



Georgian Technical University



Shota Rustaveli National Science Foundation of Georgia

## 7th International Conference “Nanotechnology”

7 – 11 October 2024, Tbilisi, Georgia

GTU nano 2024

### Program and Abstracts



7th International Conference “Nanotechnology”

7 – 11 October 2024, Tbilisi, Georgia

GTU nano 2024

Program and Abstracts

Tbilisi

2024

The book contains 120 abstracts of papers presented at the 7th International Conference “Nanotechnology”, 7 – 11 October 2024, Tbilisi, Georgia (GTU nano 2024), organized by the Georgian Technical University (GTU). GTU nano 2024 continues the regular series of nanoconferences held in Georgia since 2010. Its 7th edition brings together universities, institutes, research centers, etc., leading in the field of nanotechnology and nanoscience from 25 countries (Argentina, Armenia, Azerbaijan, Belarus, Bulgaria, Canada, Czech Republic, Egypt, France, Georgia, Germany, Hungary, Iran, Italy, Japan, Kazakhstan, Lithuania, Mexico, Romania, Russia, Spain, Turkey, Ukraine, United Arab Emirates and United States of America).

**E d i t o r s :**

**Levan Chkhartishvili**

**Mikheil Chikhradze**

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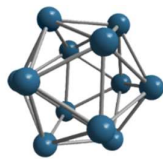
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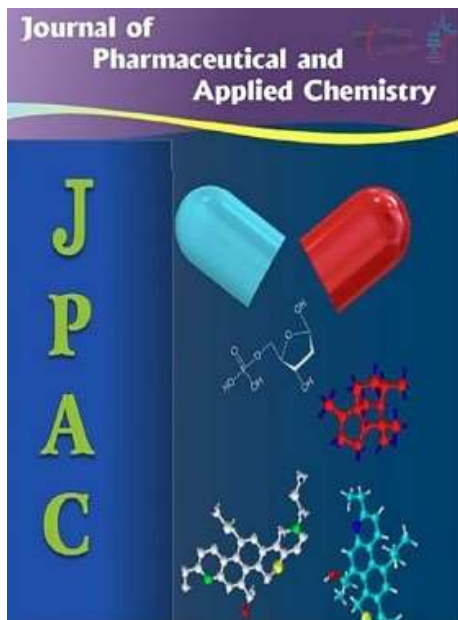
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## NANO STUDIES

INTERNATIONAL JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY



## BULLETIN OF MATERIALS SCIENCE AND METALLURGY



*nanoenergy advances*

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## FOREWORD

Since 2010, conferences on nanotechnology have been held regularly, every two years, in Georgia. Starting from the 2nd edition (2012), Georgian Technical University (GTU) took over the responsibility for their organization and successfully held conferences in 2012, 2014, 2016 and 2018. The 6th conference of this series was scheduled to take place in 2020, but due to the Covid pandemic, it was postponed to 2021 and held in the format of a virtual meeting.

According to the established tradition, the current 7th International Conference “Nanotechnology” (GTU nano 2024) will present and analyze the latest achievements not only in the field of nanotechnology itself, but also in almost all nanosciences, such as: nanophysics, nanochemistry, nanobiology, nanomaterials science, nanoelectronics, nanomedicine, nanoecology, nanosafety, nanoeducation, etc. We hope that this GTU conference will determine the main directions of future nanoresearch, and the discussion taking place here will give a significant impetus to mutually beneficial cooperation between universities and other research institutions of different countries in the development of new nanotechnologies. Professors and scientists of GTU in the field of nanotechnology are ready to take an active part in the fruitful work of the conference.

In total, the National Organizing Committee of the conference received 120 abstracts of presentations. The authors include both well-known researchers in the field and promising young specialists and students. They are representatives of a number of leading universities, institutes and research centers of 25 countries (Argentina, Armenia, Azerbaijan, Belarus, Bulgaria, Canada, Czech Republic, Egypt, France, Georgia, Germany, Hungary, Iran, Italy, Japan, Kazakhstan, Lithuania, Mexico, Romania, Russia, Spain, Turkey, Ukraine, United Arab Emirates and United States of America). All these abstracts are published in this book. The conference program includes 34 invited, 19 oral and 67 poster presentations.

We are honored that 40 leading scientists from 21 countries have agreed to join the International Scientific Committee of the conference – many thanks to them for their help and contribution. I would also like to thank the National Organizing Committee for their hard work in preparing the conference.

I cordially welcome the participants and guests of the 7th International Conference “Nanotechnology” and wish them successful work!

**Davit Gurgenzidze**

Academician  
Georgian National Academy of Sciences

Rector  
Georgian Technical University

Chair  
International Scientific Committee  
7th International Conference “Nanotechnology”

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OCTOBER 7, 2024, MONDAY

11:00 – 12:00 Registration

**Session 1**

**Chairs:** Davit Gurgenidze and Tamar Lominadze

12:00 – 12:20 Opening Speech  
*Davit Gurgenidze* – Rector of the Georgian Technical University

12:20 – 12:30 Welcome Remarks  
*Tamar Lominadze* – Vice Rector of the Georgian Technical University

12:30 – 13:00 Greetings  
*Conference Participants and Guests*

13:00 – 14:00 Opening Party

**Session 2**

**Chairs:** Laszlo Kotai and Mikheil Chikhradze

14:00 – 14:30 Invited Presentation  
“Evolution of transformative materials and role of nanomaterials and nanotechnologies on energy, environment and sustainable development”  
*Fernand D. S. Marquis* (United States of America)

14:30 – 14:45 Oral Presentation  
“Highly stable 2D MXene-based nanofluids for enhanced solar energy harvesting”  
*Shoaib Anwer*, Eiyad Abu Nada (United Arab Emirates)

14:45 – 15:15 Invited Presentation  
“Carbon-based materials for supercapacitor technologies”  
*Stefano Bellucci* (Romania – Italy)

15:15 – 15:30 Oral Presentation  
“Study of optical properties of virus-like nanostructures for biomedical application”  
*Tamar Bzhalava*, Paata J. Kervalishvili, Sergi Kapanadze, Ana Palavandishvili (Georgia)

15:30 – 16:00 Invited Presentation  
“Excitons and trions in two-dimensional materials tunable by electric and magnetic fields”  
*Roman Ya. Kezerashvili*, Anastasia Spiridonova, Shalva M. Tsiklauri (United States of America)

16:00 – 16:15 Oral Presentation  
“Strain effects in graphene oxide/silver nanowire nanocomposites exposed to gamma radiation”  
*Mahammad Baghir Baghirov*, Mustafa Muradov (Azerbaijan)

16:15 – 16:45 Invited Presentation  
“Structure and properties of photocatalysts based on titanium dioxide nanoparticles modified with silver and cerium”  
*Olena Lavrynenko*, Maksym Zahornyi, Erwan Paineau (Ukraine – France)



**16:45 – 17:00** Oral Presentation  
“Obtaining of carbon black–Fe<sub>3</sub>O<sub>4</sub> and graphene oxides–Fe<sub>3</sub>O<sub>4</sub> magnetic composites”  
**Natia Barbakadze**, Levan Chkhartishvili, Otar Tsagareishvili, Ketevan Sarajishvili, Tamar Korkia, Vakhtang Gabunia, Roin Chedia (Georgia)

**Cancelled** Invited Presentation  
“On pulse impact mechanism efficacy: The more power the less dose”  
**Volodymyr Chumakov**, Oksana Kharchenko, Zlatinka Kovacheva (Ukraine – Italy – Bulgaria)

## OCTOBER 8, 2024, TUESDAY

**10:00 – 17:00** Poster Presentations  
*Their list see at the program end*

### Session 3

**Chairs:** Fernand Marquis and Shoaib Anwer

**10:00 – 10:30** Invited Presentation  
“Synthesis of composite materials based on metal borides and aluminum oxide in solid flame combustion mode”  
**Roza Abdulkarimova** (Kazakhstan)

**10:30 – 10:45** Oral Presentation  
“Dynamics of laminar fluid in nanotube considering adhesion”  
**Tamar Berberashvili**, Vakhtang Gogichaishvili, Paata Kervalishvili (Georgia)

**10:45 – 11:15** Invited Presentation  
“Rare earth metals nano: Technologies and challenges”  
**Hossein Aminian** (Canada)

**11:15 – 11:30** Oral Presentation  
“Quantitative <sup>31</sup>P NMR spectroscopy investigation in hair of bisphosphonates as banned substance in sports”  
**Tamar Chachibaia**, Zainab Sayyed, Anfas Ahamed Rehamani, Malihah Masood Qazi, Danyaal Rehan Mir, Priya Shailesh Salunke (Georgia)

**11:30 – 12:00** Invited Presentation  
“Nonlinear interaction of novel nanostructures with strong coherent radiation”  
**Hamlet Avetissian**, Garnik Mkrtchian (Armenia)

**12:00 – 12:30** Invited Presentation  
“Structural and optical properties of GaN received by reactive magnetron sputtering”  
**Amiran Bibilashvili**, Zurab Kushitashvili, Zurab Jibuti, Zurab Kapanadze (Georgia)

**12:30 – 13:00** Invited Presentation  
“Electrochemical formation of functional iron–rhenium coatings as multifunctional materials”  
**Oksana Bersirova** (Lithuania – Ukraine)

**Cancelled** Invited Presentation  
“Molecular modeling of glycyrrhizin complexes with cortisol and anti-cortisol protein”  
**Leyla Galandarli**, Rovshan Khalilov, Gulnara Akverdieva (Azerbaijan)

**13:00 – 14:00** Coffee Break

#### Session 4

**Chairs:** Sergey Maksimenko and Yakov Enns

- 14:00 – 14:30** Invited Presentation  
“Novel 2-acetamido-2-ylidene-4-imidazole derivatives (El-Saghier reaction): Green synthesis, biological assessment, and molecular docking”  
*Ahmed El-Saghier* (Egypt)
- 14:30 – 14:45** Oral Presentation  
“New trends in enhancing biological efficacy and safety of proton therapy: Georgian experience”  
*Archil Chirakadze*, Nana Khuskivadze, Irakli Nadiradze (Georgia)
- 14:45 – 15:15** Invited Presentation  
“Explosion technologies: Problems, achievements, prospects”  
*Nikoloz Chikhradze* (Georgia)
- 15:15 – 15:30** Oral Presentation  
“Combustion synthesis of Al<sub>2</sub>O<sub>3</sub> reinforced metal carbide composite nanoparticles by aluminothermic reduction principle”  
*Ozan Coban*, Mehmet Bugdaycı, Serkan Baslayıcı (Turkey)
- 15:30 – 16:00** Invited Presentation  
“Diatomic molecular model calculations: Boron planar clusters”  
*Levan Chkhartishvili* (Georgia)
- 16:00 – 16:15** Oral Presentation  
“About Raman, ultraviolet and infrared spectroscopy methods for experimental study of viral nanomaterials spectra”  
Tamar Bzhalava, *Sergi Kapanadze*, Ana Palavandishvili, Lali Chakhvashvili (Georgia)
- 16:15 – 16:45** Invited Presentation  
“Investigating of mechanical properties and thermal behavior of modified polypropylene/nanosilica nanocomposite in presence of compatibilizer”  
*Naser Gharehbash*, Alireza Shakeri (Iran)
- 16:45 – 17:00** Oral Presentation  
“Development of luminescent dye-decorated gold nanorods and targeted drug delivery systems for visualization and treatment of cancer formations”  
*K. Chubinidze*, A. Petriashvili, M. Chubinidze, J. Markhulia, Sh. Makatsaria, Ina Burjanadze (Georgia)
- Cancelled** Invited Presentation  
“Scrutinizing of magneto-volume and magneto-caloric behavior of R<sub>2</sub>Fe<sub>17</sub> nanostructured intermetallic alloys”  
*Pedro Gorria*, Pablo Alvarez-Alonso, Jose L. Sanchez Llamazares, Jesus A. Blanco (Spain – Mexico)

OCTOBER 9, 2024, WEDNESDAY

Session 5

**Chairs:** Paata Kervalishvili and Sergei Timoshnev

- 10:00 – 10:30** Invited Presentation  
“Boron carbide in pyrolytic carbon matrix: Micro|nano composite material for medical and aerospace applications”  
M. Demidenko, D. Adamchuk, *S. Maksimenko* (Belarus)
- 10:30 – 10:45** Oral Presentation  
““Green” synthesis in low-temperature and study of luminescent properties of carbon quantum dots”  
*Oxana Kharissova*, Brayana de la Cruz Martinez, Isauro Trevino Perez, Idalia Gomez, Jose Loyola Rodriguez (Mexico)
- 10:45 – 11:15** Invited Presentation  
“Nanostructure control of silicide and boride for thermal-to-electric energy conversion”  
*Masatoshi Takeda*, Masaaki Baba (Japan)
- 11:15 – 11:30** Oral Presentation  
“Particle beam control possibilities with Field Programmable Gate Array”  
*Ana Palavandishvili*, Levan Chkhartishvili, David Chokheli (Georgia)
- 11:30 – 12:00** Invited Presentation  
“MOF-derived nanocarbons: Synthesis, properties, and applications”  
*Boris Kharissov*, Oxana Kharissova, Yolanda Pena Mendez (Mexico)
- 12:00 – 12:30** Invited Presentation  
“Non-invasive registration of magnetic nanoparticles in phantom of biological medium”  
*L. P. Ichkitidze*, O. V. Filippova, M. V. Belodedov, A. Yu. Gerasimenko, D. V. Telyshev, S. V. Selishchev (Russia)
- 12:30 – 13:00** Invited Presentation  
“Influence of DC magnetron sputtering conditions of NiO on its structural properties”  
*Yakov Enns*, Sergei Timoshnev, Alexey Kazakin, Ivan Komarevtsev, Anastasia Kondrateva, Ketevan Davitadze (Russia – Georgia)
- Cancelled** Invited Presentation  
“EPR spectroscopic studies of hexagonal boron nitride”  
*Lina Sartinska*, Vladimir Trachevsky, Igor Vorona (Ukraine)
- 13:00 – 14:00** Coffee Break

Session 6

**Chairs:** Boris Kharissov and Mustafa Muradov

- 14:00 – 14:30** Invited Presentation  
“Advanced protective coatings for power generation, oil and gas production, and mineral processing: Major processing principles, properties and applications”  
*Eugene Medvedovski* (Canada)

- 14:30 – 14:45** Oral Presentation  
 “Preparation, doping and electrophysical properties of Er<sub>2</sub>Se<sub>3</sub> films”  
**Zaur Jabua**, Akaki Gigineishvili, Erekle Bagration–Davitashvili (Georgia)
- 14:45 – 15:15** Invited Presentation  
 “Morphological changes of ZnO nano- and microstructures synthesized by different technologies”  
**David Jishiashvili**, Zeinab Shiolashvili, Nino Makhatadze, Alexander Jishiashvili, Giorgi Petriashvili (Georgia)
- 15:15 – 15:30** Oral Presentation  
 “Development and testing of nanoparticles for treatment of cancer cells by Curie temperature controlled magnetic hyperthermia”  
**Irakli Nadiradze**, Archil Chirakadze, Nana Khuskivadze (Georgia)
- 15:30 – 16:00** Invited Presentation  
 “Solid phase quasi-intramolecular redox reactions: Route to prepare nanosized metaloxide catalysts”  
**Laszlo Kotai**, Kende Attila Beres, Laura Bereczki (Hungary)
- 16:00 – 16:15** Oral Presentation  
 “*Artemisia annua* hairy roots for “green” synthesis of gold nanoparticles”  
**Nadiia Matvieieva**, Maksym Kharchuk, Anatolij Shakhovsky, Taisa Bohdanovych (Ukraine)
- 16:15 – 16:45** Invited Presentation  
 “Spintronic nanostructures and quantum devices”  
**Paata Kervalishvili** (Georgia)
- 16:45 – 17:00** Oral Presentation  
 “Nanostructural processes and nanocracks in thin films of structural steels”  
**Tamaz Eterashvili** (Georgia)
- Cancelled** Oral Presentation  
 “Demystifying arrow of time”  
**Zura Kakushadze** (Georgia – United States of America)
- 17:00 – 20:00** Gala Banquet

#### OCTOBER 10, 2024, THURSDAY

- 09:30 – 22:30** Departure for the excursion from Saakadze Square  
*Tbilisi – Ninothminda (Saint Nino) – Saint David Gareji Lavra – Tbilisi*

#### OCTOBER 11, 2024, FRIDAY

##### Session 7 – Online

**Chairs:** Levan Chkhartishvili and Mikheil Chikhradze

- 10:00 – 10:20** Invited Presentation  
 “Crystallographic transformations and nanoscale characterization of reversibility in shape memory alloys”  
**Osman Adiguzel** (Turkey)

- 10:20 – 10:40** Invited Presentation  
 “Direct production of cast multicomponent alloys from oxide raw materials by centrifugal SHS metallurgy technique. Current results and prospective research”  
**Vladmir Sanin** (Russia)
- 10:40 – 10:50** Poster Presentation  
 “Centrifugal SHS-metallurgy of cast high-entropy alloys strengthened by structural precipitations based on borides and silicides Mo and Nb”  
**V. N. Sanin**, D. M. Ikorniko, O. A. Golosova, A. O. Sivakova (Russia)
- 10:50 – 11:10** Invited Presentation  
 “Theoretical modelling of boron nitride coatings”  
**Bilgin Kaftanoglu**, Nakka Lotfy Rake (Turkey)
- 11:10 – 11:20** Poster Presentation  
 “Structural and phase features of functional coatings obtained by multichamber detonation spraying”  
**Olena Berdnikova**, Volodymyr Korzhyk, Olga Kushnarova, Petro Stukhliak, Yevhenii Titkov, Oleg Kolisnichenko, Oleg Totosko (Ukraine)
- 11:20 – 11:30** Poster Presentation  
 “Influence of external magnetic field on structure formation during water welding of structural steel”  
**Olena Berdnikova**, Sergey Maksimov, Olena Prilipko, Tetiana Alekseenko, Olga Kushnarova, Yevhen Polovetskyi (Ukraine)
- 11:30 – 11:40** Poster Presentation  
 “Study of thermal conductivity of epoxy composites modified with nanofiller”  
**Petro Stukhliak**, Oleg Totosko, Olena Berdnikova, Danylo Stukhliak (Ukraine)
- 11:40 – 11:50** Poster Presentation  
 “Nanoconjugate of hyaluronic acid carrier with cyanine-based telomerase inhibitor”  
**Larysa Dubey**, Dmytro Kryvorotenko, Igor Dubey (Ukraine)
- 11:50 – 12:00** Poster Presentation  
 “High capacity recovery of Ag(I) from aqueous solution by mesoporous silica sorbent”  
 Petra Herman, Daniel Percsi, Tamas Fodor, Laura Juhasz, Zoltan Dudas, Zsolt Endre Horvath, Vasyi Ryukhtin, Ana-Maria Lacrama, Jozsef Kalmar, **Laszlo Almasy** (Hungary – Czech Republic – Romania)
- 12:00 – 12:10** Poster Presentation  
 “Mass spectrometric characterization of molybdenum disulfide nanocomposite with polyvinyl alcohol”  
**Marina Kosevich**, Oleg Boryak, Valentina Zobnina, Vadim Shelkovsky, Pavlo Kuzema, Victor Karachevtsev (Ukraine)
- 12:10 – 12:20** Poster Presentation  
 “Electrospinning of PVP/PMMA nanofibers with incorporated silver nanoparticles”  
 A. M. Plokhotnichenko, **V. A. Karachevtsev** (Ukraine)
- 12:20 – 12:30** Poster Presentation  
 “Photoregulation of biosynthetic activity of *Lentinula edodes* (Berk.) Pegler uses colloidal solutions of biogenic metal nanoparticles and low-intensity laser radiation”  
**Oksana Mykchaylova**, Anatoliy Negriyko, Nataliia Poyedinok (Ukraine)

- 12:30 – 12:40** Poster Presentation  
 “Binding of pheophorbide-a and its derivatives to biopolymers”  
***Olga Ryazanova*** (Ukraine)
- 12:40 – 12:50** Poster Presentation  
 “Binding of two cationic porphyrins to *ds*-polynucleotides”  
***Olga Ryazanova*** (Ukraine)
- 12:50 – 13:00** Poster Presentation  
 “Inelastic electron interaction with molecular components of nucleic acids”  
***Maria Sukhoviya***, Miroslav Shafranyosh, Mykhailo Rizak, Yurii Matyovka, Ivan Shafranyosh (Ukraine)
- 13:00 – 14:00** Coffee Break

### Session 8

**Chairs:** Tamar Lominadze and Levan Chkhartishvili

- 14:00 – 14:30** Invited Presentation  
 “Repulsion driven metallic phases in one-dimensional half-filled fermion systems”  
 Gerardo Rossini, ***George Japaridze*** (Argentina – Georgia)
- 14:30 – 14:45** Oral Presentation  
 “Biologically active nanoparticles using leucine based pseudo-proteins”  
***Nino Zavradashevili***, Temur Kantaria, Nino Kupatadze, David Tugushi, Mzevinar Bedinashvili, Ekaterina Chkhaidze, Nino Neparidze, Ashot Saghyan, Anna Mkrtychyan, Artavazd Poghosyan, Ramaz Katsarava (Georgia – Armenia)
- 14:45 – 15:15** Invited Presentation  
 “Incontrovertible contribution of nanoclays to composite properties”  
***Haldun Kurama*** (Turkey)
- 15:15 – 15:30** Oral Presentation  
 “To kinetics of quantum dissipative systems: Quantum Brownian particle motion and low temperature polaron mobility problem”  
***Bezhan Kotia***, Teimuraz Berikashvili (Georgia)
- 15:30 – 16:00** Invited Presentation  
 “Effect of gamma irradiation on structure of composites based on GO/PVA”  
***Mustafa Muradov***, Mahammad Baghir Baghirov (Azerbaijan)
- 16:00 – 16:30** Invited Presentation  
 “Electronic structure of gallium nitride during sodium adsorption”  
***Sergei Timoshnev***, Andrey Mizerov, Mikhail Lapushkin, Galina Benemanskaya, George Iluridze, Tamaz Minashvili (Russia – Georgia)
- 16:30 – 17:00** Invited Presentation  
 “On Dirac cones and beyond: Featured electronic band structures of 2D materials with charge carriers mimicking massless Dirac fermions”  
***Ivane Murusidze*** (Georgia)

## Poster Session

“New condensed phosphates as inorganic polymers and possible sectors of their utilization”

**Marina Avaliani**, Elena Shapakidze, Vazha Chagelishvili, Nana Barnovi, Gulnara Todradze, Gulnara Kipiani, Mariam Vibliani (Georgia)

“High harmonic generation by strong laser radiation in fullerene molecule C<sub>180</sub>”

H. K. Avetissian, A. G. Ghazaryan, H. H. Matevosyan, **G. F. Mkrtchian** (Armenia)

“Probing mobility edges in quasi-crystals using high-harmonic generation spectroscopy”

Hamlet Avetissian, **Suren Sukiasyan**, Garnik Mkrtchian (Armenia)

“Phase transitions of graphene oxide–peroxytungstic acid composite”

**Natia Barbakadze**, Liparit Dolidze, Rusudan Tsiskarishvili, Tamar Korkia, Maia Japaridze, Maia Stephanishvili, Levan Chkhartishvili, Roin Chedia (Georgia)

“Mechanism of  $\epsilon$ -nanophase precipitation in copper-steel”

**Teimuraz Berikashvili**, Levan Chkhartishvili, Akaki Gigineishvili (Georgia)

“Chemical preparation of gold nanoparticles on GaP(001) surface”

V. L. Berkovits, V. P. Ulin, S. A. Khakhulin, **T. A. Minashvili**, A. V. Gigineishvili, G. N. Iluridze, K. D. Davitadze (Russia – Georgia)

“Silver-based electrolytic alloys with rhenium as functional nanomaterials”

**Oksana Bersirova**, Valeriy Kublanovsky, Stanislav Bersirov (Lithuania – Ukraine)

“Tungsten scrap as precursor for manufacturing advanced materials”

Levan Chkhartishvili, Otari Tsagareishvili, Archil Mikeladze, Tamaz Batsikadze, **Natia Barbakadze**, Manana Buzariashvili, Tamar Dgebuadze, Roin Chedia (Georgia)

Use of DNA for nanotechnological purposes: Study of quality of DNA double helix”

**Vasil Bregadze**, Irine Khutsishvili, Eter Gelagutashvili, Shota Gogichaishvili, Zaza Melikishvili, Tamar Giorgadze (Georgia)

“Thermodynamic investigation of nano boride’s produced via SHS technique”

**Mehmet Bugdayci**, Ozan Coban, Serkan Baslayici (Turkey)

“Static atomic charges in boron planar clusters”

**Shorena Dekanosidze**, Tornike Odishvili, Levan Chkhartishvili (Georgia)

“Photochromic liquid crystal polymer films for modern devices of optical information”

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***Lali Turiashvili***, Manana Beridze, Nino Robakidze, Gia Dagelashvili, Darejan Khocholava, Marina Shogiradze, Nona Esiava (Georgia)

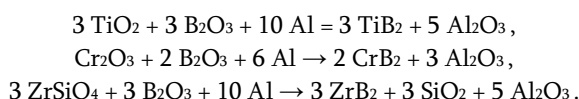
“Distinctive technological approach for preparation of dispersed and fibrous nano-structured manganese dioxide using SHS method”  
Garegin Zakharov, Archil Chirakadze, ***Mikheil Chikhradze***, Laszlo Kecskes, Zurab Aslamazashvili, David Kvashvadze (Georgia – United States of America)

# SYNTHESIS OF COMPOSITE MATERIALS BASED ON METAL BORIDES AND ALUMINUM OXIDE IN SOLID FLAME COMBUSTION MODE

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Transition metal borides with unique properties (high refractoriness, wear resistance, thermal conductivity) are of interest for the preparation of ceramic composites intended for use in high-temperature abrasive wear. However, strong covalent bonds inherent in the phases of transition-metal borides lead to low plasticity and low bending and strength, which largely limits their application in pure form. In this regard, currently much attention is paid to the technology of obtaining composite materials based on borides of transition metals in combination with more plastic materials that act as a binder. For example, aluminum can play the role of a high-temperature binder and filler, which reduces the content of expensive diboride in composite materials. The production of these materials by traditional methods of powder metallurgy is hindered by high-energy costs, multistageness complexity of process equipment and low productivity. Self-propagating high-temperature synthesis (SHS) is an efficient way of producing ceramic and metal-ceramic composites [1, 2]. Advantage of the method are fast heating (seconds) of the target product, simplicity of technology, low power consumption and low cost of the target product. An important role in the production of materials in the SHS mode is played by preliminary mechanochemical activation (MA), which can achieve a high degree of particle dispersion, change the structure, energy intensity and create a classical basis for the material [3]. Metal oxides, enriched borate ore from the Indersky deposit of the Republic of Kazakhstan and aluminum powder were used as starting components. The object of the study was a ceramic composite synthesized based on titanium, chromium and zirconium borides by the reactions:



An important stage for optimizing the conditions for studying the regularities of synthesis of boron-containing compounds in a combustion wave was carried out in a high-pressure reactor in an argon. Formation of the phase composition and microstructure of SHS-ceramic materials based on high-temperature transition metal borides and corundum ( $\text{Al}_2\text{O}_3$ ) was investigated. A possible mechanism for the procedure of SH-synthesis is proposed. Formation of submicron and nanosized crystals of titanium, chromium and zirconium borides crystals in an alumina matrix has been stated. The influence of preliminary mechanical activation, initial composition of components and synthesis temperature on the properties of the resulting nanostructured composite materials is shown.

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**Keywords:** borate ore, titanium and chromium oxides, zircon, mechanical activation, self-propagating high-temperature synthesis

## CRYSTALLOGRAPHIC TRANSFORMATIONS AND NANOSCALE CHARACTERIZATION OF REVERSIBILITY IN SHAPE MEMORY ALLOYS

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Shape memory alloys take place in a class of advanced smart materials with adaptive properties and stimulus response to the external conditions and changes, by exhibiting a peculiar property called shape memory effect. This phenomenon is initiated with thermomechanical processes on cooling and deformation processes and performed thermally on heating and cooling, with which shape of materials cycles between original and deformed shapes in reversible way in bulk level. Therefore, this behavior can be called thermal memory or thermoelasticity. Thermoelasticity is governed by the crystallographic transformations in nanoscale and atomic level, thermal and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling, with cooperative movement of atoms in  $\langle 110 \rangle$ -type directions on the  $\{110\}$ -type planes of austenite matrix, along with lattice twinning and ordered parent phase structures turn into twinned martensite structures. The twinned structures turn into detwinned structures by means of stress induced transformation with deformation. Martensitic transformations are diffusionless transformations, and movements of atoms are confined into the neighbor atom distances.

These alloys exhibit another property called superelasticity. This behavior is performed in mechanical manner with stressing and releasing the material in elasticity limit at a constant temperature in parent phase region, and shape recovery occurs instantly and simultaneously upon releasing, by exhibiting elastic material behavior. Superelasticity is also result of the stress induced martensitic transformation and ordered parent phase structures turn into the detwinned martensitic structure with stressing in parent phase region.

Copper-based alloys exhibit this property in metastable  $\beta$ -phase region, which has bcc-based structures. Lattice invariant shears are not uniform in copper-based shape memory alloys, and the ordered parent phase structures undergo the non-conventional complex layered structures with martensitic transformation.

In the present contribution, X-ray diffraction and transmission electron microscopy studies were carried out on copper-based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. This result refers to a new transformation in diffusive manner.

