Advanced Nanomaterials and Methods-ANAM2019
International Workshop and Young Scientist School
September 25 to October 2, 2019, Yerevan, Armenia

ABSTRACT BOOK
Advanced Nanomaterials and Methods-ANAM 2019
International Workshop and Young Scientist School
September 25 to October 2, 2019, Yerevan, Armenia

ABSTRACT BOOK
## Contents

ANAM2019 SCHOOL ABSTRACTS.................................................................5  
Laser induced white emission in RE doped nanocrystals.........................7  
Advanced Accelerator Driven Research in Armenia..................................8  
Advanced In-Operando Synchrotron-Based Tools for Studies of Microstructure, Thermal Transitions & Mechanical Behavior of Polymers..9  
Advanced Physics Simulations for Ni Containing Materials of Low Dimensional Systems and Clusters.................................................................11  
Optical spectroscopy of a single nano-object ........................................12  
Ultrafast acoustics and thermal responses of metallic nano-objects............13  
X-ray diffraction imaging of strain and defects in electronic materials and devices: State of the art and future trends.................................14  
High-Resolution X-ray Diffraction methods for evaluation of modern nanostructures .........................................................................................16  
The physics of viruses ................................................................................17  
Nano-/microswimmers in shear flow: from Rheo- to magnetotaxis.............17  
Nanoparticles as multifunctional systems: from synthesis to applications ..18  
Polyelectrolytes From Soft Matter Nanotechnology to Nanomedicine ......20  
ANAM2019 WORKSHOP INVITED TALKS....................................................23  
Laser stimulated white lighting of graphene..............................................25  
The amorphous-crystal transition in GeTe nanostructures: new insights from in situ synchrotron radiation measurements ......................................26  
Monitoring Crystallization and Melting with Millisecond Time Resolution: In-situ Combination of Micro-Focus X-ray Scattering and Ultra-Fast Scanning Chip Calorimetry........................................................................27  
Non-coplanar High-Resolution X-ray Diffraction to study novel materials 28  
Biological fate of Engineered Nanomaterials: tracing aggregation/degradation and nanomaterial dose in vitro and in vivo ............30  
Functionalized Noble Metal Nanoparticles: Advanced Materials for Optoelectronics and Nanomedicine Applications.................................32  
Ultrathin organic field effect transistors: from materials to devices and their applications.....................................................................................34  
Electrostatic stability of virus-like nanoparticles: Roles of metallic core and multivalent solution ions.................................................................36
Self-assemblying Systems Based on Pseudo-Proteins .......................................................... 37
A Library of Cationic Polymers as Gene Transfection Agents ........................................... 38
Stretchable and Deformable Materials and Devices for Human Machine Interface ......................... 39
ANAM2019 WORKSHOP ORAL AND POSTER CONTRIBUTIONS ........................................ 41
Fröhlich polaron formation in graphene on polar substrate ........................................... 43
X-ray dynamical diffraction Talbot effect under the condition of two-wave dynamical diffraction in crystals ................................................................. 45
The influence of electron-polar optical phonon coupling on the impurity-related optical properties in nanowire under magnetic field .................................................. 46
Multiparametric toxic gas detection with a single Langmuir-Schaefer monolayer field-effect transistor ........................................................................................................... 47
The influence of AgTOEPyP porphyrin on the stability and conformation of i-motif structure of DNA .......................................................................................................................... 50
Seeking Maxwell’s Demon in a nonreciprocal quantum ring ........................................... 52
Spongy cubic phases built through self-assembly of wedge-shaped amphiphilic mesogens ................................................................................................................................. 54
Fine structure of DMC for helix-coil transition in heterogeneous biopolymers ............................................................................................................................................... 55
Short-range disorder and electrostatic interactions in macromolecule ............................................. 57
Hard X-Ray Fourier Transform Holography Based on Two-Block Fresnel Zone Plate Interferometer with Common Optical Axis ...................................................................... 57
Investigation of Antibacterial Properties of Green Synthesized Silver Nanoparticles ............................................................................................................................................... 59
Variational calculation of impurity states in gapped graphene systems ........................................... 61
Wurtzite-nitride quantum wires under electric and magnetic fields: Polaron basic parameters ................................................................................................................................. 62
X-ray LLL interferometer with wedge-shaped mirror plate ........................................... 64
Investigation of sensory properties of organic field-effect transistors based on semiconductor-receptor Langmuir- Schaefer layers ............................................................................ 64
The features of complex formation of poly[d(A-C)]. poly[d(G-T)] with porphyrins ............................................................................................................................................... 66
Elastoplastic deformation in nanophysics ................................................................................... 67
Helix-coil transition in heterogeneous biopolymers. The GMPC ........................................... 69
Linearization of output characteristics of gas sensors based on MWCNT/SnO₂ structures ............................................................................................................................................... 70
Distortion Suppression Algorithm of Image Reconstruction in Hard X-Ray Fourier-Transform Holography Based on Two-Block Fresnel Zone Plate Interferometer with Common Optical Axis........................................72
Peculiarity of X-ray Phase Contrast at Diffraction Focusing of a Spherical Wave in a Superlattice.........................................................................................................................73
Complex Phase Transitions of Oligomer Thin Films........................................75
Influence of ZnO nanoparticles in the stability and conductivity of BLM depending on its composition..............................................................................................................................77
X-ray double refraction through nematic liquid crystals under influence of an external electric field..............................................................................................................................78
Solid-state properties of Poly(C3) polymers with closely-packed flourinated side chains .............................................................................................................................81
Investigation of drag force experienced by a moving object in granular medium...............................................................................................................................83
Comparison of methylene blue interaction with human serum albumin and DNA...............................................................................................................................85
The effect of the molecular mass of PEG on the nature of its interaction with DNA...............................................................................................................................86
Obtaining and fields of application of diamond-like carbon thin layers.....88
Zinc oxide composites in the antitumor and antibacterial drug delivery system...............................................................................................................................90
Peculiarities of the interaction of different ligands with nucleic acids ....92
Interminiband absorption in a quantum ring superlattice in transverse magnetic field.............................................................................................................................93
Morphology and optical characterization of physical vapor depositied PbI₂ films...............................................................................................................................95
Peculiarities of melting DNA from Crocker's sarcoma of a mouse treated with Ag-meso-tetra(4-N-hydroxyethylpyridyl) porphyrin in the presence of Mn²⁺ ions.............................................................................................................................97
Synthetic Analogues of Proteins – Biodegradable Polymers for Numerous Biomedical Applications..................................................................................................................98
Application of nanocalorimetry for analysis of phase behavior of azido-acetylene microparticles..................................................................................................................99
Preface

On behalf of the organizing committee, it is our pleasure to welcome you to the ANAM 2019 International Young Scientist School and Workshop in Yerevan, Armenia. The ANAM 2019 events aim to bring together leading scientists and researchers from different fields of nanostructured materials and nanocomposites as well as their characterization methods on the various scales, to create new scientific links in this novel and fast developing field in Armenia and the neighbor countries of the region.

We expect that with a strong contribution of the international experts and leading scientists, the ANAM 2019 will serve as a platform for networking and initiation of joint research projects and could help to facilitate development of young scientists and influence on a choice of the future research.

We would like to acknowledge of support received from the Volkswagen Foundation, University of Siegen, Yerevan State University and Armenian Scientific Union.

On behalf of the organizing committee,

Souren Grigorian

Chair of the ANAM2019
Laser induced white emission in RE doped nanocrystals

W. Strek, R. Tomala, M. Stefański, B. Cichy

Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland

The Stokes and anti-Stokes emission spectra of RE doped nanocrystals were investigated under irradiation with focused beam of CW laser diodes. It was found that apart of f-f transitions there appeared the intense broadband white emission the intense broadband white emission under high density excitation in IR as well as UV range. The intensity of broadband white emission was characterized by excitation density threshold. It increased exponentially with excitation power. It was observed decreasing of f-f transitions with simultaneous increasing broad band white emission. In particular the effect of excitation density and concentration of RE$^{3+}$ ions were investigated. In particular the efficient photocurrent co-occurs with appearance of white emission was investigated. It increased exponentially with excitation power density. The mechanism of white light emission is discussed in terms of intervalence charge transfer (IVCT) within the (RE$^{2+}$,RE$^{3+}$) ion pair. The possibilities of application of white light emission for optoelectronic devices are presented. The illustration of emission spectra from Yb$^{3+}$ ions in Yb$_3$Al$_5$O$_{12}$ nanocrystalline powders is shown in Fig. 1.
Fig. 1. The anti-Stokes white emission of YbAG nanocrystalline ceramic in vacuum - a; emission spectrum measured with 976nm excitation line - b; and the power dependence of emission intensity.


Advanced Accelerator Driven Research in Armenia

V. M. Tsakanov
CANDLE Synchrotron Research Institute, 0040 Yerevan, Armenia

Accelerator driven research in Armenia dates back to the early 1960s when one of the largest electron accelerators in the world at that time - the 6 Giga-electron-Volt energy electron accelerator ARUS - was built. Nowadays, a decisive role in frontier research in the fields of life and material sciences play advanced accelerator based light
sources, that enabling the deep investigation of the matter at the cell, molecular and atomic levels. To promote an advanced accelerator driven research in Armenia, a third generation CANDLE synchrotron light facility project has been developed in Armenia, the first phase of which, a laser driven AREAL electron linear accelerator has been constructed. In this report, the basics of synchrotron light facilities, experimental technique and the fields of applications will be presented along with the CANDLE project design considerations. In addition, the review of the physical bases of AREAL facility and the experimental program in the fields of ultrafast sciences will be outlined.

Figure: AREAL electron beam profiles at experimental stations.

Advanced In-Operando Synchrotron-Based Tools for Studies of Microstructure, Thermal Transitions and Mechanical Behavior of Polymers

Dimitri A. Ivanov
Institut de Sciences des Matériaux de Mulhouse - IS2M, CNRS
UMR7361, 15 Jean Starcky,
68057 Mulhouse, France
Email: dimitri.ivanov@uha.fr

The design of new polymer materials often requires a detailed knowledge of their structure and physical properties such as phase transitions (e.g., melting-reorganization) and mechanical behavior (e.g., mechanisms of deformation and rupture). In the present talk, we will dwell on the development of in-operando synchrotron-based
techniques allowing to perform:
1) Simultaneous structural and mechanical experiments with 
   resolution of the X-ray setup extending into the micrometer 
   range;
2) High-resolution scanning with nanofocused X-ray beams with the 
   beam footprint in the submicron range;
3) Combination of fast scanning chip calorimetry (FSC) with fast 
   X-ray scattering employing single-photon-counting last-
   generation detectors. The setup allows performing continuous 
   synchronous acquisition of the thermal and 2D X-ray data with 
   time exposure on the order of one millisecond.

The first topic will be exemplified for the case of newly developed 
super-soft and hyperelastic elastomers, in which the side chains 
grafted onto network strands act as both entanglement diluents and 
mechanical property regulators.[1] Precise and independent tuning of 
side-chain degree of polymerization and grafting density yields 
materials with Young’s moduli down to ~10^2 Pa and elongation-at-
break up to 10.[2] These physically crosslinked bottlebrush networks 
replicate the modulus of polymeric gels and biological tissues and 
recreate tissue’s extreme strain-stiffening behavior.[2-3]

The second and third topics will be illustrated for studies of thermal 
behavior of commodity semicrystalline polymers. In particular, the 
setup [4] allowed monitoring the early stages of crystallization of 
HDPE in order to evaluate the morphology and exact supercooling at 
the crystal growth front. To this end, the lattice parameters of the 
crystals, which are younger than 5 milliseconds were measured 
during fast cooling ramps at heating rates faster than 1000 K/s. The 
use of such rates allows bypassing the recrystallization processes on 
heating and cooling and facilitates in-depth analysis of the thermal 
behavior. By using heating and cooling rates much higher than the 
rates of recrystallization, the structural transformation corresponding 
to each of the observed thermal events can be extracted from X-ray 
data analyzed in detail.

My talk will be devoted to magnetization plateaus, magnetic susceptibility, specific heat and thermal entanglement for antiferromagnetic and ferromagnetic exchanges at low dimensional spin systems and clusters for Ni containing materials. The first part of my representation will be devoted to the spin-$\frac{1}{2}$ the Ising-Heisenberg model on connecting for measuring of $[\text{Ni}_3(\text{fum})_2(\mu_3-\text{OH})_2(\text{H}_2\text{O}_4)]_n \cdot (2\text{H}_2\text{O})_n$ as homometallic molecular ferrimagnet on a diamond chain. We demonstrate the existence magnetization plateaus, susceptibility and thermal negativity at low temperatures. By exact solution using the transfer matrix method, we show that the magnetization manifestation three plateaus at zero, mid, and $3/4$. We also present the appearance of super-stable cycles in the dynamical technique at $T \to 0$. The second part is devoted to Ni containing polymer $[\text{Ni} (\text{NN’-dmen})(\mu-\text{N}^\prime \text{ )}]_n$. We have calculated the magnetic susceptibility in zero magnetic field versus the temperature showing a peak around $T = 12.6 \text{ K}$, which is compatible with the experimental results by parallel computing (Wolfram Mathematica Language) in two pure Heisenberg blocks. We theoretically study for that polymer the behavior of magnetization plateaus, magnetic susceptibility, specific heat and thermal negativity using the transfer matrix method at low temperatures. The last part of my talk is researching of magnetic and thermodynamic properties of the high nuclearity (octanuclear $[\text{Ni}_8(\mu_3^2-\text{OH})_4(\text{OMe})_2(\text{O}_3\text{PR})_2(\text{O}_2\text{Bu})_6(\text{HO}_2\text{Bu})_8]$ and dodecanuclear $[\text{Ni}_{12}(\mu_3^3-\text{OH})(\text{HCO})_4(\text{O}_3\text{PR})_2(\text{O}_2\text{Bu})_6(\text{HO}_2\text{Bu})_6]$ nickel phosphonate-based cages (clusters). Firstly, using full exact diagonalization (ED) and quantum Monte Carlo simulations, we verify the model without anisotropic terms in order to compare our results with that of the original experimental data expressed. We
consider nickel phosphonate-based cages with Heisenberg exchanges anisotropy between interacted nickel atoms, besides uniaxial single-ion anisotropy property. We examine effects of the both anisotropy parameters on the magnetization process also the specific heat of the model and Schottky-type peaks of the specific heat. The magnetization plateaus are strongly dependent on the exchange anisotropy, as well as, single-ion anisotropy parameters.

**Optical spectroscopy of a single nano-object**

*Fabrice Vallée*

FemtoNanoOptics group, Institut Lumière Matière (iLM), Université de Lyon, CNRS – Université Lyon 1
43 Bd du 11 novembre, 69622 Villeurbanne cedex, France  
[fabrice.vallee@univ-lyon1.fr](mailto:fabrice.vallee@univ-lyon1.fr)

The strong modification with size reduction of the optical response of metal nanoparticles has led to considerable interest in the academic and industrial domains. The most conspicuous feature is the appearance of a confinement induced resonance, the surface plasmon resonance (SPR), whose spectral properties (wavelength, width, absorption and scattering cross-sections) reflect the characteristics of the particles (composition, size, shape) and of their environment. These dependencies, which will be discussed in the introduction of this talk, have been extensively exploited to design new optical materials or to create nanosensors, opening the fields of nanophotonics and plasmonics.

These optical features also constitute efficient tools to investigate the impact of size reduction on the fundamental properties of nanoparticles. However, because of the very weak optical response of a single nanoparticle, most investigations have been performed by simultaneously probing a large number of particles. Due to the unavoidable particle to particle fluctuations of the geometry and environment, only a mean response is obtained, masking the details of the individual particle behavior. These limitations can be overcome by investigating a single nanoparticle, which requires development of very high sensitivity optical detection schemes. After recalling the principles of the recently developed
methods permitting to detect light scattering or absorption by a single particle, we will focus on a far-field optical technique, the spatial modulation spectroscopy. This permits quantitative measurements of the extinction cross-section of the particle under study and precise comparison with the theoretical models when its morphology is independently determined, for instance, by electron microscopy. It opens the way to determination of intrinsic processes in nanoparticles, such as the role of quantum effect on the SPR bandwidth, and to the study of particle – surface interactions. Extension of these investigations to the nonlinear optical response of a metal nanoparticle will also be discussed.

**Ultrafast acoustics and thermal responses of metallic nano-objects**

*Natalia Del Fatti*

*FemtoNanoOptics group, Institut Lumière Matière (iLM), Université de Lyon, CNRS – Université Lyon 1*

43 Bd du 11 novembre, 69622 Villeurbanne cedex, France

natalia.del-fatti@univ-lyon1.fr

Controlling and modeling the mechanical and thermal response of nano-scale systems raise fundamental questions, which are also of central interest for many technological issues. In this size range, breaking of translational invariance leads to appearance of discrete vibrational acoustic modes of a nano-object. Investigation of their frequencies over sizes ranging from few thousand of atoms to few atoms raises the question of the limit of their description in terms of continuum elastic theory. It also yields new ways for characterizing nano-materials. Understanding of their mechanical damping is even more challenging, as this is largely dominated by energy transfer from the nano-objects to their environment for deposited or embedded ones. This mechanism, also ruling thermal
energy transfer, is thus highly sensitive to the nano-object – environment interface and the nature of the mode.

