BRITISH COUNCIL

RESEARCHER LINKS



# Russian-British Workshop
# Program

## *New Advanced Materials and Systems for Photonics and Sensors*

## Novosibirsk, Russia, March 17-20, 2014

# Monday, March 17

**Venue for the Workshop: Institute of Automation and Electrometry SB RAS, Academician Koptug ave. 1, Novosibirsk, Russia**

**$9^{30}$ Registration**

**$10^{00}$ Opening of the Russian-British Workshop**

**$10^{15}$ Optical communications and nonlinear photonics. Nonlinear photonics research at Aston University**
Sergey Turitsin
*Aston University*

## Session I New Materials for Sensors

**$10^{45}$ Functional properties of photonic crystals on the basis of single-crystal opal films including optical chemical sensors, DFB spacers**
A.I. Plekhanov
*Institute of Automation and Electrometry SB RAS, Koptyug, ave.,1, Novosibirsk, 630090, Russia, fractal@iae.nsk.su*

**$11^{15}$ Porous alumina films for sensor application**
Boytsova O.V.[1,2], Klimenko A.A. [1]
[1] *Department of Materials Science Lomonosov Moscow State University, 119992 Moscow, Russia,*
[2] *Russian Acad Sci, NS Kurnakov Gen & Inorgan Chem Inst, 119991 Moscow Russia*

**$11^{30}$ – $12^{00}$ Coffee Break**

**$12^{00}$ Gas sensing properties of fluorine-functionalized graphene**
M.V. Katkov, V.I. Sysoev, L.G. Bulusheva, A.V. Gusel'nikov, A.V. Okotrub
*Nikolayev Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences 3 Acad. Lavrentiev Ave, Novosibirsk, 630090, Russia, katkovmi@gmail.com, +7(383)333-1692*

**$12^{15}$ Porous metal-organic framework as a sensor: the guest-dependent photoluminescence**
Sergey A. Sapchenko
*Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, 3, Acad. Lavrentiev Ave., Novosibirsk, 630090, RUSSIA, ssapchenko@yandex.ru, +7(383)316 58 45*

**$12^{30}$ Sensor based on luminescent composites of pyrilocyanine dye for detection of amine-type reagents**
Viacheslav Chubakov
*Institute of Automation and Electrometry of the Siberian Branch of the Russian Academy of Sciences, Academician Koptug ave. 1, Novosibirsk, 630090, RUSSIA, chubakovsl@mail.ru, +7(383)- 3333174*

**$12^{45}$ Flow-through ordered macroporous silicon sensor for liquid detection**
Maksim A. Parashchenko, Nikolay S. Filippov, Victor V. Kirienko, Sergei I. Romanov
*A.V. Rzhanov Institute of Semiconductor Physics Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 13, Novosibirsk, 630090, RUSSIA, map@isp.nsc.ru, +7 (383) 333-26-24*

**$13^{00}$ – $14^{30}$ Lunch**

# Session II Advanced Materials for Photonics

**$14^{30}$ Thin films of liquid crystalline phthalocyanines and their composites with single-walled carbon nanotubes and metal nanoparticles: properties and applications**

Tamara V. Basova

*Nikolaev Institute of Inorganic Chemistry, 3, Lavrentiev Avenue, Novosibirsk, 630090, Russia*

**$15^{00}$ Optical properties of gold nanostructures fabricated by interference lithography**

A. Tsargorodskaya[1], A. Nabok[2], T. Basova[3], G. J. Leggett[1*]

[1]*Department of Chemistry, University of Sheffield, Brook Hill, Sheffield S3 7HF, UK,*

[2]*Material and Engineering Research Institute, Sheffield Hallam University, Sheffield, UK*

[3]*Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*

**$15^{45}$ Gold nanostructure formation in the photonic crystal matrix and investigation of their optical properties**

R.G. Parkhomenko

*Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, av. Lavrentiev 3, Novosibirsk 630090, Russia. E-mail: parkhomenko@niic.nsc.ru*

**$16^{00}$ – $16^{30}$ Coffee Break**

**$16^{30}$ Fast numerical methods for simulation of complex diffractive elements for photonics and photovoltaics**

Alexey Shcherbakov[1], A.V. Tishchenko[2]

[1] *Moscow Institute of Physics and Technology, Institutsky, 9, Dolgoprudnyi, 141707, RUSSIA, alex.shcherbakov@phystech.edu, +7(903)-5036700*

[2] *University Jean Monnet, Saint-Etienne, France*

**$17^{00}$ – Welcome party**

Tuesday, March 18

# Session III Graphene and Carbon-based Materials

**$10^{00}$ Van der Waals heterostructures**
Roman Gorbachev
*Manchester University*

**$10^{30}$ Graphene photonics and Optoelectronics**
Tawfique Hasan
*University of Cambridge, th270@cam.ac.uk*

**$11^{00}$ Nonlinear plasmonics and photonics with grapheme**
Andrey Gorbach
*Department of Physics, University of Bath, Bath, BA2 7AY, U.K.*

**$11^{30}$ – $12^{00}$ Coffee Break**

**$12^{00}$ Static polarization of donor-acceptor dyads of fullerene $C_{60}$ with porphyrin derivatives**
Pavel Krasnov
*Siberian State Technological University, 82 Mira prospect, Krasnoyarsk, 660049, Russia, kpo1980@gmail.com, +7(908)0209830*

**$12^{15}$ Fluorescent marking of double walled carbon nanotubes**
Koroteev V.O.[1], Antonova O.V.[1], Bortolamiol T.[2], Flahaut E.[2], Rakovich Y.[3], Savateeva D.[3], Bulusheva L.G.[1], Okotrub A.V.[1]
[1] *NIIC SB RAS, 630090, Novosibirsk, Lavrentiev ave. 3, Russian Federation*
[2] *Universite Paul Sabatier CIRIMAT/LCMIE, UMR CNRS 5085, Bâtiment CIRIMAT, 31062 Toulouse Cedex 9, France*
[3] *Materials Physics Center, Paseo Manuel de Lardizabal5, 20018 Donostia-San Sebastian, Spain*

**$12^{30}$ Structure and Electroluminescence Properties of Quantum Dots Nanoparticles Grown on the Aligned Carbon Nanotube Arrays**
Yu.V. Fedoseeva, L.G. Bulusheva, A.V. Okotrub, M.A. Kanygin, S.V. Larionov
*A.V.Nikolayev's Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 3, Novosibirsk, 630090, RUSSIA, fedoseeva@niic.nsc.ru, +7(383)-3305352*

**$12^{45}$ Effect of corrugation on optical properties of graphitic materials**
Sedelnikova O.V.
*NIIC SB RAS, 630090, Novosibirsk, Lavrentievave. 3, Russian Federation*

**$13^{00}$ – $14^{30}$ Lunch**

**$14^{30}$ – $16^{00}$ Excursion to the Geological Museum**

# Session IV Advanced Materials for Photonics II

**$16^{00}$ New approaches to advanced organic and hybrid photopolymer for holography recording and diffraction optics fabrication**

Vladimir Shelkovnikov

*N.N.Vorozhtzov's Novosibirsk Institute of Organic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 9, Novosibirsk, 630090, RUSSIA, vice@nioc.nsc.ru, +7(383)-3308867*

**$16^{30}$ Holographic photopolymer material using by forbidden transitions of xanthene dyes**

Evgeny Vasilyev

*N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry of the Siberian Branch of the Russian Academy of Science, Ave. Lavrentyev, 9, Novosibirsk, 630090, RUSSIA, vev@nioch.nsc.ru, +7(383)-3309642*

**$16^{45}$ Physico-chemical characteristics of photosensitive hybrid material for recording diffraction optical elements**

Dmitry Derevianko

*N.N. Vorozhtsov Institute of Organic Chemistry of the Siberian Branch of Russian Academy of Science pr. Lavrentieva 9, Novosibirsk, 630090, Russia, dmitrydereviankio@gmail.com, +7(383)- 338850*

Wednesday, March 19

# Session V Advanced Materials for Photonics III

**$10^{00}$ Study of photo desorption of rubidium atoms in hollow-core photonic band-gap fibers, generation and control quantum states of light using atomic vapours**

Sergey Atutov

*Institute of Automation and Electrometryof the Siberian Branch of the Russian Academy of Sciences, Ave. Koptuga 1, Novosibirsk, 630090, RUSSIA, atutovsn@mail.ru +7(383)-3306869*

**$10^{30}$ Engineered photonic crystal fibre single photon sources**

Dr Peter Mosley

*Department of Physics, University of Bath, Bath, BA2 7AY, U.K.*

**$11^{00}$ Lanthanide Complexes as Thermometric Contrast Reagents for MRI Diagnosing of Cancer and Control of Photo-dynamic Therapy**

Sergey Babailov

*A.V.Nikolayev's Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 3, Novosibirsk, 630090, RUSSIA, babajlov@niic.nsc.ru, +7(383)-3308957*

**$11^{30}$ – $12^{00}$ Coffee Break**

**$12^{00}$ Bioanalytical platforms based on silicon micro- and nanochannel membranes**

Nikolay Filippov, Maksim Parashchenko, Natalia Vandysheva, Sergei Romanov

*A.V.Rzhanov Institute of Semiconductor Physics of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev,13, Novosibirsk, 630090, RUSSIA, filippov@isp.nsc.ru, +7(383)-3332519*

**$12^{15}$ Gas-jet deposition of thin fluoropolymerfilm withsilver nanoparticles possessing surface plasmon resonance**

Alexey Safonov

*Kutateladze's Institute of Thermophysics of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 1, Novosibirsk, 630090, RUSSIA, safonov@itp.nsc.ru, +7(383)-3356245*

**$12^{30}$ Magnetic resonance in $CuCr_2S_4$ nanoclusters and nanocrystals**

Tugarinov V.I.