**Keywords:** shape memory effect, martensitic transformation, thermoelasticity, superelasticity, lattice twinning and detwinning

## **RARE EARTH METALS NANO: TECHNOLOGIES AND CHALLENGES**

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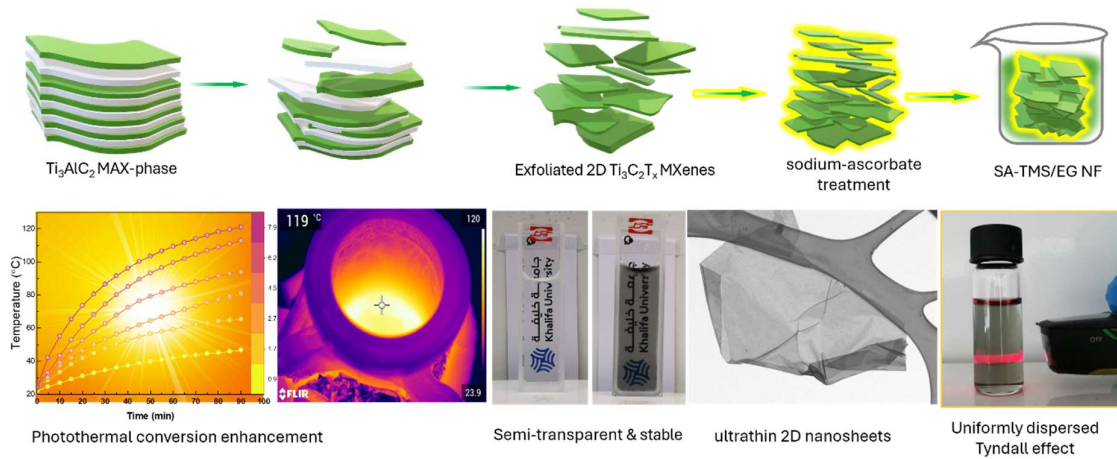
Rare Earth Metals (REMs) are used in manufacturing for a variety of important and new applications including light bulbs, hybrid, plug-in and electric vehicle, steel and aluminum industry, wind turbine, solid-oxide fuel cells etc. Because of their importance they are increasingly becoming a critical strategic resource. However, they are rarely found in economically viable quantities in the earth crust and therefore the supply chain for them is quite limited. The recovery of rare metals is technologically difficult since many of these metals are in very low concentrations and require multiple processing. In this paper, the available technologies for the recovery of rare earth metals and the challenges that exist to produce nano REMs will be discussed.

# HIGHLY STABLE 2D MXene-BASED NANOFLUIDS FOR ENHANCED SOLAR ENERGY HARVESTING

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The global push for renewable energy solutions aims to reduce dependence on finite fossil fuels and mitigate environmental impacts. Photothermal NanoFluids (NFs) play a crucial role in solar energy harvesting by balancing solar absorption, light-to-heat conversion, dispersion stability, and viscosity. This study explores the development of high-performance stable NFs using various mass fractions of Sodium Ascorbate-Treated ultrathin 2D  $Ti_3C_2T_x$  MXene nanoSheets (SA-TMS) in an ethylene glycol base fluid. We conducted comprehensive optical and photothermal analyses, focusing on dispersion, suspension stability, viscosity, and photothermal conversion. Remarkably, incorporating a trace amount of SA-TMS into ethylene glycol improved its photothermal performance by 68.73%, attributed to the high extinction coefficient and the Localized Surface Plasmon Resonance (LSPR) effect of the conductive SA-TMS nanosheets.



**Figure 1.** Preparation of SA-MXenes/EG semi-transparent nanofluids and their photothermal enhancement.

The optimized SA-TMS/EG nanofluid demonstrated semitransparency and a low effective viscosity owing to its self-lubricating properties. Additionally, the NFs exhibited excellent cycling life, no sedimentation after 90 days, and promising shelf stability. This research offers a new perspective on designing stable and efficient 2D material-based NFs (**Figure 1**) for direct solar energy harvesting, highlighting their superior photo-thermal properties.

## Acknowledgments

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**Keywords:** nanofluids,  $Ti_3C_2T_x$  MXene, 2D nanosheets, direct solar absorption, photothermal conversion

## NEW CONDENSED PHOSPHATES AS INORGANIC POLYMERS AND POSSIBLE SECTORS OF THEIR UTILIZATION

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In the frame of researches studies for new inorganic polymeric materials, certain condensed phosphates having zeolite properties are well adopted due to its special properties-as catalytic agents and adsorbents. Cyclic compounds with the general formula  $M^I M^{III} P_n O_{3n}$  have free channels and it can be predicted – they have best zeolite properties. For example, in the cycles of synthesized by our group cyclododecaphosphate of gallium–cesium  $Cs_3Ga_3P_{12}O_{36}$  the atoms of Ga are built-in within the cycle. In fact, the 12-member cycle is huge for them – is too large, they use only 6 oxygen atoms out of the total 12 atoms, the  $M^{3+}$  cations draw them to themselves, causes the chain to undulate, reducing the free space in the channel. The situation is different in the case of cyclooctaphosphate of potassium–gallium  $K_2M^{III}_2P_8O_{24}$ , synthesized by us few years ago. It is undeniably proved that cyclooctaphosphates  $M^{II}_2M^{III}_2P_8O_{24}$  are the best catalysts in the process for receiving of olefin hydrocarbons and diene combinations. The assets of this compound in the model dehydration reaction of n-butyl alcohol by the impulsion method are studied. Based on the conducted examinations, it was found that the overall conversion was up 52 to 65%. Examined compound is comparable to the activity of the sample  $BPO_3$  (50%) obtained by mixing the starting components and exceeded the activity of the zeolite catalyst (32%), practiced under analogous conditions. It has also been found that the  $C_4$  olefinic hydrocarbons were absolutely recollected by the catalyst under the same settings. Diameter of the channel in the case of Ga–K cyclooctaphosphate is 5.2 Å, which is very good performance. Thus, the double cyclooctaphosphate  $K_2Ga_2P_8O_{24}$  synthesized by us and investigated for catalytic activity shows that it has unique properties of an inorganic polymer and can be used as the best catalyst in organic synthesis reactions, in particular, for the preparation of low molecular weight diene olefins.

During the investigation of polycomponent system  $Ga_2O_3-P_2O_5-H_2O$  at the temperature range 25–500°C we synthesized an inorganic oligomer – acid triphosphate of gallium  $GaH_2P_3O_{10} \cdot (1-2)H_2O$ . The optimal temperature interval for obtaining of this oligomer is 50–380°C. It is determined that the triphosphate can be crystallized in two forms: modifications I and II. What is essential is that form I is the hydrated form:  $GaH_2P_3O_{10} \cdot (1-2)H_2O$  and the detailed study of which showed that it has pronounced properties of an excellent ion exchanger. For example, when potassium chloride solution is added to this phase, the pH quickly becomes equal to 1. When  $GaH_2P_3O_{10} \cdot (1-2)H_2O$  was titrated potentiometrically with a 0.1% NaOH solution (the content of  $Ga_2O_3$  was previously determined to be equal to 26.1%), the titration curve shows two jumps indicating interaction step by step of form I with sodium hydroxide NaOH. In the first stage, sodium triphosphate  $Na_2GaP_3O_{10} \cdot H_2O$  is obtained. In the second step (when  $pH > 7$ ), the oligomeric compound begins to dissolve and inorganic complex salts are formed. After further treatment of the double triphosphate of sodium  $Na_2GaP_3O_{10} \cdot H_2O$  with hydrochloric acid HCl and then repeated titration with NaOH, the acid triphosphate –  $GaH_2P_3O_{10} \cdot H_2O$  (form I) is obtained again. Thus, it can be concluded that the hydrated form  $GaH_2P_3O_{10} \cdot H_2O$  is a very good ion exchanger and that it is possible and justified to use it for this purpose. It is worth noting that in general the use of crystalline and non-crystalline phosphates, for example – ultra-phosphates in quantum electronics is predetermined by their specific properties, and of course, allow their application as the latest nanocomponents in modern technology. Phosphates are the greatest fertilizers, detergents, and raw components for the creation of phosphate glasses, thermo-resistant materials, effective applying nourishments, cleaners, and/or cement substances, in some cases – flame-retardants also. The thermal, vibrational, and luminescent properties of condensed compounds enable them to be employed in high-tech applications.

**Keywords:** synthesis, condensed phosphate, triphosphate, octaphosphate, dodecaphosphate, ion exchanger



# NONLINEAR INTERACTION OF NOVEL NANOSTRUCTURES WITH STRONG COHERENT RADIATION

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The synthesis of graphene has sparked a quest for novel nanomaterials exhibiting similar remarkable properties. The advancements in nanotechnology over the past two decades have enabled the creation of graphene-like nanostructures with exceptionally high carrier mobility and electrons minimal scattering making such systems new objects of manifestation of interesting physical phenomena, specifically under coherent electromagnetic radiation fields, suggesting the potential for novel nonlinear relativistic optical effects [1]. On the other hand, these nanostructures have unique high electromagnetic coefficient of nonlinearity at the interaction with strong electromagnetic fields, which is about billion times that of ordinary free electronic-atomic systems. The latter allows available high-order multiphoton effects already at moderately strong radiation fields; in particular, realization of High Harmonic Generation (HHG) phenomenon that is a direct mechanism to reach the realization of ultrashort light pulses of attosecond durations [2]. Hence, HHG is one of the most significant phenomena, which in particular leads to the formation and development of modern *attophysics*, or more general, new area in science – *attoscience*.

Taking into account the importance of above-mentioned problem, the present talk specifically concerns the problem of HHG in novel nanostructures, as one of the most active and exciting branches of modern physics – nonlinear nanophotonics. In the scope of analytically developed theory, we will consider the HHG phenomenon with underlying nonequilibrium processes in novel 1D–3D nanostructures, also revealing the role of many-body interactions and topological effects at the extreme conditions. As concrete systems, we study the nonlinear interaction of 1D chains, 2D semimetals, semiconductors, and insulators with hexagonal lattice structure, as well as 3D Dirac/Weil semimetals with the strong coherent radiation. By solving the evolutionary equations for the single particle density matrix, taking also into account the many body Coulomb interaction in the Hartree–Fock approximation, we show that the result leads to formation high-order harmonics with collective many body effects. We also study HHG phenomenon in fullerene molecules of high (more than 100) carbon molecules with the icosahedron point group symmetry. The further advancement of the issues considered in this talk will clear up our knowledge about the multiparticle dynamics in such systems of attosecond/picometer resolution and will allow us to find out the optimal conditions for operation of the new nano-optoelectronic devices, such as nanoscale frequency multipliers.

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# HIGH HARMONIC GENERATION BY STRONG LASER RADIATION IN FULLERENE MOLECULE C<sub>180</sub>

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One of the fundamental processes in intense laser-matter interaction is High-order Harmonic Generation (HHG), which allows for the production of coherent ultraviolet and X-ray radiation in atomic systems. HHG phenomenon involves highly multiphoton processes [1], offering access to extreme time resolution and enabling attosecond physics. Among nanostructured materials with potential for nonlinear extreme optical applications, carbon allotropes [2, 3], such as fullerenes [4], are of particular interest. Fullerenes being large molecules formed by closing a graphite sheet, and their stable closed topological structure makes them intriguing objects for matter-light coherent interaction with large groups of symmetry. The discovery of C<sub>60</sub> fullerene stimulated research into many other fullerene molecules with different symmetries. Large fullerenes have since been the subject of active investigation.

In this paper, the results of analytical and numerical investigation of HHG in the large fullerene C<sub>180</sub> molecule under intense laser field is presented. To model the C<sub>180</sub> molecule and its interaction with the laser field, we employ the tight-binding mean-field approach. Our detailed analysis of the HHG power spectrum reveals the multiphoton resonant nature of harmonic generation, shedding light on the underlying quantum processes involved. We examine the dependence of cutoff harmonics on both laser intensity and frequency, providing valuable insights into the optimal conditions for enhancing HHG in C<sub>180</sub> molecules. We demonstrate that the C<sub>180</sub> molecule exhibits a significantly stronger high harmonic intensity compared to the more widely studied C<sub>60</sub> fullerene.

## Acknowledgment

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**Keywords:** graphene quantum dot, fullerene, carbon allotropes, multiphoton, high-order harmonics, many particle Coulomb scattering, topological structure

# PROBING MOBILITY EDGES IN QUASI-CRYSTALS USING HIGH-HARMONIC GENERATION SPECTROSCOPY

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Quasi-crystals occupy a unique position between the ordered and disordered systems presenting a unique blend of different properties. In 3D disordered systems, phenomena such as Anderson phase transition where single particle wave functions transition from extended to exponentially localized can occur at a critical level of disorder strength, leading to a metal-to-insulator transition. Remarkably, in quasi-crystals even 1D systems exhibit metal-to-insulator transition, as demonstrated by the Aubry–Andre–Harper (AAH) model, characterized by incommensurate on-site modulations. This lattice model is crucial in exploration of Anderson localization in quasi-crystals.

The generalized AAH model that breaks self-dual symmetry introduces a mobility edge within the single-particle spectrum. This mobility edge acts as a pivotal point delineating extended eigenstates from their localized counterparts. Consequently, this model possesses a rich spectrum of physics encompassing both the energy spectrum and the spatial distribution of single-particle wave functions.

Given these properties of systems described by AAH model, there is considerable interest in developing new methodologies capable of probing their structural, topological, and dynamical characteristics. High harmonic spectroscopy (HHS) emerges as a particularly significant tool in this regard. This technique exhibits exceptional sensitivity to the properties of charged carriers.

In our study, we focus on several AAH models, highlighting the efficiency of HHS as a versatile tool for detecting localization phenomena and mobility edges in quasi-crystals. We demonstrate the utility of HHS for simplification the complicated physics of quasi-crystal systems described by AAH model.

## Acknowledgment

The work was supported by the Science Committee of Republic of Armenia, Project # 21AG-1C014.

**Keywords:** quasi-crystal, high harmonic spectroscopy, ordered and disordered systems, Aubry–Andre–Harper model, incommensurate lattice, topological Anderson localization

# STRAIN EFFECTS IN GRAPHENE OXIDE/SILVER NANOWIRE NANOCOMPOSITES EXPOSED TO GAMMA RADIATION

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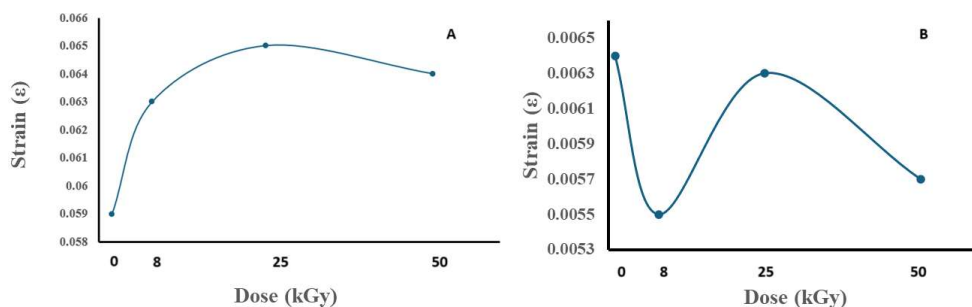
Recent advancements in metal-semiconductor-based nanocomposites have garnered significant attention, with one notable example being Graphene Oxide (GO)/silver Ag NanoWires (AgNWs) composites. This study focuses on investigating the effects of gamma radiation on the structural properties of GO/AgNWs nanocomposites.

GO was synthesized using a modified Hummers method, while AgNWs were prepared via a modified polyol method. The GO/AgNWs nanocomposites were then fabricated by mechanical stirring [1]. These nanocomposites were subsequently exposed to gamma radiation at doses of 8, 25, and 50 kGy.

Structural analysis of the samples was conducted using X-Ray Diffraction (XRD). The analysis revealed that gamma radiation decomposed the graphite in the sample. Notably, the peak positions of GO and AgNWs remained unchanged under the influence of gamma radiation. The strain within the samples, dependent on the radiation dose, was calculated using the following equation:

$$\varepsilon = \frac{\beta}{4 \tan \theta},$$

where  $\varepsilon$  represents the strain, and  $\beta$  is the half-width of the XRD peaks.



**Figure 1.** Gamma radiation dose dependence graph of strain for GO/AgNWs nanocomposite for A – GO and B – AgNWs.

The results, depicted in **Figure 1**, show the strain calculations based on signals from both GO and AgNWs components. **Figure 1A** illustrates the strain results for GO, indicating an increase in strain with higher doses of gamma radiation, likely due to defects and dislocations induced by the radiation. However, at a dose of 50 kGy, the strain decreased, suggesting a possible annealing effect that mitigated the defects caused by the gamma radiation. **Figure 1B** presents the strain results for AgNWs, demonstrating variability in strain at different radiation doses. These findings highlight the complex interplay between gamma radiation and the structural integrity of GO/AgNWs nanocomposites.

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**Keywords:** gamma radiation, nanocomposites, structure, strain

## OBTAINING OF CARBON BLACK-Fe<sub>3</sub>O<sub>4</sub> AND GRAPHENE OXIDES-Fe<sub>3</sub>O<sub>4</sub> MAGNETIC COMPOSITES

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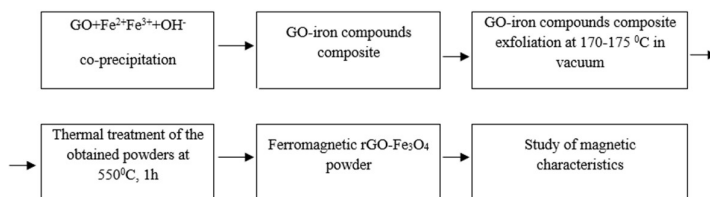
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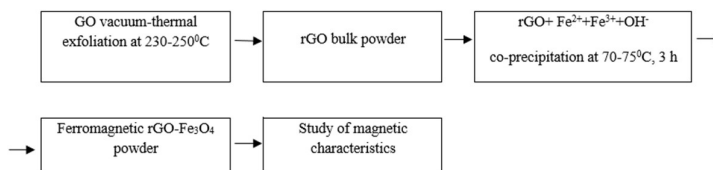
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Composites containing iron oxides are obtained by the co-precipitation of iron(II) and iron(III) compounds in the presence Carbon Black (CB) and Graphene Oxides (GOs). Therefore, there is a need to select optimal methods for obtaining magnetic composites. This article discusses two possible methods of obtaining magnetic composites using GO, which is determined by its properties. The first method includes the following steps:

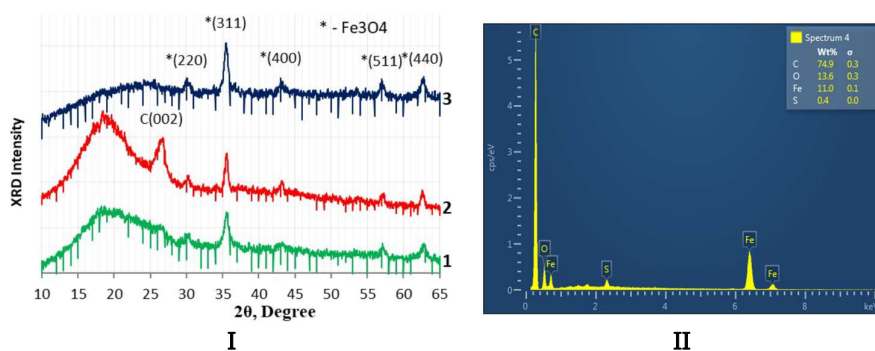


By further heating of ferromagnetic reduced Graphene Oxide (rGO) composite rGO-Fe<sub>3</sub>O<sub>4</sub> powder at 800°C, G-Fe<sub>3</sub>O<sub>4</sub> ferromagnetic composite is obtained. The second method includes the following steps:

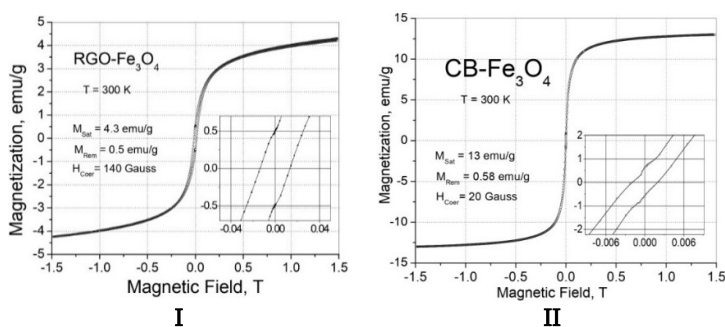


In both methods, newly synthesized GO suspensions were used, which were pre-sonicated. During the implementation of the first method, a black diamagnetic substance is formed in the co-precipitation process, the diffraction peak of GO is visible on the XRD diffractogram, and the diffraction peaks of any iron compounds (oxides, oxohydroxides) are not observed, i.e. a composite of amorphous iron compound and GO is formed.

It is determined that rGO-Fe<sub>3</sub>O<sub>4</sub> and CB-Fe<sub>3</sub>O<sub>4</sub> magnetic composites can be obtained at 70–75°C, while in the presence of GO, a non-magnetic composite containing an amorphous iron compound is formed under the same conditions. This composite, when heated in vacuum at 170–175°C, undergoes exfoliation, in result of which a powder composite rGO–amorphous iron compound is formed, the volume of which is 2.7 times greater than that of initial powder. Its partial reduction takes place at 550°C and rGO-Fe<sub>3</sub>O<sub>4</sub> is obtained (**Figure 1**).



**Figure 1.** (I) XRD patterns of (1) CB-Fe<sub>3</sub>O<sub>4</sub>, (2) rGO-Fe<sub>3</sub>O<sub>4</sub>, and (3) rGO-Fe<sub>3</sub>O<sub>4</sub> composites and (II) EDX spectrum of rGO-Fe<sub>3</sub>O<sub>4</sub> composite obtained at 550°C from GO-amorphous iron compound.



**Figure 2.** Room temperature magnetization curves for (I) rGO-Fe<sub>3</sub>O<sub>4</sub> and (II) CB-Fe<sub>3</sub>O<sub>4</sub> composites.

At the next stage the room temperature magnetic properties of CB-Fe<sub>3</sub>O<sub>4</sub> and rGO-Fe<sub>3</sub>O<sub>4</sub> (obtained at 550°C) were studied (see **Figure 2**). Vibrating Sample Magnetometer (VSM) Lake Shore 7300 was used for this purpose.

### Acknowledgments

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<https://doi.org/10.1016/j.diamond.2023.110238>

**Keywords:** graphene oxide, reduced graphene oxide, activated carbon, magnetite; magnetic composite

## PHASE TRANSITIONS OF GRAPHENE OXIDE –PEROXYTUNGSTIC ACID COMPOSITE

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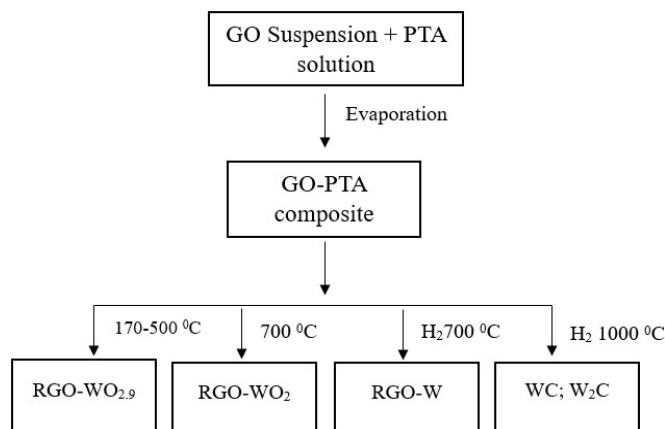
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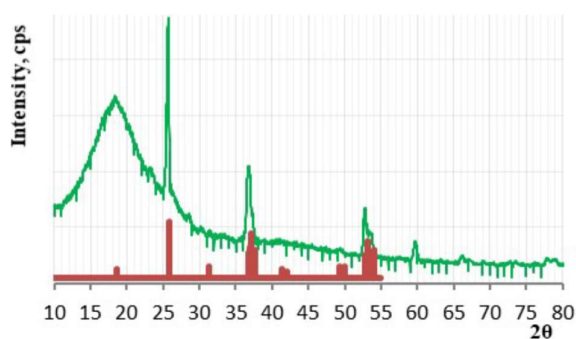
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Graphene oxides (GOs) and a metal compound composites have unique properties and they are promising materials in many fields of application [1 – 4]. GO and PeroxypolyTungstic Acid (PTA) composite GO–PTA is easily formed, because the components contain many oxygen-containing functional groups, which interact and form a stable homogeneous suspension, by drying of which the polymer films are obtained. They are flexible and can be used to coat various surfaces with tungsten oxides. We aimed to study the effect of temperature increase on the synthesized composite under vacuum, inert and reducing atmosphere. The obtained results are summarized in **Figure 1**.



**Figure 1.** Scheme of obtaining different materials from GO–PTA composite.

The specially developed methods were used for vacuum-thermal exfoliation of GO–PTA composite. It is determined that the exfoliation of the composite when using newly synthesized GO is 170–175°C and practically coincides with the temperature of vacuum exfoliation of GO (160–170°C). As a result of exfoliation, a fluffy powder is obtained, the volume of which is 200–300 times greater than the volume of the initial composite. Thus, the method of vacuum-thermal exfoliation is a new method for obtaining composites of tungsten compounds and graphene oxides. Further heating of the obtained at 170°C rGO–PTA composite up to 500°C literally does not change the phase composition and the rGO–WO<sub>2.9</sub> composite is obtained, which transforms into the rGO–WO<sub>2</sub> composite at 700°C.



**Figure 2.** XRD patterns of composite rGO–WO<sub>2</sub> obtained at 700°C, where components are shown in green and dark red respectively.

Comparing the corresponding diffractograms, it can be said that in the rGO–WO<sub>2.9</sub>–170 and rGO–rGO–WO<sub>2.9</sub>–500 composites, the WO<sub>2.9</sub> phase is not fully formed, while in the rGO–WO<sub>2</sub>–700 composite, the WO<sub>2</sub> phase is well defined (**Figure 2**).

In general, PTA gradually undergoes dehydration and deoxygenation during heat treatment, and at 600°C the WO<sub>3</sub> phase is obtained and metallic tungsten is obtained in hydrogen environment. By heating of GO–PTA composite at 1000°C to in an inert or hydrogen atmosphere, tungsten carbides (W<sub>2</sub>C, WC) are obtained.

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**Keywords:** peroxopolytungstic acid, graphene oxides, composites, vacuum-thermal exfoliation, phase transitions



## CARBON-BASED MATERIALS FOR SUPERCAPACITOR TECHNOLOGIES

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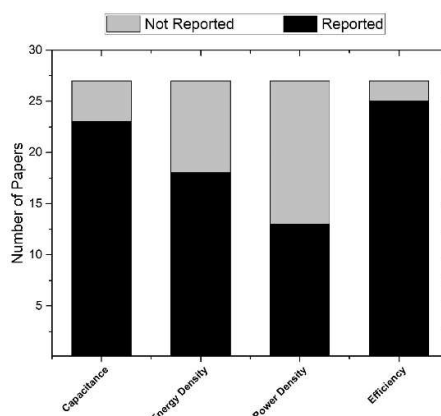
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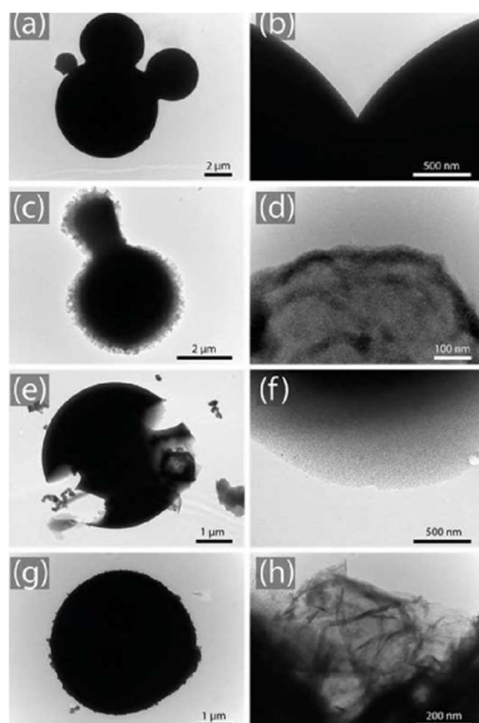
Developing efficient and sustainable energy storage systems is crucial for advancing modern technologies. This work explores the role of oxidized graphenes in Electric Double-Layer Capacitors (EDLCs) [1] and the performance of activated carbon supercapacitors derived from Italian orange juice [2].

In the first part, it is highlighted that the progress of EDLCs has greatly benefited from advancements in graphene-based materials, particularly Graphene Oxide (GO) and reduced Graphene Oxide (rGO). In fact, this work consolidates and analyzes existing research on the roles of GO and rGO in enhancing EDLC performance, focusing on synthesis methods, electrode fabrication, electrolytes, and performance metrics such as capacitance, energy density, and cycling stability (Figure 1). Key findings reveal that incorporating GO and rGO into EDLCs significantly improves specific capacitance, energy density, and cycling stability. Notable advancements include novel synthesis techniques and composite materials such as nitrogen-doped graphene, graphene/polyaniline hybrids, and various metal oxide-graphene composites, all of which exhibit superior electrochemical performance. However, challenges such as material scalability, environmental sustainability, and consistency in synthesis methods remain. To remark, this work highlights the need for continued research to address existing challenges and further optimize material properties and fabrication techniques.



**Figure 1.** Analysis of reported and non-reported metrics in research papers on the application of GO and rGO in EDLCs.

In the second part, it is scrutinized the viability of using orange juice as a promising and sustainable precursor for synthesizing activated carbon electrodes for supercapacitor technologies (Figure 2). By optimizing the carbonization-activation process and preparation parameters, such as KOH ratio and activation time, it is tailored to the Specific Surface Area (SSA) and Pore Size Distribution (PSD) of the resulting carbon materials – key factors supporting supercapacitive performance. Various spectroscopic, morphological, and electrochemical techniques characterized the obtained carbon materials. Our optimization efforts revealed that a 5:1 KOH ratio with an activation time of up to 120 min produced the highest SSA of approximately 2203 m<sup>2</sup>/g. Using these optimal conditions, we fabricated symmetric coin cell supercapacitors with Na<sub>2</sub>SO<sub>4</sub> as the electrolyte, which exhibited an impressive specific capacitance of around 56 F/g. Durability testing over 5000 cycles demonstrated excellent retention of specific capacitance, indicating the robustness of the activated carbon electrodes. This study not only advances energy storage by introducing a renewable material for electrode fabrication but also contributes to waste reduction by repurposing food byproducts.



**Figure 2.** TEM images of (a, b) pyrolyzed sample, (c, d) 4:1@120, (e, f) 5:1@120, and (g, h) 5:1@210.

### Acknowledgment

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**Keywords:** activated carbon, oxidized graphenes, orange juice, supercapacitors, electric double-layer capacitors, energy storage, renewable materials

## DYNAMICS OF LAMINAR FLUID IN NANOTUBE CONSIDERING ADHESION

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A problem of viscous fluid flow in a nanotube in connection with a boundary value problem which is depending to the flow velocity of fluid has been discussed taking into account Debye electric double layer and external friction by the authors earlier [1]. However, in the case of statistical equilibrium the sum of densities of these currents is equal to zero at any point of the double electrical layer.