In this context, femtosecond nonlinear optical techniques are key tools to analyze the acoustic and thermal responses of metal nanoparticles. These measurements are based on driving out-of-equilibrium the electron distribution of a metal nanoparticle by a pump-pulse, the induced transient change of its extinction cross-section being subsequently monitored by a time-delayed probe-pulse. In this talk, after introducing the main concepts for description of the acoustics and thermics of nano-objects, we will present experimental results obtained with time-resolved pump-probe spectroscopy and their application to the investigation of the ultrafast acoustic and thermal relaxation, on both ensembles of metal nanoparticles and at single nano-object level.

**X-ray diffraction imaging of strain and defects in electronic materials and devices: State of the art and future trends**

*Olivier Thomas*

*Aix Marseille Univ, Université de Toulon, CNRS, IM2NP, Marseille, France*

In present synchrotron radiation facilities, the trend towards fast on-the-fly experiments [1,2], made possible in particular thanks to faster low noise hybrid pixel area detectors, opens many avenues for *in situ* evaluation of structure, strain and defects in various nano-materials. Pole figure measurements can now be performed fast enough to follow intriguing texture changes during phase transformations [3]. Combination of curvature measurements with x-ray diffraction allows for a detailed understanding of strain evolution during crystallization of phase change materials [4]. Thanks to focused beams strain mapping in devices can be performed *in situ* as a function of temperature [5]. I will also show how small x-ray beams may be used for investigating the mechanical behavior of nano-
objects *in situ* during mechanical testing [6,7]. Last but not least Bragg Coherent Diffraction Imaging (BCDI), which relies on the combination of coherent illumination and phase-retrieval algorithms is becoming a mature strain and defect 3D imaging method with exquisite atomic displacement sensitivity [8]. It holds great promises for *in situ* and *operando* imaging of strain and defects during various processes (nanoindentation, catalysis …) [9,10].

All these recent evolutions will benefit a lot from the development of new and even more brilliant sources which will appear in the coming years.

**Acknowledgments**

This work is funded by ANR through ANR-15-CE24-0021 SESAME and ANR-11-BS10-01401 MecaniX projects.

High-Resolution X-ray Diffraction methods for evaluation of modern nanostructures

A. Ulyanenkov

Atomicus LLC, Seattle, WA, USA

X-rays have been proven to be a powerful and reliable tool in studying a large diversity of micro- and nanoscale objects. The wavelength of X-rays is a perfect fit to the typical sizes of basic structures used in all modern technologies and science: crystallographic lattice in semiconductor thin films; biological molecules in protein crystallography; nanoscale objects like quantum dots and quantum wires in optoelectronics; and many others. This fact initiated the intensive development of various measurement techniques and instrumentation to satisfy the large variety of requirements coming from scientific and industrial communities. There are multiple X-ray techniques used for sample evaluation, each of which is suitable for different kinds of the structures. For example, X-ray Bragg diffraction probes samples possessing a crystallographic structure and characterizes the structure on a broad scale, from micro-crystallites in polycrystalline materials to the properties of coherent epitaxial samples averaged over large areas. For the latter case of epitaxial structures, X-ray diffraction in a high-resolution mode is used. The information obtained from X-ray diffraction patterns reconstructs the sample morphology, helps in structure determination and phase identification, and may comprise such parameters as crystallinity, mosaicity, crystallographic lattice mismatch, lattice strain status, residual stresses, lattice defects, and many others.

Viruses are quintessential nanoparticles. Their proteinaceous shells are highly charged and electrostatic interactions are important for viral assembly and stability. I will describe several models of the effects of electrostatic interactions on viruses. Starting from an analysis of charge distribution and charge regulation by the bathing ionic solution, I will explore in detail several examples of the role of charge-charge interactions for capsid stability as well as the interactions between the capsid proteins and the compactified genetic cargo such as the encapsidated RNA and DNA molecules.

Nano-/microswimmers in shear flow: from Rheo- to magnetotaxis

Ali Naji

1 School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

In this talk, I will first give a broad introduction to the newly emerged and interdisciplinary field of active matter and will then briefly discuss some of the current research problems pursued on the subject in my group. Active-matter systems often comprise self-propelled (‘active’) particles that can move without the aid of external fields and by utilizing internal mechanisms to take up ambient free energy and turn it into self-propelled motion. Examples range from catalytic Janus nano-/microparticles to motile bacteria
(such as E. coli) and sperm cells. These particles often ‘swim’ in fluid media and their motion can be influenced by externally imposed shear as well as other external fields/stimuli to which the swimmer may respond by passive or active reorientation; the latter include external magnetic fields in the case of synthetic magnetic and magnetotactic bacteria, gravitational field in the case of gyrotactic microorganisms, and chemical gradients in the case of chemotactic bacteria and sperm cells. Our interests are primarily centered around computational modeling of such swimmers in confined geometries, such as cavities and narrow fluid channels. In the latter case, we have shown that a host of intriguing effects, such as population splitting, orientational pinning, net upstream swimmer flux, reverse cross-stream migration, and particle focusing can arise in the system, as a result of, e.g., the competitive interplay between the shear and external field and/or wall-induced hydrodynamic interactions. These effects can have important implications for particle separation strategies in nano-/microfluidic applications.

**Nanoparticles as multifunctional systems: from synthesis to applications**

_Ilaria Fratoddi_

*Department of Chemistry, Sapienza University of Rome, Italy*

In recent decades, nanomaterials play important roles in interdisciplinary areas that encompass (bio)chemistry, physics, biology, materials science, electrical engineering and more. Among others, Noble Metal Nanoparticles (MNPs) and Polymeric Nanoparticles (PNPs) show intrinsic properties mainly determined by their size, shape, composition, crystallinity, and structure. In principle, the control of any one of these parameters is possible to fine-tune the properties of nanoparticles. What makes nanostructures unique is that the features of the materials become strongly dependent on the surface and the laws of physics operate in an unfamiliar way. Advances in nanoscience and nanotechnology
critically depend on the development of nanostructures whose properties are controlled during synthesis [1].

In this work, we will focus on this critical concept using functionalized MNPs and PNPs, as representative examples (see figure 1). In fact, they provide the capability, through design and rational synthesis, to realize unprecedented structural and functional complexity. In particular, the bottom-up synthetic approach applied to MNPs and PNPs will be described. Briefly, functionalized MNPs (AuNPs, AgNPs, PtNPs) can be obtained by a versatile wet synthesis path comprised of sequential reduction, nucleation and growth with mono- and bi-functional hydrophilic and hydrophobic thiols as capping agents [2,3]. Polymeric nanoparticles can be easily obtained with emulsion polymerization technique starting from vinyl monomers such as MMA (methyl methacrylate) and derivatives [4]. Surface ligand molecules enabling nanoparticles to disperse in both polar/nonpolar solvents, making them a versatile tool that can be adapted to the aqueous environment as well as to hydrophobic ones. The spectroscopic and structural characterizations will be discussed. Surface techniques, morphology studies and electrical measurements are also important to completely define morphological and structural characteristics and enhance fascinating phenomena associated with nano-sized 3D structures. To leverage the reactive and tunable properties of nanomaterials, conjugation with foreign molecules such as dyes and drugs will be described. The characterization results prove that MNPs and PNPs are promising multi-functional systems, in which it is possible to combine electrical/photoelectrical and surface plasmon resonance properties (LSPR) with biological activity. Optoelectonics and nanomedicine applicative examples will be discussed.
**Figure 1**: Schematic representation of PNPs and MNPs and their surface functionalization


**Polyelectrolytes From Soft Matter Nanotechnology to Nanomedicine**

*Sergio E. Moya*

1. *CIC biomaGUNE, Paseo Miramón 182 C, 20014 San Sebastian, Spain*

Polyelectrolytes, polymers with repetitive charged units, can be considered as ideal building blocks for nanofabrication as they have a size in the nano range; they are easy to assemble, synthesize or even pattern on almost any surface; and have a responsive behaviour, changing conformation and size in response to changes in the environment such as variations in ionic strength or pH.

We have explored the use of polyelectrolytes in nanofabrication and as part of hybrid materials for the development of surface coatings, and the engineering and fabrication of nanoparticles, with a focus on biomedical applications. Work performed in the last years in our
group on polyelectrolyte multilayers, polymer brushes and other supramolecular assemblies will be reviewed. The presentation will cover different aspects of our work, such as the engineering of colloidal particles with polyelectrolytes, lipids and virus like nanoparticles for sensor fabrication; the use of polyelectrolyte multilayers for controlling cell adhesion, the fabrication of supramolecular phosphate polyamine assemblies for the delivery of silencing RNA, antibacterial coatings, etc.

**Figure 1:** Scheme of the cell uptake and degradation of polyamine/phosphate nanoparticles carrying siRNAs
ANAM2019
WORKSHOP INVITED TALKS
Laser stimulated white lighting of graphene

W. Strek, R. Tomala, B. Cichy, P. Wiewiórski
Institute of Low Temperature and Structure Research,
Polish Academy of Sciences, Wroclaw, Poland

The intense broad band of light emission in visible range were reported for graphene foam [1] ceramics [2] in vacuum upon irradiation with cw infrared laser diode. It was strongly dependent on excitation laser density. The lighting is accompanied by efficient photocurrent and electron emissions. The laser induced white light emission is the nonlinear process characterized by threshold behavior, exponentially scaled by the excitation power density. The order of scaling decreases with excitation density. The white lighting was investigated for different excitation wavelengths. It was found the lighting threshold decreased with decreasing excitation wavelength. The effect of applied voltage on intensity of white lighting was investigated. The light intensity may be tuned with applied voltage. The lighting is accompanied by efficient photocurrent and electron emissions. Applications of LIWE of graphene foam for sustained white lighting sources are presented. Moreover quite recently was observed that apart of broad band white emission earlier reported by us there appears the broad band emission in near infrared centred around 2100 nm.

![Image](image_url)

**Figure 1.** The visible and near infrared emission of graphene foam excited by 975 nm laser diode with high excitation density.

The amorphous-crystal transition in GeTe nanostructures: new insights from in situ synchrotron radiation measurements

M. Gallard$^{1,2}$, M. Amaral$^1$, C. Mocuta$^2$, N. Burle$^1$, M. Putero$^1$, S. Escoubas$^1$, C. Guichet$^1$, M.-I. Richard$^{1,3}$, L. Fellouh$^4$, M. Bernard$^4$, R. Chahine$^4$, P. Kowalczyk$^4$, C. Sabbione$^4$, A. André$^4$, N. Bernier$^4$, P. Noé$^4$ and O. Thomas$^1$

$^1$ Aix-Marseille Université, CNRS, IM2NP UMR 7334, Campus de St-Jérôme, 13397 Marseille, France
$^2$ Synchrotron SOLEIL, l’Orme des Merisiers, Saint-Aubin–BP 48, 91192 Gif-sur-Yvette, France
$^3$ ID01/ESRF, The European Synchrotron, 71 rue des Martyrs, 38043 Grenoble, France
$^4$ Université Grenoble Alpes, CEA-LETI, MINATEC campus, 17 rue des Martyrs, 38054 Grenoble, France

Phase-change (PC) memories are now considered to be the most promising technology among emerging non-volatile resistive memories to replace the current Flash memories or to achieve innovative Storage Class Memory. Chalcogenides, such as GeTe and Ge2Sb2Te5, can quickly and reversibly switch between an amorphous and a crystalline state with very different optical and electrical properties. These property changes allowed the integration of such chalcogenide materials in optical storage devices (DVD-RAM) and more recently in non-volatile memory technology (NVM) because of the high scalability of PC memories. But, for ultimate miniaturization, energy consumption becomes critical and a promising solution is the geometrical confinement of the memory points. Mastering this with Phase Change Materials at ultimate
lateral dimensions (typically 5 nm) is, however, a real challenge, which calls for a fundamental understanding of the interplay between strain (the amorphous-to-crystal transition is accompanied by a density increase of several %) and crystallization kinetics at the nanoscale.

In order to probe the influence of size, stress and confinement on the crystallization behavior of GeTe nanostructures we have developed dedicated setups that allow for a simultaneous in situ investigation of substrate curvature or electrical resistance measurement together with x-ray diffraction or x-ray reflectivity during annealing. These measurements are performed at DiffAbs beamline from SOLEIL synchrotron radiation facility. Samples are either capped thin films (thickness ranging between 100 and 5 nm) or arrays of nanopillars (diameter ranging between 200 and 50 nm) embedded in silicon nitride. Clear evolutions in crystallization behavior, crystallization kinetics or stress evolutions are observed as a function of size and confinement and will be discussed.

Acknowledgments

This work is funded by ANR within ANR SESAME ANR-15-CE24-0021 project.
A custom-made fast scanning chip calorimeter (FSC) was designed and made compatible with the environment of the micro- and nano-focus X-ray beamlines such as the ID13 beamline at the ESRF (Grenoble) [1-2]. The advent of fast single-photon-counting X-ray detectors enabled in-situ coupling of the two techniques with a possibility of conducting continuous synchronous acquisition of the thermal and 2D X-ray scattering data with time exposures on the order of one millisecond. The designed setup was used to re-explore the early stages of crystallization of HDPE in order to evaluate the morphology and exact supercooling at the crystal growth front. Also, the phenomenon of multiple melting, which constitutes one of the long-standing issues in polymer science, was revisited. In the present work, by using heating and cooling rates much higher than the rates of recrystallization, the structural transformation corresponding to each of the observed thermal events was extracted from X-ray data analyzed in detail [3-5].


Non-coplanar High-Resolution X-ray Diffraction to study novel materials

A. Ulyanenkov¹, A. Mikhalychev², A. Benediktovitch³,
T. Ulyanenkova⁴, S. Vlasenko², J. Keckes⁵, M. Myronov⁶,
V. Kaganer⁷, G. Abadias⁸, J. O’Connell⁹, A. J. van Vuuren⁹,

¹ Atomicus LLC, Seattle, WA, USA
² Atomicus OOO, Minsk, Belarus
³ DESY, Hamburg, Germany
⁴ Siemens, Karlsruhe, Germany
⁵ Montan University, Leoben, Austria
The development of structural materials for nuclear application is of great importance. Along with it, the development of radiation tolerant coatings for the application in reactors is of no less importance. One of the kinds of such protective coatings that often used is nitride-based ceramics due to their specific combination of properties suitable for the nuclear application. Radiation environment induces different kinds of damages in the materials which results in their degradation. One of the radiation-induced effects is the appearance of point defects. The presence of boundaries proved to be very effective in reducing the number of such defects. Therefore, multilayer systems are considered as coating materials.

In the present study we consider multilayer thin coatings ZrN/Si$_3$N$_4$ with different thicknesses of monolayers: unirradiated and irradiated by He$^+$ ions. In order to estimate the effect of radiation on these coatings we investigate the modification of microstructure before and after irradiation.

One of the effective methods used for structural characterizations is the X-ray diffractometry. Due to the presence of texture, performing the measurements in coplanar geometry (e.g. conventional θ/2θ scan) turns out to be not effective: it enables to obtain only two or even one reflection. In order to perform more reliable analysis of microstructure it is necessary to use more reflections. Taking into account the presence of texture one can evaluate the directions in which the best conditions for the observation of different reflections are realized. The use of noncoplanar measurement geometry [1,2] enables to obtain five reflections for the samples under consideration. Such type of measurement requires a special type of experimental data processing.
In this investigation the diffraction profile broadening is conditioned by the small grain size and instrumental function, the grains being modeled as having an ellipsoidal shape with two equal axes. The measured reflections are connected in one scan for the simultaneous fitting by the theoretical curve. In the result of the fitting procedure the microstructural parameters were estimated. The results obtained by X-ray diffraction are in good agreement with those obtained from transmission electron microscopy.


**Biological fate of Engineered Nanomaterials: tracing aggregation/degradation and nanomaterial dose in vitro and in vivo**

*Sergio E. Moya*

1. CIC biomaGUNE, Paseo Miramón 182 C, 20014 San Sebastian, Spain

There is an urgent need for a deeper understanding of the impact of engineered nanomaterials (ENMs) on human health resulting from deliberate exposure to ENMs, such as in nanomedicine, or from accidental exposure due to handling or using devices or products containing ENMs. The characteristics of ENMs, such as shape, size, degradability, aggregation, surface and core chemistry determine their interaction with biomolecules and the ENMs fate both intracellularly and at body level. Therefore, for the assessment of ENMs toxicity is necessary to correlate ENMs characteristics with their fate and biological interactions. ENMs fate *in vivo*, distribution per organ, accumulation, biodurability and dose are fundamental to assess how ENMs affect biological functions. The physical state of the ENMs, including aggregation, the interaction with biomolecules in different cellular environments, and guide the intracellular action
of nanomaterials. A fundamental aspect for understanding toxicity is to establish the relation between exposure dose of ENMs and the intracellular dose or the dose per organ. The actual dose following an exposure route is the result of the translocation of ENMs across different barriers.