*L.V. Kirensky Institute of Physics SB RAS, 660036, Krasnoyarsk, Russia*

**$13^{00}$ – $14^{30}$ Lunch**

**$14^{30}$ $17^{00}$ Academ Ski Tour**

Thursday, March 20

# Session V Fiber Optics Applications

**$10^{00}$ Light propagation, amplification and generation in fiber waveguides with micro- and nanostructures**

Sergey Babin

*Institute of Automation and Electrometry of the Siberian Branch of the Russian Academy of Sciences, Koptyug Ave, 3, Novosibirsk, 630090, RUSSIA, babin@iae.nsk.su, +7(383)-3306939*

**$10^{30}$ Development of reflection interferometers for fiber optics**

Vadim Terentyev

*Institute of Automation and Electrometry of the Siberian Branch of the Russian Academy of Sciences, Ave. Ak. Koptug, 1, Novosibirsk, 630090, RUSSIA,* terentyev@iae.nsk.su*, (383) 330-69-39.*

**$10^{45}$ Advancements in mode-locked fibre lasers and fibre super continua**

Edmund J. R. Kelleher

*Royal Academy of Engineering Research Fellow, Imperial College London, UK,*
*edmund.kelleher08@imperial.ac.uk*

**$11^{00}$ All-fibre Mode-locked fibre laser based on Carbon Nanomaterials and Fibre Gratings**

Dr.Chengbo Mou

*Aston Institute of Photonic Technologies (AIPT), Aston University,Birmingham, UK, B4 7ET*

**$11^{30}$ – $12^{00}$ Coffee Break**

**$12^{00}$ Workshop Roundtable**

**$13^{00}$ – $14^{30}$ Lunch**

**$14^{30}$ Workshop Roundtable**

# Posters

**Polarization attractors in mode-locked fiber lasers with carbon nanotubes saturable absorber**
Tatiana Habruseva
*Institute of Photonic Technologies, Aston University, Aston Triangle, B4 7ET, Birmingham, UK*

**Prediction of hydration free energies using reference interaction site model**
Maksim Misin, David Palmer, Maxim Fedorov
*Corresponding author email: david.palmer@strath.ac.uk*

**New light emitting inorganic cluster complexes for imaging and electronics**
Dr Olga Efremova
*Aston University*

**Molecular modelling, nanomaterials dispersion**
Sean O'Connor
*sean.o-connor.2013@uni.strath.ac.uk*

# Functional properties of photonic crystals on the basis of single-crystal opal films including optical chemical sensors, DFB spacers

A.I. Plekhanov

*Institute of Automation and Electrometry SB RAS, Koptyug, ave.,1, Novosibirsk, 630090, Russia, fractal@iae.nsk.su*

The development of photonic crystals (PhCs), structures with photonic band gaps (PBG) that prevent the propagation of light in a certain frequency range, has led to proposals of many novel devices for important applications in lasers, opto-electronics, sensors, and communications. The most straightforward way of achieving a PhC in three-dimensions is to use strong capillary forces at a meniscus between a substrate and a colloidal sol. It can induce crystallization of spheres into a three-dimension array of controllable thickness[1]. This method allows to fabricate the single-crystal opal films with a reflection coefficient in the photonic band gap up to 95%[2].

The lasing from artificial opal, thin single-crystal opal films and opal heterostructures infiltrated with Rhodamine 6G is studied. In the case of volume opal, we have observed random lasing. In contrast to this case, single-crystal opal films show lasing caused by distributed feedback inside PBG structure.

It was found that at the grazing incident of white-light beam on the (glass – PhC film) interface the spectrum of the Bragg backward reflection and refraction manifested the PBG, which changes its position under insignificant change of the concentration of vapor of a range of substances (isopropyl alcohol, dibutyl amine, tributyl amine, water, ammonia), filling the PhC. The effect was reversible. The spectral shift of the PBG depends on the polarity of the analyte and increases with their dipole momenta and the concentration of vapors[3]. The revealed effect can be used in the schemes of optical sensors, as well as for controlling the spectrum of refracted and reflected light in an optical demultiplexer by an external field.

We report on the low-threshold operation of nanolasers base on surface plasmon amplification by stimulated emission of radiation (spaser) fabricated of hybrid nanoparticles with a 10-nanometre gold core surrounded by a 20-40-nanometre-thick silica shell embedded with dye molecules. The spasers are introduced into the pores of the opal PhC. Owing to distributed photonic feedback, the threshold condition of the amplified spontaneous emission is the smallest threshold condition ever reported 140 kW/cm$^2$.

1. Jiang P., et al., *Chem. Mater*. **11,** 2132 (1999).
2. Plekhanov A.I. et al., *Nanotechnologies in Russia.* №1-2, 245 (2006).
3. Plekhanov A.I. et al., *JETP Letters.* **90**, 565 (2009).

# Porous alumina films for sensor application

Boytsova O.V.[1,2], Klimenko A.A. [1]

[1] *Department of Materials Science Lomonosov Moscow State University, 119992 Moscow, Russia,*

[2] *Russian Acad Sci, NS Kurnakov Gen & Inorgan Chem Inst, 119991 Moscow Russia*

Recent research trends in biosensing have been geared towards developing analytical devices that are label free, small in size and portable. The performance of these devices has been dramatically improved through the advent of new materials and microfabrication technologies. This is especially true for sensors. We put the emphasis on two specific experimental approaches so widely accessible for other groups but which can give rather specific and very important information, especially at their combined usage. The first one is the anodization of aluminium to obtain porous anodic alumina. Anodic alumina films is widely considered as one of the most promising systems possessing ordered one-dimensional technique that allows us to produce porous films with well ordered hexagonal arrays porous structure. These films will be prepared by the two-step anodization of cylindrical channels. The use of different electrolytes, voltages and anodic oxidation times allows one to adjust channel diameter, interpore distance and film thicknesses in a wide range of interests. Second, it is the wide use, in addition to the standard modification of surface, photochemical lithography.

A novel surface stress sensor is used for quantitative analysis of nanomechanical response arising from adsorption of small molecules on microcantilevers. The deflection of the microcantilever is indicative of surface stress that can be correlated with the amount of ligands bound to the microcantilever. In detail, the surface of a microcantilever is functionalized with receptor molecules that have high affinity for the ligand. In the surface stress sensor, adsorption of the ligand on the sensitized surface provides differential measurements of deflection between a sensing and reference microcantilevers. An optical interferometry is used to measure cantilever deflection that converts molecular interactions into a measureable quantitative signal with high precision and accuracy.

The sensor's principal applications would be biomedical, forensic and biosecurity areas; portability is of crucial importance in molecular recognition with high specificity and sensitivity. In current state-of-art microcantilever sensors, optical beam deflection method is utilized for the deflection measurement due to its simplistic configuration and convenience as are common in AFM instrumentation. However, the optical deflectometry requires a large optical distance for high-sensitive detection and suffers from the challenges in integration of all components in a single micro device. The sensitivity of interferometric technique, in contrast, is independent of the distance between detectors and the sensing surface of microcantilevers. Therefore, the surface stress sensor may be amenable to integrate all sensor components into a single MEMS device. One outstanding aspect of the microcantilever sensor is that the differential measurement of microcantilevers (sensing and reference pair) is inherently insensitive to environmental disturbances such as nonspecific adsorption. The use of streptavidine as receptor molecules and robust performance of the sensor because of unique features of aptamers such as long term stability and easy and straightforward chemical modification.

In order to achieve this goal, we utilized a novel microcantilever based nanomechanical sensor capable of sensitive and specific detection of chemical and biological species.

The travel was supported with the British Council.

# Gas sensing properties of fluorine-functionalized graphene

M.V. Katkov, V.I. Sysoev, L.G. Bulusheva, A.V.Gusel'nikov, A.V. Okotrub

*Nikolayev Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences*
*3 Acad. Lavrentiev Ave, Novosibirsk, 630090, Russia, katkovmi@gmail.com, +7(383)333-1692*

Chemical interaction of a graphene surface with molecules in a gas phase produces a change in its electron state. Moreover, the surface electroconductivity change can be induced by electric field or electron transfer to/from a sorbed molecule. That allows us to use graphene as a material for molecular sensors. To enhance the sensing properties of graphene, we have to create some reactive centers on its surface, such as defects and functional groups. In this case, the electrochemical graphene properties depend on the degree of its chemical modification.

We have developed a method of the functionalization of graphene layers by graphite fluoride $C_2F$ surface reduction. The degree of the $C_2F$ surface reduction was evaluated by measuring the conductivity and X-ray photoelectron spectroscopy (XPS). We showed a possibility of detecting certain types of molecules in a gas phase and measuring its concentration due to different responses of individual sensors to the molecules with different chemical structures. We noted the sensor responses to electron donor (ammonia) and acceptor (nitrogen oxide) molecules have opposite signs and different response characteristic times.

# Porous Metal-Organic Framework as a Sensor: The Guest-Dependent Photoluminescence

Sergey A. Sapchenko

*Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, 3, Acad. Lavrentiev Ave., Novosibirsk, 630090, RUSSIA, ssapchenko@yandex.ru, +7(383)316 58 45*

Metal-organic coordination polymers (or MOFs) are considered to be promising materials for gas separation and sorption, heterogeneous catalysis, luminescence and other applications.

Following the simple one-pot synthesis method we have obtained 2 permanent porous coordination polymers $[Zn_4(dmf)(ur)_2(ndc)_4]\cdot 5DMF\cdot H_2O$ and $[Zn_{11}(H_2O)_2(ur)_4(bpdc)_{11}]\cdot 7DMF$ (**dmf** = N,N-dimethylformamide, **ur** = urotropine, **$H_2$ndc** = 2,6-naphtalenedicarboxylic acid, **$H_2$bpdc** = 4,4′-biphenildicarboxylic acid). Their permanent porosity was demonstrated by the nitrogen sorption measurements. The experiments on $H_2$, CO, $CO_2$ and $C_2H_2$ sorption have shown the high selectivity of the obtained coordination polymers towards carbon dioxide and acetylene.

