy of the tube state density on the chip (Fig.2).

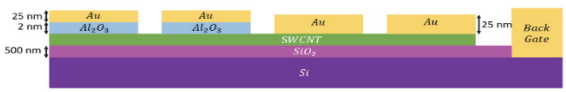


*Figure 1: Schematics of the device configuration.*

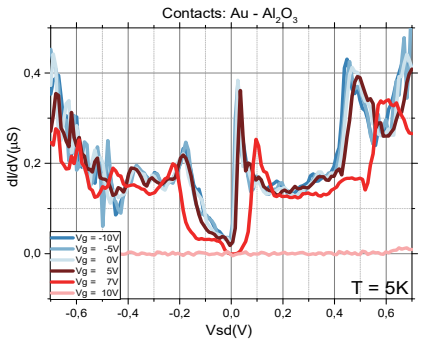


*Figure 2: dI/dV curves of one of our SWCNT obtained at different values of the gate voltage.*

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# Graphene Materials: Development, Technologies, and Production

**S07**

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Graphene materials represent a basis for progress in different areas of technology and industry. We have developed several novel graphene materials and technologies for their production. The original technology of manufacturing few- and multi-layered graphene nanoplatelets, which combines intercalation and ultrasonic exfoliation of natural graphite, has been implemented at NanoTechCenter Ltd. (Tambov, Russian Federation). Besides, we have developed a new method for synthesizing multi-layered graphene based on only chemical exfoliation, without ultrasonic treatment. This allows establishment of cheap and large-scale manufacture of multi-layered graphene. Now, the original equipment for the pilot technology is being mounted at NanoTechCenter Ltd. Chemically exfoliated graphene possesses unique properties, and can be used as electroconductive filler for polymer composite materials.

In the line of graphene materials, graphene oxide (GO) is among the most multi-purpose ones for applying in different areas of science, technology, medicine, agriculture, and construction. However, to date, it is very expensive. In this regard, we have developed a new technology of its production. The pilot reactor allows the processing of 0.2 kg graphite at once. If necessary, it can be scaled, together with supporting devices. Now, we can produce high-quality GO in any amounts.

Basing on graphene nanoplatelets and graphene oxide, we have developed hybrid nanomaterials containing nanoparticles of magnetite and cobalt ferrite immobilized on graphene layers. Two methods of preparation of these materials, chemical deposition from solution and mechanochemical treatment of GO in solutions containing metal salts, have been developed.

Hybrid films containing GO and carbon nanotubes were prepared. These films possess significant mechanical strength and interesting electromagnetic properties.

Furthermore, we have developed methods of obtaining graphene-polytetrafluoroethylene (PTFE) composite films. Films containing 10-15-20 % of graphene and 80-85-90 % of PTFE have a specific electric resistance of 0.05-0.15 Ohm.cm. These films can be used as current collectors for thin-film supercapacitors.

E18

## A New Curved Surface Wave - Photonic Hook Plasmons

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Today the surface plasmon-polariton (SPP) waves propagating along the curve trajectory are only plasmonic beams of the Airy family. In this Report, a new class of curved surface plasmon wave, called the photonic hook plasmon (PHP), is introduced [1]. The PHP is created using the in-plane focusing of the SPP wave through an asymmetric dielectric particle. This is fundamentally simpler than the generation of the SPP Airy-family beams. The PHP propagates along wavelength scaled curved trajectory with radius less than the SPP wavelength, which represents the smallest radius of curvature ever recorded for the SPP beam, and can exist despite the strong energy dissipation at metal surface.

The observed phenomenon is of potential interest in plasmonic optics and photonics, particularly, in SPP optical microscopy, photolithography and material processing, plasmonic circuitry, and in-plane SPP switches. The concept of changing structure of the PHP by changing the incident light by means of fixed coupling asymmetric dielectric structures might be adopted to dynamically control 2D SPP curved beams.

Apart from being interesting in their own right, PHPs may also hold promise for new, exciting applications in the general area of plasmonics. This field is now only beginning.