Fluid flow in nano-channels and nanoporous environments differ significantly from the general case and ordered structures are moving in pores or channels with sizes varying from one to hundreds of nanometers. The corresponding dimensionless Reynolds number  $Re$  is less than  $10^{-3}$ , therefore, the fluid flow in nano-channels is always laminar. Note that a fluid flow is referred to as laminar when  $Re < 10^2$ .

Statistical (equilibrium) processes take place in the Debye electric double layer and they ensure the existence of nonzero drifting and diffusion currents, such that their densities are different from zero.

Present paper considers the case, when the diffusion coefficient and ion mobility satisfy the Einstein relation.

We derived a solution of the boundary value problem in the form of a converging infinite series, which defines the functional relation between the viscous fluid velocity and the radius vector of a particular point.

The bulk density of electric charge in the fluid depends on the velocity variation of the fluid flow, so that by processing an appropriate empirical dependence we can perform an approximation of this functional dependence to find a solution in the form of converging infinite series.

### Acknowledgment

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**Keywords:** viscous fluid, boundary value, nano-channels, velocity variations

## STRUCTURAL AND PHASE FEATURES OF FUNCTIONAL COATINGS OBTAINED BY MULTICHAMBER DETONATION SPRAYING

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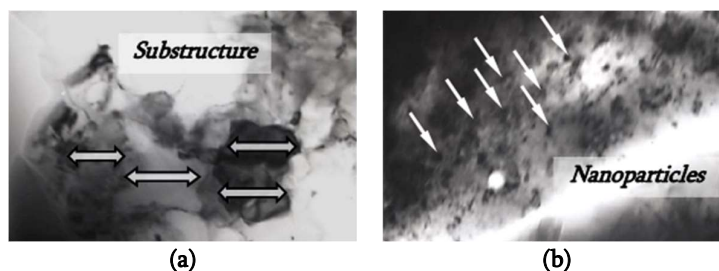
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Increasing the operational reliability and durability of parts and mechanisms used to operate under conditions of intense wear, loads, high pressure and temperatures requires the protection of working surfaces with functional coatings. The E. O. Paton Institute of Electric Welding of the National Academy of Sciences of Ukraine has developed a technology and equipment for Multi-Chamber Detonation Spraying (MCDS) of these coatings [1]. This paper summarizes the data of experimental studies of the structure of composite coatings of various systems ( $\text{Al}_2\text{O}_3\text{-Al/Ti}$ ,  $\text{Zr}(\text{SiO}_4)$ ,  $\text{Cr}_3\text{C}_2\text{-NiCr}$ ,  $\text{WC-Co-Cr}$ , etc.) for different materials. Research has established the influence of technological modes of spraying on structural and phase changes in the materials of coatings obtained by detonation spraying. Under different processing modes, the materials change: the volume fraction of phase components; microhardness; parameters of the grain and subgrain structure; size of dispersed phases; nature and distribution of dislocation density [2]. The peculiarity of the structure of coatings obtained by the MCDS method is the formation of a dispersed structure, the presence of a nanoscale substructure (**Figure 1a**) and nanoparticles of hardening phases with a size of 10–100 nm (**Figure 1b**). The formation of a nanostructural state contributes to an increase in the strength, fracture toughness, and crack resistance of coatings obtained by the MCDS method.



**Figure 1.** Thin coating structure  $\text{Cr}_3\text{C}_2\text{-NiCr}$  at (a)  $\times 50000$  and (b)  $\times 37000$ .

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**Keywords:** functional coatings, multi-chamber detonation spraying, structural and phase composition, thin structure, dislocation density

## INFLUENCE OF EXTERNAL MAGNETIC FIELD ON STRUCTURE FORMATION DURING WATER WELDING OF STRUCTURAL STEEL

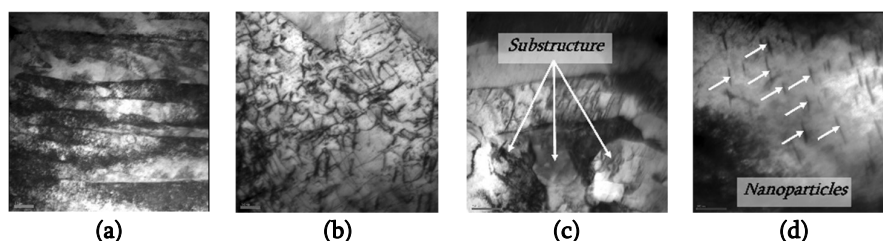
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During electric arc welding of critical metal structures in an aqueous environment, physical, chemical and metallurgical processes take place under severe, extreme conditions. One of the most relevant and promising methods for improving the quality of welds under water is forced degassing of liquid metal in the weld pool, for which External Electromagnetic Influence (EEI) is used. This paper presents the results of research on the peculiarities of the structural and phase composition of the metal of welded joints of structural steel and its influence on the physical and mechanical properties and crack resistance of the metal during underwater welding and when using EEI. In the metal of the heat-affected zone of a welded joint obtained without the use of EEI, a large-plate lath structure of upper bainite (Bu) is formed with dislocation density gradients from  $\rho = (2-4) \cdot 10^{10}$  to  $(8-10) \cdot 10^{10} \text{ cm}^{-2}$  along the boundaries of structural components. The internal structure of the packages changes significantly when using EEI: the lath structure is crushed to  $0.2-0.8 \mu\text{m}$  (**Figure 1a**) with a uniform redistribution of dislocations;  $\rho$  decreases to  $(1-3) \cdot 10^{10} \text{ cm}^{-2}$  (**Figure 1b**); a dispersed structure of the lower bainite (Bl) with a size of  $0.1-0.4 \mu\text{m}$  is formed. A characteristic feature of underwater welding and the use of EEI is the presence of a substructure with a size of  $d_s = 100-300 \text{ nm}$  (**Figure 1c**). The structure of Bl is characterized by the presence of nanoparticles of carbide phases, evenly distributed over the volume of the metal, with a size of  $(10-20) \times (30-200) \text{ nm}$  (**Figure 1d**). Such structural changes ensure the absence of zones of local dislocation hardening, a general increase in substructural and dispersion hardening, and a decrease in the level of local internal stresses – cracking concentrators.



**Figure 1.** Metal dislocation structure of welded joints obtained by use of EEI: **(a, c)**  $\times 35000$ , **(b)**  $\times 70000$ , and **(d)**  $\times 52000$ .

**Keywords:** underwater welding, structural steel, welded joints, external electromagnetic influence, microstructure, substructure; nanoparticles of carbide phases, dislocation density

## MECHANISM OF $\epsilon$ -NANOPHASE PRECIPITATION IN COPPER-STEEL

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In order to clarify the physical mechanism of decomposition of supersaturated substitution solid solutions based on  $\alpha$ -Fe with the formation of nanosized precipitates, an electron microscopic study of the structure of low-carbon copper-steel (0.05 wt.% C and 1.90 wt.% Cu), quenched in water after austenitization and tempered at different temperatures to stimulate decomposition was carried out.

It has been established that after the onset of decomposition of the supersaturated solid solution, nanosized (4–7 nm) precipitates of the fcc  $\epsilon$ -phase, i.e. iron-supersaturated copper solid solution, appear first on dislocations. Analysis of these experimental data leads to the conclusion that the nature of the decomposition is determined by the martensite substructure, which is formed from austenite one during its quenching.

In an alloy with a martensitic structure, decomposition occurs heterogeneously; both the formation and redistribution of the copper-rich  $\epsilon$ -phase and the growth of its precipitates occur primarily on dislocations and grain boundaries. Unlike martensite, in a supersaturated alloy with a polyhedral ferrite structure, decomposition occurs homogeneously, and the growth and redistribution of the copper-rich phase mainly occur in defect-free areas of the matrix.

Supersaturated iron begins to decompose, forming copper-rich isomorphic zones. With increasing copper concentration, the zones are deformed and mechanical stresses arise, which causes local tetragonal distortions of the crystal lattice. When a dislocation loop, compensating for elastic deformation, is formed around the zone, coherence is disrupted and fcc precipitates are formed in the bcc matrix.

Numerical estimates of the “set” of the total displacement required to form an incompatibility dislocation of 7.7 nm, and the size of the coherent precipitate (by the energy of its formation) of 8.0 nm are in satisfactory agreement with the proposed mechanism for the nucleation of  $\epsilon$ -phase nano-inclusions.

## CHEMICAL PREPARATION OF GOLD NANOPARTICLES ON GaP(001) SURFACE

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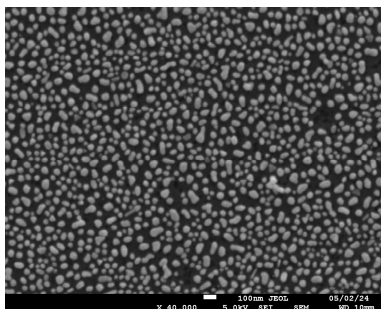
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Semiconductor-based surface structures with noble metal nanoparticles continue to be promising materials due to their practical importance and fundamental interest. We have developed a chemical procedure for obtaining the structure with gold nanoparticles on gallium phosphide surface GaP(001). The latter compound semiconductor is used in light emitting diodes and in UV radiation detectors. To prepare Au/GaP structure, we initially etch GaP(001) surface in orthophosphoric acid H<sub>3</sub>PO<sub>4</sub>. Then the etched surface is treated by 0.2 ml water solution of HAuCl<sub>4</sub>. The latter treatment, due to red-ox reaction between the solution and the semiconductor crystal, leads to formation of gold nanoparticles on the semiconductor surface. The prepared Au nanoparticles are characterized by Scanning Tunneling Microscopy (SEM). **Figure 1** presents SEM image of GaP surface after treatment in HAuCl<sub>4</sub>–H<sub>3</sub>PO<sub>4</sub> solution during 20 min at temperature 50°C.



**Figure 1.** SEM image of Au nanoparticles array chemically prepared on GaP(001) surface.

The image in **Figure 1** reveals an array of the Au nanoparticles that are randomly distributed over the GaP(001) surface. Shape of the Au nanoclusters is close to spherical, though some of them have elongated shape. From **Figure 1** we conclude that the Au clusters, whose linear sizes being in interval 40–60 nm, are dominant in the array. Optical investigation of the prepared Au/GaP structures is carried out by method of Reflectance Anisotropy (RA) spectroscopy. The measured RA spectrum of the gold nanoparticle array shown in **Figure 1** reveals a strong resonant RA line at energy of 2.1 eV. This line is attributed to the localized anisotropic plasmons of Au nanoparticles formed as a result of the developed chemical treatment. The obtained optical RA spectra clearly indicates that Au nanoparticles, prepared by the developed chemical procedure support anisotropic localized plasmons [1]. We believe that the developed chemical treatment is promising for creation various Au/A<sup>3</sup>B<sup>5</sup> plasmonic structures.

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**Keywords:** GaP(001) surface, gold nanoparticles, red-ox reaction, chemical deposition, localized plasmons

# ELECTROCHEMICAL FORMATION OF FUNCTIONAL IRON–RHENIUM COATINGS AS MULTIFUNCTIONAL MATERIALS

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The main objective of our study is to develop an electrochemical synthesis of multifunctional (magnetic and electrocatalytic) dense films of Re alloys with iron-group metals (Fe, Co, Ni). The combination of unique physical-chemical properties makes these alloys promising for use in high-technology sectors such as aviation, nuclear power engineering, electronics, biomedicine, and heterogeneous catalysis [1 – 3]. The electrochemical approach offers an eco-friendly method for synthesizing versatile materials. By co-depositing suitable compounds, this technique allows for precise tuning of properties. As a result, rhenium-based materials synthesized through this method find applications in various fields [4 – 6]. The primary focus of this study is the Fe–Re system. Electrodeposited Fe–Re alloys remain a relatively unexplored area of research despite their promising potential for various engineering applications. We developed new stable, non-toxic complex electrolytes for Fe–Re alloy deposition [7]. The dependencies of the chemical composition, current efficiency, surface morphology, and structure on the electrolyte composition (concentrations of the main components, their ratio, pH), electrolysis regimes (current density, potential), and the influence of the hydrodynamic regime were studied. High-quality nanocrystalline Fe–Re coatings with Re content ranging from 1 to 95 wt.% were obtained at temperature 20–60°C, depending on the bath composition, the concentration ratio of the main components, and deposition conditions.

## Acknowledgment

This research has received funding through the MSCA4Ukraine Project funded by the EU (Project No. 1233494).

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**Keywords:** electrodeposition, rhenium alloy, iron alloy, functional coating, nanostructure



## SILVER-BASED ELECTROLYTIC ALLOYS WITH RHENIUM AS FUNCTIONAL NANOMATERIALS

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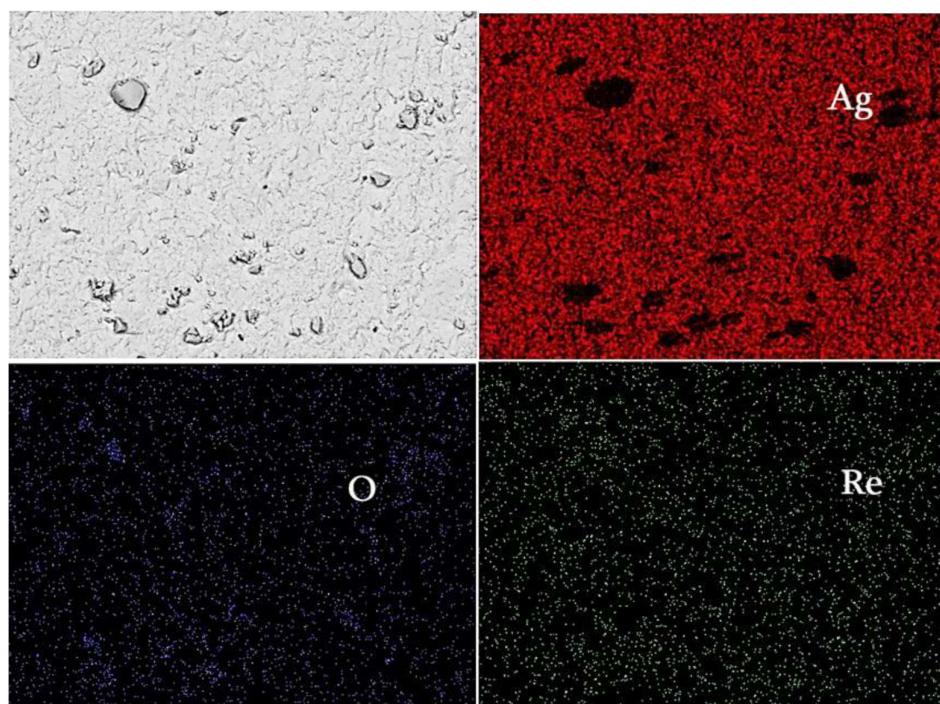
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The combination of silver's unique electrical and catalytic properties with rhenium's mechanical properties has sparked interest in developing materials based on silver–rhenium alloys [1, 2]. The electrochemical method provides an environmentally friendly way to synthesize a variety of materials, including silver–rhenium alloys, by precisely adjusting their properties, making them applicable in various fields, especially nano- and microelectronics [3, 4].

A new dicyanoargentate-perrhenate electrolyte has been developed for the electrodeposition of Ag–Re alloys [5]. The composition of the pre-cathode layer during silver electrodeposition in an electrolyte based on a dicyanoargentate complex has been modeled previously [6]. The main objective of this study was to establish the impact of bath composition, the [Ag(I)]:[ReO<sub>4</sub><sup>-</sup>] ratio, applied current density, temperature, and stirring on the alloys' composition, structure, morphology, and some properties, and compare them with electrolytic silver from the BPC dicyanoargentate bath [7–9]. Silver-white Ag–Re alloys with a thickness up to 15 μm, containing from 0.15 to 13.5 wt.% Re, were deposited from baths with [Ag(I)]:[ReO<sub>4</sub><sup>-</sup>] ratios ranging from 10:1 to 1:10. The morphology of deposits obtained from Ag-rich baths differs from those from Re-rich baths.



**Figure 1.** SEM images, corresponding elemental maps of Ag, Re, and O of sintered samples Ag–Re.

Analysis of the SEM–EDS mapping (**Figure 1**) demonstrates a uniform distribution of elements for samples deposited from an Ag-rich solution with a ratio  $[\text{Ag(I)}]:[\text{ReO}_4^-] = 10:1$ . Increasing the current density to 15 mA/cm<sup>2</sup> tended to decrease the Re content in the deposit and reduce current efficiency to 66%, irrespective of the temperature (20–60°C) and stirring. Increasing the rhenium content in the alloy resulted in a decrease in crystallite size.

### **Acknowledgment**

This research has received funding through the MSCA4Ukraine project, which is funded by the European Union (Project # 1233494).

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**Keywords:** electrodeposition, rhenium alloy, silver, functional coating, nanostructure

**STRUCTURAL AND OPTICAL PROPERTIES OF GaN  
RECEIVED BY REACTIVE MAGNETRON SPUTTERING**

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In this paper structural and optical properties of GaN polycrystalline samples received by reactive magnetron sputtering technology are presented. Deposited layers of GaN on the sapphire substrate was analysed by XRD and revealed the polycrystalline nature highly oriented with the (0002). For chemical composition was measured X-ray Photoelectron Spectroscopy (XPS) and it was found out the ratios of Ga:N to be 1.07.

The analysis of transmission spectra reveals correlation with growth temperature of GaN samples and band gap of the GaN material. By increasing temperature of samples for the formation of GaN, the edge of minimum of transmitted wavelength is shifted towards 361nm, which corresponds to the band gap 3.4 eV of the GaN material.

The band gap of GaN material can be calculated from the edge of transmission spectra minimum. This work also shows that, with the increase of growth temperature of the samples for growing GaN, the optical properties of the GaN improve, which corresponds to increasing angle of the slope of the graph transmission spectra.

## USE OF DNA FOR NANOTECHNOLOGICAL PURPOSES: STUDY OF QUALITY OF DNA DOUBLE HELIX

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The UV spectroscopic display of double proton transfer in GC pairs of DNA induced by H<sub>3</sub>O<sup>+</sup> and transition metal ions has been studied [1]. It displays itself in a red shift and broadening of the absorption band of DNA and, as a rule, in slight hypochromism. The mechanism of double proton transfer is based on a phenomenological quantum mechanical consideration of the influence of ions on the electronic configuration of atoms molecules involved in H-bonding. This consideration takes into account the specific energy of two-state H-bonds and the self-consistent transition of protons in cyclic structures that form a single electron-proton complementary molecular complex between proton-donor-acceptor groups. The latter is a necessary and sufficient condition for keto-enol and amino-imine tautomeric transformations in solutions of polar organic molecules.

The combined use of the following methods has been studied ultraviolet differential absorption spectra of DNA metal complexes, FRET [2] and atomic emission spectral microelement analysis of DNA. It comes, on the one hand, from the UV spectroscopic display of tautomeric in GC pairs induced by H<sub>3</sub>O<sup>+</sup> and transition metal ions and the associated formation of irregular Watson-Crick GC pairs and atomic emission analysis of trace elements in DNA, on the other. Quantitative analysis of irregular GC pairs in DNA is based on increasing the information capacity of the method of ultraviolet differential absorption spectra by combining it with the method of atomic emission analysis of trace elements in DNA. Thanks to this, based on the defects caused by temperature, radiation [3, 4] and various ligands it becomes possible to determine both the risk factor and the quality of DNA for use in nanotechnological purposes.

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**Keywords:** DNA, metal ions, UV difference spectroscopy, AES microelement analysis, FRET

# THERMODYNAMIC INVESTIGATION OF NANO BORIDE'S PRODUCED VIA SHS TECHNIQUE

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FactSage is a Windows™-based thermochemical computer program capable of performing complex process simulations. Thermodynamic data of hundreds of alloys, liquid and solid oxides and slags, molten and solid salts, mattes, as well as aqueous solutions and thousands of pure compounds are available in the databases of the FactSage program (Fact, FS, SGTE, etc.). Thanks to its modules, FactSage can perform chemical reaction (Reaction), pressure-temperature (Predom), Eh-Ph (Eph), balancing (Equilib) as well as phase diagram calculations (Phase Diagram) of oxides and alloys and can transfer the results to tables or graphs. FactSage addresses many fields such as pyro-, hydro- and electrometallurgy and materials engineering (plating, corrosion), chemical engineering, inorganic chemistry, environmental and geological engineering [1 – 3].

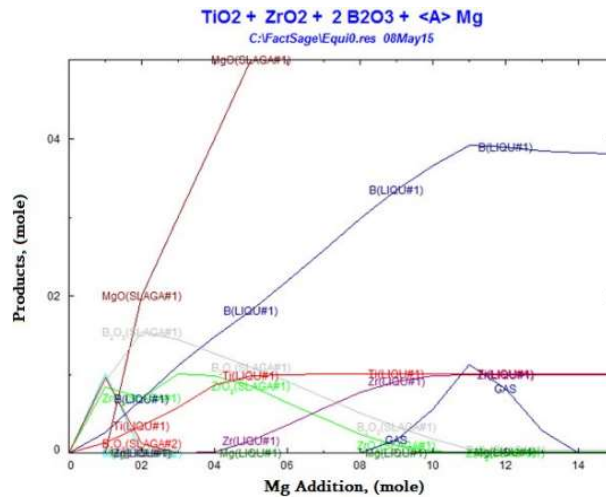


Figure 1. Probable phases of ZrO<sub>2</sub>, TiO<sub>2</sub>, B<sub>2</sub>O<sub>3</sub>, and Mg-system.

In this study, the reduction conditions of advanced ceramic materials containing boron were examined using the FactSage program. Accordingly, the reduction conditions of ZrB<sub>2</sub>-TiB<sub>2</sub> are shown in Figure 1. It was seen that it was possible to obtain the mentioned composite by adding 8 mol Mg.

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**Keywords:** B<sub>4</sub>C, ZrB<sub>2</sub>, TiB<sub>2</sub>, Self-propagating High-temperature Synthesis (SHS), FactSage

## ABOUT RAMAN, ULTRAVIOLET AND INFRARED SPECTROSCOPY METHODS FOR EXPERIMENTAL STUDY OF VIRAL NANOMATERIALS SPECTRA

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Study of spectroscopic properties of nanomaterials and nanoparticles is important and essential for development of nano-material science and nanotechnology. Spectroscopic properties of nanoparticles of biological origin, especially pathogenic nanoparticles such as viruses became actual after Covid-19 pandemic causing economic, human and social harm. Known spectra of utmost atoms, molecules and compositions are well used for identification purpose of that. In this report, we demonstrate the possibility of use spectra of viruses, viral nanomaterials or viral mixtures for sensing and identification of diseases caused by the pathogens. Raman, ultraviolet (UV) and infrared (IR) spectroscopy methods for experimental study of viral materials are proposed for consideration.

Based on experimental results, the spectroscopy methods, relevance and appropriateness of that, advantages relative to biophysical and biochemical methods, PCR-testing, immune-enzymatic and serological analysis are discussed. Spectroscopic techniques offer unique advantages, allowing non-destructive analysis in real time. It makes possible to gain the detailed information about chemical composition and structure of biomaterials, nano-/micro-biomolecules and cells by obtaining a spectral “signature” of the bio-sample and determining the characteristic absorption and scattering spectrum of biomolecules, viruses.

Analysis shows, that the spectra of viruses are strongly dependent on the virus type, the optical properties of solvent, substrate and bio-environment, the concentration of viral material in that and the wave length of light source. The intensity of the signals responded on interaction light & material, the magnitude of the peaks of absorption spectra increases, as higher is the concentration of viral material in bio-environment. We should note that the peaks (maxima) of absorption or scattering spectra observed in different solvents or bio-environments for the same virus are significantly different. Therefore, for differentiation and identification of spectra of viruses, for better understanding of experimental results is needed the comprehensive analysis, and the background signal/data processing by applying the modern statistical and computing methods.

### **Acknowledgment**

Work is supported by Shota Rustaveli National Science Foundation of Georgia (FR-23-4069).

**Keywords:** nano-biomaterial, nanoparticle, Raman spectroscopy, ultraviolet spectroscopy, infrared spectroscopy

# STUDY OF OPTICAL PROPERTIES OF VIRUS-LIKE NANOSTRUCTURES FOR BIOMEDICAL APPLICATION

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Knowledge of optical properties of nanostructures, nanomaterials and composites are very important for creation and improvement of new devices and technics applicable in biomedicine, optoelectronics, materials science and technology. Nanostructures are of different origin and compositions. The objects of our research are nanoparticles of bio-origin, such as biomolecules and bio-structures, viruses and virus-like particles (VLPs). The most of viruses are nano-sized structures, having icosahedral, helical or complex morphology. Identification and differentiation of viruses among the bio-agents of different size and composition in various environment, is significant for prevention and diagnostic of diseases, health-care and environment safety. Elaboration of new principles and basis, experimental and theoretical methods, linked to better operation of detection systems are the key in modern researches, especially after Covid-pandemic. Optical spectrum is the one of the most prominent feature, the identification signature of the atoms, molecules or composites. We consider the possibility of using spectral signatures of viruses as the main and basic identification element of detection systems. In contrast to immune-enzymatic, serological, PCR analysis, the spectroscopic methods possess opportunity to detect and identify the viruses in real time. Presently, many spectroscopic experiments carried out successfully for identification purpose of viral materials. To generate the dataset of spectral signatures of viruses will improve the detection system and become the effective tool in identification processes of bio-agents. In this paper, we consider the one of the ways to spectral dataset compilation. Methods of modelling and simulation with complement of experimental measurements, make possible to determine the viral signatures. The models of viral nanoparticles, based on their morphology are considered. Protein-capsid and DNA/RNA-core structured virion is the type of hybrid organic-organic nanoparticle, shape of model depends on virus species. Simulation study of optical properties of VLPs is based on the concept considering the virus as a particle with definite geometric, and EM parameters [1, 2].

Mathematical modeling is based on deterministic solution of physical problem, namely of electromagnetic (EM) wave & single particle interaction. EM fields inside and outside the particle are written in analytical form, which makes possible to define the scattering and absorption fields in near or far zones of the particle. Results are obtained for cylindrical and spherical structures of viral particles using the 1st and 2nd approximations of models of virions. Simulation carried out in MatLab environment for obtaining modeled "spectra" of virions. Graphical analysis shows, that modeled "spectra" are sensitive to variations of characteristic parameters of virions, bio-environment and wavelength range. The spectra are very specific for each VLPs and could be considered as the "signature" of a viral particle in a given bio-environment.

## Acknowledgment

Work is supported by Shota Rustaveli National Science Foundation of Georgia (FR-23-4069).

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**Keywords:** nanostructure, virus-like particle, modeling, simulation, spectroscopy

# QUANTITATIVE <sup>31</sup>P NMR SPECTROSCOPY INVESTIGATION IN HAIR OF BISPHOSPHONATES AS BANNED SUBSTANCE IN SPORTS

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## ***Background and Aims***

Bisphosphonates (BPs) are a class of pharmaceutical drugs approved by FDA for use in human health as well as veterinary medicine. There are many books and review articles available that describe the chemistry, pharmacology, and applications of BPs in clinical and veterinary medical use [1 – 3].

Bisphosphonates are prohibited drugs according to the International Federation of Horseracing Authorities (IFHA) [4]. Any administration of a bisphosphonate to a racehorse less than 4 years old is an unacceptable practice because of a high risk of serious injury or death from deleterious effects on bone growth and strength because of such use.

These compounds are used for the treatment of navicular syndrome and related diseases in horses and are divided in two groups: non-nitrogen-containing bisphosphonate drugs (e.g., tiludronic acid) and nitrogen-containing bisphosphonate drugs (e.g., zoledronic acid). In forensic toxicology, hair is used as a research material to detect various substances, particularly in detecting drugs for a long period of time post administration [5 – 8]. Due to their polar and strong chelating characteristics, determination of bisphosphonates represents a real analytical challenge for routine screening.

According to a recent study about successful use of hair samples for detection of BPs in horses, a method of liquid chromatography-tandem mass spectrometry was used [9].

## ***Methods***

Quantitative <sup>31</sup>P NMR spectroscopy is a valid method in analytical chemistry for detection of phosphorus containing compounds, but still not used for detection of BPs in hair as a method of choice.

<sup>31</sup>P-NMR spectroscopy is widely used to study biological structures under native conditions, which is useful for studying hair.

Preliminarily, we used an ‘in silico’ computational study of the toxicity of BPs by Yasara software to use a molecular simulation method.

## ***Results and Discussion***

Phosphorus-31 NMR, which has been widely applied since the early days of in vivo NMR. The <sup>31</sup>P isotope (with nuclear spin of I = 1/2) is 100% naturally abundant with a sensitivity of 6.63% that of <sup>1</sup>H. Computer simulation model was used to mimic in vivo <sup>31</sup>P NMR spectroscopy. Alongside with <sup>31</sup>P magnetic resonance imaging both are important applications of this nucleus. <sup>31</sup>P signals from inorganic phosphate, can be observed in whole-cell preparations, intact tissues, and whole bodies and can provide information of the cells. Both empirical and theoretical correlations between measured coupling constants, <sup>31</sup>P chemical shifts, and structural parameters have provided an important probe of the conformation and dynamics of various phosphorus-containing compounds, particularly BPs.



## ***Conclusion***

We report the results of an *in silico* investigation of the binding of a series of bisphosphonate drugs to hair keratin using  $^{31}\text{P}$  nuclear magnetic resonance spectroscopy. The  $^{31}\text{P}$  NMR simulation shows molecular dynamics quantitative results of binding interaction with hair keratin that bisphosphonate groups bind to protein.

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## EXPLOSION TECHNOLOGIES: PROBLEMS, ACHIEVEMENTS, PROSPECTS

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Explosion technologies are widely used in civil engineering and defense. Research in this direction has been conducting since the 60s of the last century at the Mining Institute in Georgia, which was then called the “Institute of Mining Mechanics, Ore Processing and Blasting Physics of the Georgian Academy of Sciences”. The work was especially expanded in the 80s, when the institute designed and built an underground semi-industrial explosive complex, which is internationally recognized as unique in the world. Completion / equipment of the base was carried out with the funds of two projects financed by the NATO scientific program in 2005–2010 and 2013–2018.