The structure of the compound $[Zn_4(dmf)(ur)_2(ndc)_4]\cdot 5DMF\cdot H_2O$ contains channels of 2 types [1]. The bigger hexagonal channels are filled with guest molecules of DMF and water, the space of the channels of the second type is filled with coordinated DMF molecules. To perform a full removal of the guest molecules from the both types of channels, a unique step-by-step activation method was proposed. The obtained biporous material $[Zn_4(ur)_2(ndc)_4]$ allowed us to separate the two-component mixture through the pores of the compound. Coordination polymer $[Zn_4(dmf)(ur)_2(ndc)_4]$ demonstrates catalytic activity as well.

Moreover this metal-organic framework can form inclusion compounds with different substrates, such as aromatic compounds. The framework itself demonstrates intense solid-state luminescence, and its spectrum contains a broad peak at 430 nm (excitation wavelength of 370 nm). Importantly, its intensity is directly dependent from the nature of the guest molecules in the pores. Thus, the inclusion of ferrocene or nitrobenzene molecules into the voids of the coordination polymer $[Zn_4(dmf)(ur)_2(ndc)_4]$ results in significant quenching of the framework's luminescence, while the presence of benzene in the internal space of the polymer results in higher luminescence intensity [2]. This phenomenon makes this coordination polymer a good candidate for sensor applications. The ferrocene inclusion compound can be used as sensor as well. It was shown, that it can change its colour, after exposure to gas oxidizers like nitrogen dioxide.

[1] Sapchenko S.A., Samsonenko D.G., Dybtsev D.N., Fedin V.P., *Inorg. Chem.*, 2013, ***52***, 9702–9704.

[2] Sapchenko S.A., Samsonenko D.G., Dybtsev D.N., Melgunov M.S., Fedin V.P., *Dalton Trans.*, 2011, *10*, 2196-2203.

# Sensor based on luminescent composites of pyrylocyanine dye for detection of amine-type reagents

Viacheslav Chubakov

*Institute of Automation and Electrometry of the Siberian Branch of the Russian Academy of Sciences, Academician Koptug ave. 1, Novosibirsk, 630090, RUSSIA, chubakovsl@mail.ru, +7(383)-3333174*

At the present time fluorescence analysis is widely used in the medical diagnostics and in bioscience. For this purpose various organic fluorophores are used as labels. Though the fluorescence analysis can be a very sensitive technique, its detection limit is usually restricted by quantum efficiency of the fluorophore and its photostability. Therefore, development of the ways for enhancing the luminescence signal of dye is an important task. Also ability to use fluorophores in the solid state systems significantly increases the list of possible application.

In this regard, nanoplasmonics provide a promising way to overcome some classic physical restrictions. Interactions of fluorophore with plasmonic nanostructured materials, such as silver, gold or cooper results in an increased fluorescence in the visible-light spectrum. Shortened fluorescence lifetime of the fluorophore increases the radiation resistance of hybrid materials based fluorophores with metallic nanostructures.

Pyrylo- and pyrydocyanine dyes belong to the organic fluorophores, which can be used as labels. It is well known that pyrylocyanine dyes interact with primary amines to form pyrydocyanines. Pyrydocyanines exhibit luminescence, which is different from the luminescence of the initial pyrylocyanines; it can be used for the luminescence detection of the organic amines.

The aim of this work is to develop a method for the preparation of a solid highly sensitive sensor based on luminescent nanostructured complexes of the functional pyrylocyanine dye. The proposed sensor should selectively react with amine-type reagents.

Our experiments are carried out with three different pyrylocyanine dyes. Spectral and luminescent properties of the synthesized dyes were measured for their solutions and films deposited on various substrates. Thickness of the films is equal to a few microns. The polymer form of the dyes is used to prepare the films, which provide an enhanced luminescence. Preliminary measurements have shown that bonding of the polymer does not affect the spectral properties of the original dyes; however spectra may shift by tens of nanometers for the films depending on the type of substrate. Some substrates, which have a structured surface, are more prospective to enhance the fluorescent response of dyes. The developed complexes of the pyrylocyanine dyes selectively react with different amine-type reagents and form pyrydocyanines, which have different spectral properties. Further development of the study assumes increase of luminescence by use of metal nanostructures.

# Flow-through Ordered Macroporous Silicon Sensor for Liquid Detection

Maksim A. Parashchenko, Nikolay S. Filippov, Victor V. Kirienko, Sergei I. Romanov

A.V. Rzhanov Institute of Semiconductor Physics Siberian Branch of the Russian Academy of Sciences, *Ave. Lavrentyev, 13, Novosibirsk, 630090, RUSSIA, map@isp.nsc.ru, +7 (383)333-26-24*

In the past few years, meso- and macroporous silicon has found usage in solving various bioanalytical problems for medicine, molecular biology, virology, and gene engineering. It was the basis for creating molecular and cell filters, biosensors, solid-state support structures with a huge internal surface and with a wide range of linear sizes of pores ranging from several nanometers to tens of micrometers. Porous silicon enables almost unlimited highly controllable modification of its extended surface, which is important for the creation of different biosensors. The principles of such sensors are similar. Test substances adsorbed on its surface caused changes in structural and electronic properties of sensor. These changes can be detected by various physical methods, for example, measuring the electrical conductivity of the structure.

In this work we have developed a flow-through sensor based on ordered macroporous silicon which was tested on different sodium tetraborate. A sensitive part of this sensor was silicon microchannel membrane created by the anodic electrochemical etching of (100) oriented p-type silicon wafer with resistivity of 40 Ohm·cm. In our study silicon membrane with 10x10μm$^2$ cell with 195 μm thickness, 0.5 cm$^2$ square and 1.3 μm thick walls was used (Fig.1). The microchannel membrane was fabricated in monolithic silicon wafer, then it was oxidized in wet oxygen at 1000ºC to create 90 nm oxide layer and finally layers of chrome and gold as electrical contacts were placed on ordered silicon surface. The fabricated sensor was set in the measuring system, which consist of input and output chambers filled with liquid. The sensor was connected to the measuring stand and all measurements were performed at room temperature. We have investigated various concentrations of the sodium tetraborate ($Na_2B_4O_7$) used in biology and medicine. The test volume of liquid in all experiments was 5 ml. Filling liquid into the inlet chamber was carried out with a graduated pipette. Then liquid passed through the sensor to the output chamber, causing a change in the high frequency conductivity and capacity of the structure. It was clearly seen that impregnation of liquid into microchannels of the sensitive element led to changes in electrophysical properties of the structure (the sensor had its own specific response), which made it possible to distinguish liquid and its concentrations in microchannels (Fig. 2).

It was established that the fabricated flow-through sensor based on ordered macroporous silicon was an effective device for electrical detection of sodium tetraborate and determination of concentrations of these liquid. These sensors appear to have considerable promise for analytical and diagnostic devices in medicine and biology.

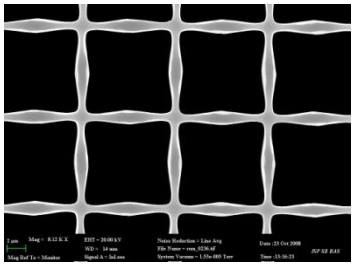

Fig. 1. Macroporous silicon membrane.

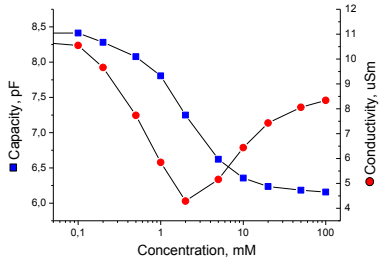


Fig. 2. Changes in conductivity and capacity depending on the concentration of sodium tetraborate.

# Thin films of liquid crystalline phthalocyanines and their composites with single-walled carbon nanotubes and metal nanoparticles: properties and applications

Tamara V. Basova

*Nikolaev Institute of Inorganic Chemistry, 3, Lavrentiev Avenue, Novosibirsk, 630090, Russia*

Disk-like molecules, typically comprising a flat rigid aromatic core and flexible peripheral substituents, self-organize into one-dimensional "supramolecular wires". Due to high charge carrier mobility along the columns, discotic mesogens are considered as realistic candidates for application in organic electronic devices [1, 2].

In this contribution, the systematic investigation of the influence of different parameters (heating and cooling regimes, substrate materials, interfaces) on the alignment of liquid crystalline (LC) metal phthalocyanines was carried out. The effect of interface on the orientation of the film of tetrasubstituted $MPcR_4$ and octasubstituted $MPcR_8$ metal phthalocyanines (M=Ni(II), Cu(II), Zn(II)) with alkoxy-, alkyltio- and polyoxo-substituents in aromatic ring, deposited on one substrate and between two substrates as well as between two conductive electrodes was studied by the methods of polarized Raman spectroscopy and polarized microscopy.

It has been shown that the phthalocyanine films confined between two substrates are characterized by homeotropic alignment while no homeotropic alignments could be obtained with an air interface if specific interaction between phthalocyanine molecules and a substrate is absent. The orientation is independent of the type of substituents in the phthalocyanine ring. The effect of the phthalocyanine films alignment and intercalation of SWCNT on their conductivity and charge carrier mobility was also demonstrated.

The composite materials of single walled carbon nanotubes (SWCNT) and gold nanoparticles with discotic phthalocyanines and distribution of SWCNT and nanoparticles in the ordered matrix of hexagonal columnar mesophase of these derivatives were studied. It was demonstrated that the nature of the mesophases was not altered in these composites. On the other hand, the films of composites exhibited enhanced electrical conductivity of about four orders of magnitude compared to the corresponding pure phthalocyanines. Plasmonic properties of gold nanoparticles distributed in the LC matrix of $CuPcR_8$ were also studied.

The dispersion of SWCNT and nanoparticles in the liquid crystalline phthalocyanine matrix provide a route for synthesizing novel materials with interesting properties useful for applications in many devices such as photoconductors, light emitting diodes, solar cells, chemical sensors, thin film transistors and so on.

## References

1. Van de Craats A.M., Stutzmann N., et. al. *Adv. Mater.* **15**, 2003, 495-499.
2. Schmidt-Mende L., Fechtenkötter A., et. al. *Science* **293**, 2001, 1119-1122.