Several aspects of ENMs fate in vitro and in vivo will be discussed mainly in relation with ENM quantification and ENMs stability. Cell uptake and intracellular fate of ENMs will be presented. The intracellular dose for metal oxides nanoparticles will be measured with Ion Beam Microscopy. Relations between exposure dose, intracellular dose and cell viability will be established.

Protein corona formation and the aggregation behavior of gold nanoparticles (Au NPs) will be investigated by means of Fluorescence Correlation Spectroscopy (FCS) in cell culture media and in live cells. The behavior in vitro will be compared with the level of aggregation of the NPs intracellularly. Diffusion coefficients of the NPs will be measured following NP trafficking at different positions in the cell: the endoplasmatic reticulum, the endocytic vesicles, the cytosol and in intracellular vesicles. Fluorescence Cross Correlation Spectroscopy (FCCS) will be applied to study the intracellular stability of protein corona.

The bio distribution, organ accumulation and fate of radiolabelled ENMs will be studied in animal models by means of Positron Emission Tomography (PET). NPs dose per organ will be evaluated. A dual radiolabelling strategy of nanoparticle core and coating will be presented using gamma emitters with non overlapping emission bands. After intravenous administration into rats, energy-discriminant Single-Photon Emission Computerised Tomography (SPECT) resolve each radioisotope independently revealing different fate in vivo for the core and coating, which will be used to evaluate NP integrity.
Functionalized noble metal nanoparticles (MNPs) depict a suitable platform for the development of efficient multi-functional responsive systems. It has been demonstrated that the synthesis by a wet chemistry method enables complete control of their optical and physical properties. A wide range of advanced applications are based on the use of MNPs, because of their unique chemical and physical properties and versatile synthesis, that allows to obtain functionalized metal surfaces with neutral or charged, hydrophilic or hydrophobic, organic or organometallic thiol molecules [1]. In particular, the research in biomedicine, catalysis, energy conversion and sensors are strongly influenced by these materials. The colloidal MNPs can be for example manipulated to induce self-assembly into complex structures, 2D or 3D networks that show collective properties. It is also noteworthy that the ease of surface chemistry of MNPs (M = Au, Ag, Pt) allows for tunable strategies to realize systems with different surface charge. Up to now these intriguing peculiarities have not been focused in a unified vision. The aim of this approach is to develop a three-dimensional nanoscopic system capped with thiol ligands that confer a different surface functionality, where every single element maintains its stability and conformation together with the chemical reactivity. In particular, the growth of AuNPs, AgNPs or PtNPs was obtained by a chemical reduction method starting from Au$^{3+}$, Ag$^{+}$ or Pt$^{2+}$ containing precursors in a single or two-phases synthesis, under ambient conditions using NaBH$_4$ as a reducing agent. The one pot synthesis is carried out in the presence of different ligands, either single or mixed thiols, bearing different ending functionalities, as schematized in figure 1.
Absorption spectroscopy measurements of the nanoparticles showed plasmonic peaks in the visible range, tunable with the metal, size, functionality and interconnection between nanoparticles. The prepared MNPs have been characterized with spectroscopic and morphological techniques and by means electrical conductivity measurements. Moreover, colloidal MNPs were prepared in the presence of hydrophilic thiols that induced suspendability and stability in water medium. These systems are particularly suitable for drug delivery applications, thanks to their cytocompatibility and easy preparation of bioconjugates with different drugs.

Figure 1: Schematic representation of functionalized metal nanoparticles

1. Fratoddi, I. Nanomaterials, 8(1), 11 (2018)
Ultrathin organic field effect transistors: from materials to devices and their applications

Sergey Ponomarenko,¹,² Oleg Borshchev,¹ Elena Agina,¹ Askold Trul,¹ Victoria Chekusova,¹ Dmitry Paraschuk¹,³
¹. Enikolopov Institute of Synthetic Polymer Materials RAS, Profsoyuznaya str. 70, Moscow, 117393, Russia
². Chemistry Department, Lomonosov Moscow State University, Leninskiye Gory 1/3, Moscow, 119991, Russia
³. Faculty of Physics, Lomonosov Moscow State University, Leninskiye Gory 1/2, Moscow, 119991, Russia

Performance of organic field-effect transistors (OFETs) strongly depends on the organic semiconducting materials structure, their purity and morphology. On the one hand, it is well-known that charge carriers in the OFETs are induced on the interface between dielectric and organic semiconducting layers by external electric field from the gate electrode. Hence, most of the charges are passed through the first monolayer of the organic semiconductor, while the following 2-3 monolayers improves the field-effect mobility somewhat further if the first monolayer is not perfect. On the other hand, mobility in OFETs is affected by the degree of ordering of organic semiconductors, with the highest mobility reported for monocrystalline OFETs. Hence, an ideal OFET should be ultrathin and monocrystalline.

Monolayer OFETs are particularly interesting due to low consumption of organic semiconductors as well as their unique sensitivity to the environment, which allows creation of ultrasensitive gas sensors.¹ Monolayer OFETs can be prepared either by physisorption or by self-assembly of various conjugated oligomers (see Figure). The former can be grown from solution of conjugated thiophene or thiophene-phenylene oligomers by drop or
spin casting with subsequent slow solvent evaporation, leading to single-crystal monolayers of unprecedented structural order, which demonstrated excellent performance in OFETs. The latter may be easily prepared from highly stable organosilicon derivatives of organic semiconductors, capable to self-assembly on the water-air interface, which allows fabrication of monolayer OFETs by Langmuir-Blodgett (LB) or Langmuir-Shaeffer (LS) techniques. Investigation of their electrical characteristics in various gas environment suggested their application as ultrasensitive gas sensors capable to detect up to hundreds ppb of hydrogen sulfide or ammonia, which pave the way of the development of an electronic nose based on this technology.

**Figure:** Examples of chemical structures of organic semiconductors synthesized and investigated in this work.

Synthetic work was made in the framework of Leading Science School supported by Russian Ministry of Science and Higher Education (grant NSh-5698.2018.3). Investigation of single crystal OFETs was supported by RSF (grant 18-12-00499), preparation and measurements of monolayer LS OFETs was supported by RSF (grant 19-73-30028).

2. V.V. Bruevich at. al., ACS Appl. Mater. Interfaces 11, 6315 (2019)
Electrostatic stability of virus-like nanoparticles: Roles of metallic core and multivalent solution ions

Ali Naji

School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

Electrostatic interactions play important roles in the formation and stability of viruses and virus-like particles (VLPs) through processes that often involve added, or naturally occurring, multivalent ions. In the context of VLPs, encapsidation of non-biological cargo, including gold and iron-oxide nanoparticles, in viral proteinaceous capsids has attracted a lot of attention in recent years, even though, from an electrostatic point of view, a consistent understanding of the intricate factors involved in the problem remain elusive. This is mainly because the existing formulations are often developed using mean-field paradigms that are however known to be severely violated in the presence of multivalent ions, causing strong electrostatic couplings with the oppositely charged macromolecular surfaces. I will give a short overview of our current understanding of such non-mean-field effects, achieved through recent computational and theoretical advances in the field. Then, by focusing on model examples of charged nanoshells, nanodroplet and, models VLPs containing an ideally polarizable metallic nanoparticle core, I will show that the combination of the competing factors involved in the problem, such as the Debye screening due to a bathing electrolyte solution, image-charge and polarization effects due, e.g., to the core particle, as well as strong-coupling effects due to multivalent ions, leads to a diverse range of effects, with counterintuitive regimes of behavior that cannot be explained by traditional approaches. The implication of these results for the electrostatic stability of the aforementioned examples, specifically, the VLPs with a metallic core, are thoroughly discussed.
The present paper deals with the synthesis and studies of two types of biodegradable self-assemblying systems based on pseudo-proteins (PPs) [1]: (i) ABA triblock amphiphilic co-polymer in which A-blocks (hydrophilic blocks) represent amino-poly(ethylene glycol) with $M_w$ 2000 Da (amino-PEG-2000), and B-block is PP labelled as 8L6, composed of $\alpha$-amino acid L-leucine (L), 1,6-hexane diol (6) and sebacic acid (8) (average MW $\approx$ 4000 Da), Fig. 1:

(ii) comb-like amphiphilic co-polymer (CLP) obtained after polymer-analogous transformation of epoxy-functionalized PP – co-polymer composed of 8L6 (50 mole %) and tES-L6 composed of trans-epoxy succinic acid, L-leucine (L), 1,6-hexane diol (6) (50 mole %) by its interaction with amino-PEG-2000.

The obtained amphiphilic polymers both ABA triblock co-polymer and CLP are of interest as micelle-forming systems, effective surfactants for fabricating nanoparticles (NPs) providing at the same time their PEGylation.
The PEGylation of the NPs decreases affinity of plasma proteins (opsonins) for adsorption on NPs - long chains of PEG form a random cloud around the NPs thereby preventing absorption of opsonins and in that way suppressing phagocytosis.


A Library of Cationic Polymers as Gene Transfection Agents

N. Zavradashvili1, C. Sarisozen2, G. Titvinidze1, G. Otinashvili1, Teng. Kantaria1, D. Tugushi1, J. Puiggali3, V. Torchilin2, R. Katsarava1

1 Institute of Chemistry and Molecular Engineering, Agricultural University of Georgia, Kakha Bendukidze University Campus, # 240 David Aghmashenebeli Alley, 0159 Tbilisi (Georgia)
2 Center for Pharmaceutical Biotechnology and Nanomedicine, Northeastern University, 360 Huntington Ave., Boston, MA (USA)
3 Universitat Politècnica de Catalunya, Av.Diagonal 647, E-08028 Barcelona (Spain)

N.Zavradashvili@agruni.edu.ge

Cationic polymers (CPs) exhibit unique physical-chemical properties and their ability that allows further modification renders them appealing for numerous applications [1]. A library of new highly
water-soluble CPs were designed and synthesized on the basis of naturally occurring building blocks such as amino acid arginine (R), endogeneous tetraamine – spermine (Spm) and synthetically made triamine N-(2-aminoethyl)-1,3-propanediamine (Apd). 12 new polyamine-based CPs of two classes - polyureas (PUs) and polyamides (PAs) were synthesized via solution active polycondensation (SAP). The cytotoxicity of all 12 CPs toward different cell lines was evaluated to select low-toxic (90% and more cell viability) candidates for in vitro transfection study. A further screening of the selected CPs was done based on the complex formation with pDNA. The samples of the CPs which formed positively charged (zeta potentials $\leq +57.4$ mV) stable nanocomplexes CPs/pDNA ($38.0 - 312.0$ nm) at low weight ratio (WR CPs/pDNA 5x - 25x) were selected for the transfection experiments on human and murine cell lines. The ability of selected CPs to deliver pDNA were investigated by flow cytometry analysis and confocal microscopy study using eGFP encoding pDNA. These studies support each other and strongly indicate the selective transfection ability profiles of the CPs tested, which means that the carefully selected CPs from a small library of polymers are able to provide all the required properties as effective transfection agents. Hence, the new CPs have a potential for the applications in gene therapy and biotechnology as nontoxic and effective agents for intracellular delivery of nucleic acids (gene carriers) [2].


**Stretchable and Deformable Materials and Devices for Human Machine Interface**

*Pooli See Lee*\(^1\)

\(^1\) School of Materials Science and Engineering, Nanyang Technological University, Singapore

*pslee@ntu.edu.sg*
The emergence of deformable devices is driven by the need of free-form properties for conformable and wearable applications. To realize these needs, approaches to fabricate flexible and stretchable devices have embraced extensive exploitation of nanomaterials for active responsive coatings, functional printing, and revolutionary modifications of the conventional rigid substrates.

We have devoted significant efforts in preparing functional nanomaterials in adapting to applications in human-machine interface. We designed and prepared flexible transparent conductor using metallic nanowires and nanocellulose for flexible transparent conductors.[1] Nanowire techtonic network provides an effective method in realizing conductive percolative pathways for electron transport on flexible substrates, making them attractive for flexible touch sensor.

Stretchable conductors using liquid metal particle based nanocomposites were designed to sustain continuous electrical conduction under extreme stretching conditions.[2] Using this strategy, a thermoplastic composite is prepared with self-healing property. It recovers 96.0% of its conductivity in healing efficiency. We fabricated an all 3D-printed triboelectric nanogenerator using this material.[3] Energy generation can be harvested even under extreme strain states. The power output performance can be recovered despite severe mechanical damage due to the self-healing properties endowed by the supramolecular hydrogen bonding of the elastomer.


ANAM2019
WORKSHOP ORAL AND
POSTER CONTRIBUTIONS
Fröhlich polaron formation in graphene on polar substrate

Arshak L. Vartanian

Department of Solid State Physics, Yerevan State University, 1, Al. Manoogian, Yerevan, 0025, Armenia

Both in technological applications and in fundamental research of graphene, polar substrates, such as SiO$_2$, SiC, HfO$_2$, e.t.c. are commonly used. The polar optical phonons which are localized near the graphene-polar substrate interface are important scattering sources for graphene carriers through the long-range Fröhlich coupling. When a graphene monolayer is in close proximity to a polar substrate, the graphene-electron interaction with surface polar optical phonons can significantly influence the optoelectronic properties of graphene [1]. An important factor in studying the interaction of charge carriers in graphene with phonons is the elucidation of features of the polaron states formed in graphene.

The structure under consideration consists of monolayer graphene located at the equilibrium distance $d$ from the dielectric of thickness $L$, which is deposited on the metal gate. It has been shown [2] that the graphene and gate plasmons can alter the dispersion relations of SO-phonon modes at graphene-dielectric interface of a considered structure (Fig.1). The carrier dynamics without phonon coupling in two-dimensional graphene is considered in frame of the
Dirac cone approximation. In Fig.2 we have represented the charge carrier energies in graphene as a function of the wave vector $k$ without (curves 1 and 2) and with (curves 3 and 4) charge carrier-surface polar optical phonon interaction in case of a) SiO$_2$ and b) Al$_2$O$_3$ substrates. The decrease (increase) in the electron (hole) energy, in general, due to interaction with surface optical phonons indicates that the formation of a surface polaron is preferred. We have also examine the screening effect on the polaron states. Our results show that the influence of the screening effect on polaron energies is significant for $k \leq k_F$.

![Figure 2](image.jpg)

Fig.2. (Color online). Charge carrier energies in graphene as a function of the wave vector $k$ without (curves 1 and 2) and with (curves 3 and 4) charge carrier-surface polar optical phonon interaction in case of a) SiO$_2$ and b) Al$_2$O$_3$ substrates.

This work has been supported by Science Committee of the Ministry of Education and Science of Armenia (SC MES RA), within the frame of the research Project No. 18T-1C247.

X-ray dynamical diffraction Talbot effect under the condition of two-wave dynamical diffraction in crystals

M.K.Balyan

Yerevan State University, Faculty of Physics, Chair of Solid State Physics

Imaging of periodic objects in free space brings to the Talbot effect in optics, for x-rays and for matter waves. In this work the Talbot effect is investigated inside a crystal under two-wave dynamical diffraction conditions. An exact formula for the diffracted wave amplitude is found. It is shown that the dynamical diffraction Talbot effect inside the crystal takes place. Expressions for polarization sensitive Talbot and corrected Talbot distances are obtained. The influences of absorption, Bragg filtration of harmonics and polarization on the dynamical diffraction Talbot effect is found. Simulated Talbot carpets inside the crystal are obtained. We present the dynamical diffraction Talbot carpets observation method by means of a wedge shaped crystal. The dynamical diffraction Talbot effect can be used for investigation of objects and crystal defects and deformations. In addition to the works [1, 2], where the dynamical diffraction Talbot effect is considered only in the diffracted and in the transmitted beams separately, in this work this effect is considered simultaneously in both beams.

The influence of electron-polar optical phonon coupling on the impurity-related optical properties in nanowire under magnetic field

Tigran Ghukasyan¹, Arshak Vartanian¹

¹ Department of Solid State Physics, Yerevan State University, 1, Al. Manoogian, Yerevan 0025, Armenia

The optical properties of a nanowire (NW) can significantly depend on the presence of impurities in NWs. Since NWs are usually made of polar materials, the interaction between electrons and confined optical (CO) as well as interface optical (IO) phonon modes must be taken into account for a reliable description of the optical properties.