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# Multiregime pulse fiber laser based on ionic liquid gated SWCNTs

**E19**

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Pulse fiber lasers are required in various areas of industry: medicine (eye surgery, tooth treatment), telecommunication, optical tomography and spectroscopy, material processing (cutting, engraving, marking). For the purposes listed above different regimes of pulse generation are needed. However, most of the commercially available lasers can operate only in one of the pulse regimes. In our approach we demonstrate multiregime pulse fiber laser, which allows to switch between the regimes of pulse generation, such as Q-switch, mode-lock and QML. Switching is achieved by an active electrochemical gating of a Fermi level of aerosol synthesized single walled carbon nanotubes (SWCNTs) implemented in fiber laser as a saturable absorber. We made electrochemical cell, based on SWCNTs transferred onto D-shape fiber and covered it with ionic liquid electrolyte. Active control of both linear and nonlinear optical absorption properties of SWCNTs is achieved by applying less than 2 V voltage to the SWCNT electrodes of the electrochemical cell.

Potentially with this approach we can replace 2-3 type of commercially available fiber lasers with a single laser operating in different pulse-generation regimes.

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# E20 Bolometric effect for detection of sub-THz radiation with devices based on carbon nanotubes

Moskotin M. V. [1,2], Gayduchenko I. A. [1], Fedorov G. F. [1,2], Titova N. A. [1], Voronov B. M. [1], Goltsman G. N. [1]

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In this work we investigate the response on THz radiation of an asymmetric FET device based on an individual carbon nanotube conductance channel. It was already shown [1], that the response of such devices can be either of diode rectification origin or of thermoelectric effect origin or of their combination. In fact, the experimental results of this work demonstrate that at room temperature the response of our device on THz radiation can be explained by a combination of diode rectification scenario and thermoelectric current scenario and there is no significant difference between inclines of IV curves with and without radiation at room temperature. But at lower temperatures we observe a strong change of the inclines of irradiated IV compared to IV with no irradiation (fig. 1), which indicates on a strong bolometric effect in the response origin. Further analysis of the IV curves leads us to estimating the responsivity of our device. Following the methodology described in [2] at 8K it appears to be ~$10^7$ V/W.

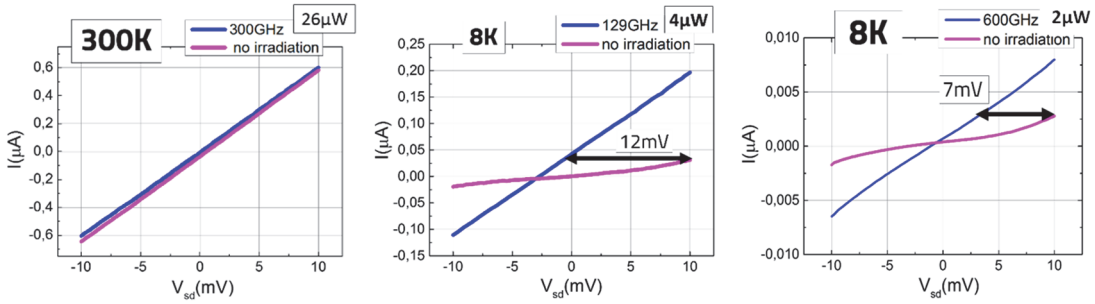


**Figure 1.** IV-curves for device type I at different temperatures (300K, 77K, 8K) measured in two conditions: with and without radiation. The response voltage is shown with the arrows.

**Acknowledgement.** This work was supported by the Ministry of Education and Science of Russian Federation (contract №14.583.21.0069, RFMEFI58317X0069).

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## Carbon aerogel from recycling paper and perspective applications

**C08**

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Besides carbon nanotubes and graphene, the carbon aerogel has attached a great deal of interest, due to its unique properties, like high conductivity and porosity, ultra-low density. With a freeze-drying method, we can get cellulose aerogel from recycling paper or some kinds of biomass with density reaches 10 mg/cm$^3$. After carbonization at high temperature in inert atmosphere, carbon aerogel shows highly porous and the density reaches 3 mg/cm$^3$. In this research we characterized this cheap material and address some perspective applications in environmental treatment, electromagnetic wave absorbing, and for electrode materials of supercapacitors and Li-ion batteries, capacitive desalination as well.