# Optical properties of gold nanostructures fabricated by interference lithography

A. Tsargorodskaya[1], A. Nabok[2], T. Basova[3], G. J. Leggett[1*]

[1] *Department of Chemistry, University of Sheffield, Brook Hill, Sheffield S3 7HF, UK*
[2] *Material and Engineering Research Institute, Sheffield Hallam University, Sheffield, UK*
[3] *Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*
*E-Mail (corresponding author): graham.leggett@sheffield.ac.uk*

Gold nanostructures were fabricated by interferometric lithography (IL) [1] with a view to their application for optical bio-sensing based on localized surface plasmon resonance. The dimensions and morphology of nanostructures obtained were characterized by AFM. The arrays of 110-200 nm wide and 300-400 nm long gold nanorods with spacing of 120-220 nm were fabricated by IL (Fig. 1).

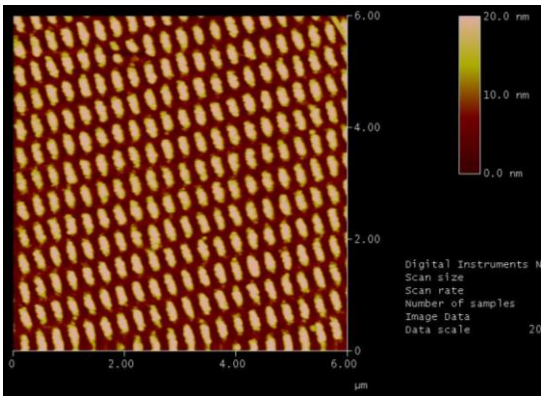


Fig. 1. Typical AFM topographical image of gold nanostructures formed by IL

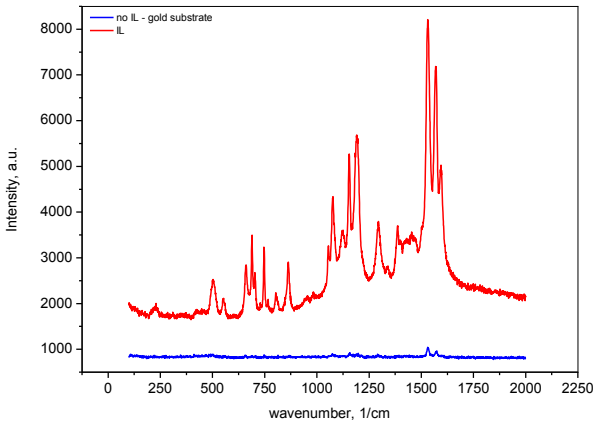


Fig. 2. SERS spectra of phthalocyanine thin film adsorbed on continuous gold film (below) and gold nanostructures (above)

UV-vis absorption spectra of fabricated gold nanostructures showed a characteristic peak at ca. 520 nm associated with localized surface plasmons similar to that observed previously in other types of gold nanostructures [2-3].

Post-lithographic processing by annealing was found to improve the optical properties of the nanostructure arrays still further. Generally, annealed samples appear higher and smaller compared to as-prepared samples. AFM topographical and SEM images show that all the samples annealed at between 500 and 550°C for 90−120 minutes retain a regular pattern. X-ray diffraction analysis of annealed gold nanostructures evinces formation of crystal clusters on the surface.

Raman spectra of a thin film of phathlocyanine adsorbed on gold nanostructures showed the enhancement of Raman scattering of up to $10^5$ times in comparison with the same film deposited on continuous gold layer (Fig. 2). These results demonstrate the potential of the IL patterning of gold layers for realization of plasmon-based sensing devices.

## References

1. H. Korre et al., *J. Vac. Sci. Technol. B* **28**, 2010, C6Q20-C6Q24.
2. M. Banaee and K. Crozier, *ACS Nano* **5**, 2006, 307-314.
3. A. Haes and R. Van Duyne, *J. Am. Chem. Soc*. **124**, 2002, 10596-10604.

# Gold nanostructure formation in the photonic crystal matrix and investigation of their optical properties

R.G. Parkhomenko

*Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, av. Lavrentiev 3, Novosibirsk 630090, Russia.E-mail: parkhomenko@niic.nsc.ru*

At the present time, gold nanoparticles (AuNP) are the subject of extensive studies, since they are of interest from the standpoint of modern materials science, creating metamaterials, microelectronics, nanophotonics offering the potentiality for the development of plasmon nanolasers.

We have investigated the formation of gold nanostructures within the matrix of a photonic crystal by means of chemical vapor deposition using organometallic compounds (MOCVD). The deposition of gold nanostructures was performed onto Si(100) substrates with applied $SiO_2$ microspheres (photonic crystal) within the temperature range of 160-250 °C. As a precursor for the deposition of gold nanoparticles with different morphology and size we used $(CH_3)_2Au(thd)$ (thd = 2,2,6,6-tetramethyl-3,5-heptanedionato). In order to obtain hollow gold nanospheres we used $(CH_3)_2Au(OAc)$ (OAc = acetate). HF solution was used for etching $SiO_2$ microspheres.

A multiple increase was revealed concerning the luminescence of fluorescein infiltrated into the photonic crystal with the deposited gold nanoparticles. Optical properties have been investigated for the photonic crystal formed from hollow gold nanospheres.

# Fast numerical methods for simulation of complex diffractive elements for photonics and photovoltaics

Alexey Shcherbakov[1], A.V. Tishchenko[2]

[1] *Moscow Institute of Physics and Technology, Institutsky, 9, Dolgoprudnyi, 141707, RUSSIA,*
*alex.shcherbakov@phystech.edu, +7(903)-5036700*
[2] *University Jean Monnet, Saint-Etienne, France*

Development of numerical methods for the light scattering and diffraction in micro and nanostructures is currently of a great interest. The main goal of the work is to implement an idea consisting in supposition that all linear phenomena can by simulated in linear time. Linear rigorous methods being developed, very accurate and fast optimization procedures of photonic structures would be possible. An implementation of the idea requires a simultaneous consideration of physical phenomena specific features, various possible mathematical representations of physical models, and facilities provided my modern computer architectures.

So far we have developed numerical methods for the rigorous grating diffraction simulation for arbitrary shaped gratings, which have linear numerical complexity [1-4]. Possible applications include optimization of diffraction gratings for spectroscopy, high-power lasers, photonic structures for photovoltaics and whole photovoltaic elements, complex diffractive optical elements (DOEs).

1. A.A. Shcherbakov, A.V. Tishchenko, D.S. Setz, B.C. Krummacher. Rigorous S-matrix approach to the modeling of the optical properties of OLEDs. // *Organic Electronics*. **12**, 654-659 (2011).

2. A.A. Shcherbakov, A.V. Tishchenko. Fast numerical method for modeling one-dimensional diffraction gratings. // *Quantum Electron.* **40**, 6, 538-544 (2010)

3. A.A. Shcherbakov, A.V. Tishchenko. New fast and memory-sparing method for rigorous electromagnetic analysis of 2D periodic dielectric structures // *JQSRT*. Vol. **113**. 158-171 (2012).

4. A.A. Shcherbakov, A.V. Tishchenko, Efficient curvilinear coordinate method for grating diffraction simulation // *Opt. Express*. **21**. No 21. 25236-25247 (2013)

# Van der Waals heterostructures

Roman Gorbachev

*Manchester University*

Research on graphene and other two-dimensional atomic crystals is intense and is likely to remain one of the leading topics in condensed matter physics and materials science for many years. Looking beyond this field, isolated atomic planes can also be reassembled into designer heterostructures made layer by layer in a precisely chosen sequence. In this talk I will review our recent progress on fabrication and investigation of such heterostructures starting from ultrahigh quality graphene encapsulated in h-BN up to complex 6-layer structures comprised of several materials. Significant attention will be paid to Moiré patterns with associated Hofstadter-like states in graphene.

# Graphene photonics and Optoelectronics

Tawfique Hasan

*University of Cambridge, th270@cam.ac.uk*

# Nonlinear plasmonics and photonics with grapheme

Andrey Gorbach

*Department of Physics, University of Bath, Bath, BA2 7AY, U.K.*

Graphene is a purely two-dimensional form of carbon, where atoms are arranged in a honeycomb lattice. Recent studies of graphene reveal its great potential for applications in photonics and optoelectronics. In particular, graphene supports surface plasmons in mid-infrared and terahertz range, where metals have no significant plasmonic response. Also, recent experimental and theoretical studies of graphene report that it could have the highest optical nonlinearity among known materials.

In this work, theoretical approach is developed for analysis of nonlinear wave phenomena in plasmonic and photonic guiding structures with graphene. The approach is based on asymptotical expansion of Maxwell equations with nonlinear boundary conditions. Self-focusing of surface plasmons and novel mechanisms of nonlinear switching are discussed for single- and multi-layer graphene structures. Also, the enhancement of effective nonlinearity in graphene-clad tapered fibres is analysed.

# Static Polarization of Donor-Acceptor Dyads of Fullerene $C_{60}$ with Porphyrin Derivatives

Pavel Krasnov

*Siberian State Technological University, 82 Mira prospect, Krasnoyarsk, 660049, Russia, kpo1980@gmail.com, +7(908)0209830*

The development of lasers capable of generating a light with high electric field strength comparable with the microscopic field strength in atoms encouraged the development of research into nonlinear optics. The subjects of this research are substances for which the dielectric polarization vector demonstrates a nonlinear response to a vector of the electric field intensity of a wave. The results of this research include the creation of optical limiters for pulsed lasers, optical communication devices and others.

Some organic materials and inorganic semiconductors are considered to be prospective candidates for applications in nonlinear optics. This result is related to various properties, including a relatively low cost, ease of creation and integration into the devices, rapid response to a change in the electric field, and a high stability to optical damage. Porphyrins, fullerenes, and its derivatives, including donor-acceptor porphyrin-fullerene dyads, are categories of materials considered for possible use. In the last case, interest arises because the dyads completely meet the special requirements: they are compounds of strong donor and acceptor molecules, and they have very extended delocalized $\pi$-electronic systems. Moreover, dyads can be created and used in crystalline form.