We considered a polar cylindrical parabolic NW, embedded into non-polar medium in a uniform magnetic field along the wire axis. The influence of impurity position, magnetic field strength and confining potential frequency on the electron and polaron binding energy as well as oscillator strength and linear and non-linear absorption coefficients (AC) and refractive index changes (RIC) for transitions from the ground state to a few excited states, have been investigated. Fig 1. shows the oscillator strength and AC for transitions for electrons and polarons. The obtained results show, that the polaron effect on the optical characteristics is noticeably manifested when the electron interacts mainly with either CO or IO phonons. We have shown that the electron-phonon interaction leads
to blue shifts of all the absorption coefficients extrema. Also, the extrema of polaron transitions have larger values than electronic ones.

Fig 2: Oscillator strengths (a) as functions of impurity position and absorption coefficients for (b) electron and (c) polaron as functions of photon energy at H=3T for 1s → 2p\textsubscript{y} transitions

Fig 2. shows the oscillator strength and RIC for transitions of electrons and polarons. A comparison of the corresponding RIC extrema in Fig 2 (b) and (c) shows that they are almost the same for electronic and polaron transitions. At the same time, it should be noted that, for electronic transitions, RICs reach their extrema near the same photon energy for all values of the magnetic field, while the extrema for the polaron transitions are somewhat distant from each other.

This work has been supported by Science Committee of the Ministry of Education and Science of Armenia (SC MES RA), within the frame of the research Project No. 18T-1C247.

**Multiparametric toxic gas detection with a single Langmuir-Schaefer monolayer field-effect transistor**

A.A. Trul\textsuperscript{1,2}, A.S. Sizov\textsuperscript{1,2}, V.P. Chekusova\textsuperscript{1,2}, O.V. Borschchev\textsuperscript{1,2}, A.A. Vasiliev\textsuperscript{1,3}, E.V. Agina\textsuperscript{1,2}, S.A. Ponomarenko\textsuperscript{1,2,4}

\textsuperscript{1} Enikolopov Institute of Synthetic Polymeric Materials RAS

\textsuperscript{2} Printed Electronics Technologies LLC

\textsuperscript{3} NRC Kurchatov Institute

\textsuperscript{4} Lomonosov Moscow State University, Chemistry department

Chemical sensors based on ultrathin organic field-effect transistors (OFETs) have garnered considerable attention in the areas
of industrial safety control, food spoilage detection and medical diagnostics because of an impressive combination of low limit of detection, low power consumption and portability. However, such type of sensors usually has two main drawbacks – poor air stability and poor restoration at room temperature. In this work [1] we have investigated sensory properties of Langmuir-Schaefer monolayer field-effect transistors (LSFETs) based on recently developed and investigated tetramethyldisiloxane dimer of non-symmetric dialkyl benzothieno[3,2-b][1]benzo-thiophene (BTBT) derivative [2]. The choice was based on outstanding electrical performance (charge carrier mobility up to $7 \times 10^{-2} \, \text{cm}^2\text{V}^{-1}\text{s}^{-1}$) of such monolayer devices as well as long-range stability of their electrical performance under normal conditions (at least six months). Sensory properties were estimated in the presence of small amount (10ppb – 10 ppm) of ammonia and hydrogen sulfide.

Detailed investigations of LSFETs electrical properties under different environment demonstrated that devices fabricated are able to operate in air atmosphere and detect ammonia and hydrogen sulfide even at very low concentrations down to 10 ppb. Moreover, we found out that direct sensor response can be splitted into the variation of different LSFET parameters, such as threshold voltage and charge carrier mobility, which are responsible for the interactions with different toxic gases. For example, charge carrier mobility variation is relatively weak under exposure of ammonia, but charge carrier mobility significantly decreases under exposure of hydrogen sulfide. Moreover, the mobility change depends on the hydrogen sulfide concentration (Figure 1). These investigations allow us to develop a special measurement routine for complete distinguishing of two different gases - ammonia and hydrogen sulfide - with a single sensing device. It should be noted that the devices investigated are reusable and can be restored to initial characteristics at room temperature after being placed in a clean atmosphere and bias stress switching off.
These findings open new perspectives for the sensing technology based on OFETs. We believe that the approach elaborated can be further improved to other toxic gases enabling the development of a system for complex air analysis based on a single device. Preliminary results of nitrogen oxide sensing with LSFETs demonstrated even different transistor parameters behavior in the presence of this gas at sub-ppm concentrations, that will be a subject of our further investigations.

This work was supported by RSF (project № 19-73-30028) and performed in the framework of Leading Science School (grant № NSh-5698.2018.3).

The influence of AgTOEPyP porphyrin on the stability and conformation of i-motif structure of DNA

L. Aslanyan¹, I. Vardanyan¹, Y. Dalyan¹

¹Department of Molecular Physics, Faculty of Physics, Yerevan State University, Yerevan, 0025, 1 Alex Manoogian, Armenia

l.aslanyan@ysu.am

The four-stranded i-motif conformation of cytosine-rich DNA is important in a wide variety of biochemical systems ranging from its use in nanomaterials to a potential role in oncogene regulation. These structures widely exist in genomes and play important roles protection of telomeres and gene regulation. I-motif structure is formed by intercalated hemiprotonated cytosine–cytosine (C–C⁺) base pairs under acidic condition or at neutral pH by molecular crowding of the cosolutes [1-3]. Recent evidences suggest that these DNA structures exist in living cells and could be involved in several cancer-related processes, thus representing an attractive target for anticancer drug discovery. It has been well known that porphyrins and related compounds have the ability to selectively interact with guanine- and cytosine-rich DNA sequences in vitro. For this reason, interaction of porphyrin derivatives with telomeric sequence is an area of great research interest.

In this study, was investigated the interaction of Ag-containing porphyrins – meso-tetra(4N-oxyethylpyridyl) (AgTOEPyP4) with intermolecular i-motif structure from a human 5’-(CCCTAA)₃CCCT-3’ telomeric sequence. Oligonucleotide was dissolved in sodium acetate buffer at pH 5.50, at a several concentrations of [Na⁺]. Using circular dichroism (CD) and UV melting methods, we studied the effect of AgTOEPyP on the folding and stability on the i-motif. The CD spectra of porphyrin/ i-motif complexes are displayed in Figure 1. The circular dichroism spectra of 5’-(CCCTAA)₃CCCT-3’ exhibit a positive band centered
at 289nm and a negative band at 255nm, which are characteristic for intermolecular i-motif structure as determined by previous studies.

![Graph showing CD spectra and changes in molar ellipticity](image.png)

**Figure 1 a.** CD spectra of complexes of AgTOEPyP4 with i-motif at 25 °C, **b.** The changes of molar ellipticity at 289nm at varies [Na+] ion and porphyrin concentrations.

The presence of AgTOEPyP porphyrin leads to decreases of the characteristic band at 289nm (Figure 1a) and shift the maximum to the low wavelengths. Which suggests that presence of porphyrin in the solution leads to conformation changes in i-motif structure. The appearance of positive ICD spectrum in Sore region at 442 nm indicates that there is an interaction between porphyrin and i-motif. It can be assumed that porphyrin has a destabilizing effect on i-motif. As the spectral changes shown, increase of [Na +] ions cause stabilization of already destabilized i-motif structure (Figure 1b).

UV melting profiles of i-motif/porphyrin complexes at 295nm also shown, that at room temperature I-motif/porphyrin complex is less stable and preferable the I-motif-to-coil transition. All of the melting curves were well fit with two-state transition. In the presence of AgTOEPyP porphyrin in the sodium acetate buffer melting temperature is lower than without it. The increasing of sodium ion concentration leads to i-motif/porphyrin complex stabilization and in the presence of 400mM [Na+] melting temperature *increases* up to 42°C.
ACKNOWLEDGMENTS

This work was supported by Grant 18T-1F055 from the State Committee of Sciences of the Republic of Armenia.


Seeking Maxwell’s Demon in a nonreciprocal quantum ring

Aram Manaselyan\textsuperscript{1}, Wenchen Luo\textsuperscript{2}, Daniel Braak\textsuperscript{3}, Tapash Chakraborty\textsuperscript{4}

\textsuperscript{1} Department of Solid State Physics, Yerevan State University, Yerevan Armenia
\textsuperscript{2} School of Physics and Electronics, Central South University, Changsha, Hunan, China
\textsuperscript{3} Max-Planck Institut für Festkörperforschung, Stuttgart, Germany
\textsuperscript{4} Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada

In the middle of nineteenth century, physicists were grappling with the implications of the newly established second law of thermodynamics, whose one profound proclamation was that, it is not possible for heat to spontaneously flow from a cold system to a hot system without external work being done on the system. Then in 1867, James Clerk Maxwell questioned [1] if the above statement was true only for a system whose properties were governed by the average behavior of the particles or whether it is still valid even at the level of individual particles. In order to test this idea, Maxwell conceived the famous gedankenexperiment where a tiny intelligent
being (demon) with exceptional capacity of being able to observe individual molecules and their speed, was assigned a very special job. The demon was to sort, in a closed box of uniformly distributed particles, the fast (hot) particles and slow (cold) particles in two compartments of the box separated by a wall with a tiny trap door. As time passes, the demon opens or shuts the door to allow the fast or slow particles in their respective compartments, thereby creating a temperature gradient from the initial uniform temperature without doing work on the system and thus violate the second law of thermodynamics.

Given the paucity of intelligent demons, for 150 years Maxwell’s demon remained an interesting idea that could never be implemented in a real world. However, in recent years, rapid progress in nanoscale physics has resulted in devices where the dynamics of even individual electron can be controlled. Examples of such systems are quantum dots and quantum rings. Experimentally, Pekola et al. [2] have reported creating Maxwell’s demon in a system of two quantum dots.

A non-reciprocal quantum ring, where one arm of the ring contains the Rashba spin-orbit interaction [3] but not in the other arm, is found to possess very unique electronic properties. In this ring the Aharonov-Bohm oscillations are totally absent because in a magnetic field the electron stays in the non-Rashba arm, while it resides in the Rashba arm for zero (or negative) magnetic field. The average kinetic energy in the two arms of the ring are found to be very different. It also reveals different “spin temperature” in the two arms of the non-reciprocal ring. The electrons are sorted according to their spins in different regions of the ring by switching on and off (or reverse) the magnetic field, thereby creating order without doing work on the system. This resembles the action of a demon in the spirit of Maxwell’s original proposal, exploiting a non-classical internal degree of freedom. Our demon clearly demonstrates some of the required features on the nanoscale.

Spongy cubic phases built through self-assembly of wedge-shaped amphiphilic mesogens

Kseniia N. Grafskaia\textsuperscript{1,2}, Denis V. Anokhin\textsuperscript{1,2}, Dimitri A. Ivanov\textsuperscript{1,2,3}

\textsuperscript{1} Moscow Institute of Physics and Technology, Russia
\textsuperscript{2} The Institute of Problems of Chemical Physics of the RAS, Russia
\textsuperscript{3} Institut de Sciences des Matériaux de Mulhouse, France

Natural and synthetic zeolites are widely used as materials for chemical separation and purification, fuel conversion and ecology. The interest is based on unique properties of porous structures with well-defined diameter. Poppe et al. have proposed an approach for fabrication of zeolite-like LC structures based on self-assembly of polyphilic molecules with pentagonal/octagonal or pentagonal/hexagonal channels [1].

The main reason of limited number studies of the organic porous materials is their tendency to collapse after removal of solvent or changes in environment. However, some molecules are suitable for design of stable molecular porous scaffold with huge variety of supramolecular morphology. The variation of organic molecule shape gives a serious advantage in formation of zeolites compare to inorganic systems. In presented work we report about formation of Cub phase in the system of non-polymerizable wedge-shaped pyridinium salts with linear side groups. The Cub phase in the system is stabilized by non-covalent interaction between alkyl chains [2]. Recently, only few examples of Cub phase formation from wedge-shaped mesogens with pyridinium as counter-ion are discussed in literature [3,4]. However, heating in the presence of methanol vapors results in formation of the Cub phase. The found cubic morphology is stable in wide temperature range and able to swell in water vapor that important for future applications.

In presented work we demonstrate a new approach for designing zeolite-like structure from small wedge-shaped mesogens. The key role of linear alkyl chains in structure formation was revealed (Fig.1). We suggest that local ordering of linear side groups prevent efficient diffusion of polar solvents like water or methanol.
through non-polar matrix. This diffusion is significantly increased for liquid alkyl chains in Colh phase above 100°C. The gyroid phase stabilized by alkyl chains can be dried from methanol by heating to 100°C. After cooling of dry Cubgyr phase to room temperature the material can efficiently swell in water vapors resulting in increase of lattice parameter by 18% compare to initial phase formed in methanol vapors.

**Figure 1:** Thermal evolution of wide-angle reflexes (left). AFM image of C8Pyr in cubic structure (right).


**Fine structure of DMC for helix-coil transition in heterogeneous biopolymers**

**Asatryan A., Tonoyan Sh., Y. Mamasakhlisov, V. Morozov**

**Yerevan State University**

Order-disorder transition often occurs in biopolymers which operate in biological systems and are in complexes with nano-materials. Problem of helix-coil transition still remains very popular. One of the main methods to investigate helix-coil transition is observation of
DMC of biopolymers. Some of our previous works concern such theoretical investigations both for homopolymers [1] and heteropolymers [2], however no fine structure was observed then. Fine structure on DMC has been observed experimentally long time ago. Mostly it concerns DMC of DNA. In experimental works DMC-s of DNA are investigated. As an explanation these works postulate assumptions that DNA contains macroscopic blocks with different G-C composition [3, 4]. We discussed DMC-s of heteropolymers with random sequences in frame of GMPC. Random sequences are generated from two types of repeated units. It is shown that fine structure of DMC of biopolymer interacting with solvent can be observed for small values of $\frac{T_B}{T_A}$, where $T_A$ and $T_B$ are melting temperatures of correspondingly “A” and “B” type homopolymers interacting with solvent. However, when short range correlation is taken into account in sequences fine structure occurs also for $\frac{T_B}{T_A} \sim 1$, which is observed in experiments [3, 4]. Our calculations show that fine structure can be obtained not only in case of block structures of biopolymers, but also for biopolymers with correlation in the sequence.

Short-range disorder and electrostatic interactions in macromolecule

Varazdat Stepanyan
Yerevan State University

We consider a generic flexible polyelectrolyte comprised of equally charged monomers with disorder is conditioned by the short-range features only (e.g. ssRNA). Interactions between chain monomers are supposed to be non-saturated to simplify calculations. We have obtained the free energy functional using the replica method and obtained the Poisson – Boltzmann and Edwards equation for the replica symmetric solution, which have been solved numerically in the no-salt regime. The polyelectrolyte density profile is obtained in the weak disorder approximation and compared with those for the pure system.

Hard X-Ray Fourier Transform Holography Based on Two-Block Fresnel Zone Plate Interferometer with Common Optical Axis

L.A. Haroutunyan* and M.K. Balyan
Yerevan State University, Yerevan, Armenia
*
levhar@ysu.am

An X-ray Fourier transform holography set-up, based on two-block Fresnel zone plate (FZP) interferometer [1] is presented. As can be seen from the figure, the reference wave is a spherical wave formed
by zero and first order diffractions on the first and second FZP, respectively, and the object wave is a plane wave formed by first order diffraction on both FZP.

**Figure:** The Experimental set-up. K – knife edge, Z1 and Z2 – first and second FZP, respectively, S – screen in the object plane.

The large-scale features of the object under investigation cause a small angle scattering of the object wave. In this case the interferometer operates in amplitude-division mode and does not impose strong requirements on the coherency of initial radiation, in contrast to the similar schemes with one FZP [2]. In contrary, the small-scale features cause a large-angle scattering. In such circumstances the interferometer does not operate in amplitude-division mode and the requirements on the coherency of initial radiation becomes stronger.

The capability of the scheme to reconstruct the amplitude transmission coefficient of the amplitude and phase objects is shown. The resolution and coherence requirements of the scheme are estimated. Examples of reconstruction of the amplitude transmission coefficient of a cosine-like grating and a two-dimensional object image are considered.


Investigation of Antibacterial Properties of Green Synthesized Silver Nanoparticles

S. Gevorgyan\textsuperscript{1}, M. Yeranosyan\textsuperscript{1,2}, R. Schubert\textsuperscript{3}, A. Trchounian\textsuperscript{1}

\textsuperscript{1} Yerevan State University, A. Manoogian 1, Yerevan 0025 Armenia
\textsuperscript{2} National Polytechnic University of Armenia, Teryan 105, Yerevan 0009 Armenia
\textsuperscript{3} European X-ray Free Electron Laser GmbH, Holzkoppel 4, 22869 Schenefeld, Hamburg, Germany

The increasing rate of antibiotic resistance of microorganisms poses a significant global concern [1]. Recent advancements in nanotechnology have led to the development of new antimicrobial compounds [2]. It is well known that among metal nanoparticles (NPs), Ag NPs have wide application in industry and medicine due to their antibacterial, antifungal and anti-parasitic properties. Therefore, there is a need to develop rapid and reliable experimental protocols for the green synthesis (GS) method of NPs, which is proposed as beneficial compared to chemical and physical approaches [3].