E21

# Massively parallel system for physical and mechanical modeling of carbon nanotube systems

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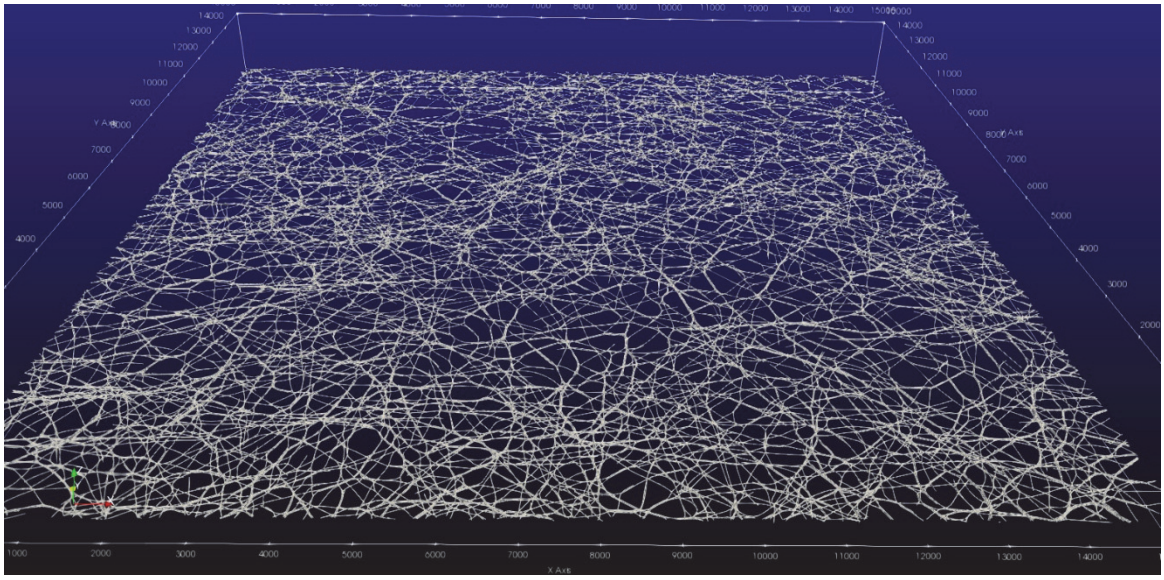
We present a universal, massively parallel framework for mesoscale modeling of carbon nanotube systems. Within our approach, individual CNTs are represented with chains of rigid bodies, linked with elastic bonds. Elasticity of the bonds utilizes recently developed enhanced vector model formalism. The van der Waals interactions between CNT segments are accounted with an anizotropic vdW potential, depending on mutual position and orientiation of the segments. The dynamics of fibers is computed using the modification of waLBerla - massively parallel rigid body dynamics engine. Time integration utilizes symplectic velocity Verlet integration schemes, and two kinds of dynamic damping, mimicking the energy transfer to implicit degrees of freedom. Our modeling system demonstrates exceptionally high parallel performance combined with the physical accuracy of the modeling. The efficiency of our modeling technique is demonstrated with illustrative examples of self-assembly of ultrathin carbon nanotube film and the mechanical test on a carbon nanotube material.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 17-73-10442.



# De-bundling of carbon nanotubes via supercritical fluid treatment

**S08**

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Most methods of carbon nanotube (CNT) usage in composite formation employ them in the form of a suspensions in water or organic solvents. The main difficulty in preparing such suspensions is reaching de-agglomeration of CNTs due to huge intermolecular attraction forces between them. The most wide-spread method for CNT de-agglomeration is high energy ultrasonication which sometimes can be harmful for CNT structure. In this work, we explore a method of bulk CNT powder de-bundling via supercritical fluid (SCF) treatment prior to ultrasonication dispersion. A portion of CNTs is suspended in a SCF in a high-pressure vessel. The suspension is then rapidly released into a collection vessel of much higher volume. Rapid depressurization leads to an abrupt density drop and volume expansion of a SCF which, in turn, leads to partial de-bundling of CNT bulk material. SCF media should be the one that is gaseous at ambient conditions to allow rapid expansion at pressure release. Nitrogen is preferred to carbon dioxide because it does not form a biphasic system during spraying and thus does not cause the collapse of the de-bundled structure due to capillary forces. Spraying can be performed either into an empty collection vessel or into a liquid. The former way can be performed repeatedly in order to increase the degree of de-bundling. 10-to-20-fold CNT bulk volume expansion is achieved by such repeated treatment. The latter way is convenient when immediate contact with the surfactant is necessary to prevent CNT re-agglomeration.

Nitrogen porosimetry revealed that the volume of micropores in bulk CNT structure was decreased. Further research using XRD and TEM showed that CNTs got less wavy and more aligned. Reduced waviness may be advantageous for the application dealing with electrical properties of CNTs.