In this report, the results are presented for quantum-chemical investigations into the static polarization of donor-acceptor dyads of fullerene $C_{60}$ noncovalently bonded to porphyrin and three porphyrin derivatives (porphyrazine, tetrabenzoporphyrin, phthalocyanine). The key problems consist of defining the influence of the relative orientation of the porphyrin to the fullerene and the nature of the porphyrin derivative on the values of the polarizability and hyperpolarizabilities of the dyads, and of defining the nature of the possible nonlinear optical properties of the dyads.

Quantum-chemical calculations of the molecular structure and the static polarization of the considered objects were performed by DFT with the B3LYP exchange-correlation potential and the 6-31G(p,d) basis set. Because the two parts of each dyad are bonded noncovalently through intermolecular interaction forces only, the intermolecular forces must be correctly described in the calculations. The potential used was not designed for such calculations; therefore, in this work, the correction of this interaction was realized by the addition of Grimme's empirical dispersion potential to the B3LYP potential. The GAMESS (US) quantum-chemical program package was employed for all the quantum-chemical calculations.

As a result of the performed calculations, the nature of the porphyrin derivative influences the nonlinear optical properties of dyad as a whole, and increases in the size of the $\pi$-electronic system lead to intensification of the nonlinear properties. In contrast, the rotation relative to fullerene of the heterocyclic molecule in the plane in these compounds has a considerably smaller impact on the polarization of the dyads in an external electric field. The dependence of the dipole moments of the separate porphyrin derivatives and fullerene on the electric field strength remains almost linear over all the studied intervals of the field strength. This type of dependence is clearly related to the significantly low values of the 1st- and 2nd-order hyperpolarizabilities rather than to the dyads. The origin of the nonlinear dependence of the dyad dipole moment on the external electric field is caused by the additional polarization of one structure part by another one, whose own electric field is induced by the external one.

# Fluorescent marking of double walled carbon nanotubes

Koroteev V.O.[1], Antonova O.V.[1], Bortolamiol T.[2], Flahaut E.[2], Rakovich Y.[3], Savateeva D.[3], Bulusheva L.G.[1], Okotrub A.V.[1]

[1] *NIIC SB RAS,630090, Novosibirsk, Lavrentiev ave. 3, Russian Federation*

[2] *Universite Paul Sabatier CIRIMAT/LCMIE, UMR CNRS 5085, Bâtiment CIRIMAT, 31062 Toulouse Cedex 9, France*

[3] *Materials Physics Center, Paseo Manuel de Lardizabal5, 20018 Donostia-San Sebastian, Spain*

Chemical modification of carbon nanotubes target different needs, such as modification of electronic structure, appearance of new properties or better bonding in composite materials. The most developed functionalization method is noncovalent functionalization, resulting molecules attachment with Van der Waals bonds and no changes in material atomic structure, but attached molecules are removed easily. Covalent functionalization, in opposite, results in formation of strong covalent bonds and changes atomic structure of materials adding functional groups. Double walled carbon nanotubes (DWNT) are perfect candidates for covalent functionalization. Attaching functional groups to outer layer doesn't affect inner layer structure, so conductivity and other properties, present due to layers structure are preserved.

Addition of fluorescent labels to track particles position in different media using simple luminescent microscopy. Attaching luminescent molecules to carbon nanotubes could cause luminescence quenching due to high nanotube conductivity. In this work, we used fluorescein as luminescent label.

For initial functionalization oxidation and fluorination techniques we used, so we could check the influence of initial functionalization step on the products. Then, 1,4-diaminodutane and 1,8-diaminooctane linkers were attached to DWNT's. Linkers, ending with amino groups, allow easily attachment of fluorescein isothiocyanate fluorescent markers.

To check the luminescence properties of reaction products we used fluorescent lifetime imaging microscopy. All the samples with fluorescein attached showed luminescence lifetimes characteristic to fluorescein with small variation.

# Structure and Electroluminescence Properties of Quantum Dots Nanoparticles Grown on the Aligned Carbon Nanotube Arrays

Yu.V. Fedoseeva, L.G. Bulusheva, A.V. Okotrub, M.A. Kanygin, S.V. Larionov

*A.V.Nikolayev's Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 3, Novosibirsk, 630090, RUSSIA, fedoseeva@niic.nsc.ru, +7(383)-3305352*

Investigation of structure and electroluminescence properties of anisotropic composite materials containing multiwalled carbon nanotubes (CNTs) and two kinds of quantum dots, nanodimonds and cadmium sulfide, have been presented. Array of vertically aligned CNTs were grown on conductive silicon substrate using an aerosol-assisted CVD method. Anisotropic nanodiamond/carbon nanotube (ND/CNT) composite material has been synthesized by immersing the array CNTs in a suspension of NDs in dimethylsulfoxide mixed with water. CdS nanoparticles have been grown on array CNTs using aqueous chemical bath containing thiourea, cadmium chloride, and ammonia. To modify the morphology of CdS/CNTs composite materials time and temperature of the synthesis of CdS was varied and the addition of polar organic solvents and electrical field were applied. Electron microscopy study shows that agglomerates of quantum dots are mainly located on the CNT array surface. Small particles and agglomerates penetrate into intertube space and attached to nanotube walls. The X-ray photoelectron spectroscopy and near-edge X-ray absorption fine structure spectroscopy reveal that applied synthetic procedure results in a non-covalent assembling of quantum dots and CNTs. The Infrared and Raman spectroscopy data indicate that composition of CNT array changes under conditions of the synthesis of NDs and CdS nanoparticles. It is demonstrated that the ND/CNT and CdS/CNT composite materials exhibit electroluminescence properties and electron field emission properties. It was found that concentration, size, crystallinity of CdS nanoparticles and their location influence on the electroluminescence properties of CdS/CNT composite.

The reported study was supported by RFBR, research project No. 14-03-31359 мол_а.

# Effect of corrugation on optical properties of graphitic materials

Sedelnikova O.V.

*NIIC SB RAS, 630090, Novosibirsk, Lavrentiev ave. 3, Russian Federation*

High mobility of π-electronic cloud of carbon nanostructures along with high value of polarizability causes a great interest in use of these materials for plasmonics and chemical and biological sensors. The properties of carbon nanostructures, which are termed structure sensitive, are greatly affected by presence of defects (vacancies, doping by non-carbon element, deformation). The aim of my investigation is theoretical study of the relationship between the geometry and the electronic and physical properties of carbon nanostructures by using quantum chemistry calculations.

Graphene has attracted a tremendous interest of physics and engineers for different practical applications. Due to high flexibility of graphene layer, its ability to match the support morphology, investigation effect of corrugation of graphene on electronic and plasmonic properties becomes an important task. Band structure calculations showed that bending of graphene layer strongly affect the local density of electronic states (DOS) [1] yielding changes in optical and plasmonic properties. Particularly, localization of π-electron around the top of corrugation of rippled graphite layers results in modulation of DOS causing favorable conditions for conduction channels. Our calculations showed that changes in optical absorption of graphene and graphite with bending are (i) appearance of new resonances due to removing restrictions on the electron transitions being forbidden in the flat material for certain light polarization and (ii) redshifting of the main absorption peaks. As a result, plasmon frequencies (π and π+σ) are also redshifted [2, 3]. Collective electron excitations in highly corrugated graphitic nanostructures were studied experimentally. Comparison of optical absorption and XPS spectra of planar graphitic structures and onion-like carbon, where the outer graphitic mantle is corrugated, revealed substantial redshift of position of optical absorption peak and π and π+σ plasmon modes. These results show that stressing the graphene mechanically or placing the layer on an artificial substrate, one could control the graphene rippling, tuning transport, sensor and optical properties of material.

1. O.V. Sedelnikova, L.G. Bulusheva, A.V. Okotrub. *Synth. Met.* **160**, 1848 (2010).
2. O.V. Sedelnikova, L.G. Bulusheva, A.V. Okotrub. *J. Chem. Phys.* **134**, 244707 (2011).
3. O.V. Sedelnikova, L.G. Bulusheva, A.V. Okotrub. *Full. Nanotubes Carbon Nanostr.* **20**, 558 (2012).

# New approaches to advanced organic and hybrid photopolymer for holography recording and diffraction optics fabrication

Vladimir Shelkovnikov

*N.N.Vorozhtzov's Novosibirsk Institute of Organic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 9, Novosibirsk, 630090, RUSSIA, vice@nioc.nsc.ru, +7(383)-3308867*

Photopolymer materials are being actively studied for practical applications such as 3D hybrid optoelectronic circuit plates, holographic storage, photoembossing including the manufacturing of refractive and diffractive optical elements, metrology, 3D displays, and direct laser write processes as preparation of photopolymer waveguides. One of the special application of the photopolymers is on holographic recording. The advantages of this material are wide possibilities to synthesize, high refractive index change and high sensitivity. For volume holograms recorded with thick materials, good optical quality and dimensional stability of the recording material are the most stringent requirements. The some problems of the photopolymer for holography and their salvations will be considered in the report.

The description of the photopolymerisation process from the chemical kinetics point of view will be done and the features of the continuous and pulse hologram recording regimes will be discriminated.

The task of finding of optimal initial optical density $D_0$ of absorbing holographic material with bleaching sensitive dye are studying theoretically and experimentally. The three holographic recording schemes are taking into account: transmitting hologram recording in following beams, reflecting hologram in counter beams, and reflecting mirror hologram recording. The optimal optical density is calculated by analysis of initial rate of photoinduced change of light wave phase $FM = \Delta n \cdot k d_{ef}$ (where $\Delta n$ – refractive index change, $d_{ef}$ – effective material thickness).

Recent holographic photopolymer materials studies have shown promising possibility of recording holograms using forbidden singlet-triplet transitions of the dye-sensitizer. Usage for holographic recording of these forbidden transitions has the advantage. The medium absorption contributes significantly less distortion in the refractive index modulation process during hologram formation in this recording mode as opposed to the conventional hologram recording. The theoretical approaches and features of the holographic recording in photopolymers by excitation of the forbidden singlet-triplet transitions of sensitizing dye are considered in the report.