The presentation will in details our main achievements and the author's personal role / contribution over the last 20 years from the multi-disciplinary work carried out at the institute, namely:

- An automatic system for protection against gas and dust explosions in mines, consisting of explosion detectors and an energy suppression module, was developed, manufactured and tested. A US patent was issued.
- A stand was developed and created, which allows determining the response of a structural element to dynamic loads generated by an explosion under natural conditions. The results are used in the calculation of the design parameters of explosive materials warehouses and special purpose buildings (fortification buildings, explosive materials production area, underground shelters, etc.).
- Innovative schemes for obtaining high-entropy, nanostructured composites by blast welding, solidification and powder compaction of metals were developed. Optimal modes were determined for specific compositions. Research is underway to obtain multi-layer armor gradient plates by explosive welding.
- A physical model of the body of an armored vehicle was created to evaluate the effectiveness of its armor under natural conditions. The results will significantly reduce the cost and duration of field / polygonal tests on armor blasting.

In the last 10 years, more than 50 articles / scientific works have been published on the mentioned topic in publications registered in international high rating databases; more than 60 reports at international conferences were presented. Since 2015, regularly have been organizing the section “Mining Engineering, Blasting and New Technologies” in the format of the World Symposium on Earth Sciences (moderator Nikoloz Chikhradze); up to the present moment 6 scientific conferences “Actual Problems of Mining and Geology” has been held.

**Keywords:** explosion synthesis, high strain rate loadings, nanocomposites, high entropy alloys, explosion technologies

## NEW TRENDS IN ENHANCING BIOLOGICAL EFFICACY AND SAFETY OF PROTON THERAPY: GEORGIAN EXPERIENCE

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Due to the super-linear growth of the number of particle (especially, proton) therapy centers in 2010–2018, many researchers forecasted the number of patients treated by proton therapy to reach 500–550 thousand before 2026 [1]. However, the real farther overall spread of hadron therapy was much slower due to its high cost, very high research intensity and very high requirements for medical and engineering staff, so that by the end of 2026 the number of patients reached only 410–415 thousand [2], clearly tending to saturation with an ever decreasing share of ion therapy and showing that the increase of the biological efficacy and safety of proton and especially heavy ion therapy is it is an urgent need of today's time. The most promising and experimentally substantiated concept of the whole body and the highly localized combination cancer therapy was developed and tested by Japanese [3] and Georgian [4] researchers in 2015–2020, which clearly demonstrated the high efficiency of the highly localized multicomponent combined therapy of cancer. Thus article reports the in vitro and in vivo data on the relative anticancer efficacy and acute toxicity of the 10 various multicomponent nanoparticle containing anticancer combinations in comparison to the widely used anticancer drugs gemcitabine, carboplatin, cisplatin and paclitaxel systematically applied against the Non-Small Cell Lung Cancer (NSCLC), clearly showing that the newly developed combinations can be several times more efficient and have a several times less toxicity than the usually applied anticancer drugs. Obtained data provide reasons to conclude that the significant increase in the effectiveness of combined formulations is caused by the super-additive synergistic interaction of nanoparticles and the active components of anticancer mixtures. It is especially important that the newly developed “cocktails” [5] reveal a 3 to 10 times increased therapeutic window due to several increased necrotic and apoptotic activity against the cancer cells in comparison to healthy tissue cells, drastically increasing the therapeutic value of the drugs due to higher efficacy and safety, significantly reduced duration and costs of treatment.

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**Keywords:** cancer, proton therapy, heavy ion therapy, efficacy, acute toxicity

# DIATOMIC MOLECULAR MODEL CALCULATIONS: BORON PLANAR CLUSTERS

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The specific (per atom) binding and vibrational energies, bonds equilibrium length, static atomic charges, electrical dipole moment, and other key ground-state parameters of boron planar clusters  $B_n$ ,  $n = 2-20$ , can be calculated in the recently introduced phenomenological diatomic molecular model [1, 2] imagining the clusters as constructions of pair interatomic chemical bonds.

In this approach, binding energy and bonds length of neutral ground-state isomorphs of  $B_n$  are found to be within the ranges of 1.48–6.26 eV/atom and 1.58–1.60 Å, respectively.

Comparison of these theoretical results with available experimental data leads to the conclusion that the developed diatomic model is able to provide realistic estimates for small boron clusters formation probabilities.

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## TUNGSTEN SCRAP AS PRECURSOR FOR MANUFACTURING ADVANCED MATERIALS

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Tungsten and its compounds are widely used in many fields of modern technology and science. China controls 80% of world production, at the same time it has partially restricted its export, due to which the price of tungsten on the world market has increased significantly. Therefore, the recycling and utilization of tungsten and its compounds from used materials, machines, or tools is of great importance [1, 2]. Unconditioned powders, plates, spirals, rods and other products of tungsten and its alloys are collected in various technological processes, which can be processed by various methods. We propose a two-step method of W-scrap recycling, which includes its grinding and dissolving of the obtained powder in hydrogen peroxide aqueous solution resulting in the Peroxypolytungstic Acid (PTA) formation. Good solubility of PTA in water and some other solvents allows to prepare homogeneous liquid charges, heat treatment of which yield WC and WC-Co in form of (ultradispersed) powders. To obtain WC-Co, we selected the system  $\text{PTA-Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}-\text{C}_{12}\text{H}_{22}\text{O}_{11}$  (sucrose), which contains water-soluble components. By mixing the component solutions and drying them by vaporization at 300–400°C, a pre-ceramic precursor is obtained, in which tungsten, cobalt and carbon compounds are homogeneously distributed, and WC-Co is obtained by their carbonization in a hydrogen atmosphere (at 1000°C). This technology does not require scarce metal powders: the target product is obtained from available reagents. PTA solution was used for tungstenizing surfaces of various nature. By reducing PTA in a hydrogen atmosphere, metallic tungsten powder is obtained, which was used to obtain sandwich composites with boron carbide B<sub>4</sub>C (W/B<sub>4</sub>C, W/B<sub>4</sub>C/W) as neutron shield materials. Composites of sandwich morphology are obtained by spark-plasma sintering method.

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**Keywords:** tungsten scrap, hydrogen peroxide, peroxypolytungstic acid, tungsten carbides and alloys, tungsten-boron carbide sandwich, spark-plasma sintering

# DEVELOPMENT OF LUMINESCENT DYE-DECORATED GOLD NANORODS AND TARGETED DRUG DELIVERY SYSTEMS FOR VISUALIZATION AND TREATMENT OF CANCER FORMATIONS

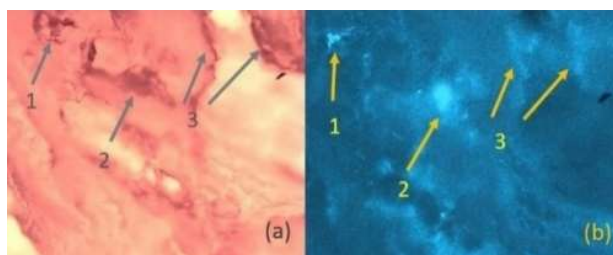
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According to the World Health Organization, cancer is a leading cause of death worldwide, accounting for nearly 11 million deaths in 2022, or about one in six deaths [1]. The combination of imaging and therapeutic agents with drug nanocarriers has received significant attention due to the number of outstanding applications in oncology and early cancer-stage diagnosis [2]. We have shown that Gold NanoRods (GNRs) conjugated with Luminescent Dyes (LD) can be considered a valuable modality for in-vitro representation of nanoparticle-mediated cancer biomarkers for cell labeling and tracking in biological tissues through luminescence. This method can be highly advantageous for early-stage cancer detection and visualization because of the reduced scattering and absorption of Near-Infrared (NIR) irradiation, which results in the deep penetration of light in the biological tissues. In cancer cells, the ratio of extracellular and intracellular pH values differs. Next, we have demonstrated a novel, light, and pH-controlled drug delivery system based on the SpiroPyran (SP) and pH-sensitive LD-doped Liquid Crystal (LC) microcontainers (Figure 1).



**Figure 1.** GNR/LD-doped cancer tissue as it looks under (a) optical and (b) confocal microscopes equipped with NIR CCD camera

Experimental results have shown that upon exposure to UV/violet light and variation of pH value, the photochromic and pH-responsive molecules inside the LC microcontainers experience an interconversion from the hydrophobic, oil-soluble, non-polar state to the hydrophilic, water-soluble, highly polar condition. The light and pH-induced isomerization destabilize the LC water interface, stimulate its translocation across the LC-water barrier, and result in their homogeneous distribution throughout an aqueous environment. The proposed strategy can be considered a novel platform for early-stage cancer cell labeling and photo-damaging. In addition, the photo and pH-stimulated drug delivery systems offer the possibilities of the controlled delivery and release of a wide variety of drugs into the body at a suitable time and desired sites to fight different kinds of diseases, including cancer.

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**Keywords:** gold nanorods, luminescent dye, cancer, drug delivery

## ON PULSE IMPACT MECHANISM EFFICACY: THE MORE POWER THE LESS DOSE

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(1) The resulting effect of electromagnetic radiation interaction with different physical objects is determined, as a rule, by the radiation power. In this case, two impact mechanisms are divided: cumulative, which takes place at continuous low-power radiation, when the reaction of the object is caused by accumulation of a certain dose of radiation within a certain period of time, and pulse, when the reaction is a consequence of a shock, short-term impact. The fundamental difference between both mechanisms is determined by the radiation power. By example of the biological action effect of UV radiation, the peculiarities of the impact mechanism are considered [1 – 6]. The results of UV sterilization studies show that the efficiency of process  $I$  is described by the expression

$$\log I = \exp(-H_{bac}/H_0), \quad (1)$$

where  $I = N_r / N_0$  is the ratio of residual infection population  $N_r$  to initial population  $N_0$ . Besides, the relation  $N_0 = N_r + N_k$  takes place, where  $N_k$  is the number of pathogens destroyed. The asymptotic dependence of the cumulative continuous radiation mechanism efficiency determines its main disadvantage, which in the case of UV exposure is the principal impossibility to realize complete 100% sterilization. At the same time residual infection is the cause of hospital-acquired infection forming, e.a. of resistant to disinfecting effect viral or pathogenic microflora development, or formation of new biological forms due to induced mutagenity. It follows from dependence (1) that the radiation dose required to destroy  $\Delta N$  viruses at the beginning of the process is rather small, while at its final segment it is equal to infinity. Notice that the cumulative dependence of pathogen destroying is identical to the quantum efficiency of radiation impact on a semiconductor [7]:

$$\eta(\lambda) = \frac{(1-r)[1-\exp(-\alpha d)]}{1-r\exp(-\alpha d)}, \quad (2)$$

where  $\alpha$  is the optical absorption coefficient,  $r$  is reflection coefficient. The value  $d$  in this case can be considered as the seeded pathogens monolayer thickness [5, 8, 9]. At  $r=0$ , the expression (2) turns into cumulative dependence  $N_k/N_0 = 1-I$ . This means that in the continuous radiation there is almost complete absorption of radiation in the monolayer.

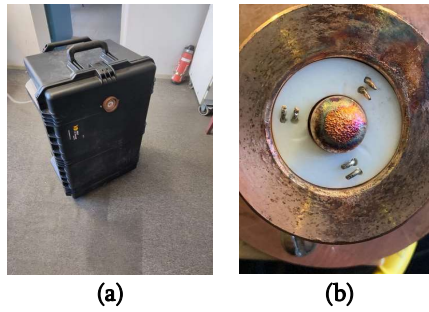
(2) In the pulse mode the process reduces to the following [8 – 10]. It is easy to show that dependence (1) takes the vertical line shape when power increases. Besides, there is a ratio connecting the power required to realize the sterilization effect with the duration of the complete destruction pathogens process  $t_k$  [11]:

$$P(t_k) = \frac{P_0}{1 - \exp(-t_k/t_0)}, \quad (3)$$

where  $P_0 t_0$  is the specific energy that determines the pathogens resistivity. Function (3) reflects the two most important features of the pulse impact mechanism:

- Threshold effect, i.e. at  $P t_k < P_0 t_0$  full sterilization is basically impossible;
- Dependence  $P t_k$  reflects a fundamental feature of pulse impact – the more radiating pulse power the less integral energetic dose required for complete sterilization.

(3) For experimental studies, a source of pulsed UV radiation based on a magnetoplasmatic compressor was developed (Figure 1). The device generated power about 3.6 MW in UV bactericidal band.



**Figure 1.** Pulse high-power UV source based on (a) magnetoplasma compressor and (b) design of UV irradiator.

**Table 1.** Experimental results of sterilizing efficacy (pulse duration 30  $\mu$ s).

Pathogen	Bacteria			Viruses					Spore
	<i>S. epidermidis</i>	<i>S. aureus</i>	<i>E. coli</i>	Flu N1H1	Flu A/PR8/34/H0N1/	Herpes II type	BVD	TVG	<i>Bacillus Anthracis</i>
Exposition (number of pulses)	10/15	5	5	2/5	2	2	5	5	15
Sterilizing efficacy, %	99,99999/100	100	100	94/100	100	100	100	100	99,99

The high efficiency of pulse sterilization was confirmed by a series of experiments, as a result of which, for the first time, the effects of complete destruction of the coronavirus family viruses were obtained, as well as of the *B. anthracis* (Table 1).

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**Keywords:** pulse mechanism, UV radiation, sterilization, pathogen, virus



# COMBUSTION SYNTHESIS OF $\text{Al}_2\text{O}_3$ REINFORCED METAL CARBIDE COMPOSITE NANOPARTICLES BY ALUMINOTHERMIC REDUCTION PRINCIPLE

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The synthesis of advanced technology ceramics and composite nanoparticles is of importance for advanced technology applications such as in the defense and aerospace industry. The Self-propagating High temperature Synthesis (SHS) method, a type of combustion synthesis, enables the synthesis of carbide and boride ceramic nano powders from oxide raw materials [1]. In this study, which focuses on the synthesis of composite nanoparticles to improve negative aspects such as low sinter ability and low toughness, the use of Al as a reductant instead of the commonly used Mg, and the direct production of  $\text{Al}_2\text{O}_3$ -reinforced composite powders from oxide raw materials, is presented. For the synthesis of  $\text{TiC-Al}_2\text{O}_3$ ,  $\text{ZrC-Al}_2\text{O}_3$ , and  $\text{TiC-ZrC-Al}_2\text{O}_3$  composite powders, after thermodynamic evaluation and thermochemical simulation processes, the stoichiometries of the reductant and oxide raw material charges for the SHS method were optimized, and an innovative chemical route to control the amount of  $\text{Al}_2\text{O}_3$  formed as a by-product was proposed [2, 3]. **Figure 1** presents experimental set up.



**Figure 1.** Experimental setup of aluminothermic reduction.

Characterization was performed using XRD and SEM-EDS analyses. The results revealed that, by using the more cost-effective Al reductant instead of Mg, it is possible to achieve in-situ synthesis of  $\text{Al}_2\text{O}_3$ -reinforced composite nanoparticles with particle sizes ranging from 200 to 400 nm, eliminating separate processing steps such as the synthesis of carbides,  $\text{Al}_2\text{O}_3$  production, and mechanical alloying, and that the amount of  $\text{Al}_2\text{O}_3$  can be controlled with a novel chemical route which includes pre-acid leaching, caustic fusion and water leaching steps.

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**Keywords:** self-propagating high temperature synthesis, nano composite, zirconium carbide, titanium carbide, aluminum oxide

## STATIC ATOMIC CHARGES IN BORON PLANAR CLUSTERS

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Due to the finiteness of the structure, the constituent atoms even of a cluster composed of identical atoms may have non-zero static electric charges. Since the coordination numbers of the atoms located on the periphery of the cluster are less than those of its central part, the valence electrons will move from the periphery to the center. As a result, the peripheral and central atoms will be, respectively, charged positively and negatively. And if the symmetry of the cluster structure is such that the centers of distribution of positive and negative static charges do not coincide, then it will have a non-zero electric dipole moment as well. Hence, there is a quite high academic interest in the topic.

The topic is also of practical interest, because planar boron nanoclusters are the building blocks of borophene – a promising two-dimensional nanomaterial. The electric dipole moment affects the interaction of the clusters with each other and with the borophene growth substrate. Borophenes and boron clusters themselves can be used in such areas of techniques and technology as nanoelectronics, radiation protection (from neutron fluxes and gamma-rays), hard and corrosion-resistant coatings, etc.

In the diatomic model of structures constructed from atoms, a cluster binding energy is expressed as the sum of binding energies between pairs of nearest neighboring atoms in its structure. In addition to the corresponding diatomic molecule binding energy related to the exchange of valence electrons, the interatomic binding energy also includes the energy of electrostatic interactions caused by the non-zero static electric charges of the atoms associated in the cluster.

In small boron clusters, the unequal distribution of the valence electronic charge between identical atoms is due to the different coordination numbers of the peripheral and central atomic sites. The constituent atoms non-zero static electric charges can also cause the inducing of a non-zero electric dipole moment of the cluster. In this work, coordinates and static effective charges of constituent atoms of  $B_n$ ,  $n = 1 - 20$ , planar cluster are calculated and then, using these data, values of boron nanoclusters electric dipole moment are estimated. Calculations were performed only for isomorphs with the highest symmetry, because it was assumed that they correspond to the ground state. It is confirmed that the electric dipole moment for all clusters with rotational symmetry is identically equal to zero, and it is established that only the clusters without rotational symmetry –  $B_5$ ,  $B_8$ ,  $B_{11}$ ,  $B_{14}$ , and  $B_{17}$  – have non-zero electric dipole moments.

In addition to chemical interactions, in vacuum these clusters can physically interact with each other and, relatively more weakly, with clusters without a dipole moment and also with surfaces. Thus, the electric dipole moments of small boron clusters affect the growth kinetics of borophenes and other boron nanostructures. The values of the static electric charges of the atoms constituting the planar boron clusters and, accordingly, their dipole electric moments influence such key characteristics of the clusters as the molar binding energy and the chemical bonds equilibrium length, as well as the vibrational energy.

The obtained results are compared with the available literature data and a good agreement between them is confirmed. This circumstance means that both the diatomic model of the cluster and the estimation of static electric charges of atoms, according to their coordination numbers, give correct estimates.

**BORON CARBIDE IN PYROLYTIC CARBON MATRIX: MICRO|NANO  
COMPOSITE MATERIAL FOR MEDICAL AND AEROSPACE APPLICATIONS**

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In this talk we report the synthesis methodology and material properties of the boron-enriched pyrolytic carbon (B-PyC). In the research we aimed to propose a material demonstrating high strength characteristics and heat resistance, durability, chemical inertness and biocompatibility making it attractive for advanced biomedical and engineering applications. The material has been synthesized by high temperature low pressure CVD method. The synthesis the process takes place on the inner surface of a hollow graphite hexagonal prism heated to the temperatures 1450–1570°C. Controlled low-density flows of nitrogen, boron trichloride and carbonaceous gas react in this zone producing B-PyC film deposited on the graphite substrate. A homogeneous and fairly dense composite material with a small number of micropores is deposited in the upper part of the reaction zone and mainly consists of agglomerates, which are rather thin flaky carbon structures. In turn, these structures are compositions of thin graphite layers, randomly stacked on top of each other and highly entangled, with a rather low degree of crystallinity. Morphology, mechanical and physical properties of this material was investigated using X-ray diffraction, Raman spectroscopy, scanning and transmission electron microscopy. It was found that during the synthesis a two-phase composite system is organized comprising fragments of graphene layers (pyrolytic carbon) and boron carbide B<sub>4</sub>C. Such a structure provides high mechanical properties of the material and their stability in a wide temperature range, heat resistance, chemical inertia and biocompatibility. Depending on the synthesis conditions, the micro hardness may vary in a wide range and reach the values of 100–135 HV. This makes the material promising for the heart surgery prosthesis. Corresponding operational life testing of the valve with cusps made of B-PyC has been successfully carried out.

## PHOTOCHROMIC LIQUID CRYSTAL POLYMER FILMS FOR MODERN DEVICES OF OPTICAL INFORMATION

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Qualitatively new polymer films, consisting of photochromic SpiroPyran (SP) doped in the nematic-chiral Liquid Crystal (LC) matrix, have been obtained using the technological process of the microencapsulation method, improved by the authors [1]. SPLC polymer films contain nematic-chiral mixtures, the helix pitch of which weakly depends on the temperature. Such polymer films are characterized by an insignificant temperature shift of the selective reflection of the light in the long-wavelength region of the visible spectrum, and is distanced from the absorption band of the short-wavelength colored merocyanine form of SP. Exposure to UltraViolet (UV) light can be controlled not only the process of photochromic transformations, but also the structure of the LC matrix. Hence, the combination and preservation of the properties of LC and SP in one system, interaction between them give qualitatively new optical properties to the nanostructured polymer films, received by the authors [2]. Spectral and microscopic research has shown that by regulating technological characteristics – sizes of microcapsules, thickness, and stretching of the film – at the stages of the microencapsulation process, the authors obtained technologically perfect reversible SPLC polymer composites in the form of films with improved photosensitivity and with high intensity of the selective reflection (**Figure 1**).



**Figure 1.** Optical recording images with high contrast by the UV light in SPLC polymer films.

Presented SPLC polymer films are photochemically stable-over time, technological characteristics determine the engineering properties of the optical parameters of polymer films, which is very important for practical use. The creation of multifunctional photosensitive LC rewritable materials based on SPLC polymer films are promising to record, display, and storage information in modern high-performing photo-optically controlled devices, such as UV irradiation dosimeters, holograms, light-controlled molecular and fluorescent switches, etc. [3, 4].

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**Keywords:** liquid crystal, photochromic, microencapsulation, polymer film

# NANOCONJUGATE OF HYALURONIC ACID CARRIER WITH CYANINE-BASED TELOMERASE INHIBITOR

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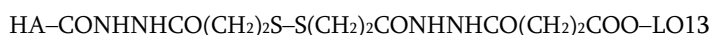
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Telomerase is an enzyme synthesizing the telomeric DNA. High telomerase activity is observed in a majority (85–90%) of cancer cells, in contrast to normal somatic cells. This tumor-associated enzyme is a promising target for anticancer drugs. The majority of antitumor telomerase inhibitors act by binding and stabilizing the G-quadruplex (G4) structures of telomeric DNA. G4s are specific four-stranded nano-sized assemblies formed by the stacks of guanine quartets linked by non-canonical systems of hydrogen bonds. G4 ligands are usually based on large planar heteroaromatic systems containing the cationic / basic groups [1, 2].

Anticancer drugs often suffer from low specificity, toxicity and low water solubility. To overcome these problems, the drugs can be covalently attached to nanocarriers, including the biocompatible hydrophilic polymers, either natural (polysaccharides) or synthetic (polyethylene glycol, polylactic acid, dendrimers, etc.). Such nanoconjugates allow the targeted delivery of drugs and releasing the bioactive compound inside the tumor cell [3].

The biological screening of a series of our cyanine dyes revealed the monomethine cyanine LO13 as G4 ligand and telomerase inhibitor with submicromolar antiproliferative activity in vitro. This cationic dye contains the basic substituent increasing the ligand affinity to anionic G4-DNA. Here, we prepared a nanoconjugate of LO13 with Hyaluronic Acid (HA). This natural COOH-containing polysaccharide is a well-established carrier for drug delivery [4]. To obtain the conjugate, both inhibitor and polymer were first functionalized. COOH group was introduced into the cyanine, whereas HA (average MW 130–150 kDa) was modified with a bifunctional reagent DTP, 3,3'-dithiodipropionic acid dihydrazide, in the presence of water-soluble carbodiimide EDC to form a hydrazide derivative.

The conjugation was performed via the activation of COOH group of LO13 succinate with phosphonium reagent BOP in the presence of 1-hydroxybenzotriazole in dry DMF followed by the coupling with hydrazide-modified HA at ambient temperature to provide the polymer–drug conjugate of the following structure:



HA-cyanine conjugate was purified by ethanol precipitation followed by the dialysis. LO13 content in various samples of the lyophilized product was in the range 10–20  $\mu\text{mol/g}$ . The linker contains the biolabile S–S bond that can be easily cleaved inside the cell by reducing agents like glutathione to release the bioactive agent. Indeed, the conjugate treatment with dithiothreitol (DTT, 100 mM, pH 7.5, r.t. overnight) resulted in LO13 cleavage from the polymer. Cyanine can also be cleaved from the carrier in alkaline medium. The nanoconjugate is well soluble in water and sufficiently stable (no decomposition was observed in 4 months upon dry storage at 4°C). The study of its biological activity is in progress.

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**Keywords:** telomerase, G-quadruplex DNA, inhibitor, cyanine, hyaluronic acid, nanoconjugate

NOVEL 2-ACETAMIDO-2-YLIDENE-4-IMIDAZOLE DERIVATIVES (EL-SAGHIER REACTION): GREEN SYNTHESIS, BIOLOGICAL ASSESSMENT, AND MOLECULAR DOCKING

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El-Saghier reaction is the novel, general, and green reaction of various amines with ethyl cyanoacetate and ethyl glycinate hydrochloride. A new series of imidazolidin-4-ones and bis-N-(alkyl/aryl) imidazolidin-4-ones was synthesized in a sequential, one-pot procedure under neat conditions for 2 h at 70°C. Excellent high yields (90–98%) were achieved in a short period of time while avoiding issues related to the hazardous solvents utilized (cost, safety, and pollution). The spectrum analyses and elemental data of the newly synthesized compounds helped us to clarify their structures.



The obtained compounds were tested for antibacterial activity in vitro and compared to the standard antibiotic chloramphenicol as the standard, measuring the inhibition zone (nm) and activity index (%). With an antibacterial percentage value of 80.0 against *Escherichia coli*, N,N'-(propane-1,3-diyl)bis(2-(4-oxo-4,5-dihydro-1H-imidazole-2-yl)acetamide) proved to be the most effective. Antimicrobial activity was confirmed by a molecular docking investigation to investigate how chemicals bind to the bacterial FabH–CoA complex in *E. coli* (PDB ID: 1HNJ).

## INFLUENCE OF DC MAGNETRON SPUTTERING CONDITIONS OF NiO ON ITS STRUCTURAL PROPERTIES

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Currently, nickel oxide (NiO) has shown itself to be a promising semiconductor material. This material is a wide-bandgap p-type semiconductor that is highly promising for the creation of heterojunctions for rapidly developing applications based on GaN and Ga<sub>2</sub>O<sub>3</sub> [1]. At the same time, this material itself can be in demand in various sensors, such as semiconductor gas sensors. One of the features of NiO is the strong dependence of the structural, electrical and optical properties of films on deposition methods and parameters, which is typical for many oxide semiconductors. This allows for controlled operation of film parameters depending on its application. There are several basic methods for deposition of NiO films, such as pulsed laser deposition, sol-gel, electron beam, radio frequency and direct current magnetron sputtering [2, 3]. Films produced by magnetron sputtering are of high quality and have high potential for mass production. The work reports on the influence of DC magnetron sputtering conditions of NiO in a gas mixture of Ar and O<sub>2</sub> on the structural properties of the resulting thin films. NiO films were obtained in two different deposition modes with deposition powers of 100 W (0.3 A, 330 V) and 265 W (0.5 A, 530 V). In this case, the fundamental difference between the sputtering processes is whether the nickel target is in a passivated or unpassivated state.

The work shows the transition between deposition modes, where a sharp increase in current occurs with a gradual increase in the discharge voltage. With a subsequent increase in power, there is a lack of oxygen and the formation of a metal coating. Analysis of the film structure by XRD showed for both cases the presence of a polycrystalline NiO phase, but with different main pronounced diffraction directions. In this case, for the high-power mode, the formation of a film with a large crystallite size is observed. Comparison of the phase composition results obtained by XPS showed a decrease in the Ni<sup>3+</sup>/Ni<sup>2+</sup> ratio with increasing sputtering power. The observed difference in the structure and composition of the films was observed in the transparency and conductivity of the films. Films obtained in the 100 W deposition mode showed a transparency of no more than 5% and a low resistivity of 0.01 Ω·cm. For other mode, high transparency (up to 85%) and resistivity of 10<sup>6</sup> Ω·cm are observed.

### Acknowledgments

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**Keywords:** wide bandgap semiconductors, NiO, magnetron sputtering

# NANOSTRUCTURAL PROCESSES AND NANO CRACKS IN THIN FILMS OF STRUCTURAL STEELS

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Recently, much attention has been paid to nano cracks and their formation mechanism. Even theoretical works have already appeared, in which they study where and by what mechanism nano cracks are formed at the modeled boundary [1]. The reason is clear, because nano structures are already actively used in many fields of industry. It is natural that nano cracks are formed in them, which also require investigations. Accordingly, it is necessary to investigate the mechanism of formation of nano cracks, both by theoretical and experimental methods [2]. In our work, the course of nano structural changes in austenitic chromium-nickel steel used in nuclear power is studied after Low-Cycle Fatigue (LCF) deformation. In particular, the nano-cracks formed as a result of relaxation in the areas of localization of residual internal stresses in slip bands. The causes and mechanism of their formation are discussed. Formation locations and distribution of LCF slip bands during low-cycle fatigue microplastic deformation. It is shown that the course (development) of micro deformation during LCF depends on the microstructure of the material. It is established that the cause of both non-localized and localized microplastic deformation is the structural inhomogeneity of the material. During the redistribution of residual internal micro-stresses, in areas of high concentration, nano cracks are formed during their relaxation [3]. The geometric size of the crack depends on both the magnitude of the concentrated internal stresses and the places of concentration.

## Acknowledgments

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**Keywords:** nano cracks, micro strains, cyclic, deformation, fatigue



# MOLECULAR MODELING OF GLYCYRRHIZIN COMPLEXES WITH CORTISOL AND ANTI-CORTISOL PROTEIN

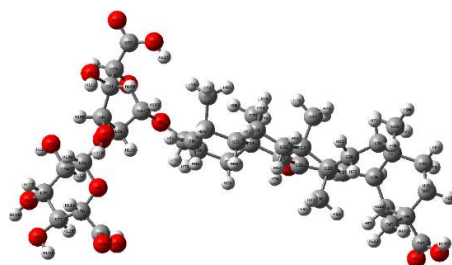
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Glycyrrhizin and its aglycon, glycyrrhetic acid, which is an active metabolite in licorice, has inhibitory properties on the metabolism of cortisol- stress hormone, that increases glucose level in the bloodstream [1]. Our work represents the molecular interaction of glycyrrhizin (ChemSpider ID: 14263) (**Figure 1**) and cortisol in complex with anti-cortisol Fab fragment (PDB ID: 8cbv) using the molecular docking software AutoDock Vina.



**Figure 1.** Molecular structure of glycyrrhizin.

It was found the ligand forms an interaction with the active site of the anti-cortisol complex with affinity values – 7.4 kcal/mol (**Table 1**). Based on the calculated results and SAR data analysis the pharmacophore model for the glycyrrhizin interaction with the specified receptor was proposed [2].