The aim of current research was to study the influence of GS Ag NPs on specific growth rate of Gram-negative \textit{E. coli} BW25113 and Gram-positive \textit{E. hirae} ATCC9790. Royal Jelly as a source of oxidizing/reducing and stabilizing agents has been used in the GS of Ag NPs. UV-Vis and Fluorescent spectroscopy show a maximum absorption at a wavelength of 430 nm and fluorescence emission peaks at a wavelength of 487 nm confirmed the presence of Ag NPs. The shape and size of the NPs, as well as the effect of ultrasound on the NPs, were analysed using Transmission Electron Microscopy and Atomic Force Microscopy. Obtained data reveal: i) the presence of particles mainly with a size of 20-100 nm, as well as few small particles below 20nm in size and larger clusters up to 1 \textmu m, ii) ultrasonic treatment helps to reduce the size of the NPs and increase the homogeneity of the solution (Fig.1).
The growth properties of *E. coli* and *E. hirae* strains, grown under anaerobic conditions in the presence of GS and ultra-sonicated Ag NPs (from 5 to 30 μg/mL), have been investigated. Preliminary growth data analysis shows that all above mentioned concentrations of green synthesized and ultrasound treated Ag NPs have an inhibitory effect on both *E. coli* BW25113 and *E. hirae* ATCC9790.

**Figure 1:** TEM visualization of size (a) and diameter distribution (b) of Ag NPs. AFM images of non-treated (c) and ultrasound-treated (d) Ag NPs.

In conclusion, green synthesis plays an important role on properties of Ag NPs and further research is needed to better understand of their biological activity.

**Acknowledgements**

This work was partially supported by SC MES RA, within the frame of the research Project No. 18T-1C247, ANSEF research grant (condmatth-5214), CANDLE Synchrotron Research Institute and European XFEL.
Variational analysis of impurity states in gapped graphene systems

A.P. Djotyan, A.A. Avetisyan

Department of physics, Yerevan State University

The interest on mono- and few layer graphene systems with opened energy gap derives from its great potentials for applications in nano- and optoelectronics, e.g. for creation of new spintronic devices, novel lasers and quantum information processing. Bilayer graphene, which consists of two stacked monolayers and where the quasiparticles are massive chiral fermions, has a quadratic low-energy band structure. Theoretical and experimental investigations have shown that a perpendicular electric field applied to bilayer of graphene modifies its band structure near the K point and may open an energy gap in the electronic spectrum, which is tunable by the gate voltage [1] and depends on stacking order of graphene layers [2].

Here we develop a variational approach for calculation of an impurity electron binding energy in graphene systems with an energy gap opened by external gates. The dependencies of the ground state, binding energy and oscillator strength of the impurity electron on the gap value and tight binding parameters, describing the interaction between two layers, have been found.

The suggested method can be developed for three layer graphene systems with different stacking orders as well as in the presence of an external magnetic field.

Various aspects of polaronic properties in quasi-one-dimensional quantum wire systems are still of interest from a theoretical and experimental perspective. The characteristics of polaron for wurtzite structure are substantially different from zinc-blende structure due to anisotropy effects. The picture becomes more complicated in the presence of external fields. The presence of a magnetic field, as it is well known, introduces another electronic confinement which superposes the geometrical one. The electric field applied perpendicular to the interfaces leads to both a polarization of the carrier distribution and an energy shift of the quantum states introducing a considerable change in the energy spectra of carriers (quantum Stark effect), and this property is very useful for optoelectronic devices.

In the present work, we have studied theoretically the effects of both applied electric and magnetic fields on Fröhlich polaron properties in a wurtzite nitride quantum wire (QWR). We have calculated the polaron self-energy (SE) and the relative change in the effective mass (RCEM) due to confined (CO) and interface (IO) optical phonons by using the Lee-Low-Pines variational approach. Numerical calculations have been performed for GaN QWR embedded in a non-polar matrix. The dependences of the polaron SE and RCEM are obtained as functions of the cylindrical wire radius, the strength of the electric field applied perpendicular to the wire axis, and the induction of magnetic field applied parallel to the wire axis. In Fig.1, we present the CO polaron SE (a) and the RCEM (b) as a function of the electric field strength $F$ for different values of the magnetic field. One can see that the SE increases with the increase of the electric field (Fig.1a) and RCEM decreases to a minimum value first and then increases. This behaviour is qualitatively analogous to...
the one obtained in Ref.[1] for the same system without a magnetic field.

![Figure 1: The CO polaron self-energy (a) and the relative change in the effective mass (b) as a function of the electric field for different values of the magnetic field ($E_R \approx 32.4\text{meV}$).](image)

Fig.1 also shows that the polaron SE decreases with the increase of the magnetic field while the RCEM increases for the lower values of $F$ and decreases for the higher ones. It should be noted that in cubic CdSe cylindrical QWR CO polaron basic parameters increase with the increase of magnetic field [2]. This difference is apparently due to the structure anisotropy of wurtzite crystals.

This work has been supported by the Science Committee of the Ministry of Education and Science of Armenia (SC MES RA), within the frame of the research Project No.18T-1C247 and the Armenian National Science and Education Fund (ANSEF) research grant (condmatth-5214).

X-ray LLL interferometer with wedge-shaped mirror plate

Tigran H. Eyramjyan, Tamara S. Mnatsakanyan and Minas K. Balyan

Faculty of Physics, Chair of Solid States, Yerevan State University,
Alex Manoogyan 1, Yerevan, 0025, Armenia
email: tigeyro@ysu.am

Experimentally obtained interference patterns of X-ray LLL interferometer with wedge-shaped mirror plate show that the moiré fringes are superposed on pendellozung fringes and the period of pendellozung fringes is not changed after passing the analyzer plate. The predictions of the developed eikonal theory of interference fringes formation in interferometer with wedge-shaped mirror plate coincide with experimentally obtained results. Possible applications of the suggested interferometer for object investigations is discussed.


V.P. Chekusova, A.A. Trul, A.S. Sizov, M.S. Polinskaya, A.N. Kiselev, E.V. Agina, S.A. Ponomarenko

1 Enikolopov Institute of Synthetic Polymeric Materials RAS
2 Printed Electronics Technologies LLC
3 Lomonosov Moscow State University, Chemistry department
The purpose of our work was to develop high-sensitive reusable gas sensors, which can allow to detect NH3 and H2S gases in real-time mode in humid air atmosphere.

Our previous investigations demonstrate that monolayer films based on BTBT-derivatives possess high sensitivity to toxic gases such as NH3 and H2S due to strong dependence of the OFET electrical properties on the environment [1]. Such devises have several advantages: inexpensive fabrication techniques, low energy consumption as well as the opportunity of easy scale up to the industrial application without losing performance of the devices. These facts allow to use them as gas sensors for multiparametric real-time detection [2]. However, the main flaw of these devises is strong dependence of the OFETs electrical performance to water vapor presence in the atmosphere.

In order to reduce the influence of humid air as well as to improve selectivity of gas sensors the modification of LS OFETs by additional porphyrin receptor layers was undertaken.

Figure 1. Schematic representation of LS OFET architecture (semiconducting layer (blue) with additional receptor layer (orange))

Here we present new developed easy, fast and technological approach of porphyrin layer LS transfer from water surface to BTBT semiconducting monolayer without losing OFET electrical characteristics. Modification of OFETs by receptor layers allows to amplify sensor response in a humid air (up to 60% of humidity) as well as to decrease limit of detection (LOD) up to two times as compared with non-modified LS OFETs. All fabricated sensors demonstrated high reproducibility, fast response and full recovery after finishing gas exposure that paves the way to their use as chemo-sensors in real gas analyzing systems [3].
This work was supported by RSF (project № 19-73-30028) and performed in the framework of Leading Science School (grant № NSh-5698.2018.3)

2. A. Sizov et al. ACS Appl. Mater. Interfaces 2018, 10, 43831–43841

The features of complex formation of poly[d(A-C)].poly[d(G-T)] with porphyrins

Gayane V. Ananyan, Nelli H. Karapetyan, Yeva B. Dalyan

Chair of Molecular Physics, Faculty of Physics, YSU, 1 Alex Manoogian str., 0025 Yerevan, Armenia

The features of complex formation of water soluble cationic meso-tetra-(4N-oxyethylpyridyl) porphyrin (H$_2$TOEPyP4) and it's Cu- and Co-derivatives with synthetic double-stranded alternating polynucleotide poly[d(A-C)].poly[d(G-T)] was studied by UV/Vis and CD spectrosopes. The sequences (dA-dC).(dG-dT), which are often repeated in the eukaryotic genome, can regulate transcription [1]. Hence, double-stranded synthetic polynucleotide poly[d(A-C)].poly[d(G-T)] is a good model for physico-chemical studies that can provide additional insight into the structural requirements for the functionality of these natural repeats.

Binding mode of investigated porphyrins with double helix was determined by sign of induced circular dichroism (ICD) spectra in visible range [2]. In the case of H$_2$TOEPyP4 and CuTOEPyP4 observed both ICD: negative band at lower relative concentrations (intercalation, r<0.1) and positive band at higher relative concentrations (outside binding mode). In the case of Co-derivatives observed strongly pronounced positive bands. These results suggest that H$_2$TOEPyP4 and CuTOEPyP4 are intercalated into poly[d(A-C)].poly[d(G-T)], but CoTOEPyP4 binds only via external manner [1]. In high concentration range all porphyrins binds with duplex poly[d(A-C)].poly[d(G-T)] preferably via outside self-stacking mode regardless of the planarity of the porphyrin molecules. CD spectra in
UV range demonstrate the ability of poly[d(A-C)].poly[d(G-T)] to adopt a Z-type conformation.

The effect of the studied porphyrins on the melting parameters of poly[d(A-C)].poly[d(G-T)] has also been studied. Melting experiments of the studied complexes showed that the thermal stability of poly[d(A-C)].poly[d(G-T)] increases in presence almost all porphyrins. In addition, differential melting curves reveal two-stage melting of polynucleotides.

All experiments were performed in a phosphate buffer 0.1BPSE (BPSE=6mM Na$_2$HPO$_4$+2mM NaH$_2$PO$_4$+185mM NaCl+0.1mM EDTA), pH 7.0, ionic strength [Na$^+$] = 0.02M.

This research has been supported by grants SCS of RA 18T-1F055.


Elastoplastic deformation in nanophysics

Arakelyan M.M.

Yerevan State University, dep. of Physics

The study of the physical regularities of behavior of materials of various physical nature at the micro and nano level in a wide range of changes in external parameters is one of the actual problems of the experimental mechanics of a deformable solid. The Bauschinger effect is one of the main effects that determine the elastoplastic deformation and destruction of materials under alternating loading. From the point of view of the dislocation mechanism of plastic deformation, the Bauschinger effect indicates that when re-deformed, it is easier for dislocations to move in the direction opposite to their movement during pre-plastic deformation.
Dislocations are blocked in their place, so that when unloading they can not move until a reverse sign stress is applied. For single crystals of pure metals, the Bauschinger effect is explained by the theory of dislocations. A one-dimensional Frenkel – Kontorova dislocation model was used to describe the motion of a dislocation. Its motion in aluminum was considered taking into account the Peierls relief and friction forces in the presence of an external variable elastic field for various values of external parameters. The inhomogeneous Gordon sine equation is obtained in dimensionless variables with friction and a periodic external elastic field \( F(t) = F_0 e^{i\Omega t} \)

(\( F_0 \) the amplitude of the external force, \( \Omega \) its frequency):

\[
\ddot{\varphi}_n + \sin \varphi_n - \dot{\varphi}_n + \beta \varphi_n = \gamma \sin \frac{\Omega t}{\omega},
\]

\[
\omega^2 = \frac{2\pi f_0}{ma}, \quad \beta = \frac{\mu_0}{m\omega}, \quad \gamma = \frac{2\pi F_0}{ma\omega^2}, \quad \mu_0 - \text{coefficient characterizing friction, } \varphi_n \text{ is the displacement of the atom from the equilibrium position, and } a \text{ is the lattice constant. In this case, dissipation is understood as radiation friction. The boundary conditions are accepted in the form } \left[ \frac{\partial \varphi}{\partial x} \right]_{x=0} = \left[ \frac{\partial \varphi}{\partial x} \right]_{x=1}, \text{ where } l \text{ is the dimensionless length of the sample.}
\]

The dislocation displacement field is simulated at equal time intervals when the friction force and the presence of an external mechanical field are taken into account. As a result of numerical experiment it is received: dislocation at first moves to the right, then some time is blocked on the place owing to hardening, at change of a sign of an external mechanical field dislocation moves to the left. When the external alternating mechanical field is switched off, there is no effect of dislocation rotation. A stress-strain curve is obtained (hysteresis). It consists of elastic and plastic parts and illustrates the Bauschinger effect. The dislocation velocity before and after the rotation is periodic, which reflects the periodicity of the crystal structure at the micro level. When overcoming the Peierls barrier, the dislocation moves nonuniformly, accelerating in front of the barrier and slowing down after overcoming the barrier. The amplitude of the dislocation velocity before and after the turn changes as a result of
radiation friction, it decreases in absolute value after the turn. When a dislocation stops as a result of blocking its motion, the mechanical stress increases, and hence hardening occurs. The stress-strain curves are obtained for various temperatures. At low temperatures (-196°C), intense hardening occurs, while at the same interval of deformation at high temperatures (-78°C) the material goes into a state of perfect ductility. The long stage of hardening at low temperatures can be explained by the fact that in this case there is no noticeable rearrangement of the crystal microstructure. Thus, the Bauschinger effect is one of the main effects that determines the processes of elastoplastic deformation and fracture of materials under alternating loading at micro and nano levels, which is of considerable interest in nanophysics, the aerospace industry.

**Helix-coil transition in heterogeneous biopolymers.**

**The GMPC.**

**Asatryan A., Tonoyan Sh., Y. Mamasakhlisov, V. Morozov**

*Yerevan State University*

The problem of helix-coil transition has been investigated since 1960-s. There are many interesting results obtained [1]. However, number of essential problems still remain unsolved. One of such problems is connected with description of helix-coil transition in heteropolymers. The last we investigated in frame of GMPC, where various approaches were applied [2, 3, 4]. No additional approximation was used in straight multiplication approach and all the calculations were done in frame of GMPC by multiplication of transfer-matrices each of which corresponds to the exact type of repeated unit [3]. Free energy was calculated while using constrained annealing method [2]. And all the other parameters such as helicity degree, correlation length and others were obtained correspondingly. DMC-s were gained according to these approaches for bimodal heteropolymers with random sequences, block systems, regular heteropolymers and heteropolymers with correlation in sequence.
The results are qualitatively in agreement with experimental ones [5].


**Linearization of output characteristics of gas sensors based on MWCNT/SnO₂ structures**

*B.O. Semerjyan*

*Center of Semiconductor Devices and Nanotechnologies, YSU, 0025 Yerevan, Armenia*  
E-mail: semicsemer@ysu.am

One of the major advantages of gas sensors (GSs) based on multi-walled carbon nanotube (MWCNT) MWCNT/SnO₂ nanocomposite is the relatively high variation of the output parameters [1,2]. However, this type of GSs has several specific features making the processing of gas registration and measurement results difficult. These features involve distribution of resistance at very low registration values of gas concentration and considerable non-linearity of load characteristic as a result of inversely proportional character of transformation function from gas concentration to resistance. Elimination of these unfavorable characteristics is possible to perform in input measurement circuits
through proportional changing of GS conductivity to electrical signal.

In this study, for linearization of output characteristics of MWCNT/SnO$_2$ gas sensors, we propose to use the Wheatstone bridge circuit. GS resistance ($R$) shunting by constant resistance $R_{sh}$ leads to significant change in loading characteristics. Index of shunting is a ratio: $g=R/R_{sh}$, which is determined at $R=R_o$. From analysis of GS shunt effect on its output characteristic, it is obtained that along with reduction of shunt resistance (with increasing $g$) the nonlinearity of characteristic is sharply reduced at values $g < 5$ (at $g=5$ nonlinearity decreases twice). Further increase in $g$ will lead to slow decrease of nonlinearity. Essential distinguishing feature of nanocomposite-based high resistance GS (HRDS) with no use of Wheatstone bridge circuit is the instability of $R_o$ and high values of $\Delta R/R_o$. Consequently, application of the Wheatstone bridge circuit design for HRGS, at optimal $R_{sh}$, mainly results in highest sensitivity at lowest nonlinearity of the load characteristic. The bridge output characteristic $N(m)$ is determined according to [3] (m is the Wheatstone bridge circuit parameter). The theoretical results obtained in this study are also applicable to low resistance GSs owing to their “internal shunting”.