The synthetic approaches to new two chemistry photoinitiators and to oxygen termination free photopolymers on the base of hybrid of siloxan-oxirane moeties oligomers and hybrid thiol-ene oligomers will be discussed.

# Holographic Photopolymer Material using by Forbidden Transitions of Xanthene Dyes

Evgeny Vasilyev

*N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry of the Siberian Branch of the Russian Academy of Science, Ave. Lavrentyev, 9, Novosibirsk, 630090, RUSSIA, vev@nioch.nsc.ru, +7(383)-3309642*

Optical information recording in volume media occurs by means of recording of the hologram the entire thickness of recording medium. A significant problem to obtain a uniform recording throughout the thickness of the medium is its absorption. Absorption of photopolymer is usually due to the absorption of the dye-sensitizer, which is a main photosensitive component. This leads to a non-uniform distribution of coherent recording radiation throughout the thickness of medium.

There is a contradiction between the desire to reduce the photopolymer layer absorption to ensure uniform recording radiation throughout thickness of the layer and the need to use the maximum possible concentration of dye-sensitizer for high sensitivity and large photoinduced refractive index changes. Thus, the absorption of the dye-sensitizer is the principal barrier to effective holographic recording the throughout layer thickness in volume medium.

One way of solving this problem is use for holographic recording forbidden singlet-triplet electronic transitions of the dye. It is known that in some organic molecules under excitation from the ground state occur forbidden singlet-triplet ($T_1 \leftarrow S_0$) transitions than those allowed by the multiplicity singlet-singlet ($S_1 \leftarrow S_0$) transitions. Extinction coefficients corresponding $T_1 \leftarrow S_0$ transitions are small (from $10^{-4}$ to 1 $mol^{-1}cm^{-1}$), and the transition frequencies are shifted to the red region relative to the ground singlet-singlet transition. For xanthene organic dyes such a shift is 100-150 nm relative allowed singlet-singlet transition in the visible region of the spectrum.

We have developed a new holographic photopolymer material for recording holograms using the forbidden singlet-triplet transitions dyes. This photopolymer material provides a level of diffraction efficiency about 50 % for transmission holograms, sensitivity no more than 300 $mJ/cm^2$ to radiation with a wavelength of 633 nm.

A number of xanthene dyes-sensitizers (eosin, 2,4,5-triiodfluorescein, erythrosine, 2,4,5-tribromthiofluorescein, thioeosin and thioerythrosine) were investigated. Thioerythrosin is the most effective sensitizer for free radical polymerization in the recording mode using of the forbidden $T_1 \leftarrow S_0$ transition dye.

The influence of used solvents (ethanol, dichloroethane, acetone, acetonitrile, water, chloroform and methylene chloride) on the efficiency of the holographic recording was investigated. Solution of thioerythrosine in acetone shown the highest luminescence. By replacing chloroform (previously used) to acetone photopolymer sensitivity was increased 3 times.

Optimal concentrations of the acceptor (iodonium salt ~ 0.1 mol/liter), and heterocyclic donor (about 0.14 mol/liter) were determined.

It was found out that the cross-linking monomer 1,4-bis(acryloyl)piperazine has a significant effect on the rate of hologram formation as well as make the polymer structure more "rigid". With increasing concentration of the 1,4-bis(acryloyl)piperazine decreases of the induction period of 7 s (at 0 mol/liter) to 3.5 s (at 0.54 mol/liter). Further increasing the concentration of cross-linking monomer is difficult due to its crystallization in the photopolymer drying process during preparation.

# Physico-chemical characteristics of photosensitive hybrid material for recording diffraction optical elements

Dmitry Derevianko

*N.N. Vorozhtsov Institute of Organic Chemistry of the Siberian Branch of Russian Academy of Science, pr. Lavrentieva 9, Novosibirsk, 630090, Russia, dmitrydereviankio@gmail.com, +7(383)-338850*

At present, the actual problem is the fabrication of diffraction optical elements. These elements are thin relief-phase structure and are widely used in optical storage system, displays, sensors, etc. To make them on a smooth surface is necessary to obtain the surface micro-relief with a continuous profile.

Nowadays, the widespread hybrid (inorganic-organic) materials, which were called organic modified silicate (ORMOSIL) or organic modified ceramics (ORMOCER). These materials combine the properties of their constituents, such as low processing temperatures, high optical transparency, refractive index, thermal stability and other properties of the material. Due to the wide variation in chemical structure that is possible for hybrid polymers, their properties can be adjusted in a wide range.

A hybrid photopolymer material for recording of the diffractional optical elements and was elaborated in the Laboratory of Organic Photosensitive Materials N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry SB RAS. The hybrid materials are synthesized by cohydrolysis in various proportions of thiobis[4,1-phenyleneoxy(2S)propane-3,1,2-triyl]tetrakisacrylate and product of condensation diphenylsilanediol and 3-mercaptopropyl-trimethoxysilan. In presence photoactivator the acrylate group of organic part of the hybrid materials polymerized when exposed to UV-light, by free radical mechanism, formed crosslinked polymer. The thiol groups that are presented in the linker compound protect from oxygen inhibition during photopolymerization.

The purposes of my research is studying photopolymerization and physico-chemical characteristics of the synthesized compounds, containing siloxane units, thiol and acrylate units with different ratios of siloxane and acrylate units and fabrication of photonics integrated circuits and diffractive optical elements on hybrid materials.

The exposure conditions of the composition were selected to get a solid relief of diffractive optical element copy. The curing compositions were studied using 1H NMR spectroscopy, mass spectrometry, ultraviolet spectrometry, refractometry. The curing process was monitored by IR spectroscopy. The degree of conversion of the cured film was determined by absorption of acrylat double bond. In average the degree of conversion is 80 percents. Also were studying thermomechanical properties of hybrid material, in depending on the qualitative and quantitative content of the original photopolymer compositions. Refractive index of curing hybrid material was measured, equal to n = 1.511.

The high aspect ratio pillars and microchannels were obtained on the hybrid materials by the exposure of X-ray synchrotron radiation at the LIGA-technology station in Institute of Nuclear Physics SB RAS.

# Study of photo desorption of rubidium atoms in hollow-core photonic band-gap fibers, generation and control quantum states of light using atomic vapours

Sergey Atutov

*Institute of Automation and Electrometryof the Siberian Branch of the Russian Academy of Sciences, Ave. Koptuga 1, Novosibirsk, 630090, RUSSIA, atutovsn@mail.ru +7(383)-3306869*

The atomic photodesorption process and atomic diffusion inside dielectrics are interesting fields of investigation as they give useful insights into both the knowledgeof atom-dielectric interactions and to important practical applications. They have been recently enriched by the recent and unexpected observation of a new effect consisting of a huge atomic desorption from transparent silane films when weak visible or UV light which illuminates the surface. The diffusion of atoms or molecules in a bulk within to a surface onto which the particles have been absorbed can also be involved in photo desorption process.

When the diffusion of the particles in the film bulk is important, the bulk of the coating together with the coating surface can act as a container for a large number of stored particles. If the adsorption energy of atoms or molecules to the surface is small, these particles can be desorbed by a weak light. Because of the photodesorption, the density of particles in a bulk within to the surface of polymer organic film is decreased to zero. This leads to a transportation of the particles from the inside of the coating towards the surface, where, finally, the desorption from the coating to the vapor phase is accomplished. The density of the photo desorbed atoms in the vacuum depends to the size and form of the cell where photodesorption is performed. The maximal peak density of the desorbed gas is attainable in a cylindrical cell with reflecting walls, with a pulse light source placed inside of the cell used. When a coherent desorbing light (which can be tightly focused on the end of glass cylindrical cell) is used, the diameter of the chosen cell can be extremely small. This fact opens up the possibility of the use of photodesorption for the generation of controlled high density gases in photonic-band-gap fibers. This is of significant interest in performing experiments on low-light-level optical nonlinearities.

Low-light-level optical nonlinearities are of significant interest for performing of generating and controlling quantum states of light using atomic vapors. For this optically thick an atomic ensemble, which is pushed to be transparent by a weak, resonant probe field has to be created, to perform experiments on electromagnetically induced transparency in which a coherent superposition of atomic states is created. This effect has been expanded to schemes that allow one to exploit two extremely weak fields, which in an extreme case, can consist of strongly interacted single photon light. This is perspective for quantum network applications.

To obtain strong nonlinearities from single photons, one can enhance the matter-photon interaction using strongly nonlinear dense alkali vapors confined a hollow-core photonic band-gap fiber. This kind of fibers filled by atoms provides a long interaction length while maintaining a small light mode area. Hollow-core photonic band-gap fiber filled by alkali atoms through effect of atomic photo desorption allow one to obtain very large optical depths and electromagnetically induced transparency with control light with much lower power than those used for hot vapor cells in a common focused beam geometry.

# Engineered photonic crystal fibre single photon sources

Dr Peter Mosley

*Department of Physics, University of Bath, Bath, BA2 7AY, U.K.*

Single photons and entangled photon pairs are a vital resource for optical implementations of quantum-enhanced technologies such as quantum cryptography and quantum computation. A variety of different techniques can be used to create photons individually or in pairs, but the most widely used are based on high-power pulsed lasers driving parametric interactions in nonlinear materials. Photonic crystal fibre (PCF) provides an ideal platform for the generation of photon pairs by four-wave mixing. Firstly I will explain how, by fabricating bespoke PCF with specific dispersion, we can engineer the properties of photon pairs produced as a laser pulse propagates along the fibre. Secondly I will discuss our current work to combine the outputs of several fibres in an actively multiplexed photonic network to create a PCF-based single-photon source beyond the current state-of-the-art in terms of generation rate and signal-to-noise ratio. This requires the integration of ultrafast photonics, high-speed switching, and electronics to build a system that can be interfaced with on-chip photonic quantum-information processing units.