**Table 1.** Comparison of binding energies of glycyrrhizin and anti-cortisol Fab in complex with cortisol (8cbv).

#	Affinity, kcal/mol)	Distances from best mode, Å	
		Rmsd l.b.	Rmsd u.b.
1	– 7.4	0.000	0.000
2	– 7.1	3.000	12.224
3	– 7.1	3.025	12.265

Molecular docking that as effective method for drug design and discovery, reveals bimolecular interactions between the target protein and the docked ligand. In this work, molecular docking was used to examine the interaction mechanism of the glycyrrhizin molecule with complex cortisol–anti-cortisol Fab fragment by AutoDock Vina software [3].

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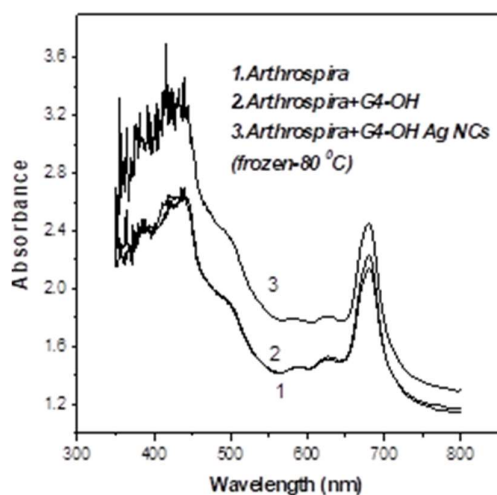
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**Keywords:** glycyrrhizin-1, cortisol-2, anti-cortisol Fab fragment-3, molecular docking-4, pharmacophore model-5.

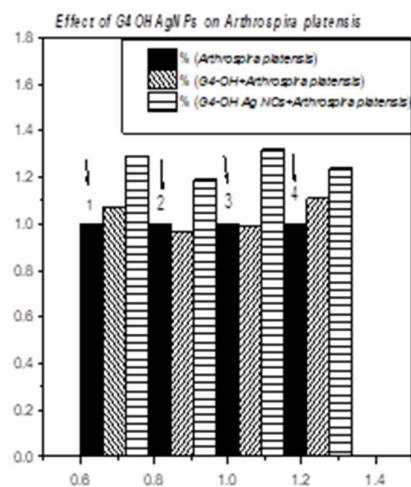
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Gold and silver NanoParticles (NPs) are widely used in the therapeutic and the diagnostics fronts. Many questions about the risks of the interaction between NPs and plants, as a basic component of all ecosystems unknown. The purpose of this study is to investigate the effect of PAMAM–Au and Ag NanoComposits (NCs) on algae (cyanobacterium) *Arthrospira platensis*, as a model at various conditions using UV–visible spectrometry.



**Figure 1.** Influence of PAMAM (G4–OH)–Ag NCs on frozen at  $-80^{\circ}\text{C}$  and then re-cultured *Arthrospira platensis*.



**Figure 2.** Graphical presentation of effect of PAMAM (G4–OH)–Ag NCs on *Arthrospira platensis* at various conditions: (1) freezing, (2) intact cells, (3) irradiation, and (4) fermentation (all cases after cultivation).

In **Figure 1**, as an example, are presented effect of PAMAM–Ag NCs on frozen at  $-80^{\circ}\text{C}$  and then re-cultured *Arthrospira platensis*. It is seen from **Figure 1** that PAMAM (G4–OH) do not influence on the *Arthrospira platensis*, but PAMAM–Ag NCs increasing silver nanoparticles absorption intensity. Analogue effects were observed at various conditions (**Figure 2**). Influence of PAMAM–Au NCs on *Arthrospira platensis* also was investigated.

#### Acknowledgment

The work was supported by Shota Rustaveli National Science Foundation of Georgia (Grant # STEM-22-1347).

**INVESTIGATING OF MECHANICAL PROPERTIES AND THERMAL  
BEHAVIOR OF MODIFIED POLYPROPYLENE / NANOSILICA  
NANOCOMPOSITE IN PRESENCE OF COMPATIBILIZER**

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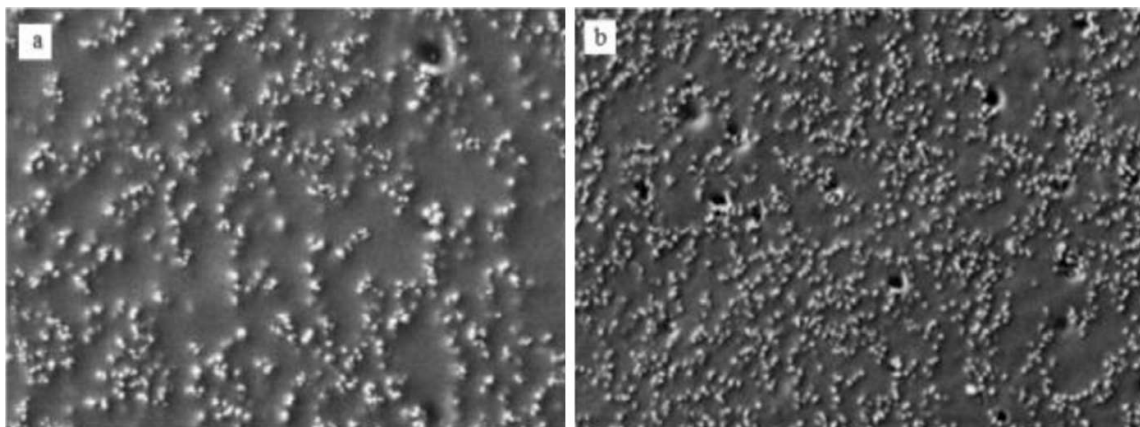
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In this research, the effect of nanosilica modified with vinyltris (2-methoxy, ethoxy) silane and its effect on the thermal behavior and mechanical properties of polypropylene/nanosilica nanocomposite [1 – 3], in the presence of maleic anhydride (PP-g-MA) compatibilizer, were investigated. Two sets of nanocomposites were prepared with different filler ratios (1, 3, and 5%) in the presence of maleic anhydride compatibilizer and without compatibilizer. Scanning Electron Microscope (SEM) and ThermoGravimetric Analysis (TGA) techniques were used to check the morphology of the prepared nanocomposites and standard tests were used to check the mechanical properties of the nanocomposites (Figure 1).



**Figure 1.** SEM image of nanocomposites: (a) 1.0, and (b) 3.0 and 5.0% modified nanosilica.

The SEM images showed that the addition of maleic anhydride PP-g-MA improved the dispersibility of the modified nanosilica in the polypropylene matrix and created a homogeneous structure. The results of thermal and mechanical tests showed that their heat resistance and tensile and Flexural strength increases. These thermal and mechanical properties show a significant increase in the nanocomposite prepared with 3% by weight of modified nano silica filler in the presence of maleic anhydride compatibilizer (Table 1).

**Table 1.** Findings for nanocomposites  
mechanical properties by measuring of strength.

Sample	Flexural Strength, MPa	Flexural Modulus, GPa	Tensile Strength, MPa
Pure polypropylene	37.1 ± 1.0	1.4 ± 1.0	29.7 ± 1.0
Nanocomposite (1% nanosilica)	43.7 ± 4.0	1.9 ± 0.3	31.8 ± 4.0
Nanocomposite (3% nanosilica)	58.1 ± 3.0	2.5 ± 0.2	38.5 ± 3.0
Nanocomposite (5% nanosilica)	51.5 ± 4.0	2.3 ± 0.3	35.1 ± 2.0

With an increase in the amount of modified nanosilica by 3wt.%; bending strength, tensile strength and bending modulus will increase. However; if there is a 5wt.% increase, these properties will reduce.

Examining the morphology of nanocomposites by SEM showed that addition of modified nanosilica will improve the interaction between particles and the matrix; and specimens with 3wt.% of nanosilica have a larger intercalation space and 5wt.% nanosilica compared to specimens with 1wt.% nanosilica. And XRD confirms the formation of intercalation structure in the resulting nanocomposite.

#### **Acknowledgment**

Thanks to the Nanocomposite Research Department, University of Tehran, for support.

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**Keywords:** nanosilica, nanocomposite, thermal resistance, tensile/bending strength

## PROCESS OF PROPAGATION OF ELECTRICAL IMPULSE IN NEURAL NETWORK BY ELECTRODYNAMIC ANALYSIS

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Based on the principles of thermodynamics and electrodynamics [1 – 8], the authors of the study seek to provide a simplified explanation for the process of electrical impulse transmission in the neural networks of multicellular animals. For this purpose, a rigid coaxial cable is considered as a nerve fiber (axon), the membrane of which acts as an insulator and its resistance is one-millionth of the insulation resistance of a real electrotechnical coaxial cable. Its contents are electrolytes, the resistance of which is much lower than that of the sheath (myelin), but it is many times higher than the resistance of the metal “core” (central conductor) of the real electric cable. Because of this, a nerve fiber in its resting state is uneconomical to transmit an electrical signal over long distances.

The paper presents the electrical scheme of the axon, that is, the active and capacitive resistance of the membrane in the form of parallel-connected elements interconnected by intracellular electrical resistance. In this scheme, the magnitude of the potential during propagation inside the myelin sheath is higher than the excitation potential before the Ranvier constriction. At the Ranvier constriction, a short circuit occurs and the potential quickly rises to zero, due to the direct connection between the membrane and the extracellular electrolyte solution. This means that in an inanimate environment, the process would end, but local changes in the membrane occur. The potential inside the biocell stimulates the opening of ion channels, which further increases the potential and causes an action potential. As a result, the flow of current between the resting and active parts allows the nerve impulse to propagate at high speed along the axon of the neuron.

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**Keywords:** sheath (myelin), electrical impulse, nerve fibre (axon)

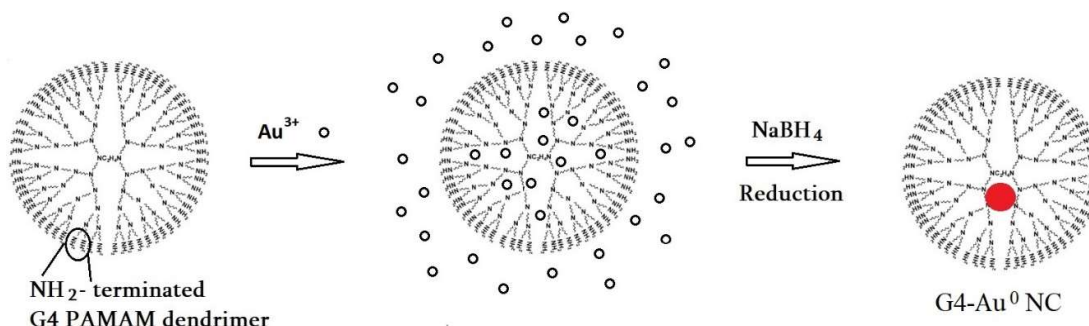
## STUDY OF REDUCTION PROCESS OF GOLD IONS ON G4 PAMAM DENDRIMERS

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Organic nanoparticles G4 PAMAM (polyamidoamine) dendrimers have important characteristics, such as: chemical content, huge surface, spherical form, “pockets” full of water between the branches, therefore in modern research, dendrimers are used for synthesis of various metal nanoparticles. This means that the metal ions enter the existing hollow space in the structure of the dendrimer, and when the reductant is added, they reduce to atoms and form a nanoparticle. In this case, the distribution of nanoparticle sizes is narrow.



**Figure 1.** Creation of G4–Au<sup>0</sup> NC.

The main goal of the research was to study the reduction process of gold ions on G4 PAMAM dendrimers with different terminal functional groups (**Figure 1**): NH<sub>2</sub> and OH, to create new, stable nanosized (~ 5 nm) metalorganic NanoComposites (NC). The investigation of the catalytic properties of the G4 PAMAM in the reactions of reduction of gold ions, was performed using spectroscopic and thermodynamic methods.

### Acknowledgment

The research was supported by Shota Rustaveli National Science Foundation of Georgia (Grant # STEM-22-1347).

**Keywords:** PAMAM dendrimers, metal ions, metalorganic nanocomposites, absorption spectroscopy

## DETECTION OF PHASE TRANSFORMATION IN BINARY Ti-Ta ALLOYS BY MEANS OF ELECTRICAL RESISTANCE AND DIFFERENTIAL THERMAL ANALYSIS

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Titanium alloys have low density, high solidity, heat stability and steadiness towards a number of aggressive environments. However, there are often some difficulties in the way of using titanium alloys. They are associated with chemical heterogeneity, instability of mechanical properties, low temperature stability and others. The presence of two allotropic modifications in titanium, low-temperature hexagonal ( $\alpha$ ) and high-temperature cubic volume-centered ( $\beta$ ), is the basis for creation alloys having shape memory effect. In our time, special attention is paid to the study of these issues.

Despite the large number of works on the metastable state of titanium alloys, a number of questions concerning both the structure of some metastable phases and the mechanism of their formation remain unanswered. Some details of phase transformation kinetics in titanium alloys have not yet been fully explored. The nature and mechanism of martensitic transformation, as well as the structure and properties of metastable structures, are poorly studied.

The use of multi-component alloys in production with chemical elements that affect the phase composition and kinetics of phase transformation in different ways creates the need to study the formation of metastable phases and the processes of transformations, both in binary and compositionally more complex systems, since during heat treatment the influence of individual elements and their combination on the nature of transformation is less studied.

The aim of the research is creation of the titanium-based binary alloys with shape memory effect, ductility and maximum damping ability. The solution of the problem lies in determining of the concentration of the components in the alloy that provide the outlined goal. Ti-Ta binary alloys are chosen as the research material. The concentration of stabilisation for Ta is determined from the critical metastability concentration of the  $\beta$ -phase “on both sides” (the minimal concentration at which the  $\beta$ -phase can still be fixed by tempering).

Experiments have been performed on electrical resistivity and differential thermal analysis instruments of our own design, and our data are in good agreement with calorimeter results obtained by other methods.

**Keywords:** titanium, binary alloy, shape memory effect, phase transformation, damping

# SCRUTINIZING OF MAGNETO-VOLUME AND MAGNETO-CALORIC BEHAVIOR OF $R_2Fe_{17}$ NANOSTRUCTURED INTERMETALLIC ALLOYS

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The so-called ‘invar effect’, discovered at the end of XIX century, is still today an intriguing topic at the crossover between solid state and materials science that stimulates a lot of research work. This effect, primarily investigated by Guillaume in a ferromagnetic fcc  $Fe_{65}Ni_{35}$  binary alloy, consists of an almost constant ‘invariant’ lattice parameter or unit cell volume of the material (nearly zero or Low Thermal Expansion – LTE) in a wide temperature range just above the Curie temperature [1]. Invar alloys are commonly exploited as functional materials for applications requiring temperature-independent geometry (i.e. precision sensors for aerospace technology or high-resolution screens). Therefore, the search for new invar materials and/or new processing methods to enlarge the temperature range for LTE above room temperature is a current challenging issue [2, 3]. Moreover, ferromagnetic invar materials display other anomalies in their physical properties, such as the negative pressure dependence of the Curie temperature and the hyperfine field distribution, the elastic moduli or the heat capacity among others, which are commonly referred to as magneto-volume anomalies [1].

$R_2Fe_{17}$  compounds (R = rare earth) exhibit a variety of magnetic behaviors (ferro-, antiferro-, or ferri-magnetic and more complex magnetic orderings such as helimagnetism or fan magnetic structures) depending on the rare earth element [4]. Likewise, all of them display large magneto-volume anomalies induced by the strong dependence of the magnetic exchange interaction on the Fe-Fe interatomic distances [5 – 7]. In addition, these binary intermetallics show a moderate Magneto-Caloric Effect (MCE), with values of the magnetic entropy change  $\approx 6 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$  (for  $\mu_0\Delta H = 5 \text{ T}$ ) at room temperature (for R = Nd, Pr) [8 – 10].

In this talk, we will show our investigations on the magneto-volume anomalies and the magnetocaloric properties of  $R_2Fe_{17}$  alloys in polycrystalline, nanostructured and rapid quenched samples with special emphasis given to the advantage of using neutron and synchrotron X-ray diffraction under extreme conditions (T and P).

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**Keywords:** nanostructured materials, Fe-rich intermetallic alloys, magnetic properties, invar behavior



## INVESTIGATION NANOCOMPOSITES BASED ON PTFE MATRIX FILLED WITH Fe-DOPED CARBON NANOPARTICLES

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The present work is dealing with the study of a nano-compositional material which was obtained on the basis of PTFE with 2.5–10.0wt.% of core-shell type Fe-doped Carbon NanoTubes (CNTs) and carbon nano-particles as fillers [1]. The PTFE samples without the fillers were prepared too.

Weight wear, friction coefficient and temperature were measured after passing some velocity steps, and afterwards the linear wear was calculated. The obtained results have shown that the incorporation of about 2.5–5.0wt.% of Fe-doped CNTs into PTFE matrix drastically improves the antifrictional properties in comparison to the unfilled PTFE. Namely, the wear resistance of these nanocompositions increased by the factor of 500–150 in the range of friction velocities 0.25–1.25 m/s. Increase of the filler portion up to 10wt.% transforms the obtained nanocomposite from antifrictional to friction material with the enhanced coefficient of friction up to 0.32, but with the unexpectedly ultra-low wear.

SEM–EDX analyses of the worn surfaces of the tested nanocomposites and the cast iron samples after working as a tribological pair, revealed some favorable effects of the Fe-doped CNTs filler on the formation mechanism of a transfer film and its role in promoting very low wear of the obtained new nanocomposites.

The mechanical, electrically conductive and thermophysical properties of nanocomposites were also studied.

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**Keywords:** Nanocomposite polymer, PTFE, Fe-doped CNT

# ELECTROLESS SYNTHESIS OF COBALT NANOWIRES IN EXTERNAL MAGNETIC FIELD AND THEIR CHARACTERIZATION BY NMR AND RESONANT RADIO-FREQUENCY MAGNETOMETRY METHODS

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A simple and effective low-temperature electroless chemical method provides the synthesis of cobalt micro- and nanowires due to the processes of self-organization of magnetic cobalt nanoparticles under the influence of a magnetic field, using the low-temperature technology of chemical synthesis of magnetic nanoparticles and nanowires [1].

Cobalt nanoparticles have magnetic dipole moments. The presence of an external magnetic field forces them to be oriented parallel to the field. Dipole–dipole interactions between magnetic nanoparticles lead to attraction between cobalt nanoparticles leading to their self-organization into nanowires, reducing their total energy.

The magnetic and structural properties of the synthesized nanowires were studied by the resonant Radio-Frequency (RF) magnetometry, NMR and electron microscopy methods [1, 2]. The characteristics of Domain Wall (DW) pinning (fixing) centers in cobalt nanowires were studied by the NMR spin-echo method using an additional Magnetic Video-Pulse (MVP) acting in between two radio-frequency pulses in two-pulse spin echo method [2].

It was shown in [2] that the use of nuclear spin echo of cobalt nanowire nuclei located in DWs in combination with MVP is a convenient method for studying DW pinning centers and their dynamics. The coercive force of cobalt nanowires was studied by the macroscopic resonant RF magnetometry method complimentary to the microscopic NMR method. These methods are of interest for optimizing the synthesis of cobalt nanowires with a view to their possible use to create permanent magnets that do not use rare earth elements, as well as in information processing devices and sensors. As is known, the magnitude of the coercive force of a magnetic sample is directly related to the efficiency of pinning of a DW and, consequently, to the difficulty of its detachment from the pinning (fixing) centers.

## Acknowledgment

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**Keywords:** electroless, cobalt, nanowire, NMR, magnetometry

# HIGH CAPACITY RECOVERY OF Ag(I) FROM AQUEOUS SOLUTION BY MESOPOROUS SILICA SORBENT

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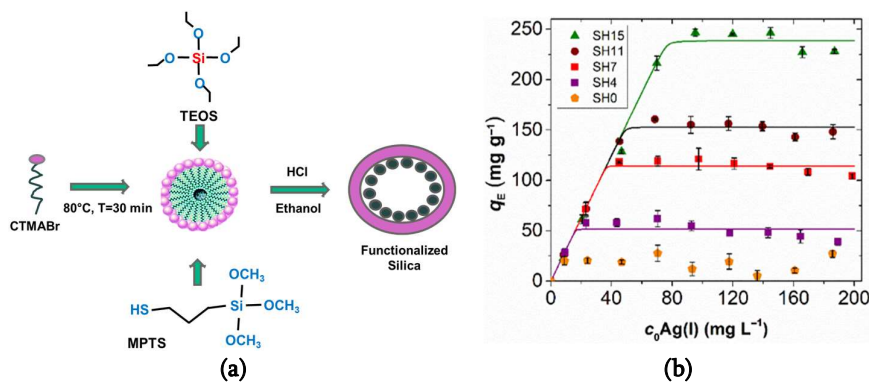
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A simplified sol–gel method was developed for the preparation of thiol functionalized porous silica particles using (3-mercaptopropyl)-trimethoxy-silane (MPTMS) for co-gelation in the presence of micellar templates. The resulting short range ordered porous silica microparticles are exceptionally effective sorbents of aqueous Ag(I) (Figure 1).



**Figure 1.** Synthesis scheme (a) and Ag(I) sorption isotherms (b) of thiol-functionalized mesoporous silica.

The binding of aqueous Ag(I) is almost stoichiometric in the broad pH range between 4.0 and 9.0 even at low Ag(I) concentrations until reaching the limiting ca. 200 mg·g<sup>-1</sup> sorption capacity. The sorbent displays high selectivity towards Ag(I), which was tested in the simultaneous presence of several different metal compounds. The practically complete recovery of Ag(I) and the regeneration of the sorbent was achieved by washing with a Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution. X-ray Photoelectron Spectroscopy (XPS) revealed that silver is not reduced on the surface of the sorbent. The reason for the strong and selective binding of Ag(I) is the formation of layered thiolate coordination compounds on the functionalized silica surface that display characteristically high stability [1].

## Acknowledgments

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**Keywords:** mesoporous silica, adsorption, sol–gel, nanoparticle, functional material

## LOW-VOLTAGE ACTUATORS BASED ON ION-POLYMER MATERIALS

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Compared to traditional actuators (drives), polymer actuators have many advantages, such as versatility, optimal power-to-weight ratio of the material, lack of inertia, noiselessness, and the possibility of direct connection with the actuator (there is no need to use a transmission) [1, 2]. Ionic Polymer-Metal Composites (IPMCs) exhibit low electrical voltage (1–10 V) actuation, high deformation, light weight, silent operation, and similar flexibility to biological muscles. One of the promising materials for IPMC actuators is the so-called nafion polymer. It is a fluoropolymer-copolymer based on sulfonated tetrafluoroethylene and is considered one of the main components in the actuator. The structure of nafion has an important role on the electromechanical characteristics of the actuator, such as elastic modulus, conductivity, capacitance, water content, migration channel and cationic degree of hydration of its matrix membrane.

IPMC actuators with a nafion membrane are capable of operating effectively in both air and water environments. Thus, it becomes possible to implement various forms of deformation (tension, compression, bending, etc.). The actuator independently generates movement and does not contain additional moving elements used in traditional drives (internal combustion engines, electric motors, etc.), in particular, levers, rotating and sliding parts. The following general limiting factors were identified that need to be eliminated in IPMC actuators with a nafion membrane: metal electrodes increase the rigidity of the IPMC, as a result of which the range of its movement is limited; the realized output force is weak <50 mN; the achieved ratio of the developed force to the mass of the actuator is less than the same parameters for the human heart or other muscle.

It has been shown that the deterioration of the electromechanical characteristics of actuators is significantly influenced by the properties of the metal electrodes of the membrane. Therefore, much attention is paid to promising other materials that are suitable as electrodes in membranes. It is believed that they should contain non-metallic fillers, in particular oxidized graphite, carbon nanotubes, fullerenes, etc.

It is noted that the use of biocompatible composite nanomaterials based on carbon nanotubes as Nafion membrane electrodes can significantly improve the characteristics of the IPMC actuator. For example, such an example is an implant to correct drooping upper eyelid [3].

### Acknowledgment

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## NON-INVASIVE REGISTRATION OF MAGNETIC NANOPARTICLES IN PHANTOM OF BIOLOGICAL MEDIUM

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Magnetic NanoParticles (MNPs) are being actively studied for wide application in biomedicine, in particular, in the diagnosis and treatment (theranostics) of oncological diseases, as well as for tumor hyperthermia and magnetically controlled targeted delivery of drugs to pathological sites.

This work examines the physicochemical properties of MNPs and the possibility of their registration at localization sites in a biological environment, as well as the prospects for their use in theranostics.

MNPs were synthesized in an aqueous medium by chemical coprecipitation (Massart reaction). This method involves the co-precipitation of iron hydroxides by adding an excess of ammonia solution to a solution of iron (III) and (II) chlorides in a 2:1 ratio in an aqueous solution with vigorous stirring. The main product of the reaction is Fe<sub>3</sub>O<sub>4</sub> magnetite nanoparticles, the sizes of which are in the range of 10–25 nm. To stabilize and prevent coagulation and oxidation of the obtained MNPs, their surface was coated with Polymeric Materials (PM).

In this work, the coprecipitation reaction was carried out both in the presence of polyvinyl alcohol as a stabilizer and without it. The resulting MNPs powder was mixed with MicroCrystalline Cellulose (MCC) powder in a ratio of 3wt.% MNPs to 97wt.% MCC. From this powder, tablets with a diameter of 13 mm and a thickness of 2.2–5.8 mm were made by pressing (press 200 bar). Suspension samples were a mixture of liquid PolyMethylSiloxane (PMS) and MNP in the ratio: 3wt.% MNPs to 97wt.% PMS. The suspension was considered a phantom of a biological medium since their viscosities practically coincided (~5 mPa·s). Tablets and suspensions were used as samples on which measurements were carried out to study the magnetic properties of MNPs.

A magnetic field  $B_0$  was used, the value of which was controlled by a Honeywell HMR2300 magnetometer. The magnetic field  $\Delta B$ , which is the difference between the measured values of the magnetic fields without the sample and with the sample, was used to estimate the values of magnetization  $J$  and the specific magnetic moment  $p_m$  inside the sample. It was believed that the measured  $\Delta B$  is correlated with the values of  $J$  or  $p_m$ , i.e.  $\Delta B \sim J, p_m$ .

It has been established that in a weak field  $B_0 \leq 2$  G, samples (MNPs without coating and with PM) exhibit the properties of an ideal superparamagnet. The magnetic susceptibility is higher for MNP samples than for MNPs with PPM. In the second case, the samples were placed in a high magnetic field  $B_0 = 600$  G for 1 min and their magnetic susceptibility and magnetization relaxation were studied.

In these studies, the susceptibility of the samples turned out to be more than an order of magnitude lower than in the field  $B_0 = \pm 2$  G, and the behavior of their remanent magnetization was similar to that of a ferromagnetic material. At the same time, the relaxation time (estimated by the exponential law) for the MNPs samples was approximately greater than for MNPs with PM. The samples had sufficient residual magnetization, which allowed them to be reliably recorded at a distance of up to 5–6 cm from the magnetometer sensor, which had an

operating temperature corresponding to room temperature and a resolution of  $\pm 0.1$  mG. All measurements took into account the influence of the Earth's magnetic field.

Thus, the synthesized magnetic nanoparticles and the technique for their registration make it possible to use them as theranostic agents for targeted delivery of various ligands and markers in a biological environment. The considered concentrations (3wt.% MNPs) are sufficient for their complete and non-invasive control under in vivo conditions in small laboratory animals.

Examples of the use of magnetic nanoparticles in theranostics of osteoarthritis, oncology, etc. are considered.

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## HIGH-VOLTAGE ACTUATORS WITH ELECTRODES WITHOUT METAL MATERIALS

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Since electrodes are an important element of DEA, they must be able to simultaneously track large deformations of the elastomer without creating counter-voltage or loss of conductivity.

Soft robots, in which the main elements are soft materials and/or stretchable materials with a significant number of degrees of freedom, provide an opportunity to bridge the gap between machines and humans. Large deformation, high energy density and short response time can be considered as the main problems, the solutions of which will allow creation of soft robots for large-scale applications in science, technology and medicine [1].

In soft robots, the most promising is the use of Dielectric Elastomer Actuators (DEA) as actuators, which can perform various forms of mechanical movement and action. Particularly positive properties should be noted that DEA can convert electrical energy into mechanical movement with fairly high efficiency (more than 60%), and its active elements contain inexpensive and accessible materials such as silicone, acrylic, natural rubber, polyurethanes, etc. [2]. However, they have some disadvantages, in particular, to achieve a significant change in shape (deformation) and a high efficiency value, it is necessary to use strong electric fields ( $\geq 100$  MV/m) or high operating electrical voltages ( $\geq 4$  kV) [3]. In this case, at some points of the membrane, dielectric breakdown may occur and the DEA fails.

As usual, films of noble metals (Pt, Au, etc.) are used as electrodes, but they worsen the mechanical properties (hardness, elastic modulus, elasticity increase) and the efficiency of DEA. In medical applications, the flexibility and high degree of biocompatibility of all elements in the DEA, including the electrodes, are especially important. These issues are discussed and several types of DEA-free metal electrodes are described, their parameters are analyzed, and pictures and descriptions of actuators intended for soft robotics and medicine are presented.

From the literature analysis it follows that layers of single-walled carbon nanotubes (SWNT) can be a good replacement for metal electrodes [4]. With a dielectric membrane thickness of 31  $\mu\text{m}$ , the optimal electrode thickness is considered to be  $\sim 60$  nm based on SWNTs. Such electrodes also have acceptable transparency ( $\geq 65\%$ ) in the optical range, and have high physical and mechanical parameters, for example, electrical conductivity, thermal conductivity and relative stretchability. These properties are necessary for the creation of flexible transparent DEAs with prospects for their use in flexible electronics and medicine.

### Acknowledgment

The work was carried out within the framework of the state assignment of the Russian Ministry of Education and Science (Project # FSMR-2024-0003).