Absorbance measurements of CNT dispersions in water revealed moderate signal increase after SCF treatment. One can assume that apart from de-bundling partial de-agglomeration occurs during spraying. Subsequent co-precipitation of SCF-treated CNTs with polycarbonate led to a composite material having simultaneously increased tensile strength and elasticity compared to the same composite obtained using untreated CNTs.

**Acknowledgement.** This work was supported by the Russian Foundation for Basic Research, grant 18-29-06071.

# E22 Single walled carbon nanotubes-polymer composite/amorphous silicon hybrid thin film solar cells with novel top contact

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In this work, we utilize the effective approach of combining single-walled carbon nanotube (SWCNT) film and poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) to form heterojunctions with thin film hydrogenated amorphous silicon (a-Si:H) [1,2]. We put forward flattened highly conductive SWCNT fibers on top, to form a SWCNT-PEDOT:PSS/a-Si:H hybrid solar cell. The SWCNT fibers act as self-similar top electrodes, like conventional metal grids. The fibers condensed from the SWCNT films, not only improve the SWCNT-PEDOT:PSS/a-Si:H junctions, but also enhance the conductivity of top electrodes without introducing any contact barrier. The power conversion efficiency (PCE) for the as-designed PEDOT:PSS-SWCNT/a-Si:H HSC with SWCNT fibers is 8.3%. Further, by placing the HSC on a reflecting mirror the PCE improves to 8.8%. This record performance for such a hybrid device is reported for the first time.

**Acknowledgement.** This work was supported in the framework of ERA.Net RUS Plus. The author PMR would like to thank DORA Plus Action 2 for financing the research in Tallinn University of Technology.

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# Synthesis of silver nanoparticles (AgNPs) using *E. crassipes* extract as a reducing agent and its antimicrobial activity

**S09**

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Metal nanoparticles are widely used in different areas such as biotechnology and biomedical, for example, to control bacterial growth in a variety of applications, including dental work, catheters, burns, cosmetics, food packaging and more. The antimicrobial effects of silver salts (Ag) have been identified since ancient times. However, the effects of Ag nanoparticles on microorganisms and the antimicrobial mechanism have been validated for different microbiological strains. Therefore, the synthesis of silver nanoparticles (AgNPs) is investigated by the green route using solutions of silver nitrate ($AgNO_3$) at a concentration of 0.1 mM and a natural extract of *Eichhornia crassipes* as a reducing agent. The reaction of the synthesis is carried out at different temperatures (75, 80, 85 and 95oC), examining the morphology and size of the nanoparticles as a function of time (0, 30, 60, 120 and 180 min).

The behavior of the nucleation during the synthesis was monitored by means of the technique of visible ultraviolet spectrophotometry (UV-Vis) where maximum absorption peaks are presented between 350-450 nm, by transmission electron microscopy (TEM) the morphological characteristics of the nanoparticles being generally spheroids between 20-40 nm., the colloidal solutions are composed of approximately 2.5% of AgNPs predominating the $Ag^0$ and $Ag^{+1}$ species, this through the photoelectron spectroscopy technique emitted by X-rays (XPS).

The antimicrobial activity of these nanomaterials was evaluated in *Escherichia coli (E. coli)* and *Staphylococcus aureus (S. aureus*) according to the guidelines set out in the manual of antimicrobial susceptibility testing by the FDA (*Food and Drug Administration*). The antimicrobial effect was analyzed in the presence of sensidiscs with nanoparticles observing inhibition zones from the contact zero time for *E. coli,* being the most effective at 95oC and 120 minutes, while the effect is null for *S. aureus.*

**Acknowledgement.** This work was supported by SIP-IPN (20171515 and 20171217 projects). CNMN-IPN and María de Lourdes Palma Tirado (UNAM, Campus Juriquilla).

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E23

# Intersubband plasmon excitations in doped carbon nanotubes

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Experimental studies of highly-doped single wall carbon nanotubes (SWNTs) demonstrated the presence of a prominent peak in NIR-Vis range both in optical [1] and EELS spectra [2]. It was shown that the peak is observed when the light is polarized in the direction perpendicular to the nanotube axis (no peak for parallel polarization), whereas its position depends on the doping level. The origin of the peak was predicted to be collective electronic oscillation (plasmon) rather than single-particle excitation or electron-hole pair (exciton) [3,4]. The Drude model and semiclassical theory were applied to predict how plasmon frequency in a SWNT depends on its diameter and Fermi energy, with particular examples that were only provided for zigzag and armchair SWNTs [5]. However, calculations of plasmon excitations for many different chiral (*n*,*m*) nanotubes are not available yet. Such a study is important to understand general plasmonic nature of light absorption in SWNTs.