# Lanthanide Complexes as Thermometric Contrast Reagents for MRI Diagnosing of Cancer and Control of Photo-dynamic Therapy

Sergey Babailov

*A.V.Nikolayev's Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 3, Novosibirsk, 630090, RUSSIA, babajlov@niic.nsc.ru, +7(383)-3308957*

Magnetic Resonance Imaging (MRI) is routinely used in the clinic to visualize the structure and function of organs. For several applications, including tumor and cardiovascular imaging in clinic and *in vivo* studies, an enhancement in contrast is an absolute requirement to improve the sensitivity and the diagnostic contents of the images. For this, several contrast agents (CAs) have been developed over the past years, most of which incorporates paramagnetic gadolinium ions ($Gd^{3+}$). Currently, complexes of the different lanthanides (Ln, other than Gd), remain largely unexplored as probes for nuclear magnetic resonance spectroscopy (NMR) and MRI.

Recent studies by us and others have demonstrated that MRI can be used as a tool for noninvasively assessing temperature changes in tissues associated with absorption of nonionizing radiation. As an example, we initially proposed the use of special NMR thermosensitive contrast reagents (NMR-TSCR) based on paramagnetic Ln complexes. This technique can diagnose conditions such as inflammatory reactions and cancer. The mechanism of action of NMR-TSCR is based on the substantial dependence lanthanide-induced shifts (LIS) in NMR spectra of the ligands studied complexes Ln. This new approach is characterized by: (a) Non-invasive in comparison with the known methods of temperature microprobe, (b) the possibility of the temperature determination on almost any depth from the surface of the body as opposed to, for example, the fluorescence-based diagnostics (FD) and infrared (IR) diagnostics; (c) compatibility directly with the photo-dynamic therapy (PDT), neutron and proton capture therapy. According to our evaluations, temperature determination error ($\Delta T$) is ~0.3 K and 3D resolution ($\Delta L$) is ~30 mkm.

The aim of this proposal is to apply Ln complexes for measurement of variations in the local tissue temperature and to investigate chemical processes mechanisms at PDT. The main objectives of the current project include: (a) molecular design of nanoscale paramagnetic NMR-TSR Ln complexes with a number of complexing agents; (b) development of the technique of *in vitro/in vivo* magnetic resonance thermometry; (c) development of the NMR technique of *in vitro/in vivo* investigation of chemical processes mechanisms at PDT; (d) development of the NMR technique of *in vitro/in vivo* control of temperature at influence of light radiation pulse related with PDT. Our preliminary data include (1) development of the method of the molecular structure determination of paramagnetic Ln complexes in solution according to the combined analysis of LIS and increase of the paramagnetic spin-lattice relaxation enhancement in the presence of conformational dynamics; (2) development of the methods for NMR investigation of reversible and irreversible photochemical processes; (3) development of the technique for the kinetic parameters determination of conformation of the intramolecular and intermolecular dynamics in paramagnetic Ln complexes based on the study the NMR signals lineshape (with temperature changes of LIS); (4) initial experimental with model paramagnetic Ln complexes on the possibility of addressing the interconnected challenges of determining molecular structure, dynamics and paramagnetic properties of organic and aqueous solvents.

# Bioanalytical platforms based on silicon micro- and nanochannel membranes

Nikolay Filippov, Maksim Parashchenko, Natalia Vandysheva, Sergei Romanov

*A.V.Rzhanov Institute of Semiconductor Physics of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 13, Novosibirsk, 630090, RUSSIA, filippov@isp.nsc.ru, +7(383)-3332519*

Modern medicine needs relatively small cheap and rapid diagnostic systems which enable analysis of biomaterial right here and right now, so called point-of-care testing devices. Bioanalytical platform based on silicon micro/nanochannel membranes can be used as such devices. It is microfluidic device consisted of three different parts: transporting, filtering and sensing (Fig. 1). Silicon channel membranes are used as a basis of each part of the device.

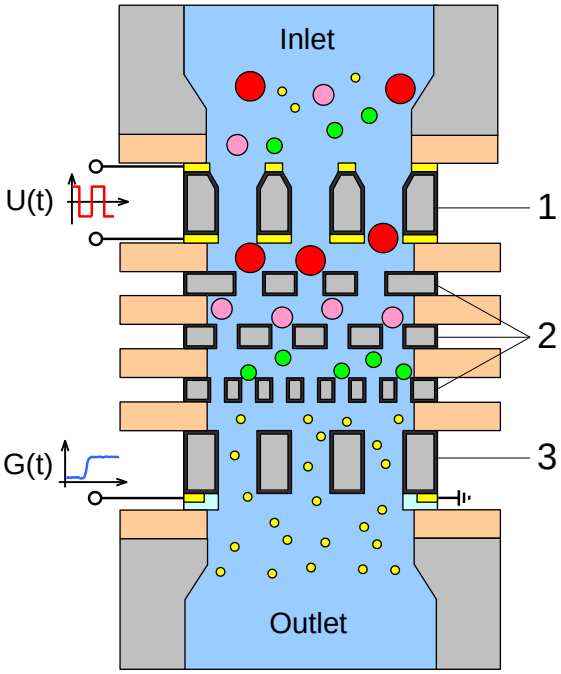


Fig. 1 Scheme of the device consisted of electroosmotic pump (1), set of filters (2) and chemical sensor (3)

The nano- and microchannel membranes made of biocompatible silicon by patented technology hold much promise for their integration with advanced electronic, optical, and biochemical devices. Conceptually the structure of obtained membranes comprises a monolithic connection of a nanochannel array with rigid supporting microchannel one and has an ordered profile of open through channels with diameter varying from nanometers to tens of micrometers. These membranes could be used as a basis structure for electroosmotic pump, filter or sensor fabrication with a slight modification of production technology and additional postprocessing operations. Combining all these three devices into a single one we obtain a complex platform for microfluidic analysis. Each part of the device performs its own function. Electroosmotic pump transports solution of interest through a set of filters to sensor. By means of the set of filters analyte can be purified and separated into fractions each of which can be transported further to be detected by the sensor. Coupled with needed electronics such device is intended for separation, concentration, and detection of nanoparticles, cells, polynucleotide and protein molecules, their conjugates and associates.

# Gas-jet deposition of thin fluoropolymerfilm withsilver nanoparticles possessing surface plasmon resonance

Alexey Safonov

*Kutateladze's Institute of Thermophysics of the Siberian Branch of the Russian Academy of Sciences, Ave. Lavrentyev, 1, Novosibirsk, 630090, RUSSIA, safonov@itp.nsc.ru, +7(383)-3356245*

In recent years, the methodsare developed to obtain the inexpensive solar cells. The decrease of cost is to usesolar cells based on thin-films of amorphous silicon. Relatively recently, for enhancing the absorption of light and thus improve the efficiency of solar cells of amorphous silicon thin-film has been proposed to use a coating having a surface plasmon resonance (SPR) [1]. Such coatings containing of metal nanoparticles and usually a dielectric matrix can increase the efficiently of the solar cell. The researches have shown that the intensity and width of the absorption of light essentially depend on: material, size, shape and concentration of nanoparticles in the coating [2]. Same an important role plays the matrix material surrounding the metal nanoparticle. In this work for this aim, we offer to use the silver nanoparticles deposition in the fluoropolymer matrix. The silver nanoparticles in the fluoropolymer matrix does not coagulate, their concentration can provide the conditions of full electrical isolation from each other.

The work is devoted to the method of vacuum gas-jet deposition on a surface of silicon the thin-films of fluoropolymer with silver nanoparticles having surface plasmon resonance (SPR). The main idea of the method consists in simultaneous deposition in vacuum on the rotating target composites from two high-speed gas jets [3].The first jet is precursor of fluoropolymer film matrix the second jet is argon carrier nanoparticles of metal. The method allows controlling the size and concentration of the silver nanoparticles in fluoropolymer matrix. Initially, the silver nanoparticles of different average size on the glass and silicon substrates were deposited. Further the composites of fluoropolymer matrix and silver nanoparticles different size was deposited.

The deposited samples were examined for the transmission of light in the visible frequency range. The measurements were made of the spectrograph DFS-485C.The morphology of the surfaces of obtained composite coatings was investigated by the method of scanning electron microscopy (SEM) with the aid of the electron microscope JEOL JSM-6700F.The obtained coatings of fluoropolymer film with silver nanoparticles possess the peak of SPR in the area of wavelengths 470-550 nm.

The results of the research might be of interest in the production of coatings for solar cells, sensors and other electronic devices.

The work was financially supported by the Russian Foundation for Basic Research (Grant 12-08-00441-a).

**Reference**

1. S. Pillai, K.R. Catchpole *et all*. Surface plasmon enhanced silicon solar cells. // *J. Appl. Phys.*, V. 101, P. 093105 - 8p, (2007).

2. S. Linic, P. Christopher, D. B. Ingram. Plasmonic-metal nanostructures for efficient conversion of solar to chemical energy. // *Nature Materials* **10**, P. 911–921, (2011).

3. A.K. Rebrov, A.I. Safonov, *et all*. Gas-jet synthesis of silver-polymer films // *Journal of Applied Mechanics and Technical Physics*, V.51, No. 4, pp. 598-603, (2010)

# Magnetic resonance in $CuCr_2S_4$ nanoclusters and nanocrystals

Tugarinov V.I.