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## EFFICIENCY OF FILM SUPERCONDUCTING WEAK MAGNETIC FIELD CONCENTRATOR

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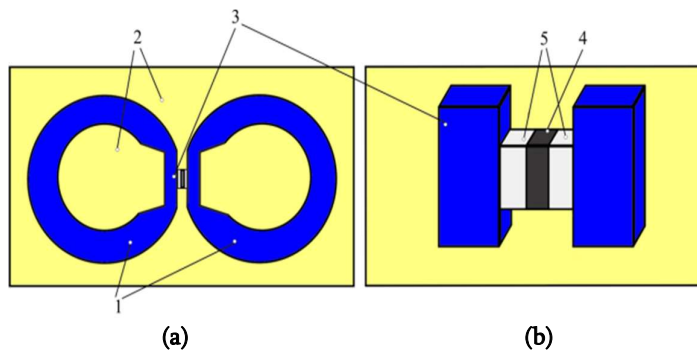
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Most combined magnetic field sensors (CMFS) have high resolution, i.e. low threshold sensitivity ( $\delta B \leq 1$  nT), achieved through the use of superconducting film Magnetic Field Concentrators (MFC). They repeatedly lower the resolution threshold of the magnetic field  $\delta B$  and thereby increase the efficiency of the MagnetoSensitive Element (MSE) in the CMFS or in other magnetic field sensors (SQUIDs, Hall sensors, spintronic structures, etc. [1, 2]).

CMFSs, like SQUIDs, are also promising for use in ultra-low-field MRI [3, 4], or for non-invasive monitoring of weak biomagnetic fields, including for studying the activity of the nervous system or brain.

Optimal fragmentation of the Active Strip (AS) of the concentrator into alternating superconducting branches and slits leads to an additional increase in its concentration coefficient and a decrease  $\delta B$  in the MSE [5, 6]. However, in a planar CMFS (the MFS and MSE are located on the same plane – **Figure 1**), the concentrated magnetic field on the MSE has a high degree of inhomogeneous distribution  $i_h$  on the MSE, which reduces the efficiency of the CMFS.



**Figure 1.** Sketch of a planar CMFS: (a) 1 – receiving rings of CMFS, 2 – substrate and 3 – AS, and (b) 4 – MSE and 5 – gap between nearest edges of AS and MSE.

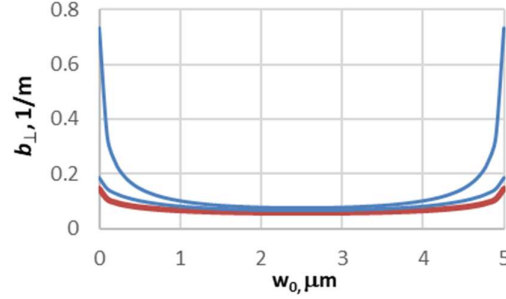
The efficiency of the  $E_{MFC}$  concentrator was determined as the implementation of the maximum average value of the magnetic field at the MSE, with a minimum degree of its inhomogeneity, i.e.  $E_{MFC} = B_{av} / i_h$ ,  $i_h = B_{max} / B_{min}$ , where  $B_{av}$ ,  $B_{max}$  and  $B_{min}$  are the magnetic fields at the MSE (average, maximum and minimum, respectively). The calculations took into account the conditions that the film thicknesses ( $< 10$  nm) of the MFC and MSE are negligible relative to other dimensions: the penetration depth  $\lambda_{\perp}$  of the perpendicular magnetic field in the superconducting films of the MFC, and the widths  $w_s$  of the AS and  $w_0$  MSE, and the gaps  $w_a$  between the edges of the AS and MSE. Calculations were carried out according to the formulas:

$$B_{\perp} = \mu_0 I b_{\perp}, \tag{1}$$



$$b_{\perp} = \frac{1}{2\pi\lambda_{\perp}} \left[ k_1 \int_0^{w_s/2} \frac{e^{-x/\lambda_{\perp}} dx}{(w_s + w_o + w_a - x)} + k_2 \int_{w_s/2}^{w_s} \frac{e^{-(w_s-x)/\lambda_{\perp}} dx}{(w_s + w_o + w_a - x)} \right], \quad (2)$$

where  $\mu_0 = 4\pi \cdot 10^{-7}$  H/m is the magnetic constant,  $k_1, k_2$  are the coefficients that determine the fractions of half the widths of the strips in which the corresponding fractions of the shielding current  $I$  flow. The origin of coordinates  $x = 0$  is considered to be the left edge of the left AS. The nonuniform distribution of the shielding current in the AS is determined by the exponential parts in (2). The final value of the magnetic field on the MSE took into account the fields created by the left and right AS.



**Figure 2.** Dependency  $b_{\perp}(w_o)$ . From top to bottom: heterogeneous, homogeneous and heterogeneous, when cutting into AS.

**Figure 2** shows a typical distribution of the concentrated magnetic field on the MSE, obtained with the following parameters:  $w_s = 7.5 \mu\text{m}$ ,  $w_a = 20 \text{ nm}$ ,  $w_o = 5 \mu\text{m}$ ,  $\lambda_{\perp} = 0.25 \mu\text{m}$ . From this figure it follows that the values  $i_h$  are significantly higher ( $\sim 9.9$ ) in the case of a non-uniform distribution of the shielding current in the AS, relative to its uniform distribution ( $\sim 2.5$ ), and a non-uniform distribution ( $\sim 2.8$ ) in the case when the current near the cut of the active strip near the edge of the distance  $x = 7.0 \mu\text{m}$  (cut width  $\leq 10 \text{ nm}$  and was not taken into account in the calculations). The corresponding values  $E_{MFC}$  have a ratio of 0.014:0.029:0.031. It can be seen that the optimal location of the slot in the AS increases the efficiency of the concentrator by more than 2 times. It should be noted that uniform current distribution in “wide” superconducting films ( $w_s \gg \lambda_{\perp}$ ) is possible by using an additional shielding layer on which the MFC is located.

It was shown that with increasing AS width in the range  $w_s = 7.5\text{--}240 \mu\text{m}$  decreases, but its rate of decrease  $E_{MFC}$  is greater in the case of a uniform distribution than in the case of a non-uniform distribution. At  $w_s = 60 \mu\text{m}$  their values  $E_{MFC}$  are approximately equal. At large  $\lambda_{\perp} = 1 \mu\text{m}$  this situation is achieved at  $w_s = 15 \mu\text{m}$ .

Thus, to achieve high efficiency of MFC based on films of low-temperature superconducting material ( $\lambda_{\perp} \leq 0.25 \mu\text{m}$ ,  $w_s \leq 7.5 \mu\text{m}$ ), an additional shielding superconducting layer should be used, but for the case of films of high-temperature superconducting material ( $\lambda_{\perp} \geq 1 \mu\text{m}$ ,  $w_s \geq 15 \mu\text{m}$ ) such a need disappears.

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## LAYERS OF BIOCOMPATIBLE COMPOSITE NANOMATERIAL AS TACTILE SENSING ELEMENT

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Tactile perception is an important function of the human skin that facilitates human interaction with the environment. Nevertheless, it is possible that impaired tactile sensation may be observed subsequent to damage to the skin or the wearing of gloves. This may result in difficulty with regard to body control and force application, particularly in instances where minor deformities are concerned. It is established that carbon nanotubes in a polymer matrix can serve as a basis for the creation of deformation sensors, including strain-sensitive elements in tactile sensors. This type of sensor exhibits several advantages. Primarily, the presence of exceptional mechanical and electrical properties [1] provides a sensitive and robust basis for sensors. Secondly, polymers are easily manufactured, economical, flexible, and their physical parameters (hardness, elasticity, etc.) can be readily adjusted over a wide range [2].

This study examines composite material layers comprising biocompatible microcrystalline cellulose (MCC) and Multi-Walled Carbon NanoTubes (MWCNTs). The layers were evaluated as sensing elements for various forms of deformation, with a specific focus on their potential as a tactile sensing element (TSE). This report outlines the parameters of the prototype tactile strain sensor and explores its potential applications.

The following materials were used in the experiments: MWCNTs “Taunit MD” by “NanoTechCenter” LLC, Russia [3], MCC in the form of a medicinal preparation (tablets) by “Evalar” [4], polyethylene food film PET from primary raw material with thickness of 30  $\mu\text{m}$ .

Aqueous suspensions comprising MCC, MCC and MWCNT (MCC/MWCNT) were thoroughly mixed using a magnetic stirrer for 50 min, then the MCC/MWCNT suspension was dispersed by a powerful ultrasound source. The suspensions contained 2wt.% MCC, 2wt.% MCC and 0.8wt.% MWCNT, the rest was distilled water. The aqueous suspension was applied to a flexible PET substrate by the sputtering method. Prior to application, the substrates were pretreated in various organic solutions (alcohol, acetone) and an ion-plasma beam, which significantly increased their hydrophilicity. Laser irradiation was characterized by the following parameters: mode – continuous, wavelength – 970 nm, irradiation power – 0.001–0.005 W/mm<sup>2</sup>, irradiation time – 20–150 s. After completion of the preparation process, the substrate together with the deposited layer was cut into samples of ~3–5 mm width. The thicknesses of the deposited layers were in the range of ~0.20–22  $\mu\text{m}$ , and characterized by a length of 12–15 mm.

The deformation and measurements of the physical parameters of TSE were conducted automatically on a specialized machine [5], which was operated via a computer interface. The unit measured and automatically stored the parameters: resistance, measurement temperature, time, bending angle, and number of bending cycles. The bending angle was varied in the range  $\pm 100^\circ$ .

The investigated MCC//MWCNT composite nanomaterial films showed acceptable specific electrical conductivity ( $\sim 10^3$  S/m) at layer thicknesses  $\leq 1$   $\mu\text{m}$ . High specific conductivity was realized after exposure to laser irradiation. It is shown that TSE based on thin composite layers (thickness  $\leq 1$   $\mu\text{m}$ ) exhibit the properties of a bipolar strain sensor, and thick layers (thickness  $\geq 10$   $\mu\text{m}$ ) exhibit the properties of a unipolar strain sensor.

It has been found that strain-resistive measurements can capture a tactile pressure of  $\sim 0.2$ – $20$  Pa, which corresponds to the order of tactile sensitivity of human fingers [6]. For a film thickness of  $0.023$   $\mu\text{m}$  MCC/MWCNT nanomaterial realized a transparency of  $\geq 70\%$  in the optical range. The potential applications of the results are considered, including their use in flexible electronics, minimally invasive surgery, and the development of T-sensors and electronic skin (e-skin).

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## PREPARATION, DOPING AND ELECTROPHYSICAL PROPERTIES OF $\text{Er}_2\text{Se}_3$ FILMS

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Chalcogenides of Rare Earth Elements (REE) are widely used in various branches of science and technology (electronics, mechanical engineering, aviation industry, biomedicine, etc.). But not all compounds of this class are studied rather fully. There is no data in the scientific literature on the technology of preparing erbium sesquelenide films, their doping and physical properties. It is known that the properties of films often differ from the properties of bulk materials, which allows to study the physical compounds more deeply.

The purpose of this work was to develop a technology for the preparation of thin films of  $\text{Er}_2\text{Se}_3$  on various substrates by vacuum-thermal evaporation from two independent components, their doping and the studying the electrophysical parameters, specific electrical resistance and Thermo-ElectroMotive Force (TEMF), in a wide temperature region.

Thin  $\text{Er}_2\text{Se}_3$  films 0.6–1.3  $\mu\text{m}$  in thickness, 6 mm in length, and 5 mm in width were grown by vacuum-thermal evaporation from two separate sources, Er and Se, the source materials with 99.99at.% of main material contents. During the film growth process the residual pressure in the deposition chamber was  $\sim 10^{-6}$  Pa. The Er source was evaporated using an electron beam evaporator, and the Se evaporator source, by Joule heating. The Er evaporation temperature was 1620 K, and the Se evaporation temperature – 540 K. The evaporator-substrate separation was  $\sim 60$  and  $\sim 55$  mm, respectively, and the axes of the evaporators were tilted  $\sim 30$  и  $\sim 50^\circ$  about the normal to the substrate. The film growth rate was varied in the range  $\sim 35$ – $50$   $\text{\AA}/\text{s}$ . The substrate temperature in our experiments was varied within range of 650–1200 K. As substrates, we used plates having the shape of a rectangular parallelepiped with  $15 \times 8 \times 0.5$  mm twists were used. The substrate materials were glass–ceramic, sapphire, fused quartz and single-crystalline silicon with plane orientation (111).

To examine the effects of substrate temperature and substrate material on the crystallinity and phase composition of the films, we carried out experiments in which the substrate temperature was varied from 700 to 1200 K. The results indicated that the substrate material had no significant effect on the phase composition and crystallinity of the films. The films grown at substrate temperatures under 1100 K contained metallic erbium inclusions as a separate phase. The films grown at substrate temperature above 1145 K were two-phase: they consisted of  $\text{ErSe}_2$  and  $\text{ErSe}$ . Only the films grown at substrate temperatures in the range 1100–1145 K were of single phase, and their composition corresponded to  $\text{Er}_2\text{Se}_3$ . In subsequent measurements, we used the films grown at substrate temperatures in this range. All the films prepared by us on all substrates corresponded to the  $\gamma$  modification (cubic structural type  $\text{Th}_3\text{P}_4$ ), with lattice constant  $a = 8.52$   $\text{\AA}$ , which well matches with the literature data [1]. X-ray microanalysis showed that all prepared films contained 38.85at.% Er and 60.15at.% Se.

Sesquelenides films of REE, due to their fairly wide band gap, are promising materials for use in optoelectronic devices in the visible region of the spectrum. Their practical use is difficult due to the very high electrical resistance – about  $10^{10}$  Ohm-cm. In this regard, the selection of the alloying element and the alloying method is an urgent task. Based on geometric and electrochemical factors, we chose element Zn as the alloying agent, and the alloying method was diffusion in a closed volume from the gas phase.

In this work, for the first time,  $\text{Er}_2\text{Se}_3$  film was doped with Zn atom and measured temperature-dependence of specific electrical resistance. TEMF was measured in the temperature region of 90–650 K. According to the measurements, with increasing temperature, resistivity decreases, while TEMF increases with increasing temperature. All doped films have n-type conductivity and the quantity of heating-cooling cycles does not cause

the recovery of the initial electrical parameters, as is observed in the Sm, Dy and Yb sesquisulfides films, every doped with cadmium atoms [2, 3], in which 8–12 heating–cooling cycles during measurements cause restoration of the initial value of electric resistivity and thermo-emf.

As is known in the cationic sublattice of REE sesquifides, every ninth node is vacant [4, 5], and the fact is given that the ionic radius of Zn –  $1.42 \cdot 10^{-10}$  m is less than the ionic radius of Cd –  $1.61 \cdot 10^{-10}$  m [6]. So, it can be assumed that Zn atoms occupy vacant nodes stronger than cadmium atoms that are in the lattice interstitials.

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**Keywords:** film, substrate, evaporation, doping, thermo-emf, electro resistance

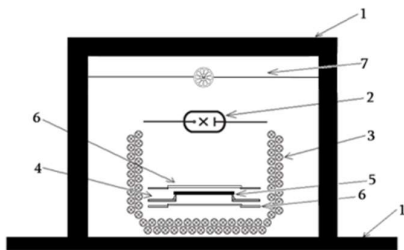
## METHOD AND SYSTEM OF PULSED PHOTON IRRADIATION FOR MODERN ELECTRONICS TECHNOLOGIES

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Activation-diffusion methods of modification of physical properties of semiconductor materials in traditional technologies are carried out by thermal effects in a furnace, i.e. by heating the material for many hours at a temperature close to the melting temperature. Accordingly, carrying out these processes in nanoscale films becomes particularly challenging. Rapid thermal annealing has proven to be an effective means of defect elimination. Despite the efforts of researchers, it has not been possible to see and thoroughly evaluate such factors as high concentration of formed antibonded electron-hole pairs, selective absorption of photons by impurities and defects, changes in their charge state, etc., as well as other factors. These factors, in our opinion, play an important role in the processes of photostimulated crystallisation, annealing of defects, activation or diffusion of introduced impurities. Indeed, the various ‘fast thermal annealing’ systems existing today are ‘fast’ furnaces that completely ignore the importance of the lamp irradiation spectrum and the associated series of photostimulated athermal processes occurring in materials. The purpose of the presented system and the proposed design are based on the theoretical model of photostimulated processes in materials that we have developed [1]: conduction band electrons and valence band holes are anti-bonding quasiparticles that “soften” bonds in the crystal and contribute to its low-temperature melting. Thus, we came to the conclusion that if in the process of pulsed photon irradiation (PPI) a critical concentration of nonequilibrium charge carriers ( $n_{cr}$ ) (antibonding quasiparticles) generated by light is achieved, the melting of the surface layer of the semiconductor should occur already at  $T < T_{mel}$  with subsequent recrystallization, leading to complete annealing of structural or radiation defects as well as to accelerating the diffusion and activation processes. We offer a wide-spectrum pulsed photon irradiation instrument IMNE 9 (Figure 1).



**Figure 1.** Pulsed photon irradiation unit of the PPI system.

It has sources of radiation of electromagnetic waves in a wide range of the spectrum (190–4100 nm), which is located in a housing with internal reflection surfaces (1). In the upper part of the housing there is an ultraviolet lamp, which ensures continuous irradiation of the sample with electromagnetic waves 190–400 nm (2). In the bottom and side part there are halogen lamps in two rows, which provide irradiation in pulse mode with electromagnetic waves in the range of 400–4100 nm (3). Standard filters operating at low temperatures ( $<300^{\circ}\text{C}$ ) located on both sides of the sample are used as optical filters (6). The cooler (7) provides cooling of filters and sample by air flow.

Lamp power supplies are connected to a computer from where irradiation modes (duration, power, temperature) are controlled. Effective application areas of the device can be: various synthesis processes, diffusion and activation processes.

Practical application of the presented device will give researchers new opportunities to effectively carry out diffusion processes at temperatures relatively lower than traditional ones; to avoid negative factors associated with technological processes involving high thermal effects.

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**Keywords:** rapid thermal annealing, pulsed lamp annealing, pulsed photon irradiation, photostimulated processes

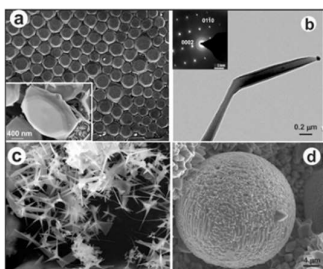
# MORPHOLOGICAL CHANGES IN ZnO NANO- AND MICRO-STRUCTURES SYNTHESIZED BY DIFFERENT TECHNOLOGIES

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The electrical, optical and chemical properties of nanomaterials strongly depend not only on their sizes but also on their morphology and surface area of exposed crystal facets [1, 2]. ZnO nanomaterials and nanostructures with different morphologies were synthesized using pyrolytic and arc-plasma technologies. Some of the produced nanomaterials are presented in **Figure 1**.



**Figure 1.** SEM and TEM images of ZnO (a) hexagonal plates, (b) nanobelts, (c) tetrapods and (d) microspheres.

The ZnO nanobelts (**Figure 1b**) were growing by the Vapor-Liquid-Solid (VLS) mechanism using the Zn droplets as self-catalysts. The synthesized nanomaterials were growing in [0001] direction. For nanomaterials depicted in **Figures 1a-c** we have evaluated the activity for photocatalytic decomposition of methylene blue dissolved in water.

The results clearly show the morphology dependence of the catalytic activity. The study of decolorization of methylene blue solution under solar light simulator revealed that the ZnO hexagonal plates had maximum activity followed by ZnO tetrapods and nanobelts. The highest activity of hexagonal disks was explained by the high exposure of energetic (0001) facet in these nanomaterials compared to tetrapods and nanobelts.

ZnO nanowires with altering cross-sections were produced by VLS method using Sn catalyst at a linearly increasing temperature, ranging from 250 to 500°C. The nanowires with hexagonal cross-sections were grown in the [0001] direction at temperatures below 370°C. At higher temperatures, the cross-section was transformed into a dodecagonal one with well-distinguished {01-10} and {11-20} facets. We explain this morphological change by the temperature dependence of surface free energies. The normal surface energies of ZnO prism planes are quite close (1.12 J/m<sup>2</sup> for 01-10 plane and 1.06 J/m<sup>2</sup> for 11-20 plane [3]). We suppose that at elevated temperatures these values become closer enabling the revealing of both prism planes and the appearance of the dodecagonal cross-section.

One more morphology of the synthesized ZnO nanomaterials was the spherical, micron-sized mesocrystals presented in Fig. 1 d. Depending on the process parameters two types of microspheres were produced. The first one was the hollow microsphere, and the second was the microsphere with filled inner space. The possible mechanisms of their formation were proposed.

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**Keywords:** zinc oxide, nanomaterials, morphology

## THEORETICAL MODELLING OF BORON NITRIDE COATINGS

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The Direct Simulation Monte Carlo (DSMC) method is used to model the MS of the Boron Nitride (BN) coating. DSMC enables the calculation of probabilistic collisions. The Lorentz force, which is created by an electric field, magnetic field and particle collision, is utilized to model the BN coating. The Physical Vapour Deposition (PVD) method is used for the coating process. This study helps improve our understanding of PVD mechanisms and suggests optimal parameters for coatings.

The current research aims to improve the coating deposition rate and thickness. Three distinct bias voltages are used to generate three different BN coating models under the same conditions. The bias voltages are 0, 100 and 250 V. The modelling of BN coatings at various substrate voltages reveals that the deposition rate decreases as the substrate voltage increases. The thickness of the coating is also reduced when the deposition rate is decreased. The results from the models are compared with experiments in this investigation. The model and experimental results demonstrate a good correlation.



## DEMYSTIFYING ARROW OF TIME

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Scientific discussions of the arrow of time often get quite confusing due to highly complex systems they deal with. Popular literature then often conveys messages that tend to get lost in translation. The purpose of this note is to demystify the arrow of time by stripping off the unnecessary complexities and thereby simplifying the discussion.

We do this by providing examples that are exactly solvable and make it easy to see the root cause of the apparent “time-irreversibility”. We also discuss “time-reversal” solutions, where the initial state evolves such that it reaches the state which is the same as the initial state moving backward in time. These solutions are simple enough to be comprehensible to a highschooler.

We discuss the arrow of time both in the classical and quantum settings, including in the cosmological context.

## STRATEGIES FOR DEVELOPMENT OF GELATIN-BASED BIOCHIPS FOR DETECTING MATRIX METALLOPROTEINASES ACTIVITY

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The development of biochips and biosensors for the production of early-prognostic biochemical markers represents the cutting-edge of biomedical technology. Matrix MetalloProteinases (MMPs) are involved in the breakdown of ExtraCellular Matrix (ECM) in normal physiological processes as well as play a negative role in a variety of disorders such as cancer metastasis, diabetes, cardiovascular diseases, stroke, etc. [1]. The application of MMP-9 as a biomarker for several illnesses was evaluated. Detecting MMPs may be done in a number of ways. The most commonly used technique is ELISA, which quantifies proteins in biological samples using subsequent antibodies. The zymography approach is the alternative. Using a sensitive polyacrylamide gel-based electrophoretic technique, gel zymography measures the protease activity of MMPs to break down their substrates, gelatin (a denatured form of collagen, a structural component of the ECM) in the case of MMP-9 and MMP-2, the two most abundant MMPs in blood. A zymography method distinguishes the pro-MMP and active MMP forms but does not quantify MMP. ELISA quantifies total MMP. Numerous innovative biosensors, including MMP-9 biosensors based on peptide cleavage and those without, were created recently [1]. This kind of biosensors require much effort and complex technology and has no translational application into real clinical use. We are developing a new protein-biochip technology based on the copolymerization of gelatin and polyacrylamide gel, which enables the quick measurement of MMP activity. Rhodamine-B-conjugated gelatin-polyacrylamide arrays have been designed to detect MMP activity. The MMP activity is determined by measuring the decrease in fluorescence intensity that results from the MMP-induced degradation of Rhodamine B-conjugated gelatin. Fluorescence intensity is measured in the MMP activation buffer both before and after the plasma incubation.

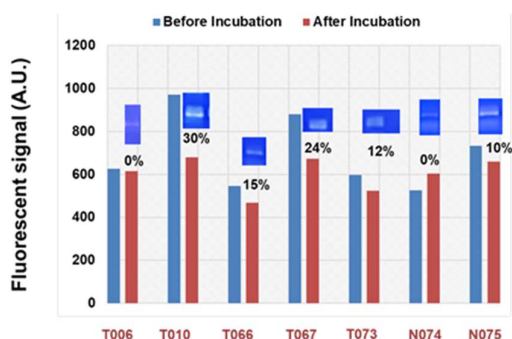


Figure 1. Comparative analysis of MMP activity using zymography and gelatin-biochip approaches.

As follows from Figure 1, the analysis of the plasma of seven alcohol- and opioid-dependent patients by biochip (columns) and zymography approach (gel cut of MMP-9 activity) is in good congruity. A strong decline in fluorescent signal intensity correlates with high MMP-9 activity, which is shown as white lanes on a blue background, and vice versa.

### Acknowledgment

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**Keywords:** protein-biochip, MMP, blood, rhodamine B-conjugated gelatin

# SPINTRONIC NANOSTRUCTURES AND QUANTUM DEVICES

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Recent progress in nanosystems development has generated significant enthusiasm for the creation of high-aspect-ratio nanostructures – the elementary blocks of energy-efficient, non-volatile spintronic devices. Nanowires, nanorings, and nanodots are some of the most extensively explored nanostructures for various technologies [1 – 3]. Most of the research has primarily focused on two-dimensional 2D planar nanostructures where the film thickness is significantly smaller than the planar dimensions. With advances in nanofabrication techniques and the increasing demand in the field, it is possible to exploit the effect of film thickness towards 3D spin and quantum electronics. The presence of chiral structures can help in the design of topologically protected memory elements. Compared to planar nanodots, the model for thicker nanodots includes a mass term (inertia term) to the vortex equation of motion. Spin wave modes were also detected in a perpendicularly magnetized thick nanodot array. This innovative method ensures geometrical integrity along the thickness for thick nanostructures across a large area pattern. The convergence between quantum materials properties and prototype quantum devices is especially apparent in the field of 2D materials, which offer a broad range of properties, high flexibility in fabrication pathways and ability to form artificial states of quantum matter. Along with their quantum properties of as solid-state platforms for quantum- dot qubits, single- photon emitters, superconducting qubits and topological quantum computing elements it is necessary to select the best method of their preparation.

On the basis of our previous investigations, we are developing and using the laser-plasma method which enables preparation of nanostructured layers with fine and perfect structures and high purity [4]. The usage of resonance light heat creates the opportunity to energize the selected atoms as well as their groups (assemblies) and to produce plasma with the necessary properties relevant to structures which must be prepared. This technique was successfully used by the authors to study the conditions for obtaining diamond-like films, as well as thin 2D layers of B<sub>4</sub>C and SiC, the both homogeneously doped GaAs:Mn layers and 2D structures, including a  $\delta$ -doped GaAs:Mn layer and a In<sub>x</sub>Ga<sub>1-x</sub>As quantum well separated by a GaAs spacer. At room temperature, the formed structures have magnetic and magneto-optical properties and in the low-temperature region (~30 K), the anomalous Hall Effect was observed. In this study, we showcase the fabrication of nanostructures by laser plasma method reaching thicknesses of up to 50 nm, accomplished through the creation of nano trenches in the different substrates. Subsequently, the evolution of spin texture and spin dynamics as a function of parameters of laser plasma process plus nanostructure thickness have been presented. The results are substantiated with computing simulations. Our results open horizons in the utilization of the third dimension for emerging spin textures and their potential applications in future spintronic devices.

## **Acknowledgment**

I'm sincere thankful to my GTU colleagues for their high-level help and support.

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**Keywords:** nanosystems, fabrication, laser-plasma, spintronics, spinquant devices

# EXCITONS AND TRIONS IN TWO-DIMENSIONAL MATERIALS TUNABLE BY ELECTRIC AND MAGNETIC FIELDS

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The studies of direct and indirect magnetoexcitons in Rydberg states in monolayers and heterostructures of emerging 2D materials: Transition Metal DiChalcogenides (TMDC), Transition Metal TriChalcogenides (TMTC), and phosphorene in an external magnetic field, applied perpendicular to the monolayer or double layer heterostructures, in the framework of a Mott–Wannier model of excitons [1 – 3] are presented. We consider direct and indirect magnetoexcitons in Rydberg states in monolayers and double layer heterostructures of Xenos (silicene, germanene, and stanene) in the external parallel electric and magnetic fields applied perpendicular to the monolayer and heterostructure [4]. Calculations of Binding Energies (BEs) of magnetoexcitons for the Rydberg states 1s, 2s, 3s, and 4s by the numerical integration of the Schrödinger equation, using the Rytova–Keldysh (RK) potential for direct magnetoexcitons and both the RK and Coulomb potentials for indirect magnetoexcitons, are given. Using two different potentials allows to investigate the role of the screening in these 2D materials and their heterostructures. We report the magnetic field energy contribution to the binding energies and diamagnetic coefficients for direct and indirect magnetoexcitons. We demonstrate the tunability of the binding energy of direct and indirect magnetoexcitons by the external magnetic and electric fields and the possibility to control the binding energy of magnetoexcitons in double layer heterostructures by the manipulation of numbers of hBN monolayers.

We develop the theoretical formalism and study the formation of valley trions in two-dimensional monolayers within the framework of a nonrelativistic potential model using the method of hyperspherical harmonics (HH) in four-dimensional space [5]. The numerical solution of the three-body Schrödinger equation with the RK potential by expanding the wave function of a trion in terms of the HH is obtained. Our approach yields the analytical solution for binding energies and wave functions of trions in the diagonal approximation for these two limiting cases: the Coulomb and logarithmic potentials. We obtain exact analytical expressions for eigenvalues and eigenfunctions for  $X^-$  and  $X^+$  trions that can be considered as the lower and upper limits for the trions BEs. We apply the proposed theoretical approach to trions in TMDC [5] and predicted the possible existence of  $X^-$  and  $X^+$  in Xenos [6]. Results of numerical calculations for the BEs with the RK potential for TMDC are in the good agreement with similar calculations and in the reasonable agreement with experimental measurements of trion binding energies. Controllable ground-state energies of intravalley and intervalley trions in Xenos by the external electric field are presented. BEs of trions formed by A and B excitons have a non-negligible difference that increases slightly as the electric field increases. It is demonstrated that trion BEs can be controlled by the external electric field, and the dielectric environment has a significant effect on the trion BE. The capability to control the BE and compactness of trions in buckled 2D materials by the external electric field suggests a possible trion crystallization in Xenos. In summary, we demonstrate that 2D monolayers and their heterostructures provide a unique platform for novel optoelectronic applications. They offer the tunability of magnetoexciton BEs by means of the external magnetic and electric fields and the number of hBN layers separating two monolayer sheets, and the tunability of trions binding energies by the electric field in Xenos.