The Wheatstone bridge characteristics dependent on parameters $g$ and $m$ (the nonlinearity of output characteristic, the common resistance, the power supply voltage of circuit, and the output signal voltage) are calculated with the two-terminal “HRGS-Shunt” included in one of the bridge arms. We have obtained terms for HRGS performance linearization at preserved sufficiently high gas sensitivity and stability that permit application of standard electronics for registration of bridge readings.

Distortion Suppression Algorithm of Image Reconstruction in Hard X-Ray Fourier-Transform Holography Based on Two-Block Fresnel Zone Plate Interferometer with Common Optical Axis

L. A. Haroutunyan
Yerevan State University, Yerevan, Armenia
levhar@ysu.am

A hard X-ray Fourier-transform holography set-up, based on two-block Fresnel zone plat (FZP) interferometer is suggested in [1]. Being a diffraction grating the FZP has multiple diffraction orders. This is the reason for their usage as blocks of the interferometer. However, the same reason leads to difficulties in the interferometry due to the appearance of multiple wave propagation channels. The distortions in the lower half of the reconstructed image in [1] are caused by this “unwanted” channels of wave propagation.

Figure: The reconstructed images of the grid-like test object, carried out by (a) conventional and (b) “strip-by-strip” algorithms.

In the presented work the mechanism of formation of mentioned distortions is investigated and, based on it, the so called “strip-by-
strip” multistep algorithm of image reconstruction is suggested to suppress the distortions. According to this algorithm, the image reconstruction is carried out not by one step, but in a multistep way, reconstructing just one thin horizontal strip in each step. The reason for such approach is to darken the part of the hologram that form the distortions in the considered strip, at each step of the reconstruction. The narrower the reconstructed strip, the smaller the darkened part of the hologram and, consequently, higher reconstructed image resolution. Efficiency of the suggested algorithm is demonstrated in the figure, where the reconstructed images of test object, carried out by both conventional and “strip-by-strip” algorithms, are presented.


**Peculiarity of X-ray Phase Contrast at Diffraction Focusing of a Spherical Wave in a Superlattice**

*L.V. Levonyan, H.M. Manukyan*

*Yerevan State University, Armenia*

The study of the internal structure of weakly absorbing noncrystalline materials, as well as of biological samples, is usually carried out using the method of X-ray phase contrast. In [1] the possibility of reconstructing the internal structure of one-dimensional phase objects at diffraction focusing of X-ray spherical wave was investigated. As a crystal analyzer, a strongly absorbing wedge-shaped superlattice with a rib parallel to the diffraction vector was used in symmetric Laue geometry case. It is known that in this geometry, the diffracted radiation is focused inside the crystal, as well as behind the crystal, in vacuum. In [1] focusing inside the superlattice was used. In this work, we investigate the possibility of studying the internal structure of phase objects by means of
diffraction focusing of radiation behind the superlattice in vacuum. It is assumed that prior to the incidence on the crystal the radiation passes through phase object in which it is refracted according to the optical law $\sin \alpha / \sin \beta = n = 1 - \delta$, where $\alpha$ is the angle of incidence, $\beta$ is the angle of refraction, $\delta$ is the unit decrement of the refractive index $n$. The value of $\delta$ is directly proportional to the density of the material and for hard X-ray radiation is of the order of $10^{-5}$. According to the presented law of refraction, it is not difficult to estimate the change in the direction of the refracted ray $\gamma = \beta - \alpha \approx \delta \tan \alpha$, which is also of the order of $10^{-5}$ for not very large angles of incidence. A characteristic property of the diffraction of X-rays on superlattices is the presence of satellites around the main diffraction maximum, the position of which are determined by the relation $\Delta \theta_m = m/(kz_0)$, where $m$ is the satellite number, $z_0$ is the superlattice period, $k$ is the wave number in vacuum. For superlattice with $z_0 \sim 10^{-4}$ cm the angular distance of neighboring satellites for hard X-ray radiation will be of the order of $10^{-4}$. In the absence of phase object, the radiation incident from a point source has all possible directions near the Bragg angles $\theta_0$ and diffraction satellites $\theta_m$, so the focusing conditions are satisfied in all these directions. At the propagation of radiation through phase object, the conditions of focusing are violated, since as a result of refraction on inhomogeneities the rays change their directions and the wave front is deformed. Moving the phase object in the direction of diffraction vector will restore the focusing condition for a particular section or can lead to the appearance of new focus areas. By measuring the lateral width and coordinates of the reflex behind the crystal at two different distances, we can determine which satellite it corresponds to and calculate its focal length. According to the obtained data, it is possible to restore the internal structure of the corresponding section of the phase object.

Complex Phase Transitions of Oligomer Thin Films

Eduard Mikayelyan\textsuperscript{1}, Linda Grodd\textsuperscript{1}, Viachaslau Ksianzou\textsuperscript{2},
Daniel Wesner\textsuperscript{1}, Alexander I. Rodyn\textsuperscript{3,4}, Holger Schönherr\textsuperscript{1},
Yuriy Luponosov\textsuperscript{5}, Sergei Ponomarenko\textsuperscript{3,5}, Dimitri A. Ivanov\textsuperscript{3,4,6,7},
Ullrich Pietsch\textsuperscript{1}, and Souren Grigorian\textsuperscript{1}

\textsuperscript{1} University of Siegen, Germany
\textsuperscript{2} Technische Hochschule Wildau, Germany
\textsuperscript{3} Lomonosov Moscow State University, Russia
\textsuperscript{4} Moscow Institute of Physics and Technology, Russia
\textsuperscript{5} Enikolopov Institute of Synthetic Polymeric Materials RAS, Russia
\textsuperscript{6} Institut de Sciences des Matériaux de Mulhouse, France
\textsuperscript{7} Russian Academy of Sciences, Russia

A combination of in-situ electrical and Grazing-Incidence X-ray Diffraction (GIXD) is a powerful tool for studies of correlations between the microstructure and charge transport in thin organic films. The information provided by such experimental approach can help optimizing the performance of the films as active layers of organic electronic devices.

In this work [1], we have investigated the phase transitions in vacuum-deposited thin films of a common organic semiconductor dihexyl-quarterthiophene (DH4T) [2]. The initial crystalline structure exhibits a large number of Bragg reflections allowing assigning it to a monoclinic phase (see Figure). A transition from the initial highly-crystalline phase to a mesophase was detected upon heating, while only a partial backward transition was observed upon cooling to room temperature.

In-situ electrical conductivity measurements revealed the impact of both transitions on charge transport. This is partly accounted for by the fact that the initial crystalline phase is characterized by inclination of molecules in the plane perpendicular to the $\pi-\pi$ stacking direction whereas the mesophase is built of molecules tilted in the direction of $\pi-\pi$ stacking. Importantly, in addition to the two
phases of DH4T characteristic of the bulk, a third interfacial substrate-stabilized monolayer-type phase was observed. The existence of such interfacial structure can have important implications for the charge mobility, being especially favorable for lateral two-dimensional charge transport in the OFET geometry.

**Figure:** GIXD patterns of the highly crystalline vacuum deposited DH4T film with overlaid simulated Bragg reflections (red circles) for a monoclinic unit cell. Intensity line profiles measured along $q_\perp$ of 11 ± L (b) and 12 ± L (c) reflection families are given in purple and green color, respectively

Influence of ZnO nanoparticles in the stability and conductivity of BLM depending on its composition

Gayane V. Ananyan, Suzi M. Grigoryan, Tsovinar Jomardyan, Ishkhan V. Vardanyan, Valery B. Arakelyan

Chair of Molecular Physics, Faculty of Physics, YSU, 1 Alex Manoogian str., 0025 Yerevan, Armenia

In recent years, nanotechnologies and nanoparticles have been increasingly used in many fields of science and practice. Metal oxide nanoparticles have wide applications in biomedical applications as drug delivery systems for treatment and diagnosis. Currently they are widely used in medicine as targeted carriers of drugs for damaged tissue. Nanoparticle-cell interaction begins with their primary interaction with biological membranes [1]. Lipid bilayer is the basic structural element of biological membranes.

This work is devoted to the study of the effect of zinc oxide nanoparticles (ZnO), with an average size of 50 nm, on the stability and conductivity of BLM. The experiments were performed on BLM obtained from a mixture of 1,2-dipalmitoyl-sn-glycero-3-[phospho-1-serine](DPPS) and 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) of the company Avanti Polar Lipids in a ratio 1:1. Voltage, in the range of 0.20-0.55V, was applied to the BLM using chlorine-silver electrodes connected to the ADC and controlled by a computer. Experimental points were obtained depicting the dependence of the average BLM lifetime on the potential in the absence and presence of zinc oxide nanoparticles in solution. The parameters characterizing the BLM stability (BLM tension, the linear tension of the pore edge in the BLM and the pore diffusion coefficient in radius space) were determined from fitting the experimental data with a theoretical curve for the dependence of the average lifetime of the BLM on the potential [2].

The dependence of BLM stability in an electric field on the BLM composition is investigated. It was shown that the stability of BLM depending on the composition is in the following order: DPPS > mixture of DPPC and DPPS in a ratio of 50:50 > DPPC. The effect of ZnO nanoparticles on the stability of BLMs of various compositions was studied. It was shown that the presence of ZnO
nanoparticles in the surrounding BLM solution leads to an increase in BLM stability both in the case of BLM from DPPC and in the mixture of DPPC and DPPS in a ratio of 50:50. Moreover, the stability of BLM from a mixture (50:50) is higher than the stability of BLM only from DPPC.

It was shown that the electric capacitance and conductivity of BLM from phosphotidylcholine decrease in the presence of ZnO in the surrounding BLM solution. It has been shown that the electric capacitance and conductivity of BLM from both DPPC and a mixture of DPPC and DPPS in a ratio of 50:50 decrease in the presence of ZnO nanoparticles in the surrounding BLM solution. It was also shown that the conductivity of BLM from phosphotidylcholine in the presence of ZnO is higher than the conductivity of BLM from a mixture of DPPC and DPPS in a ratio of 50:50.


**X-RAY DOUBLE REFRACTION THROUGH NEMATIC LIQUID CRYSTALS UNDER INFLUENCE OF AN EXTERNAL ELECTRIC FIELD**

*V.P. Mkrtchyan, L.G. Gasparyan, T.K. Dadalyan*

*Yerevan State University*

Influence of an electric field on the refractive indices of the normal beam \( n_o \) and the abnormal one \( n_e \), as well as X-ray optical anisotropy of a nematic liquid crystal (NLC) of type E7 by X-Ray interferometrical method were investigated.
The NLC sample of 20 µm thickness was installed in a cell composed of two transparent glass plates and an electric field was applied to the NLC through the cell. The molecules of the NLC were oriented parallel to the cell plates by smearing a polymer layer over the NLC. To disorient the NLC molecules an electric field of 1kHz was applied by a signal generator; the applied field vector was perpendicular both to the polarization vector and the wave front. To measure \( n_o \) and \( n_e \) the experiment was carried out for the cases shown on the Pic. 1a and Pic. 1b. In the first case, the initial orientation of molecules, that is, the optical axis (\( N \)) had been perpendicular both to the polarization vector (\( \sigma \)) and the wave vector (\( K \)). When an electric field perpendicular to the optical axis was applied, the molecules were reoriented parallel to the field vector (\( E \)) and the wave vector, staying perpendicular to the polarization vector.

In the second case, the initial orientation of molecules (the optical axis) had been parallel to the polarization vector and perpendicular to the wave vector. When an electric field was applied, the molecules were reoriented parallel both to the field vector and the wave vector, staying perpendicular to the polarization vector; that is, the orientation of the LC optical axis under the electric field influence was the same for the both cases, \( (N \parallel E \parallel K \perp \sigma) \). Consequently, the refraction indices must go to the same value when the electric field increases.
To investigate the influence of an external electric field on the refraction indices of normal and abnormal waves the Moire pattern were obtained for various values of the electric field. The periods of these Moire fringes are the same, but their displacements depend on the electric field value, that is, on the NLC molecules orientation. Measuring the period and displacement of Moire pattern for different electric field values and using the formulae presented in [1-3], it is possible to find the decrements of the refraction indices, \( \delta = \frac{\lambda \Delta \Lambda}{t \Lambda} \), where \( \lambda = 0.709 \text{ Å} \) is the wavelength of MoK\( \alpha_1 \) radiation; \( \Delta \Lambda \) is the Moire patterns relative displacements; \( \Lambda = 620 \text{ µm} \) is the Moire period; \( t = 20 \text{ µm} \) is the thickness of the NLC layer. The results are presented on the Pic.2. One can see that when the electric field value increases, the decrements of the normal and abnormal beams increase too, going to the same value. This is due to the fact that the NLC molecules begin to gradually reorient under the influence of the electric field and, at a certain value of the electric field, the optical axes of the molecules of both cases have the same orientation (\( \mathbf{N} \parallel \mathbf{E} \parallel \mathbf{K} \perp \sigma \)).

\[ \delta = \frac{\lambda \Delta \Lambda}{t \Lambda} \]

Pic.2. Dependences of the decrement values of normal and abnormal beams on the electric field.

It is also shown that the difference of the mean values of the refraction indices, \( n_0 - n_e > 0 \), that is, the NLC of E7 type is a positive X-Ray optical anisotropic medium.
Solid-state properties of Poly(C3) polymers with closely-packed flourinated side chains

E. Bersenev$^{1,2}$

$^1$Moscow Institute of Physics and Technology (National Research University), Institutskiy per. 9, Dolgoprudny, Russian Federation
$^2$Institute of Problems of Chemical Physics, Russian Academy of Sciences, Semenov Av.1, Chernogolovka, Moscow Region, 142432, Russian Federation

In this contribution, we investigate properties of polymers with two closely packed –C$_8$F$_{17}$ side chains attached to every third carbon atom in main chain. This arrangement provides a side-chain positioning that allow lateral units to spread out efficiently and prevent steric crowding, while maintaining a very high degree of substitution along the backbone. Solid-state samples were systematically studied with DSC and SAXS. DSC curves obtained for homopolymer exhibit two major characteristic transitions: one between 60 and 70 °C and one between 90 and 115 °C on heating. The same two transitions appear during cooling with a significant hysteresis on their temperature position[1].

SAXS variable-temperature study reveal two sets of equidistant peaks that can be ascribed to two different smectic phases: one with larger (38.5 A) interlayer distance exhibiting much stronger peak intensities can be identified as SmB phase, second phase with interlayer distance of 28.6 A can be identified as SmC. In the latter case one should expect that a bilayer of mesogens, i.e. the side chains are inclined with respect to normal to the smectic layers.

In order to check the assignment of the dominant SmB phase, a thin film was formed on a Si substrate from melt, which
cause the planes of the smectic layer to orient parallel to substrate. At a room temperature, one can observe smectic diffraction peaks positioned in meridional direction on GIWAS pattern. In addition, a strong equatorial peak is observed at a distance of 5Å. This corresponds to packing of PTFE-like chains[2]. It can be therefore concluded that the pendant fluoro carbon chains packed in a hexatic structure are standing upright in the film. Experiments show a coexistence of two smectic phases SmB and SmC. The reason for such coexistence could be attributed to the fact that the distance between carboxylic oxygens bonded to the same carbon are very close to the ones between the neighboring carboxylic oxygens alongside the backbone. This results in the formation of two independent conformers with different packing modes for the pendant fluoroalkyl chains arranged in an hexatic order.

**Figure:** Variable temperature SAXS pattern and presumable polymer conformation for different phases

Investigation of drag force experienced by a moving object in granular medium

Salar Abbasi Aghda 1, Ali Naji 1,2*

1 School of Nano Science, Institute for Research in Fundamental Sciences (IPM), Tehran 19395-5531, Iran.
2 School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran 19395-5531, Iran.
*Corresponding authors: a.naji@ipm.ir

Amorphous materials are attracting considerable interest due to repulsion and dissipative particles feature such as randomness [1]. This material can be classified to colloidal suspensions, granular materials, emulsions, and foams. During the last decade, granular materials have been considered for their special applications more than other amorphous families. Specifically, granular matter is a collection of macroscopic solid particles like sand, coal, and coffee, whose behavior is important to numerous industrial applications (e.g., storage in silos, transport and processing, drilling for oil recovery, and mixing and segregation problems, etc.) [2-4]. Unlike traditional continuous matter such as Newtonian fluids, the rheology of granular materials is complicated by inhomogeneity in internal force transmissions [5]. The force applied is transmitted through force chains in a granular media. A particular example where such force transmissions become important is the motion of an object (intruder) in a granular bath. This behavior in a simple viscous fluid is especially well-established in the regime of low Reynolds numbers (large viscosity), where the fluid flow and the drag forces are described by Stokes equations [6]. However, it remains much less explored in the context of granular systems [7]. There are considerable researches –both experimental and simulation- that have tried to characterize the drag force experienced by a solid intruder moving in a granular media. Nevertheless,
previous works have only focused on characterizing the drag force experienced by a solid intruder moving in a granular media. Despite this interest, no one to the best of our knowledge proposed the efficient design.