In this work, we show the calculation of plasmon frequencies for doped SWNTs being as a function of chirality (*n*,*m*), diameter ($d_t$), and the Fermi energy ($E_F$). The calculated plasmon frequencies for many nanotubes within 0.5 nm< $d_t$ < 2 nm exhibit a diameter dependence of $d_t^{-0.7}$ and they also increase with $E_F^{0.25}$ [6]. We find that the light absorption at plasma frequency is dominated by intersubband energy transitions (within valence band or conduction band for $E_F < 0$ or $E_F > 0$, respectively), whereas the most dominant transition changes with Fermi level shift. In contrast to the optical $E_{ii}$ excitations in undoped SWNTs, plasmon excitations are shown to arise from $E_{ij}$ transitions, where *i* and *j* are band indices. The intersubband plasmon appears at a given Fermi energy for each (*n*,*m*) nanotube. The smaller (larger) SWNT diameter needs higher (lower) doping to excite the plasmon. Using the analytical formula of plasmon frequency, we expect that researchers in this field can quickly estimate the doping level present in the doped SWNTs.

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## Design of electroconductive and vacuum-tight MWCNT-$Al_2O_3$ ceramic composites

**S10**

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A method for production of conductive, vacuum-tight α-$Al_2O_3$ ceramic composites modified by multiwall carbon nanotubes (MWCNT) has been developed. We use acid treated MWCNTs with hydrophilic surface to introduce them into α-$Al_2O_3$ powder (particle size 100 nm) using their sonication in water suspensions. Sodium dodecyl sulphate (SDS) and Triton X-100 were used as surfactants during homogenization. While consolidating the nanosized powder mixtures of the α-$Al_2O_3$ (particle size 100 nm) and MWCNTs with and without surfactants, the composites with high density (~ 99%) and conductivity in the range from $10^{-12}$ to $10^{-3}$ S/cm have been obtained by cold isostatic pressing followed by sintering and by hot isostatic pressing. We have shown that the mixing of MWCNTs with surfactants is the most effective way for dispersing them in the α-$Al_2O_3$ powder at a microscopic level. Other things being equal, the composites obtained by mixing the α-$Al_2O_3$ powder and MWCNT with TX-100 in aqueous solution exhibit the highest conductivity and vacuum-tightness. Furthermore, the electric conductivity increasing by 12 orders of magnitude compared with pure alumina ceramics. During synthesis, MWCNT-$Al_2O_3$ composites obtained without surfactants and prepared in the same conditions exhibit decreased sintering behavior, which leads to a significant decrease in density, vacuum-tightness, and conductivity of the composites.

**Acknowledgement.** This work was conducted within the framework of budget project No. 0303-2016-0004 for Boreskov Institute of Catalysis

E24

# Magneto-Optical Properties of the Magnetite-Graphene Oxide Composites in Organic Solvents

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Graphene oxide (GO) is a two-dimensional material, derived from the graphene backbone by oxidation. Due to its unique physical and chemical properties, it was successfully tested in numerous applications ranging from selective membranes and water remediation through electrode materials in energy harvesting and storage devices. The presence of the oxygen functional groups on the surface allows this material to form stable colloidal solutions in water and some polar organic solvents. The functional groups are also responsible for the GO ability to form coordinate-covalent bonding with transition metal cations, and potentially with any Lewis acids. This property is actively employed in the design and production of composite materials with metals and metal oxides.

Graphene oxide aqueous solutions are known to form liquid crystals that can switch in electric fields. Magnetic fields as external stimuli are inefficient toward GO due to its diamagnetic properties, and GO is known to be insoluble in most of the organic solvents.