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**Keywords:** 2D materials, binding energy, exciton, trion, magnetoexciton

## ABOUT FORMATION OF GOLD THIN FILMS ON POLYMER BASE

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The authors have been conducting research for years on mercury-sensitive gold thin films formed on a dielectric solid substrate (sapphire, sial, etc.), with the prospect of creating a mercury-sensitive sensor [1, 2]. As a result of these studies, the sensitivity of gold thin layers to mercury was confirmed. However, the resulting structures were not sufficiently stable to create a reliable functioning sensing device in the future. The instability of the structure was mainly due to the poor adhesion of the gold thin films to the solid dielectric layers (substrates).

The innovativeness of the studies in the presented paper is that the formation of thin gold films will not take place on a solid dielectric layer, but on the contrary, a polymer layer will be formed on a thin layer of gold, which after polymerization will turn a substrate. In this technological process, a gold film is formed on a metal plate (foil), which will not be difficult to chemically poison later. In order to obtain the best results, various metals (nickel, copper, aluminum, etc.) were tested, the etching technology of which is well known and available. Based on our research, the sensitivity of the sensor increases dramatically when the thickness of the sensitive layer is reduced, so the goal was to the deposit thinnest film possible (no more than 1000 Å). Finally, it was obtained the structure thin gold film–wpolymer.

At first glance, thin films should have the same structure as massive crystals, but in reality, the structural order, i.e., the size and orientation of crystals in thin films is significantly different from that of massive crystals, depending on the degree of movement of adatoms at the time of deposition and can vary from strong chaos to complete order. Therefore, it was necessary to thoroughly study the structure of the obtained gold thin films. To refine the technological and construction parameters the following were studied: morphology and structure of gold layers of different thickness deposited by different methods; their adhesion to the polymer base; dependence of adhesive strength on gold layer thickness; annealing modes are set.

According to the primary data of the conducted studies, the adhesive strength increased, a structure with fairly good stability in the temperature range  $-25 - +350$  °C was obtained. Which gives us a reason to assume that on the basis of this structure it will be possible to create a more stable mercury sensitive sensor.

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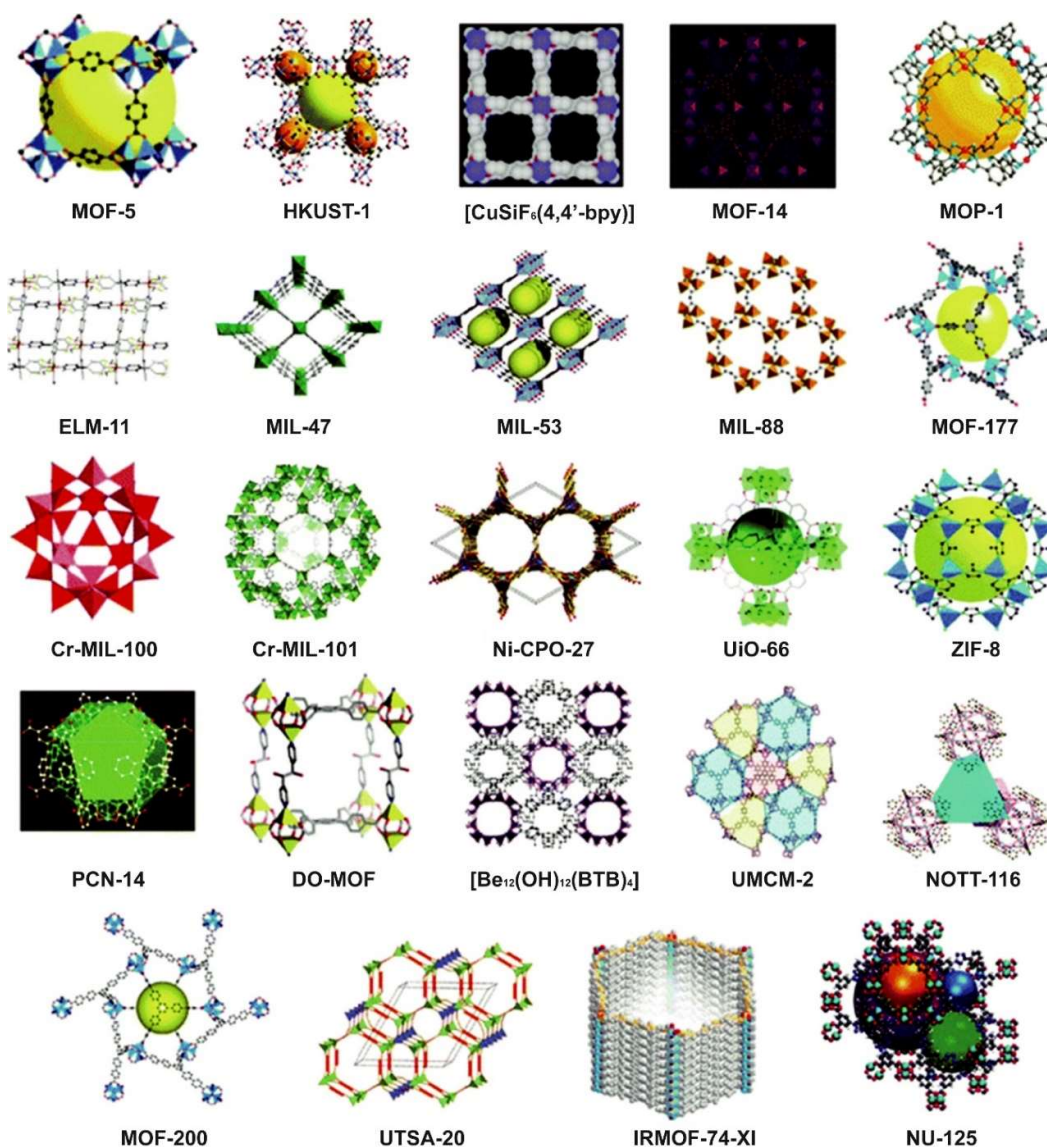
**Keywords:** gold film, mercury, polymerization, substrate, adhesive strength

## MOF-DERIVED NANOCARBONS: SYNTHESIS, PROPERTIES, AND APPLICATIONS

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Metal-organic frameworks (**Figure 1**, MOFs) are multi-dimensional nanoporous structures composed of metal ions (or clusters) coordinated to rigid organic molecules (linkers). The choice of the metal ion and linker species completely determines the structure and functionality of the resulting MOF. Common organic linkers include bidentate carboxylics (e.g., HOOC–COOH), tridentate carboxylates (e.g., C<sub>9</sub>H<sub>6</sub>O<sub>6</sub>), 1,4-benzenedicarboxylate (BDC), and azoles (e.g., C<sub>2</sub>H<sub>3</sub>N<sub>3</sub>) molecules. The great freedom with which the linkers and metal ions can be chosen and combined is reflected in the more than 20,000 MOF species that have been reported in the last two decades. Numerous MOF composites have been prepared by assembling MOFs and functional species, including graphene and carbon nanotubes [1].



**Figure 1.** Nanoporous structures of different MOFs. Reproduced from [2].

At the same time, the MOFs built from metal ions and polyfunctional organic ligands have proved to be promising self-sacrificing templates and precursors for preparing various carbon-based nanomaterials, possessing high BET surface areas, abundant metal/organic species, large pore volumes, and extraordinary tunability of structures and compositions [3]. In comparison with other carbon-based catalysts, MOF-derived carbon-based nanomaterials have great advantages in terms of tailorable morphologies, hierarchical porosity, easy functionalization with other heteroatoms and metal/metal oxides, which make them highly efficient as catalysts directly or as catalyst supports for numerous important reactions.

Among most recent reviews in this area, we note MOF-derived heteroatom-doped carbon-based electrocatalysts, including non-metal (such as N, S, B, and P) and metal (such as Fe and Co) doped carbon materials [4]. In addition to the catalysis, as it will be seen below, the uses of MOF-derived carbons include other electrochemical applications, for example for batteries.

In whole, heat treatment of metal-organic frameworks, resulting MOF-derived carbons, belongs to green energy applications [5]. There are a lot of opportunities in creating novel metal-containing nanocarbons due to a variety of already existing multifunctional nanoporous MOFs.

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# “GREEN” SYNTHESIS IN LOW-TEMPERATURE AND STUDY OF LUMINESCENT PROPERTIES OF CARBON QUANTUM DOTS

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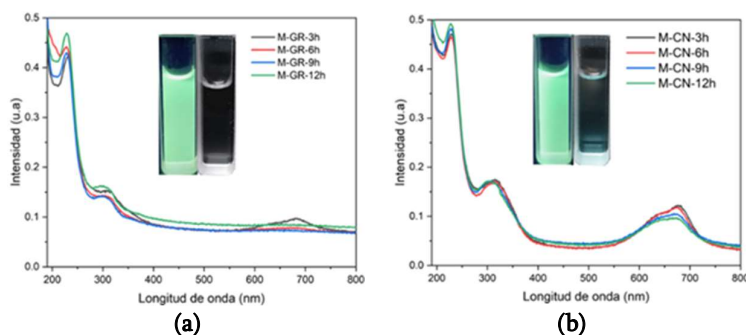
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Carbon Quantum Dots (CQDs) with a modified surface can be used in semiconductor electronics as a basis for organic diodes, light emitting diodes, biosensors and chemical sensors. Some of their advantages are high luminosity, good biocompatibility and low toxicity. One of the problems is that many production methods use harmful substances (HNO<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>, KMnO<sub>4</sub>, sodium borohydride, hydrazine hydrate and dimethylhydrazine) [1], which is associated with risks to the environment and human health. However, it has been shown that by producing ROS groups it is possible to make structural changes in carbon allotropes [2]. The aim of this research was the synthesis of CQDs by a “green” method and the study of their properties. For sonification, The Fisher Scientific FS30 ultrasonic cleaner (1 gallon capacity, 40 kHz operating frequency at 135 W power) was used for 1–12 h to carbon precursors such as carbon black and graphite with reducing agents (theraphthal (4,5-octacarboxyphthalocyanine cobalt salt) and ascorbic acid). The obtained nanoparticles were characterized by Thermo Scientific™ FT-IR Nicolet™ iS™ TM 10 spectrometer, Thermo Scientific™ Evolution™ 600 UV-vis equipment and transmission electron microscopy (TEM). The results (Figure 1) have shown that it is possible to obtain CQDs with luminescent properties from carbon black and graphite.



**Figure 1.** Analysis of the samples by UV-vis spectra at different ultrasound application times: (a) graphite raw material (M-GR) and (b) raw material carbon black (M-CN) (show how samples look under UV light of 365 nm (left image) and under white light (right image)).

Analyzing the results of the samples, it was observed that both precursors can be used for the synthesis of carbon quantum dots. It was observed that in aqueous medium it is possible to synthesize quantum dots with luminescent properties by applying ultrasound. The luminescence is stable and does not disappear after half a year. The photoluminescence properties depend mainly on the quantum confinement effect (QCE) and the surface states in GQDs and CQDs due to their crystal lattices such as edge states, defects and functionalities.

## Acknowledgment

The authors thank the UANL PROACTY program for supported the work.

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**Keywords:** carbon quantum dots, green synthesis, carbon black, theraphthal, luminescent properties



## DNA AS BASIS FOR REDUCTION OF SILVER AND GOLD IONS

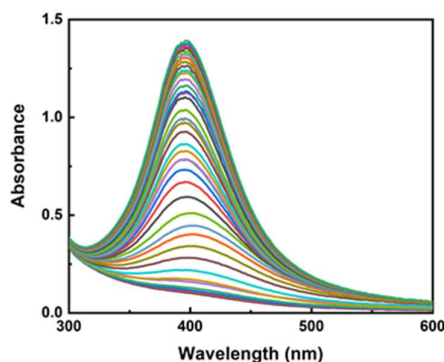
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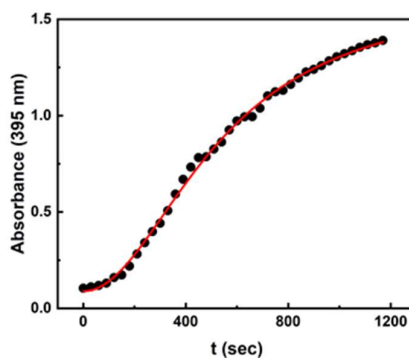
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Using different organic materials, it is possible to obtain various types of clusters during the reduction of metal ions. For example, the unique structural features and powerful recognition capabilities of DNA can be of interest for assembling artificial structures for a variety of applications in nano-photonics. A DNA helix is, itself, a nano-object that can be manipulated in various ways, but it can also be treated as a versatile molecular scaffold for building nanoscale devices from the bottom up. The unique properties of DNA's are being intensively studied from different points of view: as a molecular wire, as a drug delivery system, as a ladder for ordered arrangements of various nanostructures, as a spacer to control distances between nano-objects, etc.



**Figure 1.** Silver ions reduction process on DNA,  $t = 0\text{--}20$  min;  $\Delta t = 30$  sec.  $\text{Ag}^+/\text{bp} = 3/1$ ,  $[\text{DNA}] = 2.5 \cdot 10^{-4}$  M (bp).



**Figure 2.** Kinetic curve of reductions for silver ions on DNA for ratio  $\text{Ag}^+/\text{bp} = 3/1$ .

The main goal of the research was to study the reduction process of silver and gold ions on calf thymus DNA, using reductant borohydride, to create one dimensional structure of silver (**Figure 1**) and gold atoms. The S-shape of kinetic curve of reduction on DNA (**Figure 2**), indicates conformational changes of DNA during the reduction of silver ions.

### Acknowledgment

The research was supported by Shota Rustaveli National Science Foundation of Georgia (Grant # FR-23-21749).

**Keywords:** DNA, metal ions, nanowire, spectroscopy

## NOTIFICATION SYSTEM FOR LANDSLIDE PRONE AREAS

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The solution is proposed to the existing situation is the construction and production of flexible early warning systems in Georgia, which will cost the state ten times cheaper and we will have the opportunity to cover all critical areas of natural hazards.

The notification system developed by us for landslide-prone areas provides:

1. Measurement of ground displacement and relative slope;
2. Measurement of construction deformation and bulge; and
3. Transfer and visualization of information in the center.

When installing the sensors in the ground, their reading is taken as a baseline. In other words, we are interested in the change with respect to the initial state, where  $X_0$  are the initial values and  $X$ , the current values, and  $dx$ , the absolute values of their change. The program provides regulation of the maximum threshold value of changes. Since fluctuations are always observed in the soil should be ignored by the system, and if the change exceeds the set limit, the system in this case gives an alarm message, which will be received by both the central server and the residents registered in the surrounding area. Information is transmitted through the system.

This notification system requires very little power. Magnets are located on the ground surface (in a shallow trench). Hall sensors are mounted a few millimeters above the magnets. A change in the ground surface causes a change in the magnetic field which is detected by the sensor. The Hall sensor is free from all kinds of harmful fluctuations, it is characterized by high reliability and accuracy. If we place a semiconductor or conductor strip in a magnetic field of a certain induction, in which a current flows, then moving charged particles will move in the direction of movement under the influence of the Lorentz force, as a result of which a voltage will appear on the directed ends of the plate.

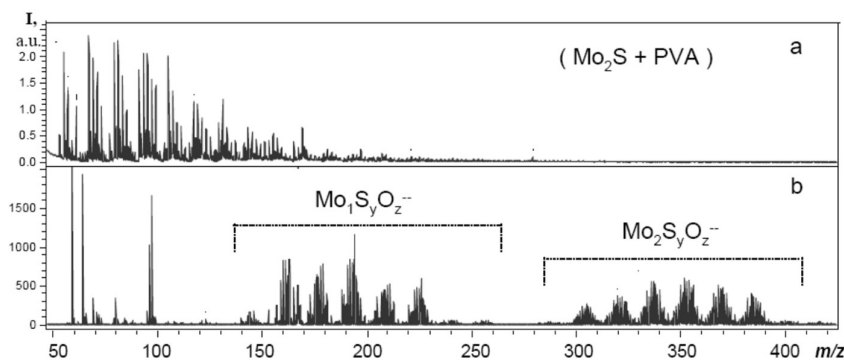
# MASS SPECTROMETRIC CHARACTERIZATION OF MOLYBDENUM DISULFIDE NANOCOMPOSITE WITH POLYVINYL ALCOHOL

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Some applications of 2D nanomaterials molybdenum disulfide, MoS<sub>2</sub>, involve its interactions with organic compounds. In our previous studies of nanocomposites of MoS<sub>2</sub> flakes with organic molecules prepared by sonication it was noticed that the type of intermolecular interactions in the composite may vary from noncovalent physical sorption to chemical sorption and chemical interactions in dependence of the type of organic compound. In the present work we investigated aqueous system of MoS<sub>2</sub> treated by ultrasound with PolyVinyl Alcohol (PVA). Upon mixing of these two components, both of them were rapidly assembled into a dark viscous clot which separated from its aqueous environment. This effect may be accounted in water purification technology.



**Figure 1.** Laser desorption / ionization mass spectra of MoS<sub>2</sub>-PVA nanocomposite recorded in (a) positive and (b) negative ion modes.

Thus formed MoS<sub>2</sub>-PVA nanocomposite was probed by Laser Desorption / Ionization (LDI) mass spectrometry (Figure 1). In the positive ion mode a spectrum of organic component of the composite was recorded: a set of ions with enhanced abundances for odd mass species was present in the small masses range. These ions may be tentatively attributed to products of hydrogenolysis of PVA polymeric chains, which can occur due to catalytic activity of MoS<sub>2</sub>. Full identification of these products necessitates further investigations. In the negative ion mode sets of clusters characteristic of MoS<sub>2</sub> with proper isotopic distribution were recorded: Mo<sub>x</sub>S<sub>y</sub>O<sub>z</sub><sup>-</sup> (x = 1, y = 2–5, z = 0, 1; x = 2, y = 3–7, z = 0, 1; and x = 3, y = 5–8, z = 0, 1). In contrast to the LDI mass spectrum of pure MoS<sub>2</sub>, any clusters with x>3 were absent. This may point to the effect of encapsulation of MoS<sub>2</sub> flakes by PVA polymer. Thus, LDI mass spectrometry allows revealing certain features of MoS<sub>2</sub> interactions with PVA.

## Acknowledgment

This work was supported by Grant # 0123U100628 of the NAS of Ukraine.

**Keywords:** molybdenum disulfide, polyvinyl alcohol, laser desorption/ionization mass spectrometry

## SOLID PHASE QUASI-INTRAMOLECULAR REDOX REACTIONS: ROUTE TO PREPARE NANOSIZED METALOXIDE CATALYSTS

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Synthesis of transition metal compounds (Ag, Cu, Zn, Cd, Co, Ni, Fe, Cr) with reducing ligands (ammonia, pyridine, urea or their substituted derivatives) and oxidizing or oxygen-containing anions (permanganate, chromate, dichromate, perrhenate, perchlorate, nitrate, sulfate, selenate, persulfate) is a challenging task, for example, due to the redox interactions might exist between the ligands and the oxidizing anions during the solution phase synthesis. The preparation of these kinds of compounds led to the realization that, in addition to their specific structural properties, these materials show a special reaction, a solid-phase quasi-intramolecular (ligand-anion) redox reactions at low temperatures (<150°C). These reactions lead to amorphous, defect-structured nano-sized oxides or in the case of metal-containing anions (permanganate, perrhenate, dichromate) mixed metal oxides. Furthermore, by formation of isomorphous solid solutions (e.g. [(Fe,Cr)(urea)<sub>6</sub>]<sub>3</sub> or [Ag(NH<sub>3</sub>)<sub>2</sub>(ClO<sub>4</sub>,MnO<sub>4</sub>)] or with mixed anions (e.g. [Me(urea)<sub>6</sub>](CrO<sub>4</sub>)(MnO<sub>4</sub>), Me = Fe(III), Al, Cr, Ir, Rh) opens up new possibilities to prepare doped or supported oxides in situ.

The ammonia ligand-containing complexes mostly resulted in nanosized MMn<sub>2</sub>O<sub>4</sub> spinel-type oxides from their permanganate anion-containing salts (M=Cu, Zn, Co, Cd, Ni). However, by changing the valence of the central metal ion and outer and/or inner sphere ligands, spinel oxides with variable metal: manganese ratio can also be prepared. For example, using (Co(NH<sub>3</sub>)<sub>6</sub>)(MnO<sub>4</sub>)<sub>3</sub> (Co:Mn = 1:3), (Co(NH<sub>3</sub>)<sub>5</sub>Cl)(MnO<sub>4</sub>)<sub>2</sub> (Co:Mn = 1:2), (Co(NH<sub>3</sub>)<sub>6</sub>Cl<sub>2</sub>)(MnO<sub>4</sub>), and (Co(NH<sub>3</sub>)<sub>4</sub>CO<sub>3</sub>)(MnO<sub>4</sub>) (Co:Mn = 1:1) complexes mixed metal oxide spinels with a nominal ratio of Co:Mn = 1:(1–3) can be produced. The Co:Mn ratios can be modified by removing the water-soluble cobalt compounds from the primary decomposition products by washing them with water. The decomposition of these complexes typically takes place with the formation of the ammonium nitrate intermediate, which is the product of the selective oxidation of the ammonia ligand. The ammonium nitrate intermediate melts and further reactions take place in this melted phase.

If the ammonium nitrate is removed by washing with water, oxides with different properties as that are formed without the removal of ammonium nitrate can be prepared. For the safe decomposition of these explosive substances, we have developed a decomposition process with an isothermal heat removal process in refluxing inert solvents. The structure of the resulting spinels (normal, inverse, cation and valence distribution in the tetrahedral and octahedral sites, the number of defects), and the particle size of the oxides (2–100 nm) can be adjusted by the appropriate selection of the precursor complexes and the decomposition conditions. The production of alkali metal-doped materials is also in progress, we have successfully synthesized and decomposed a special material, the compound (Co(NH<sub>3</sub>)<sub>6</sub>)(KCl<sub>2</sub>(MnO<sub>4</sub>)<sub>2</sub>), which contains a tridentate coordinated permanganate ion, and the central metal ion of the complex anion is potassium, with a chloride and permanganate coordination and a 2D permanganate linked polymer structure.

In addition to the structural, spectroscopic (IR, Raman, UV, Mössbauer, ESR) and thermal analysis (TG–MS, DSC) studies of the complexes, the properties of the resulting oxide products were also examined (BET, XPS, SEM, HR–TEM). Furthermore, the catalytic properties of these oxides were also investigated in CO oxidation and CO<sub>2</sub> reduction reactions or in photocatalytic decomposition reactions.

# TO KINETICS OF QUANTUM DISSIPATIVE SYSTEMS: QUANTUM BROWNIAN PARTICLE MOTION AND LOW TEMPERATURE POLARON MOBILITY PROBLEM

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New, exact generalized quantum evolutionary (kinetic) equations for the equilibrium double-time correlation functions (Green's functions: advanced, retarded and causal) and statistical operator (density matrix) of a quantum dynamical system interacting with a phonon field (thermostat) were derived in the case of linear as to the Bose-amplitudes.

The Random Phase Approximation (RPA), factorizing initial condition, has not been used to derive these equations. In the initial moment of time for the correlation functions a thermal initial conditions (mixed Gibbs state) were used. The projection operator technique and generalized Bogolubov's lemma for a dynamical system interacting with a boson field is proved and used for the excluding the dynamical variables of the phonon field from the derived evolutionary equations. The collision integrals of these equations include explicitly both the dissipative terms describing the dynamics of the system and the terms responsible for the time evolution of initial correlations.

The derived kinetic equations are used to analyze the kinetic and linear transport phenomena in exactly soluble model of the quantum dissipative system: A quantum Brownian particle dynamics of which is described by Caldeira–Legget Hamiltonian. It is asserted that there is no quantum regression theorem in the sense of Onsager. This is shown by explicit calculation of quantum Brownian motion of an oscillator. The specific form of kinetic equations of correlation functions and the mobility of Brownian particle were calculated.

As an application of this approach, the uniform theory of Froeclhlich's polaron low-temperature mobility – in the wide range of frequency of the weak external electric field – is developed as well. It reproduces the generalized Osaka result at low frequencies of external electric field and Feynman–Hellwarth–Iddings–Platzman (FHIP) result at high frequencies.

Such an uniform theory of low-temperature polaron mobility was not yet developed until.

**Keywords:** kinetics, dissipative systems, polaron mobility

# INCONTROVERTIBLE CONTRIBUTION OF NANOCLAYS TO COMPOSITE PROPERTIES

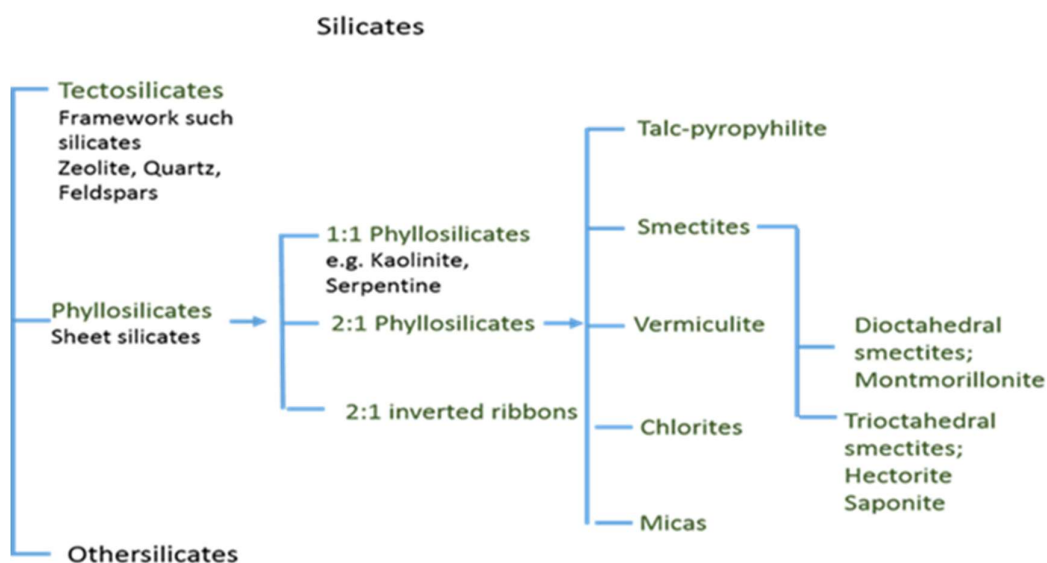
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The synthesis of composite materials, whose strength, durability and functionality are significantly increased with the contribution of nano-sized materials, and their usage in industrial applications have attracted great attention as a valid alternative in recent years. As given in **Table 1**, nanocomposites have many advantages compared to composite structures. In this context although various nano additives exist in inorganic or organic forms, nanoclays in the form of 2D layered mineral silicate composed of a large number of nanoparticles are distinguished from other counterparts by their individual properties, making them outstanding products for use in industry.

**Table 1.** Properties of composite and nanocomposite materials.

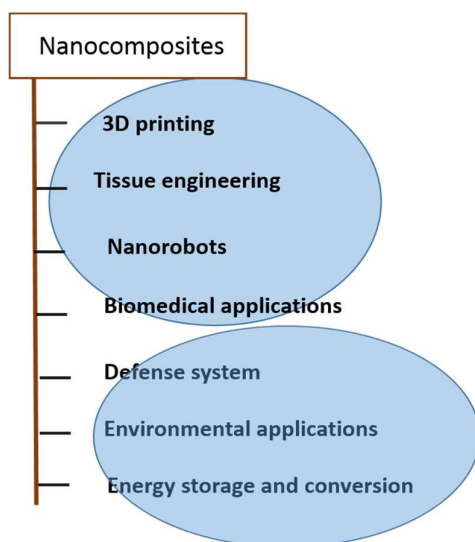
Composites	Nanocomposites
Stiffness and strength	Mechanical properties (strength, bulk modules, withstands limit, etc.)
Low coefficient of expansion	Thermal stability
Resistance against fatigue	Hinders flame and reduce smoke generations
Ease in manufacturing complex shapes	Permeability of gases, water, and solvents are reduced
Simple repair of damaged structures	More surface appearance, enhance optical clarity as compared to conventionally filled polymers
Resistance to corrosion	Improved electrical conductivity and chemical resistance



**Figure 1.** Silicates classification (adopted and redrawn from [1]).

Among other inorganic substances, clay minerals are natural, abundant, inexpensive, and nontoxic. Also important for practical use, clay nanocomposites have outstanding thermal stability, improved mechanical

properties, flame retardancy, high dimensional stability, anti-corrosion and reduced gas permeability, making them stand out as innovative materials attracting significant commercial interest. The most generally used clays for the preparation of nanocomposites belong to the family of phyllosilicates, that is, layered or sheet like structures more commonly referred to as layered silicates (**Figure 1**). Montmorillonite, hectorite, illite, and chlorite can be given as most widely used examples of this 2:1 phyllosilicates groups [1].



**Figure 2.** Application areas of nanoclay composites.

Nowadays, nanoclays in different composite forms, especially nanocomposite gels, have many applications such as food packaging, water purification, biomedical applications (tissue engineering, regenerative drugs and therapeutic antibodies), catalysis, energy storage and conversions and environmental remediation (**Figure 2**) – see [2, 3]. The basic approach in these applications is not only to produce alternative solutions to the difficulties encountered in practice, but also to make the sector and the country's economy sustainable.

In this review, structures, chemical compositions, surface modification methods before use, synthesis techniques of nanoclay composites and their usage for innovative applications in various fields regarding the latest developments are summarized.

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**Keywords:** nanoclay, nanocomposites, synthesis, application

# NONCOVALENT INTERACTION OF GRAPHENE NANOMATERIALS WITH 1-PYRENEBUTANOIC ACID SUCCINIMIDE ESTER AND GLUCOSE OXIDASE

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Maintaining the functionality of the recognizing molecule at immobilization on the graphene surface is a key question of the development of biosensor based on graphene nanomaterials. This problem can be solved using a molecular interface. A 1-Pyrenebutanoic acid Succinimide Ester (PSE) is often used as molecular interface for the carbon surface [1]. PSE is a bifunctional molecule containing a succinimide ester that is covalently bound to amines of proteins (enzymes, DNA/RNA) by forming an amide bond and a pyrene residue that interacts with the carbon surface through  $\pi$ - $\pi$ -stacking. In spite of several studies devoted to the PSE adsorption on graphene nanomaterials, there is necessary additional study to further understand the mechanism of the PSE adsorption on the carbon surface.