The present paper aims to propose and validate the characterization of the effective force experienced by an external intruder moving in a granular bath which is a common motif in many applications in fluid dynamics, geophysics, and robotics. As an example, for the latter case, investigation of the motion of certain living organisms in grains, such as sand snakes, has been of interest in relation to designing artificial robotic devices able to perform efficient motion in granular beds [8].

We believe that we have developed and designed an innovative simple setup to define the role of those different parameters (grains and intruder size, packing fraction, penetration velocity, wall effects, and etc.) on the drag force.

Comparison of methylene blue interaction with human serum albumin and DNA

Shahinayan M.A., Mikaelyan M.S., Vardevanyan P.O.

Department of Biophysics, Faculty of Biology, Yerevan State University, A. Manoogian 1, Yerevan, Armenia 0025

Study of methylene blue (MB) interaction with DNA and human serum albumin (HSA) has been carried out. MB is known to possess anti-fungal, anti-bacterial, antiviral, anti-malarial activities and widely used in photodynamic therapy. Besides, MB is a ligand that specifically binds to DNA. In the present work the binding of MB with DNA and HSA was studied by absorption spectroscopy method [1]. In the fig. 1 the absorption spectra of MB-HSA (a) and MB-DNA (2) complexes were presented. From the given figure it is obvious that the absorption spectra of MB-albumin complexes practically coincide with MB spectrum, while in the case of this ligand interaction with DNA an apparent decreasing of absorptions of the complexes and a shifting to the relatively long wavelengths are obvious.

The specific binding of MB with proteins is not revealed. Absence of MB specific binding to albumin is maintained based on the spectral studies. In the case of MB interaction with DNA, a relevant alteration of the absorption spectra takes place (fig. 1b), while in the case of this ligand interaction with HSA the change is insignificant (fig. 1a). Apparently, in the bound state with albumin, MB has practically the same spectral characteristics as in free state, while in the case of DNA these characteristics noticeably differ. Particularly, at the intercalation (or semi-intercalation) the heterocyclic aromatic molecule of MB transits from the solution to hydrophobic, internucleotide space and enters to stacking interaction with DNA azotic bases. It leads to considerable weakening of the ligand molecule oscillation strength, in the consequence of which the absorption spectra maxima of MB-DNA complexes decrease and a little shift of the spectra of the complexes to long wavelengths occurs as well. At the binding with albumin the oscillation strength change of the ligand chromophore group does not occur, which indicates that the surrounding of MB bound molecules to protein is practically the
same as the surrounding of free molecules. Based on this fact we assume that MB does not interact with albumin by any specific mechanism.

**Figure:** Absorption spectra of MB (1) and its complexes with albumin (2-37) (a) and DNA (2-17) (b). MB concentration was equal to \(~7.1 \times 10^{-6}\) mol/l at the interaction with albumin and \(~6.01 \times 10^{-6}\) mol/l – at the interaction with DNA.


**The effect of the molecular mass of PEG on the nature of its interaction with DNA**

*Ani A. Avetisyan, Gayane V. Ananyan, Vigen G. Barkhudaryan*

*Chair of Molecular Physics, Faculty of Physics, YSU, 1 Alex Manoogian str., 0025 Yerevan, Armenia*

We studied the influence of the molecular mass of polyethylene glycol (PEG) on the nature of its interaction with DNA. PEG is a
very common food supplements, used as thickeners in many fields, also for condensation of DNA. The effect of oligomers and polymers at various masses of PEG on the conformation of DNA was studied by spectrophotometry and viscosity methods.

The viscometric measurements show that PEG oligomers (mol. mass 400, 1000, and 2000) have absolutely no effect on DNA macromolecule’s size in the studied concentration ranges. The condensing properties of PEG on DNA macromolecule sizes are observed at presence of PEG with molecular masses of 6000, 7000, 10000, 20000 and 40000. The insignificant increasing of DNA macromolecule sizes was observed at interaction with PEG6000 and PEG7000, which is interpreted as a consequence of the complexation of PEG-DNA. In high concentration range of PEG the solution viscosity decreased, which may be caused by decrease of DNA macromolecule sizes. This effect can be explained by a change in the balance of hydrophilic-hydrophobic interactions or by the redistribution of DNA surface negative charges as a result of interaction with PEG. The linear dependence of the viscosity of DNA and PEG on the composition of the solution corresponds to the principle of additivity.

The presented results were confirmed by spectrophotometric studies too.

At the Heliotechnics laboratory of the National Polytechnic University of Armenia a vacuum equipment for growth of preferred thin carbon cover layers is constructed using the effect caused by intersection of electric and magnetic fields. Layers based on diamond-like carbon as well as metal oxides are obtained by using equipments of plasma enhanced ion plasmon and magnetron techniques simultaneously. It is well known that these layers differ greatly depending on method of producing plasma flow and on the origin of used hydrocarbon. In case of decomposition of complex hydrocarbons, neutral or ionized atoms along with complex radicals are formed in the electromagnetic field maintained by the ion source. The main cause for the origin of complex radicals are the low power of the ion source and the high flow density of Hydrogen. For this reason the choice of ion source power and the content of gas mixture is of prime importance and the proper choice can allow obtaining of needed plasma flow which form structures with predicted composition. DLC layers exhibit great mechanical strength, flexibility, high optical transmission in the visible light range as well as they are indifferent to chemical media. During the process of synthesis in case of doping the structures with Nitrogen or Hydrogen or with other components the layers obtain the wide range of refractive index [1] and brighten up which is a valuable property for application.
A route to further application of such layers is their application in photoelectric conversion devices [2]. The application of different methods and technical regimes will make possible to obtain structures with diverge optical, electrical, mechanical and surface properties.

By deposing such thin layers on substrates of semiconducting materials such as Si, Ge, GaAs as well as on the surface of solar energy converters made of these semiconductors, in addition to abovementioned protecting properties the reflection of light decreases multiple times and increase carrier mobility [3]. DLC as well as thin metal layers can be deposed on the surface of window glasses for reflecting back the heat to living room. This technique can be used to cover car windows for both decorative and energy saving purposes, and the surface sunglasses for skiing etc.

To succeed in application of our ideas currently we need companions with whom the frontier of co-operation could be different:

• Foundation of an international company for covering different surfaces with DLC;

• Our laboratory can cover the surface of flexible organic and inorganic films and protect them for a long period of time, or provide rolled films for applying on any surface.

• To develop the business and to penetrate the business market we intend to find collaborators and investors, who are interested in the research and obtained results.


Zinc oxide composites in the antitumor and antibacterial drug delivery system

Emma R. Arakelova¹, Stepan G. Grigoryan², Ashot M. Khachatryan¹, Anahit A. Mirzoian¹, Zoya M. Farmazyan¹, Susanna L. Grigoryan¹, Mkrtich A. Yeranosyan¹,³, Flora G. Arsenyan², Rafayel Muradyan²

¹National Polytechnic University of Armenia, Yerevan, Armenia
²Scientific Technological Center Organic and Pharmaceutical Chemistry, Yerevan, Armenia
³Yerevan State University, Yerevan, Armenia

Currently nanomedicine is dominated by nanoparticulate drug delivery systems because of their ability to cross biological barriers and increase the solubility of drugs. The use of metal oxide, in particular zinc oxide nanoparticles(ZnONPs) has made a significant contribution to diagnostics and therapy of various diseases. Semiconductor ZnO films have a wide practical use in optoelectronic and sensing devices, medicine and shows photocatalytic, antibacterial, antitumor activity.

This work is devoted to a novel drug delivery platform based on zinc oxide composites of antitumor as well as antibiotic drugs formed by DC magnetron deposition of nanosize ZnO particles on the surface of drug coatings and composite films. For example, doxorubicin (DOX) zinc oxide composites in the form of coatings (DOX+ZnO) on glass and composite films with polyvinyl alcohol (DOX+PVA+ZnO) have shown in vivo experiments on mice on the model of ascetic Ehrlich's carcinoma higher (by a factor 2) antitumor activity at much lower doses in comparison with the initial preparations at therapeutic doses.

Presently in vivo study on Staphylococcus aureus 5 (on mice) has shown that zinc oxide compositions of the antibiotic drug, doxycycline (DOXY), in the form of coatings (DOXY+ZnO) and composite films with PVA (DOXY+PVA+ZnO) at the lower doses (50mg/kg) show higher/or same activity (90% and 80%) in
comparison with the initial drug at higher doses (100mg/kg) (76% and 80%). Much the same difference was observed for *Sh Flexneri* 6858 strain. Using the methods of spectroscopy, atomic force microscopy (AFM) and X-ray Powder Diffraction (XRD), the role of ZnO NPs size on the antitumor and antibiotic activity of DOX and DOXY zinc oxide compositions is shown. The antitumor and antibiotic drug delivery system based on the thin film technology for obtaining zinc oxide composite drugs has several basic advantages: purity of zinc oxide compositions formed in vacuum, controlling the process of formation of the compositions at low deposition temperature without undesirable side transformations, simplified techniques of controlling of ZnO NPs size deposited on the surface of antitumor and antibiotic drugs which allows formation of composites with optimal technological characteristics and target delivery of the composites to affected tissues.

![AFM pictures](image)

**Figure:** AFM picture: (a) morphology sample DOX+ZnO, (b) morphology sample DOXY+PVA+ZnO

Peculiarities of the interaction of different ligands with nucleic acids

Antonyan A.P., Parsadanyan M.A., Vardevanyan P.O.

Department of Biophysics, Faculty of Biology, Yerevan State University, A. Manoogian 1, Yerevan, Armenia 0025

During the recent years the quick and efficient method of preparation of new biologically active compounds has been elaborated using nanoparticles on the basis of branched molecules of DNA. Meanwhile, DNA molecules serve as a “skeleton” of the complicated molecule that plays the role of a carrier of these compounds [1]. Dendromers are the important components of this nanosystem that can carry themselves various biologically active molecules: drugs, protein markers, fluorescent agents. From this point of view, the nanoparticles become an ideal measure to import drug or bioactive preparations into a cell. Consequently, the problem of the interaction mechanisms of biologically active molecules – ligands with DNA-nanoparticles becomes an important topic.

It is necessary to mention that ligands bind to nucleic acids (NA) by more than one mode, since their classification into intercalators and non-intercalators is quite conditional. Thus, the results of our experimental data reveal that EtBr is a classical intercalator, though, it may be considered also as a classical multimodal ligand due to the ability to bind to NA by several modes, which in turn does not depend on both the ionic strength and pH of the solution [2]. Moreover, EtBr at the interaction with NA shows multimodality in the presence of the other, competitive ligands. Analogous studies, carried out on MB interaction with NA indicate that the multimodality of this ligand is conditioned by the medium factors, particularly by the solution ionic strength, since at the low ionic strengths the real multimodality is displayed, while at the relatively high ionic strengths not all binding modes of this ligand to NA are performed. This fact is important, since MB is considered to be an intercalator and it is thought that one of its binding mechanisms is the intercalation. As our data show the main binding mode for this ligand actually is a semi-intercalation. MB owns some peculiarities, particularly, fluorescence properties, that make different this ligand
from the others possessing the same characteristics. Nonetheless, the experimental data on MB interaction with NA allows to classify this ligand as a multimodal one.

The same thoughts are not justified in the case of non-intercalator, groove-binding compound H33258. The experimental data reveal that the ionic strength of the solution radically changes the binding mechanism of this ligand to DNA, moreover, at the certain conditions this ligand can bind to DNA by two, controversial mechanisms, one of which corresponds to the principle “key to lock” (groove binding), another – so called “fit-to-fit” (intercalation, at which the ligand molecules should fit to DNA molecule), which indicates that this ligand is also a multimodal one.


**Interminiband absorption in a quantum ring superlattice in transverse magnetic field**

V. Aziz-Aghchegala¹, V. Mughnetsyan², A. Atayan³, A. Kirakosyan²

¹Department of physics, Urmia university of technology, Urmia, Iran

²Department of solid state physics, Yerevan state university, Yerevan, Armenia

³Department of Medical Physics, Yerevan State Medical University

Nanostructured materials in which the system of conduction electrons can be considered as two-dimensional are subject of an extensive investigation during the last two decades. Among them graphene [1–3] and other atomic monolayers are of great interest. The intraband optical absorption in QRs has attracted an enormous interest in recent years [4] because of large optical nonlinearity observed in these structures and potential applications in photodetectors and high-speed electro-optical devices [5].
The miniband Aharonov-Bohm oscillations and the interminiband absorption coefficient have been considered theoretically for one-layer superlattices of square and rectangular symmetries, composed of cylindrical quantum rings in the external transverse magnetic field with a periodic vector potential by the lattice constants:

\[
\begin{align*}
A_x &= -(B/2) \sum_{C_y}(y-C_y) \Theta \left( a_y/2 - |y-C_y| \right) \\
A_y &= (B/2) \sum_{C_x}(x-C_x) \Theta \left( a_x/2 - |x-C_x| \right) \\
A_z &= 0
\end{align*}
\]

where \( C_{x(y)} \) and \( a_{x(y)} \) are the \( x(y) \) components of the lattice vector, and lattice constant, respectively, \( B \) is magnetic field induction and \( \Theta(\xi) \) is the unite step function. The crossings and anticrossings of the energies corresponding to different values of quasimomentum are observed. It is shown that the energy gap between the minibands and
the sequence of the energies in each miniband can be tuned by the magnetic field. The interminiband absorption coefficient qualitatively depends on the symmetry of the superlattice, magnetic field induction and the incident light polarization. The obtained results indicate on the possibility to control the electronic and optical characteristics of the devices based on quantum ring superlattices.

2. A.K. Geim, K.S. Novoselov, Nat. mater. 6, 183 (2007).

Morphology and optical characterization of physical vapor depositied PbI$_2$ films

H. Dashtoyan$^1$, M. Yeranosyan$^{1,2}$

$^1$ National Polytechnic University of Armenia
$^2$ Yerevan State University

Attention to the Lead Iodide (PbI$_2$) is mainly caused by the possible use as a material for flat-panel x-ray imagers [1]. Also, PbI$_2$ occupies a highly prominent role in the field of photovoltaics as a key precursor in the synthesis of organo-lead halide absorber layers [2]. As well PbI$_2$ is a well-known layered semiconductor and may be used as a convenient model object for studying the features of physical phenomena in quasi-two-dimensional systems due to the weak Van der Waals interaction between layers.
Nanostructured micron-sized optical quality PbI$_2$ films were synthesized on a glass substrate at room temperature by the physical vapor deposition method (vacuum level $\sim 10^{-5}$ torr). Basic investigations of deposited films were carried out. The shape and size of the nano-sized particles (NPs) were analysed using Atomic Force Microscopy (AFM). Independent measurements of T and R at the near-normal incidence of light (spectral range 400-1000 nm with spectrophotometer Filmetrics F20) showed that fabricated films are void-free and mainly consist of close-pack NPs with the length and height 238nm and 50nm respectively (Fig. 1). Also, a complete set of optical parameters: refractive index (n), extinction (k) and absorption coefficient (a), optical band gap (2.46 eV) of fabricated films were determined via calculations based mainly on Swanepoel's (envelope) [3] method (Fig. 2).

![AFM image of PbI$_2$ nanostructured film surface.](image)

**Fig. 1** AFM image of PbI$_2$ nanostructured film surface.

![Optical characteristics of PbI$_2$ film.](image)

**Fig. 2** Optical characteristics of PbI$_2$ film (thickness 1 µm).
Acknowledgements

This work was partially supported by SC MES RA, within the frame of the research Project No. 18T-1C247, ANSEF research grant (condmatth-5214).


Peculiarities of melting DNA from Crocker's sarcoma of a mouse treated with Ag-meso-tetra(4-N-hydroxyethylpyridyl) porphyrin in the presence of Mn^{2+} ions.

Nelli H.Karapetyan*, Gayane V.Ananyan, Yeva B.Dalyan,

Chair of Molecular Physics, Faculty of Physics, YSU, 1 Alex Manoogian str., 375025 Yerevan, Armenia

The melting futures of DNA isolated from liver and spleen of healthy, tumor-diseased and treated by Ag-meso-tetra(4-N-hydroxyethylpyridyl)porphyrins (AgT4OEPyP) mouse’s were investigated in presence of Mn^{2+} ions.

In the present work we used a method that allows reveal the conformational state of DNA by investigating the influence of transition metal ions, such as Mn^{2+} on the intra-molecular melting. The DNA melting was performed in the presence of different stoichiometric concentrations of Mn^{2+} ions. It is known that in DNA samples isolated from tumor cells defects in the secondary structure are found. So, this method allows evaluate structural changes in DNA molecule. The structural changes may influence the character of the DNA-Mn^{2+} ion interactions, which allows one to reliably detect the structural differences of DNA isolated from normal and tumor cells.