In this study, composites consisting of nano-sized magnetite and flakes of graphene oxide were prepared by mixing solutions of graphene oxide and oleate-protected magnetite nanoparticles in different ratios in the mixed isopropanol-chloroform solvents. Analysis of these mixtures for the presence of birefringence in the flow and in a magnetic field revealed formation of the two types of composites ("A" and "B") having different shapes and structures, which lead to a difference in their optical properties. Thus, Composite "A" could not form optically anisotropic media, and its structure was defined as multi-layered sandwich. Alternatively, solutions containing composite "B" exhibited birefringence both in the flow and in the magnetic field. The microscopy method analyses confirmed conclusions about the structure of the two types composites made based on their optical properties: the composite "A" particles are multilayered and geometrically isotropic, while the particles of composite "B" are mostly single-layered and geometrically anisotropic. Dispersions of composite B possess unique magnetooptical properties. The light transmission and the direction of light scattering respond momentarily to the applied magnetic field. This property paves the way for fabricating functional magneto-responding materials.

**Acknowledgements.** The work is performed with support of the subsidy provided to Kazan Federal University for a performance of the Russian Federation Government task in a research area (Grant No. 4.7094.2017/8.9).

# Aerosol coating approach for controllable doping of single-walled carbon nanotubes

**C09**

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Precise control of nanoparticle formation on top of the adsorption doped carbon nanotubes is a highly desirable tool for both theoretical studies and emerging mass production technologies of such thin film materials [1,2,3]. First, will allow to understand the nature of doping mechanism, including the role of nanoparticle size and its aggregation. The second, will positively influence the overall morphology, film uniformity and of cause – the resulting transmittance and sheet resistance. To realize the mentioned, we introduced and utilized a novel approach using aerosol coating process for doping of single-walled carbon nanotubes. The doping level of the films was confirmed at each step of the doping process. Finally, we optimized the aerosol doping set-up for transparent and conductive applications and obtained the sheet resistance value of as low as 81 Ω/□ at the transmittance of 90% (at 550 nm).

**Acknowledgement.** This work was supported by Russian Science Foundation No. 17-19-01787 (synthesis, measurements and characterization of the thin films) and Russian Foundation for Basic Research No. 18-32-00246 (THz measurements and analysis of the samples).

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# E25 Deep Elastic Strain Engineering for Optimization and Exploration of Semiconductors Electronic Properties

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Large deformation of a material without inelastic relaxation can result in unprecedented properties [1, 2], which are experimentally achievable [3]. However, the optimal deformation state is buried within the vast continua of choices available in the strain space [4]. Here we advance a unique and powerful strategy to circumvent conventional trial-and-error methods and adopt artificial intelligence techniques for rationally designing the most energy-efficient pathway in the space of admissible strains to achieve a desirable material property such as the electronic bandgap. In addition to the conventional approach of optimizing the materials composition, we present the broad framework for tailoring any target figure of merit for any material using machine learning, which opens up new opportunities [5] to adapt elastic strain engineering of properties and performance in devices [6] and systems in a controllable and efficient manner for potential applications in microelectronics, optoelectronics, photonics and energy technologies.

**Acknowledgement.** This work was supported by the Skoltech NGP Program No. 2016-7/NGP.

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# The Influence of CNT network functionalization in gaseous media $Cl_2$ , $NO_2$ , $O_3$ on their electrical properties

**E26**

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In this work we investigate the influence of CNT treatment in gas media of chlorine ($Cl_2$), nitrogen dioxide ($NO_2$), and ozone ($O_3$) on their electrical properties. The nanotubes are synthesized by the aerosol chemical vapor deposition with used ethanol as source of carbon, which allows producing thin films (networks) based on single-walled CNTs (SWCNTs) immediately at the reactor outlet [1].

The results of investigate using the method of Fourier-transform infrared and Raman scattering spectroscopy show the effective functionalization of single-walled carbon nanotubes. The study by 4-point probe measurement gives us the information on the decreases sheet resistance of the SWCNT films after treatment in gaseous media. The proposed methods of functionalization of CNT networks in the atmosphere of chemically active gases contribute to the improvement of conductivity permitting to apply the obtained films as an electrode material.

**Acknowledgement.** The reported study was funded by RFBR according to the research project № 18-29-19169.

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# S12 A spark discharge generator for high-yield aerosol CVD production of single-walled carbon nanotubes for biomedical applications

Zabelich B. Yu. [1], Krasnikov D. V. [1], Iakovlev S. Ya. [1], Romanov S. A. [1], Tsapenko A. P. [1] Alekseeva A. A. [1], Jiang H. [2], Kauppinen E. I. [2] and Nasibulin A. G. [1,2]

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Small size, high ratio of the surface area to volume and chemical stability make single-walled carbon nanotubes a promising material for drug delivery. However, for their application, certain conditions must be met, such as degree of aggregation, length of tubes, catalyst residues, *etc*.