*L.V. Kirensky Institute of Physics SB RAS, 660036, Krasnoyarsk, Russia*

Magnetic materials with critical dimensions on the order of nanometer scale display unique properties such as superparamagnetism, high field irreversibility, and high saturation field due to surface anisotropy contributions. Tailoring of the nanomaterial properties and applications is primarily dictated by their size and shape, which can often be controlled by the synthetic methodology. Among the chalcospinels, Cu- and Cr-based systems are unique in that they are ferromagnetic at room temperature with Curie temperatures (TC) of 377, 430, and 360 K for $CuCr_2S_4$, $CuCr_2Se_4$, $CuCr_2Te_4$, respectively. As concerned Cu-Cr-S system depending on the synthesis conditions one can obtain pure disulphide $CuCrS_2$, mixture of the $CuCrS_2$ and $CuCr_2S_4$ phases or pure $CuCr_2S_4$ spinel phase [1]. At that, for example, formation of the $CuCr_2S_4$ phase in bulk $CuCrS_2$ matrix also depends on the synthesis conditions. It may forms volume regions, thin plates or nanoparticles randomly distributed among $CuCrS_2$ matrix. It was shown [2] that by choosing a specific growing method it is possible to obtain a pure $CuCr_2S_4$ spinel phase in the form of nanocrystals or nanoclusters. In this paper we present the extension of the investigation of the resonance and magnetic properties of $CuCr_2S_4$nanoclusters and nanocrystals first reported in [2].

In the temperature range 77-370 K, the resonance spectra were collected with Brucker spectrometer Elexsys E580 operating at X- and Q-band ($\nu$ = 9.7 and 36 GHz respectively). With temperature lowering, the single line with almost Lorentzian form was observed for the nanocubes at all temperatures, while two resonance peaks can be seen at temperatures below 280 K for the nanoclusters spectra.

At low temperatures, the resonant properties of nanocluster and nanocubeswere studied in a wide frequency band with a magnetic spectrometer with pulse magnetic field [3]. The frequency-field and temperature dependencies of the magnetic resonance were investigated. For both nanocluster and nanocube samples, the dependencies are linear at both temperatures and gapless at T = 80 K. At T = 4.2 K, the energy gap of the resonance spectra $\nu_c \approx 7$ GHz for both samples.

1. G. Abramova, A. Pankrats, G. Petrakovskii et al. *Journal of Applied Physics*. 2010. **107**, No. 9, pp. 093914–+
2. K. Ramasamy, D. Mazumdar, Z. Zhou, Y. Wang, and A. Gupta. *J. Am. Chem.Soc.* 2011, **133**, 20716−20719.
3. V. Tugarinov, I. Makievskii, A. Pankrats, *Instruments and Experimental Techniques*, 2004, **47**, 4, 472-476

# Light propagation, amplification and generation in fiber waveguides with micro- and nanostructures

Sergey Babin

*Institute of Automation and Electrometry of the Siberian Branch of the Russian Academy of Sciences, Koptyug Ave., 3, Novosibirsk, 630090, RUSSIA, babin@iae.nsk.su, +7(383)-3306939*

A brief review of recent developments in studies of nonlinear interactions of light with micro- and nanostructures in fiber waveguides is given. Techniques of refractive index modification in the fiber core by CW ultraviolet and femtosecond infrared radiation are described. Obtained characteristics are measured. Various photonics devices based on in-fiber micro- and nanostructures formed by these techniques are presented including fiber Bragg gratings with phase shifts, periodically poled fibers, long period gratings, diffraction interferometers. Interaction of light with such periodic as well as with random structures is studied. As a result, new regimes of light propagation, amplification, generation and nonlinear conversion in all-fiber configurations have been obtained and explored, namely tunable single-frequency lasing, frequency self-scanning, parametric and second harmonics generation, random lasing, dissipative soliton generation and its Raman conversion. Potential applications of the obtained results for practical purposes are also discussed.

# Development of reflection interferometers for fiber optics

Terentyev Vadim

*Institute of Automation and Electrometry of the Siberian Branch of the Russian Academy of Sciences, Ave. Ak. Koptug, 1, Novosibirsk, 630090, RUSSIA,* terentyev@iae.nsk.su, *(383) 330-69-39.*

Modern fiber and diode lasers can have wide spectral range of generation (more than 100 nm). Fiber lasers used for interrogation sensor systems need to have wide wavelength and high frequency of tuning with narrow spectrum of generation. Fiber Bragg gratings and distributed feedback technique are often used to obtain single mode regime in fiber lasers. But the range and frequency tuning of such devices are limited because of slow mechanical stretching of silica fibers. For that purposes reflection multiple-beam interferometer (RI) with wavelength tuning range more than 100 nm and frequency more than 1kHz gives more benefits.

RIs can filter incident light in reflection. It is useful for laser intracavity mode selection applications and for cases when light detection in transmission is unavailable. RIs were widely applied in bulk optics for these purposes. In the report a development of RI for fiber optics will be considered.

One of the conventional variants of fiber RIs is a Fox-Smith interferometer, based on three mirrors cavity with one of the mirrors acting as an optics coupler. It has so called "transmission-like" response function in reflection. Well known fiber Fabry-Perot multiple-beam interferometer has the same response function, but only in transmission (Airy function).

Recently [1, 2] it was numerically and experimentally shown that it is possible to fabricate RI in single-mode fiber basing on simple two-mirror optical scheme. The fabrication technology is based on conventional thin film vacuum evaporation technique. Advantages and disadvantages of some RI designs will be discussed. New interferometer schemes and fabrication methods will be examined in order to improve characteristics of fiber RI.

1. V.S. Terent'ev. Numerical Simulation of a Reflective Diffraction Fiber Interferometer // *Optoelectronics, Instrumentation and Data Processing*, 2012, Vol. 48, No. 4, pp. 358–368

2. V.S. Terentiev, A.V. Dostovalov and V.A. Simonov. Reflection interferometers formed on the single-mode fiber tip // *Laser Physics*, v.23 (2013) 085108 (5pp)

# All-fibre Mode-locked fibre laser based on Carbon Nanomaterials and Fibre Gratings

Dr. Chengbo Mou

*Aston Institute of Photonic Technologies (AIPT), Aston University, Birmingham, UK, B4 7ET*

Mode locked fibre lasers are the next generation compact ultrafast light sources. All-fibre structure offers unique compact format in the real applications. Various approaches have been developed to achieve the all-fibre structure. Novel nanomaterials enabled ultrashort pulse generation have attracted a significant attention in the last decade. We have recently studied the polarisation dynamics for the first time using carbon nanotube mode locked fibre laser. Various polarisation patterns have been observed. Furthermore, we studied nanotube mode locked fibre laser based on in-fibre microfluidic devices. Over the past few decades, fibre gratings have been studied majorly for telecom, sensing applications. At AIPT, we have recently explored the unique tilted fibre grating structure in laser mode locking which facilitate all-fibre ultrafast lasers.

# Advancements in mode-locked fibre lasers and fibre super continua

Edmund J. R. Kelleher

*Royal Academy of Engineering Research Fellow, Imperial College London, UK,*
*edmund.kelleher08@imperial.ac.uk*

# Polarization attractors in mode-locked fiber lasers with carbon nanotubes saturable absorber

Tatiana Habruseva

*Institute of Photonic Technologies, Aston University, Aston Triangle, B4 7ET, Birmingham, UK*

Harmonic mode-locked fiber lasers based on carbon nanotubes (CNTs) saturable absorber are stable sources of sub-picosecond pulses at high repetition rates, which can be used in optical communications, metrology, optical sampling or sensing applications. When compared to active mode-locking techniques, passive mode-locking has reduced complexity and a potential to obtain shorter optical pulses at high repetition rates. The polarization insensitivity of CNTs based saturable absorber extends the possibility of studying polarization dynamics in mode-locked fiber lasers. Polarization dynamics in MLFLs is important to reveal the pulse train stability, which is vital for fiber optic communications and all-optical cock recovery.

We study polarization dynamics in the erbium-doped mode-locked laser for fundamental and harmonic mode-locking and multi-pulse operation. We report new types of vector solitons with locked, switched and precessing states of polarization. The results have potential applications for increased capacity in coherent communications using various polarization-based modulation schemes, such as polarization division multiplexing, polarization switching, and modified coded hybrid subcarrier-amplitude-phase-polarization multiplexing.

# Prediction of hydration free energies using reference interaction site model

Maksim Misin, David Palmer, Maxim Fedorov

*Corresponding author email: david.palmer@strath.ac.uk*

We have recently developed a new method for accurate prediction of hydration free energy based on the 3D Reference Interaction Site Model (3DRISM) [1]. The proposed methodology allows for quick prediction of hydration free energy of organic molecules with root mean square error of 1.5 kcal/mol: a result comparable to the best existing models [2]. On this poster we analyse the strengths and weaknesses of the new model, compare it to existing methodologies and explore its additional applications.

1. S. Palmer, A.I. Frolov, E.L. Ratkova, and M.V. Fedorov. Towards a universal method to calculate hydration free energies: a 3D reference interaction site model with partial molar volume correction. *J. Phys. Condens. Matter*, **22**, No. 49, p. 492101, Nov. 2010.
2. M.T. Geballe and J.P. Guthrie. The SAMPL3 blind prediction challenge: transfer energy overview. *J. Comput. Aided Mol. Des.*, **26**, No. 5, pp. 489–496, May 2012.

# New light emitting inorganic cluster complexes for imaging and electronics

Dr Olga Efremova

*Aston University*

Octahedral rhenium and molybdenum metal cluster complexes have recently attracted interest of researchers due to their excellent potential as materials for many light emitting applications. This is due to the strong phosphorescence of these inorganic species in the red and also in the near infrared regions. Along with the high photoluminescence quantum yields and microsecond(s) long excited state life times these complexes also possess the capability for reversible oxidation and have tremendous chemical stability. Collectively, such properties make them attractive for exploiting in biological (bioimaging, cancer treatment via singlet oxygen generation) and materials-based applications (light-emitting devices and solar cells). The most advantageous way to exploit the properties of octahedral cluster complexes is to embed them into an appropriate bespoke organic polymer matrix to target a desired application. Recent advances made in our laboratories include the development of polystyrene microspheres doped with a novel highly photoluminescent molybdenum cluster; irreversible doping of conventional linear polymers with rhenium clusters to obtain readily processable, photoluminescent polymers; characterisation of the electroluminescent properties of rhenium cluster complexes and their hybrids with organic polymers, which has led to the realisation of the first organic light-emitting diodes (OLED) based on rhenium cluster complexes.

## Molecular modelling, nanomaterials dispersion

Sean O'Connor

*sean.o-connor.2013@uni.strath.ac.uk*