The melting parameters (the melting temperature and the melting interval) of DNA isolated from the tumor-diseased mouse’s tissues
differed from the healthy DNA. In DNA samples of healthy animals the Mn$^{2+}$ ion binds to the sites of excess charge density at the guanine bases, leading to selective destabilization of GC base pairs, which leads to equalization of the thermal stabilities of AT and GC pairs and, consequently, to the narrowing of the melting interval ($\Delta T$). In presence of defects in the secondary structure of tumor DNA the access of metal ions to the defective areas is difficult, which leads to a smaller narrowing of the melting interval of tumor DNA compared to healthy. The melting parameters of the DNA isolated from the treated by AgT4OEPyP mouse liver and tumor tissues were approaching to the norm. The obtained results revealed that AgT4OEPyP4 porphyrins have a antitumor effect.

This effect was observed in DNA from tumor and liver cells. However, in the DNA isolated from the spleen, the described effect was less pronounced.

The experimental studies were conducted within the framework of RA MES Committee of Science Project no 18T-1F055.


**Synthetic Analogues of Proteins – Biodegradable Polymers for Numerous Biomedical Applications**

*Ramaz Katsarava*

*Institute of Chemistry and Molecular Engineering, Agricultural University of Georgia, Kakha Bendukidze University Campus, # 240 David Aghmashenebeli Alley, Tbilisi 0131, Georgia*

*r.katsarava@agruni.edu.ge*

Biodegradable polymers (BPs) - “green materials” of the future, have an innumerable uses in biomedicine, particularly in the fields of
tissue engineering and drug delivery. Among this kind of materials highly suitable are naturally occurring polymers - proteins which are constituted of one of the most important “bricks of life” - \( \alpha \)-amino acids (AAs). A wide biomedical applicability of proteins is due to special properties such as a high affinity with tissues and releasing AAs upon biodegradation that means a nutritive potential for cells. Along with these positive characteristics proteins have some limitations such as batch-to-batch variation, risk of disease transmission, and immune rejection. The last limitation is connected with the molecular architecture of proteins. Furthermore, the content of only peptide bonds in protein molecules significantly restricts their material properties. Synthetic analogues of proteins made of AAs look by far more promising as biodegradable biomaterials since they are free of the limitations of proteins retaining at the same time their positive features – a high tissue compatibility and nutritive potential. The present review deals with a brief description of different families of the synthetic analogues of proteins such as poly(amino acid)s, pseudo-poly(amino acid)s, polydepsipeptides, and pseudo-proteins - relatively new and broad family of synthetic AA-based BPs. Most of these polymers have a non-proteinaceous architecture and contain in the backbones various types of chemical links along with peptide bonds that substantially expands properties of materials destined for sophisticated biomedical applications [1].


Application of nanocalorimetry for analysis of phase behavior of azido-acetylene microparticles

*E.V. Komov\(^{1,3}\), A.A. Piryazev\(^{1,3}\), D.V. Anokhin\(^{1,3}\), D.A. Ivanov\(^{1,2,3}\)*

\(^{1}\) Faculty of Fundamental Physical and Chemical Engineering, Lomonosov Moscow State University (MSU), GSP-1, Leninskie gory - 1, 119991 Moscow, Russia

\(^{2}\) Institut de Sciences des Matériaux de Mulhouse - IS2M,
Over the past few years, much attention has been paid to the synthesis, study of properties and investigating the ways of using hyperbranched polymers with azide and ethynyl groups, as well as with triazine and triazole rings [1]. Monomers of AB\textsubscript{2} type are the best ones to produce such kind of polymers. The main feature of AB\textsubscript{2}-compounds is carrying out of reactions under mild conditions, besides they are very susceptible to chemical aging, so the study of this issue is important for their practical usage. In this study we used three different monomers of that type: 2-azido-4,6-bis(propyne-2-yloxy)-1,3,5-triazine (ABPOT), 2,4-diazido-6-(propyne-2-yloxy)-1,3,5-triazine (DAPOT) and 2-azido-4-(propyne-2-ylamyno)-6-bis(propyne-2-yloxy)-1,3,5-triazine (APAPOT). The last one is much more stable in the studied temperature range.

Using standard methods of thermal and structural analysis such as TGA, DSC and X-Ray analysis, we observed the processes of melting, polymerization and decomposition of bulk samples and made conclusions about their thermal behaviour and stability. Due to the local heating effect which can make an impact on its phase state in bulk, it is necessary to explore phase transitions of their microparticles with nanocalorimetry and polarization optical microscopy for studying the effect of chemical aging.

Nanocalorimetry has proven itself for the study of energetic substances [2, 3]. The combination of a nanocalorimeter with an ultrahigh-speed camera makes it possible to interpret more accurately the thermal effects that occur to microparticles during ultrafast heating: for aged samples, one can see the decrease of an enthalpy of melting, as well as the appearance of peaks of thermal decomposition at high temperatures (Fig. 1). Nanocalorimetry data for non-oligomerized samples demonstrates the appearance of evaporation steps and the absence of polymerization peaks.
Figure 1: Nanocalorimetric curves of ABPOT (left) and aged DAPOT (right) with microphotographs made with fast CCD camera.

Thus, we studied the processes occurring during thermal treatment of triazine-based monomers. The obtained results give us an additional insight into the thermophysical processes in azido-acetylene monomers based on energy-intensive triazines, as well as their interactions and effect on each other.

Boron nanoparticles: production, properties, various applications

1. Polina Khaptakhanova¹, Sergey Uspenskii¹, Tikhon Kurkin¹

¹ Enikolopov Institute of Synthetic Polymeric Materials, Russian Academy of Sciences, Moscow, 117393 Russia
2. khaptakanova@ispm.ru

The use of boron nanoparticles as additives in various materials is becoming increasingly widespread due to the unique structural complexity, valuable properties of nanoparticles, as well as a wide range of existing and potential applications.

Basically, the options for the synthesis of boron nanoparticles are the methods of chemical deposition from the gas phase. Such methods may be classified as follows: electron beam method, laser method, plasma method, arc evaporation method, or a combination of thereof. The advantages of precipitation method are tonnage, high yield of the target product (close to 98%) and a high degree of purity of elemental boron (99.6-99.9999%). By using most of precipitation methods, it is possible to obtain crystalline powders of elemental boron, in which micron-sized particles predominate as a result of the sintering process. The transition to nano-objects is due to a change in the surface area of the particles, which itself leads to the appearance of unique size effects. Ultrasonic technology is a new approach to improving the implemented methods of chemical deposition from the gas phase, i.e. the dispersion of sintered powder with micron particles to nanoscale. The proposed method is economical and technically easy to implement. By using this method and by means of specifically selected technological conditions it is possible to obtain a sufficient amount of boron nanoparticles in a short period of time. By using prolonged (400 minutes) exposure to ultrasound and cascading fractionation the lines of particle dispersions of less than 100 nm were obtained. As a result of repeated exposure of the ultrasound to the 80 nanometer fraction the particles of less than 20 nm were obtained, while it should be noted that, there was a tendency to a decrease in size and their ovalization. The structural parameters (size, shape) of the obtained particles were characterized using dynamic light scattering, electron microscopy. To assess the effect of ultrasound on the crystal structure of elemental boron – X-ray diffraction analysis was used. The degradation of the initial crystal structures is observed under the influence of cavitation flows
generated in liquid media in the presence of ultrasonic waves, and the dispersion of the initial micron boron powder increases [1]. The implementation of boron nanoparticles obtained by ultrasonic dispersion technology may find new various applications. In medicine: in boron neutron capture therapy of malignant neoplasms, where due to the property of the boron-10 isotope to absorb neutrons, nanoparticles based on it can be used as a target agent. The advantage of nanoparticles in comparison to the practiced clinical drugs is a high content of boron-10 atoms in one nano-particle, which will allow achieving the necessary therapeutic concentration of the isotope in the affected area [2]. High energy biofuel supplement. An alternative application of boron nanoparticles is their use as an additive in fuel which is possible due to the large volumetric heat of reaction with oxygen - 138 kJ / cm3. According to x-ray diffraction analysis, after prolonged treatment of micron boron powder with ultrasound in a liquid medium, the reflection of the B2O3 boron oxide was not detected in the diffractogram of the nanosample, which increases the potential for using nanoparticles as an additive to fuel. The presence of an oxide layer in the surface of the particles significantly complicates the ignition of elemental boron, which limites the scope of nanoparticles. Nanoscale filler in polymeric materials. The presence of a developed specific surface for boron nanoparticles opens the potential for their use as a nucleating additive in polymers. Studies have been conducted on the effect of boron nanoparticles on polylactide. According to X-ray diffraction analysis, the crystallinity of the final nanocomposite increased, i.e., a developed crystalline structure of macromolecules is formed in the boundary layer between the nanoparticle and the polymer due to the structuring activity in the surface of the boron particle, which leads to an increase in the thermodynamic conditions of crystallization of macromolecular chains.

The nanoparticles of elemental boron boron obtained by such new technological method are a promising material for further scientific research in various fields of technology.

Change of charge transport type in thiophene-phenylene co-oligomers via terminal substitution

D.I. Dominskiy*, V.A. Trukhanov¹, A.Yu. Sosorev¹, L.E. Yakushkin¹, A.S. Komolov², O.V. Borshchev³, S.A. Ponomarenko²,³, D.Yu. Paraschuk¹,³

¹Faculty of Physics & International Laser Centre of Lomonosov Moscow State University, Russia
²St. Petersburg State University, Russia.
³Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences, Russia
⁴Chemistry Department, Lomonosov Moscow State University, Russia
*e-mail: di.dominskiy@physics.msu.ru

Thiophene-phenylene co-oligomers (TPCO) are promising optoelectronic materials for light-emitting devices and lasers as they combine efficient charge carrier transport and high luminescence¹,². These organic materials exhibit mostly p-type charge transport; whereas the n-type transport is not easy to realize. Fluorination is a well-known approach to alter the electronic properties of p-type semiconductors. For example, common p-conductive organic semiconductors such as pentacene, copper phthalocyanine, diethynyl naphthalene and oligophenylenevinylenes can be converted to the n-conductive ones via fluoro-substituents³,⁴.

Here, we study the impact of fluorination of the methyl terminal group on the structural and electronic properties of single- and polycrystals of TPCO with the phenylene-thiophene-thiophene-phenylene (PTTP) conjugated core using x-ray diffraction, DFT and dipole moment calculations, total current spectroscopy (TCS) and field-effect transistor (FET) measurements.
Figure: Transfer characteristics of single-crystal TPCO based OFET devices with Ca and MoO$_3$/Ag top electrodes (a) CH$_3$ and CF$_3$ at $|V_d|=50$ V, (b) TMS at $|V_d|=100$ V.

Our experimental data show that fluorination of the methyl terminal group in CH$_3$-TPCO results in an insignificant impact on the crystal habit and on the molecular orientation vs their basal plane but switches the conductivity from the p-type to the n-type (Fig. 1a). We suggest that the terminal groups control the charge injection type into the FET active layer.

*This work was partially supported by RFBR (project № 18-03-00020), by RSF (project № 18-12-00499) for material synthesis and device fabrication and studies, and by the Foundation for the advancement of theoretical physics and mathematics «BASIS».*

2. L. Kudryashova et al.: ACS Applied Materials & Interfaces, 8, 16, (2016)
Recently ultrathin (2D) organic electronics became a topic of great interest for research and applied development in pursuit to create superlightweight, transparent, ultraflexible and inexpensive electronic devices based on organic semiconductor films with a thickness of one or more molecular layers. However, luminecent properties of 2D semiconductor single crystals are unknown, despite the fact that they would be useful because of their high structural order. Thiophene-phenylene materials are promising for organic optoelectronics because of lucky combination of decent charge-carrier mobility and high luminescence. Linear conjugated thiophene-phenylene molecules with long alkyl terminal substituents easily form large-area 2D single-crystal monolayers.

This work is focused on photoluminescence (PL) properties of 2D samples based on (Dec-P)₂-BTBT molecules (Fig.1, top). 2D samples were prepared from solution and studied with interference, atomic-force, and confocal PL microscopies. We found polarization anisotropy in PL of (Dec-P)₂-BTBT monolayers. (Fig. 1, bottom) and thus helped us to identify differently oriented monolayer domains. The PL properties of 2D (Dec-P)₂-BTBT single crystals are discussed.
Fig 1. Top: chemical structures of (Dec-P)₂-BTBT (right) molecules. Bottom: panels (a)-(b) show PL maps with different laser polarizations marked by thick white arrows. Panel (c) plots the difference between intensity maps presented in (b) and (a). AFM profiles show the borders between (a) mono- and bi-layer, (b) substrate and mono-layer and (c) between the monolayer domains.

This work was supported by Russian Science Foundation (#18-12-00499)
The investigation of electronic structure and optical properties of YGa$_2$

Mane Sahakyan$^1$ and Vinh Hung Tran$^1$

$^1$Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P. O. Box 1410, 50-422 Wroclaw, Poland

E-mail for corresponding author: m.sahakyan@intibs.pl

First principles calculations were performed to study the electronic structures of YGa$_2$ compound with different layer in order to understand the influence of layer number on electronic and optical properties for this compound, using the projector augmented wave (PAW) method [1] with the Generalized Gradient Approximation (GGA). First-principles electronic structure calculations were performed within the framework of density functional theory (DFT) by means of VASP Simulation Package [2]. The exchange-correlation potential of Perdew–Burke–Ernzerhof (PBE) for electron–electron interactions is used [3]. The accuracy for the total energy convergence after the self-consistent calculations has been set at $10^{-8}$ eV. The tetrahedron method of k-integration has been applied for the self-consistent calculations with the (8; 8; 12) k-mesh of the Brillouin zone, according to the Monkhorst–Pack grid scheme [4]. The optical anisotropy in YGa$_2$ is analyzed through the optical functions such as refractive indices and static dielectric constants along the principal axes. Our calculated band structure and optical spectra have also been compared. In addition, we have compared our results with the theoretical results of MgB$_2$ and AlB$_2$ [5], which crystalize with the same space group ((AlB$_2$ type structure at NTP, space group P6/mmm)).

Acknowledgments

This study was supported by the National Science Centre in Poland under grant No 2016/21/B/ST3/01366.

INFLUENCE OF CATION PORPHYRINES ON DNA DAMAGE DURING ELECTRON BEAM IRRADIATION

L.R. Aloyan, Y.B. Dalyan, S.G Haroutiunian
Yerevan State University, Al. Manoogian 1, Yerevan, 0025, Armenia.

Radiation therapy uses electrons beams to treat tumors. The fast electrons directly ionize the DNA molecule, causing damage. The understanding and study of DNA damage mechanisms causing by ionizing radiation is one of the important problems in the development of new cancer therapies and effective radiosensitizers. The usage of the porphyrin-based Photodynamic Therapy (PDT) in conjunction with electron beam radiation therapy can be one of the effective methods for cancer. Porphyrins have attracted the attention of researchers globally for application as photosensitizing agents in medicine. However, our recent studies shown that some porphyrins (Fe cationic metalloporphyrins) have protective effect on DNA during radiation. The goal of our investigations was to continue previous investigations, to examine DNA damage in the presence of different amounts of water soluble cationic meso-tetra- (4N-oxyethyl-pyridyl) porphyrin and it’s Fe and Cu - containing analogs induced by 3-4 MeV electron radiation depending on radiation doses in vitro. The samples with different relative concentrations of porphyrins were irradiated by the electron beam. And then revealed the possible protective or sensibilizing effects depending from quantity of porphyrins and radiation doses.

It is known, that the melting parameters ($T_m$ and $\Delta T$) of DNA is sensitive to the structure of double helix. Conclusion about the changes occurred in DNA can be done from melting parameters of the DNA ligand complexes. Therefore, it can be used as an indicator of strand breaks of DNA molecules after radiation. After samples radiation the melting curves of DNA-porphyrin complexes were obtained.
The water soluble cationic 4-N meso-tetra-oxyethyl-pyridyl, 4-N meso-tetra-allyl-pyridyl porphyrins and their Cu and Fe analog were used in this work. The samples with different relative concentrations of porphyrins per base pair were irradiated by the electron beam. After samples irradiation, the melting curves (the dependence of denaturized DNA percentage on temperature) of investigated complexes were obtained. It was shown that at the radiation dose equal 1Gy, the metall free porphyrins and Cu containing metalloporphyrin causes a stronger radiation effect on the DNA structure, which grows with increasing porphyrins concentration. While the effect on DNA structure of Fe containing metalloporphyrin is non-essential that can be result of the protective effect of these porphyrins. At the higher radiation dose (2 Gy) for all porphyrins we abtaind the same rezult, depending on the dose increases the damage effect is incerasing. For FeTOEPyP4 porphyrins we suggest that at the 2 Gy the effect of radiation exceeds the porphyrins stabilizing and protective effect on DNA at all examined relative concentrations of porphyrins.

The experimental studies were conducted within the framework of RA MES Committee of Science Projects no 18T-1F055.