In this work, we integrated a spark discharge generator as catalyst source for high-yield production of single-walled carbon nanotubes of controlled length and diameter distribution. Using a comprehensive set of physical methods: TEM, Raman and UV-vis-NIR spectroscopy, differential mobility analyzer, 4-probe technique, - we show the interplay between the specific parameters of spark generator (*i.e.* breakdown voltage, current between electrodes, carrier gas type, carrier gas flow) and the intrinsic properties of carbon nanotubes. For example, there is a direct dependence of the breakdown voltage and the yield of the synthesized single-walled carbon nanotubes (Fig. 1A,B) due to complementary growth of catalyst concentration (Fig. 1C) while the shape of diameter distribution of single-walled carbon nanotubes is maintained (Fig. 1D). The results obtained will be used for development of biocompatible magnetic species for enhanced diagnostics.

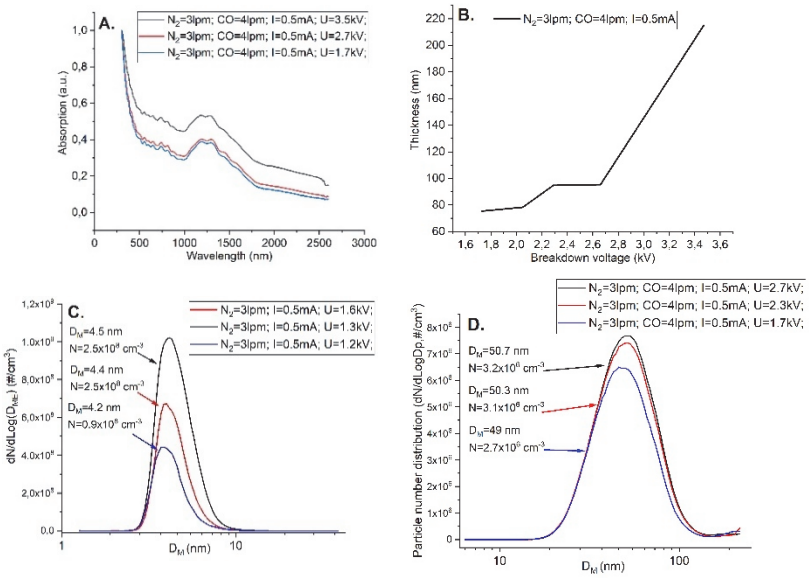


**Figure 1.** Influence of a breakdown voltage of spark-discharge generator on: (A) - optical spectra of SWCNTS; (B) – thickness of films (1cm filter, 30min collection time); (C)- diameter distribution of catalyst particles; (D) - mobility diameter distribution of single-walled carbon nanotubes.

**Acknowledgement.** This work was supported by the Skoltech Biomedical Initiative, project Assignment No 2017-7/SBI.

## Tailoring of electronic properties of SWCNT films by doping

**C10**

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Stable doping of single – walled carbon nanotube (SWCNT) films for application in transparent flexible electronics is a complex scientific task. There are two approaches of SWCNT doping. The first one is p-type doping, the second is n-type doping. SWCNTs are intrinsically p-doped by oxygen which is present in the environment. Due to this fact, stability of p-doped SWCNT films is higher in comparison with n-doped SWCNTs, in which oxygen from the air mitigates n-type doping effect. Although there are a lot of publications on p-type doping of SWCNT films for application in transparent conductive films (TCF) [1], few works were dedicated to n-type doping [2]. In this work both p- and n -type doping of SWCNT films were employed. In the case of p-type doping, SWCNTs were transferred onto the glass substrates, thermally annealed at different temperatures: 100 $^{o}$C, 200 $^{o}$C, 300 $^{o}$C, 400 $^{o}$C, 500 $^{o}$C and doped by drop-casting of 15 mM solution of $HAuCl_4$ in ethanol. The resistance of 31 Ohm/sq was obtained under annealing at 400 $^{o}$C with immediate doping. Furthermore, SWCNTs were deposited by dry transfer technique onto PEN substrate, in which gold electrodes were patterned previously in order to measure resistance, and doped with polyethyleneimine PEI with consequent spin-coating of PMMA passivation layer. Concentrations of PEI dopant were varied: 1 w%, 5 w%, 10 w%, 20 w%. The electronic properties of SWCNT films after n- and p-doping were characterized by UV-vis-NIR adsorption, Raman spectroscopy, SEM and four point probe resistivity measurements.

**Acknowledgement.** This work was supported by the Russian Science Foundation, grant 12-34-56789.

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# E27 Electric and Magnetic Optical Resonances for Spherical Crystalline Single Nano- and Microparticles Fabricated by Femtosecond Laser Printing Approach

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Single Ge and $Si_{1-x}Ge_x$ ($x \approx 0.6$) spherical particles with the diameter from 100 to 1500 nm were fabricated using femtosecond laser printing approach based on laser-induced forward transfer process [1, 2]. Corresponding amorphous thin films deposited by e-beam evaporation on transparent substrates were employed as donors for the particle transfer. The size and shape of particles were estimated using scanning electron microscopy. The phase composition was studied by Raman spectroscopy measurements, which revealed a crystalline structure of all transferred particles. The experimental scattering spectra of single particles in visible and near IR ranges were obtained by dark-field microscopy. It is shown that the observed resonances in the scattering spectra may be explained by the electric and magnetic dipole and quadrupole contributions, as results from the theoretical simulations performed on the basis of Mie theory. The demonstrated optical and structural properties of synthesized nano- and microparticles make them the promising candidates for the needs of integrated photonics.

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# The Hollow $Fe_3O_4$ Microspheres: the lightweight radar absorbing material

**E28**

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We present the investigations of the radar absorbing properties of the hollow magnetite microspheres. They were produced in one short-time process of the plasma dynamic synthesis [1]. The synthesized particles was separated into fractions with sizes from 3 µm to 30 µm (sample No. 1), from 30 µm to ~100 µm (sample No. 2) and the fraction with size greater than 100 µm (sample No. 3). In order to investigate the microwave characteristics of materials, the selected fractions of the hollow microspheres were placed in an epoxy compound. The weight content of the filler in the compound was equal to ≈ 50 %. The electromagnetic response of the samples was studied on the toroidal samples with the same thickness t = 2.2 mm.

From Fig. 1a it is evident that particles with sizes ≤ 30 µm provide the greatest signal attenuation up to – 40 dB at the frequency ~ 10.5 GHz. There is also a shift of the absorption maxima in the region of low frequencies with increase in the size of hollow spheres. The samples provide a reflection coefficient smaller than – 10 dB in following frequency ranges: 8.8 ÷ 16.2 GHz (No. 1), 7.4 ÷ 11.3 GHz (No. 2) and 3.7 ÷ 5.0 GHz (No. 3). The sample on the base of initial (none separated) powder (see Fig. 1b) allows attenuating the EMW (below – 10 dB) in the frequency range from 3.7 to 15.6 GHz, due to the presence of particles with a broad size distribution. The ground spheres have rather small attenuation of EMW.

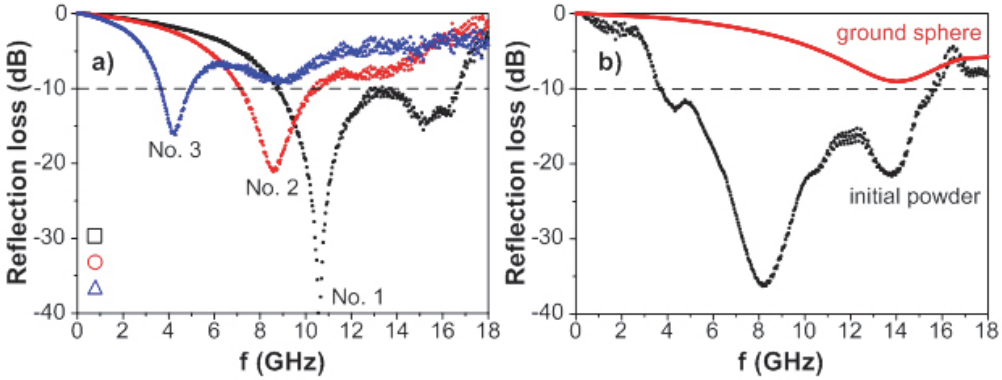


Figure 1. The frequency dependencies of the reflection losses (a) – for samples No. 1, No. 2, No. 3 and (b) – for samples from not separated powders (initial and ground spheres). Measurements are carried out in "reflection" mode using short-circuited load.

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