In this work, we present results of the Raman spectroscopy study of adsorption of PSE on reduced graphene oxide (rGO) and simulation of an immobilization of glucose oxidase ( $GO_x$ ) on graphene using PSE in an aqueous environment by exploiting molecular dynamics study. The structures of the nanobiohybrid and the interaction energy between components were determined. The interaction energy between graphene and  $GO_x$  through PSE interface was revealed to be about  $-30$  kcal/mol. It was shown that at least two PSE molecule are needed to keep stably  $GO_x$  near the graphene surface in the water surrounding and prevent the strong interaction between graphene and  $GO_x$ .

The Raman spectra registered in the range of  $1100$ – $1700$   $cm^{-1}$  displayed two broad bands peaked at  $1300$  and  $1603$   $cm^{-1}$  which correspond to defect (D) and tangential (G) vibrational modes of rGO. Experimental spectra were fitted to a sum of Lorentzian functions. We have revealed slight changes of frequency of maximum, spectral width and intensity ratio (D/G) at comparison between rGO sample and rGO–PSE– $GO_x$  one. Both D and G bands are shifted towards lower frequencies (by  $1$  and  $0.5$   $cm^{-1}$ ) in the rGO–PSE– $GO_x$  spectrum, such a shift is qualitatively similar to that observed in earlier studies of interaction between PSE and carbon nanotubes [1]. The obtained results can be used in the biosensor elaboration for the detection of glucose, lactate, and other compounds.

## Acknowledgment

This work was supported by Grant # 0123U100628 of the National Academy of Sciences of Ukraine.

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**Keywords:** noncovalent interaction, graphene, glucose oxidase, pyrenebutanoic acid succinimide ester, Raman spectroscopy



# ENHANCED THERMOELECTRIC PERFORMANCE OF SOL-GEL PROCESSED $\text{Bi}_2\text{Ca}_2\text{Co}_2\text{O}_y$ COBALTITE BY $\text{BiBO}_3$ AND $\text{NaF}$ CO-DOPING

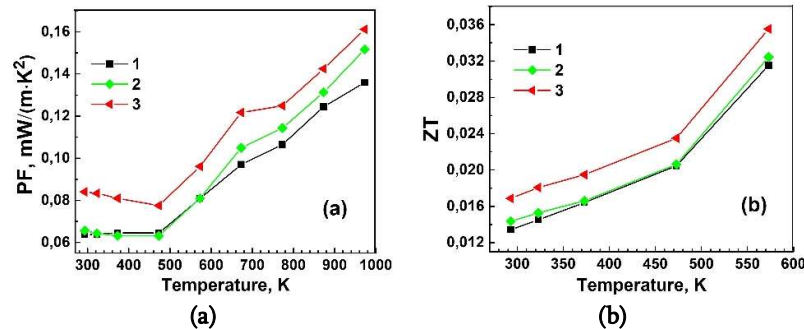
Iamze Kvartskhava<sup>1</sup>, Masatoshi Takeda<sup>2</sup>, Vakhtang Zhghamadze<sup>1</sup>,  
Giorgi Mumladze<sup>1</sup>, Giorgi Kakhniashvili<sup>1</sup>, Nikoloz Margiani<sup>1</sup>

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Renewable energy technologies are increasingly important due to the world's growing energy needs and environmental degradation. In this context, extensive research focuses on thermoelectric materials that can directly convert waste heat into electric power. Doping through sol-gel chemistry, which yields materials with very high chemical homogeneity, is an attractive method to fine-tune their thermoelectric properties. The layered cobaltite  $\text{Bi}_2\text{Ca}_2\text{Co}_2\text{O}_y$  with p-type electrical conductivity is a promising material for thermoelectric applications. This work examined the combined impact of  $\text{BiBO}_3$  and  $\text{NaF}$  co-doping on the thermoelectric characteristics of  $\text{Bi}_2\text{Ca}_2\text{Co}_2\text{O}_y$  ceramics. Samples with a nominal composition of  $\text{Bi}_2\text{Ca}_2\text{Co}_2\text{O}_y$  (reference),  $\text{Bi}_{1.9925}(\text{BiBO}_3)_{0.0075}\text{Ca}_2\text{Co}_2\text{O}_y$ , and  $\text{Bi}_{1.8925}(\text{BiBO}_3)_{0.0075}(\text{NaF})_{0.1}\text{Ca}_2\text{Co}_2\text{O}_y$  were prepared using the sol-gel method with citric acid and ethylene glycol as chelating agents. The temperature dependence of electrical resistivity, Seebeck coefficient, and thermal conductivity was measured to calculate the Power Factor ( $\text{PF} = S^2/\rho$ ) and figure of merit ( $\text{ZT} = S^2T/\rho k$ ), with  $S$ ,  $\rho$ ,  $T$ , and  $k$  representing Seebeck coefficient, electrical resistivity, absolute temperature, and total thermal conductivity, respectively (Figure 1).



**Figure 1.** Temperature dependence of (a) power factor and (b) figure of merit. 1 –  $\text{Bi}_2\text{Ca}_2\text{Co}_2\text{O}_y$  (reference), 2 –  $\text{Bi}_{1.9925}(\text{BiBO}_3)_{0.0075}\text{Ca}_2\text{Co}_2\text{O}_y$ , and 3 –  $\text{Bi}_{1.8925}(\text{BiBO}_3)_{0.0075}(\text{NaF})_{0.1}\text{Ca}_2\text{Co}_2\text{O}_y$ .

The  $\text{NaF}$ -doped sample has a much lower electrical resistivity ( $\rho$ ) than the reference  $\text{Bi}_2\text{Ca}_2\text{Co}_2\text{O}_y$ . This result is due to the partial substitution of  $\text{NaF}$  for  $\text{Bi}_2\text{O}_3$ , which increases the concentration of charge carriers. Although this sample has a slightly lower Seebeck coefficient and higher thermal conductivity than the ones studied, the decreased resistivity has a greater impact on the thermoelectric properties, leading to a higher power factor (PF) and figure of merit (Figure 1b). The maximum PF and ZT values achieved in the  $\text{NaF}$ -doped composition are approximately 16% and 13% higher, respectively, compared to the reference  $\text{Bi}_2\text{Ca}_2\text{Co}_2\text{O}_y$ .

## Acknowledgment

This work was supported by the ISTC Project Grant # GE-2776: “Enhancing the Thermoelectric Conversion Performance of Cobalt-Based Oxide Materials through Doping and Microstructure Modulation”.

**Keywords:** thermoelectricity, doping, sol-gel technique, power factor, figure of merit

IMPACT OF Lu<sub>2</sub>O<sub>3</sub>/Bi<sub>2</sub>O<sub>3</sub>, Lu<sub>2</sub>O<sub>3</sub>/BiF<sub>3</sub> and Lu<sub>2</sub>O<sub>3</sub>/NaF CO-DOPING ON THERMOELECTRIC PROPERTIES OF CaMnO<sub>3</sub> CERAMICS

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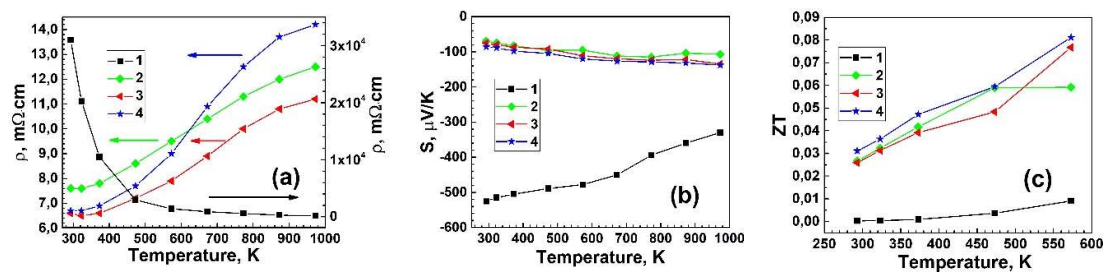
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Thermoelectric technology can provide clean energy by directly converting waste heat from various systems into electricity via the Seebeck effect. Both p- and n-type materials in which holes and electrons participate in the electrical conductivity are necessary for this process. The thermoelectric conversion efficiency of materials is quantified by the dimensionless figure of merit:  $ZT = S^2T/\rho k$ , where  $S$ ,  $T$ ,  $\rho$ , and  $k$  are the Seebeck coefficient, absolute temperature, electrical resistivity, and total thermal conductivity, respectively. Calcium manganite (CaMnO<sub>3</sub>) is the most promising n-type material because of its high Seebeck coefficient. However, the electrical resistivity of this compound is too high to be practical. The thermoelectric performance of CaMnO<sub>3</sub> can be improved by suitable aliovalent doping of various elements at the Ca and/or Mn sites. In this work, we attempted to optimize the thermoelectric performance of CaMnO<sub>3</sub> through co-doping with Lu/Bi, Lu/BiF, and Lu/NaF. For this purpose, samples with a nominal composition of CaMnO<sub>3</sub> (reference), Ca<sub>0.875</sub>Lu<sub>0.1</sub>Bi<sub>0.025</sub>MnO<sub>3</sub>, Ca<sub>0.875</sub>Lu<sub>0.1</sub>(BiF<sub>3</sub>)<sub>0.025</sub>MnO<sub>3</sub> and Ca<sub>0.875</sub>Lu<sub>0.1</sub>(NaF)<sub>0.025</sub>MnO<sub>3</sub> were prepared using the solid-state reaction method. The temperature dependences of electrical resistivity, Seebeck coefficient, and thermal conductivity were measured to calculate the figure of merit. The reference sample with semiconducting temperature dependence exhibits high resistivity ( $\rho$ ) of  $3.1 \cdot 10^4$  and  $144 \text{ m}\Omega \cdot \text{cm}$  at 293 and 973 K, respectively (Figure 1a). Figures 1a and 1b display a notable decrease of the electrical resistivity and Seebeck coefficient values in doped samples, attributed to the increase in charge carrier concentration (n-type electrical conductivity).



**Figure 1.** Temperature-dependence of (a) resistivity, (b) Seebeck coefficient, (c) figure of merit. 1 – CaMnO<sub>3</sub> (reference), 2 – Ca<sub>0.875</sub>Lu<sub>0.1</sub>Bi<sub>0.025</sub>MnO<sub>3</sub>, 3 – Ca<sub>0.875</sub>Lu<sub>0.1</sub>(BiF<sub>3</sub>)<sub>0.025</sub>MnO<sub>3</sub>, and 4 – Ca<sub>0.875</sub>Lu<sub>0.1</sub>(NaF)<sub>0.025</sub>MnO<sub>3</sub>.

Dual doping of CaMnO<sub>3</sub> with Lu/Bi lowers thermal conductivity from 1.04 to 0.92 W/m·K, while co-doping with Lu/BiF<sub>3</sub> and Lu/NaF increases  $k$  value by 9–13% at 573 K. Overall, enhanced  $ZT$  values in doped materials resulted from significantly reduced electrical resistivity. Figure 1c shows that the Lu/BiF<sub>3</sub> and Lu/NaF co-doped compositions achieve the highest  $ZT$  values of around 0.08 at 573 K.

### Acknowledgment

This work was supported by the ISTC Project Grant # GE-2776: “Enhancing the Thermoelectric Conversion Performance of Cobalt-Based Oxide Materials through Doping and Microstructure Modulation”.

**Keywords:** thermoelectricity, CaMnO<sub>3</sub>, co-doping, power factor, figure of merit

## DROPLET EPITAXY OF InGaP NANOSTRUCTURES

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Quantum Dots (QDs) are semiconductor nanocrystals with remarkable potential for high-performance photonic and electronic devices, particularly those based on semiconductor alloys of III–V elements.

This review briefly covers the fabrication methods of InP/GaP quantum dots, including Stranski–Krastanov growth mode, droplet epitaxy, and the chemical synthesis of colloidal QDs.

Additionally, it discusses the technological advancements in growing III–V nanocrystal layers, such as the electrochemical deposition of Group III metals on III–V semiconductor surfaces followed by annealing in an inert gas atmosphere. The electrical and photonic properties of the fabricated InGaP/GaP nanomaterials are examined, and a model for the formation mechanism of the InP nanostructured layer on the GaP surface is proposed.

### Acknowledgments

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**Keywords:** nanocrystals, quantum dots, droplet epitaxy, III–V semiconductor

## SEMICONDUCTOR NANOSTRUCTURES FOR PHOTONIC DEVICES

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Semiconductor nanostructures, particularly quantum dots, are excellent materials for photonic and electronic devices. Among the various research and technological domains, quantum communication is notably the most advanced [1]. Recent studies indicate that Droplet Epitaxy (DE) can generate highly entangled photon pairs with excellent photon indistinguishability, suggesting that DE may complement or even surpass conventional Stranski-Krastanov (SK) InGaAs quantum dots (QDs) as quantum emitters [2].

DE is an epitaxial technique, primarily used for III–V semiconductors, to fabricate a variety of nanostructures, such as QDs, Quantum Rings (QRs), and nanoholes. The DE method leverages the controlled crystallization of metal nano-droplets into III–V semiconductors [3].

This paper provides a detailed description of the DE method for III–V nanostructures, emphasizing its applications in quantum communication and solar cells.

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**Keywords:** quantum dot, droplet epitaxy, nanostructure, III–V semiconductor, quantum communication

# STRUCTURE AND PROPERTIES OF PHOTOCATALYSTS BASED ON TITANIUM DIOXIDE NANOPARTICLES MODIFIED WITH SILVER AND CERIUM

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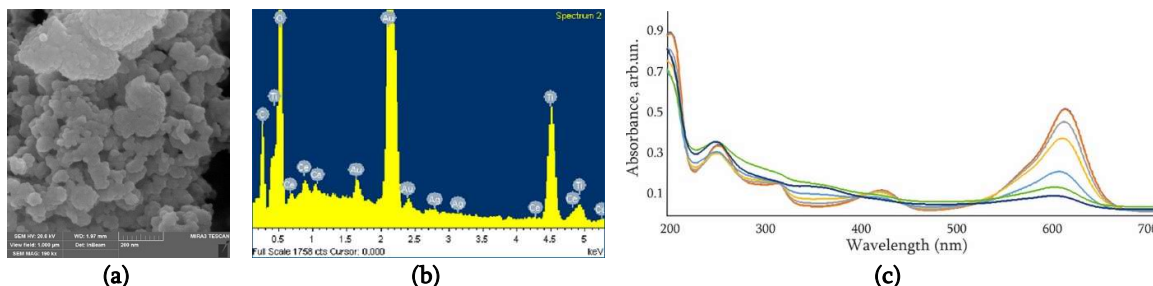
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Today, among the numerous strategies aimed at improving the photocatalytic properties of nanosized particles of titanium dioxide, their modification with Noble Metals (NM), particularly silver, and REE, among which nanoceria occupies a special place, has gained considerable popularity. In our previous works, a method of chemical synthesis of binary and ternary nanocomposites based on anatase was developed using titanium tetraisopropoxide, auxiliary substances, inorganic salts of noble metals, and REE. The composition, structure, morphology, optical properties, and photocatalytic activity of titania-based binary nanocomposites modified with NM or cerium were studied. The indicated binary structures showed high activity in the destruction of the chromophoric and aromatic components of several organic dyes of anionic and cationic nature. The presence of cerium and NM in the structure of composites contributes to reducing the time of processing dye solutions under the influence of UV irradiation and visible lights, providing an opportunity to increase the efficiency of the destruction of dyes by combining catalytic and photocatalytic processes. Some our works were published based on the results of the conducted research [1, 2]. The purpose of this work was to study the structure, catalytic and photocatalytic properties of ternary TiO<sub>2</sub>&CeO<sub>2</sub>&Ag nanocomposites and to analyze their efficiency in the destruction of the organic dyes: Malachite Green, Methylene Blue, Rhodamine B, Methyl Orange, Orange G. **Figure 1** shows the morphology of TiO<sub>2</sub>&CeO<sub>2</sub>&Ag composite particles doped with 3wt.% Ce and Ag (a), the EDS spectrum (b) and the UV–VL spectra obtained during the interaction of the Malachite Green solution with the composite particles (c). It will be noted that Au in the spectrum **Figure 1b** corresponds to metal-atomizer, which was used during SEM studies. The optimal conditions for the destruction of organic dyes were determined by combining sorption, catalytic, and photocatalytic processes, which ensures both an increase in the efficiency of the destruction process and a reduction in the time it takes.



**Figure 1.** Characteristic of TiO<sub>2</sub>&CeO<sub>2</sub>&Ag (3wt.%) composite particles: (a) morphology, (b) EDS spectrum, (c) typical UV–VL spectra obtained during destruction of Malachite Green solution.

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**Keywords:** TiO<sub>2</sub>-photocatalysts, nanoceria, silver, cationic and anionic dyes, dye destruction, UV irradiation

## SURFACE FUNCTIONALIZATION OF FLUORESCENT NANO-DIAMONDS (FNDs) FOR BIOMEDICAL APPLICATIONS

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NanoDiamonds (ND), nanometer-sized carbon structures, have exceptional chemical, optical and biological properties. In particular, nanodiamonds (NDs) are characterized by their biocompatibility, low toxicity to cells, chemical inertness, large surface area relative to their volume, and small size, allowing them to have potential value for medical and biological applications. Fluorescent NanoDiamonds (FNDs) have revolutionized research and innovation in cell imaging and tracking, showing great promise as drug delivery vehicles, fluorescent markers, protein transport, and in technological applications such as fiber optic technologies.

In this work, the surface of nanodiamonds was modified by the ultrasonic method and the addition of an extract of the medicinal plant *Cissus Genus* in order to improve their luminescent properties. The optical properties of such nanodiamonds placed in aqueous suspensions were studied and compared with the resulting classical detonation nanodiamonds. To obtain nanodiamonds functionalized with *Cissus Genus* plant extract, NDs were treated by one of the following methods: 1) mixing with a solution distilled water and 30% hydrogen peroxide in several ratios, 2) bubbling ozone, 3) mixing with theraphthal (soluble cobalt phthalocyanine containing COONa groups) aqueous solution, 4) mixing with theraphthal and urea. Then, the formed mixtures were subjected to ultrasonic treatment (35 kHz) for 1–12 h. Finally, the samples were washed with distilled water and *Cissus Genus* extract was added to the resulting samples in different quantities.

The formed nanoparticles were characterized by FTIR spectroscopy, UV-visible spectroscopy, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The presence of red luminescence was observed in NDs functionalized with an extract of the *Cissus Genus* plant (nanoparticle size of 4–7 nm). The resulting nanostructures are non-toxic and can be used to develop more effective and selective drug delivery systems, including fluorescent markers.

### Acknowledgment

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**Keywords:** nanodiamonds, fluorescence, theraphthal

# IMPACT OF Fe<sub>3</sub>O<sub>4</sub> NANOPARTICLES ON FERTILIZATION PROCESS OF COMMON CARP (*Cyprinus carpio* Linnaeus, 1758) AND EMBRYONIC DEVELOPMENT STAGES

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There is insufficient information in the scientific literature on rapid development of nanotechnology and its impact on hydrocele, particularly to embryonic development stages, which are more sensitive to external environmental factors in connection with its application to various fields. Therefore, the main purpose of the current research is to investigate the effect of nanoparticles current research is to investigate the effect of Fe<sub>3</sub>O<sub>4</sub> (20–30 nm) nanoparticles on sexual cells (sperm, egg cell) of common carp (*Cyprinus carpio* Linnaeus, 1758) before fermentation in the aquaculture process and the effects of embryonic developmental stages after fermentation, as well as absorption of nanoparticles by feedstuffs and entry into the food chain and investigating possible bioaccumulation.

The research material was carried out in June 2021 at the farm “Samukh-fish” located in the Barda district and June 2023 at the fishery located in the Neftchala district of the Republic of Azerbaijan. During the experiment caviar was taken from the reproductive fish, smoothing its abdomen with the thumb, and placed in porcelain vessels with a smooth surface according to the number of experimental options. Experiments were carried out on different variants on given topics. The quality of sperm taken from male was initially assessed visually, and the sperm activity in the samples was determined on a 5-point scale in accordance with the obtained methodology [1 – 3]. Skyspring Nanomaterials in the course of experiments. Inc, USA, Houston TX. Fe<sub>3</sub>O<sub>4</sub> (20–30 nm) nanoparticles from the company were used. The Fe<sub>3</sub>O<sub>4</sub> (20–30 nm) nanoparticles were added to the germ cells of common carp (*Cyprinus carpio* Linnaeus, 1758) before fertilization in different amounts (0.0001, 0.001, 0.005 and 0.05 g), as well as to the fertilized egg and their embryonic. The effect on developmental stages was studied with the help of Carl Zeiss Axio Imager M2 binocular by magnifying them for 200 times. Every day in the incubation proses, dead embryos are removed from the apparatus in every version, noted in special book, and the free embryos are then counted.

Studies have shown that when Fe<sub>3</sub>O<sub>4</sub> (20–30 nm) nanoparticles were added to the yeast of common carp before fertilization, during the process the fertilization rate of the eggs was higher and the yield of free embryos was higher than in other variants. Fe<sub>3</sub>O<sub>4</sub> (20–30 nm) nanoparticles have a stimulating effect in the amount of 0.05 g. It can be assumed that these nanoparticles in the specified doses have a catalytic effect on the acrosomes of sperm, accelerate energy activity and, consequently, increase the activity of sperm, which leads to an increase in the fertilization rate of eggs. Correspondingly, the results that obtained can be used to reduce weights, especially in the process of carp aquaculture, to reduce losses during embryonic development and increase overall productivity.

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**Keywords:** common carp, nanoparticles, sexual cells, fertilization, embryonic stages

# SYNTHESIS AND CHARACTERIZATION OF h-BN@SPIONs MAGNETIC NANOCOMPOSITES FOR POTENTIAL BIOMEDICAL APPLICATIONS

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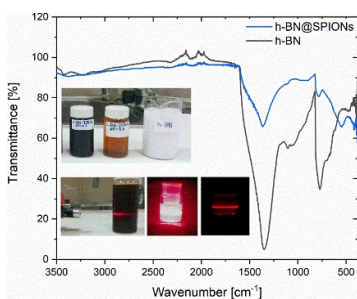
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This study reports the successful synthesis and characterization of h-BN@SPIONs (hexagonal Boron Nitride @ SuperParamagnetic Iron Oxide Nanoparticles) magnetic nanocomposite, designed for potential biomedical applications. The nanocomposite was synthesized using a controlled sonochemical co-precipitation method, where magnetite nanoparticles were formed in an aqueous suspension of pre-synthesized hexagonal boron nitride under an inert (N<sub>2</sub>) environment to prevent undesirable oxidation of Fe<sup>+2</sup>. The resulting nanocomposites, h-BN@SPIONs, were characterized using Dynamic Light Scattering (DLS), Electrophoretic Light Scattering (ELS), Fourier Transform Infrared Spectroscopy (FTIR), Vibrating Sample Magnetometry (VSM), and Ultraviolet-Visible (UV-Vis) Spectroscopy. The hydrodynamic size distribution and zeta potential of the nanocomposites were measured to ensure colloidal stability in aqueous suspensions, a critical factor for biomedical applications. FTIR spectra confirmed the successful encapsulation of SPIONs by h-BN (**Figure 1**), while VSM analysis demonstrated the superparamagnetic properties of the composites.



**Figure 1.** FTIR spectrum of h-BN and h-BN@SPIONs samples. Inset shows photograph of h-BN@SPIONs and h-BN aqueous dispersion with laser pointer beam passing through colloid (Tyndall effect).

The potential biomedical applications of h-BN@SPIONs are numerous and promising. The unique combination of h-BN's fluorescence properties and SPIONs' magnetic responsiveness makes this nanocomposite an excellent candidate for multimodal imaging [1, 2]. Furthermore, the good biocompatibility of both components, coupled with the ability to functionalize the surface, opens up possibilities for targeted drug delivery and cancer therapy, particularly in Boron Neutron Capture Therapy (BNCT) [1]. The stability of the h-BN@SPIONs aqueous dispersion was demonstrated through the observation of the Tyndall effect and long-term sedimentation studies (**Figure 1**), indicating its suitability for biological applications. Additionally, the antibacterial properties of BN nanoparticles suggest potential use in developing antimicrobial coatings for medical devices [2]. The unique combination of h-BN's biocompatibility and SPIONs' magnetic properties makes these nanocomposites promising candidates for advanced biomedical applications. Further research will focus on in vitro and in vivo studies to fully elucidate the biocompatibility and efficacy of this nanocomposite in specific biomedical contexts.

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**Keywords:** h-BN, SPIONs, magnetic nanocomposites, sonochemical co-precipitation, biomedical applications



# EVOLUTION OF TRANSFORMATIVE MATERIALS AND ROLE OF NANOMATERIALS AND NANOTECHNOLOGIES ON ENERGY, ENVIRONMENT AND SUSTAINABLE DEVELOPMENT

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Sustainable development is a comprehensive and complex system of systems requiring multidisciplinary and interdisciplinary science and technology inputs with economic, environmental, and social objectives and goals. In broad terms, sustainable development is achieved when the present needs and challenges are met without placing in jeopardy the ability of future generations to meet their own needs and challenges. The trade space is very wide, and the multitude of trade-offs generate considerable challenges and make it often difficult to achieve an effective balance, most beneficial to all concerned.

During the last sixty years the planet's population has grown exponentially, from 2 to almost 8 billion people, and the technological progress achieved has been tremendous, especially in the industrialized countries. These trends are expected to continue, even at faster rates. However, all these associated technological activities in the pursuit of better living standards have created a considerable depletion of resources and pollution of land, water, air, and natural resources, for the global population.

During this period considerable achievements have been obtained in the development and deployment of transformative materials such as light weight metallic alloys, metal matrix composites, intermetallic and carbon fiber composites, and hybrid materials. Nano, nano-structured and nano-hybrid carbon-based materials systems and nanotechnologies are now being deployed with considerable impact on energy, environment, and sustainable development.

This presentation presents perspectives on the evolution and global impact of transformative materials with a focus on nanomaterials and nanotechnologies, and with examples from several domains of sustainable development.

**Keywords:** transformative materials and technologies, advanced materials, nanomaterials, nano-hybrid materials, carbon base nano materials systems, nanotechnologies, sustainable development, energy, environment

**TO STUDY INFLUENCE OF RADIOACTIVE SUBSTANCES  
ON GROWTH AND DEVELOPMENT OF ANNUAL GRAIN  
CROPS: SALINE SOILS OF SHIRAK VALLEY (GEORGIA)**

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In the Project described here, we would like to study the influence of radiation on the development of one-year grain crops in the saline soils of Shirak Valley (Georgia). To the extent that the growth and development of the plant depends on both the soil and the climate change, the latter is constantly changing both seasonally and during the day and night. Among the many components of climate change, the study of radiation has an important place. It is constantly updated and changing. These changes require a special study in the soil, because there is an accumulation of various radioactive substances, both from the atmosphere and from the ground water.

In the process of forming the root system of annual cereal crops, detailed studies should be carried out in the soil during the relevant season. Special attention should be paid to the investigation of doses of radon, cesium, strontium and potassium. Each of them has a significant impact on plant development. Their slightly increased dose may not have much effect on the suitability of grain for food, but it is known that the yield of irradiated grain is reduced by half, and it is not recommended to use them as seed. The issue requires study with agronomists. It is possible to identify various diseases of cereal crops in the researches, which are caused by the radioactive substances listed above.

In terms of solving the posed problem, it will be useful to determine the irrigation norms under the given radiation conditions, in order to eliminate the undesirable result for obtaining the yield.

## *Artemisia annua* HAIRY ROOTS FOR “GREEN” SYNTHESIS OF GOLD NANOPARTICLES

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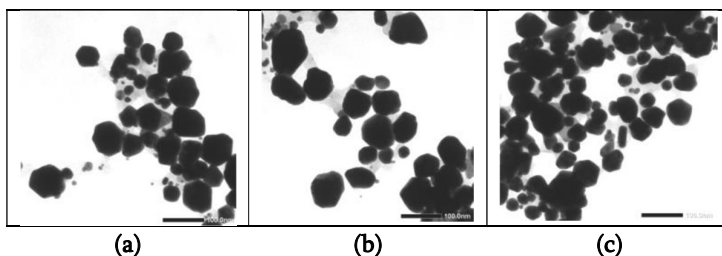
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“Green” synthesis of metal nanoparticles is one of the modern methods of obtaining nanomaterials. In this process extracts from plant material that have reducing activity are used. Hairy roots are the roots that form on various parts of plants when they come into contact with soil bacteria *Agrobacterium rhizogenes* and are a manifestation of plant disease caused by microorganisms. However, at the end of the 20th century, a new, simple, and effective method was developed to use the ability of these bacteria to infect plants and transfer their genes to the plant genome, thereby transforming them. The result of this biotechnological process is the formation of roots that are grown in sterile conditions (in vitro). Cultivation of such roots can be long-term and does not require specific conditions (heating, lighting, etc.). The ability to synthesize plant-specific compounds in an amount that significantly exceeds that of the original plants is the feature of hairy roots. In addition, hairy roots can also synthesize compounds that are not characteristic of the original plants, as well as have a different ratio of various secondary metabolites. Accordingly, the bioactivity of such roots, in particular, reducing activity, can be changed [1]. That is why extracts from hairy roots with reducing activity can be used for the “green” synthesis of metal nanoparticles. In our work, we used ethanol (70%) extracts from *Artemisia annua* hairy roots and extracts from the roots of the control nontransformed plants. The extracts were diluted to the same concentration (0.5 mg RE/ml). The reducing activity of the extracts was studied by the reaction with FeCl<sub>3</sub>. For gold NanoParticles (AuNPs) formation the extracts were added to the solution of HAuCl<sub>4</sub>. Nanoparticles were visualized using microscope JEM-1400 (Jeol, Japan), accelerating voltage of 80 kV. The samples were prepared by applying a suspension of NPs to a copper grid with a formvar coating, which is reinforced by carbon sputtering.



**Figure 1.** TEM images of AuNPs obtained with *Artemisia annua* extracts: (a) extract of control roots, (b) and (c) extracts of two lines of transgenic roots (hairy roots).

To obtain AuNPs, three extracts were used, which had the same content of flavonoids and comparable reducing activity. However, TEM analysis revealed some differences in the nanoparticles obtained after adding these extracts to HAuCl<sub>4</sub> solution (Figure 1). Such differences may be due to the fact that the bacterial *rol* genes, which are transferred to the plant genome during transformation, can affect secondary metabolism in transgenic roots. Such influence can lead to qualitative changes of secondary metabolites, which is reflected in the formation process of gold nanoparticles. Such features allow the selection of extracts from different lines of transgenic roots from our in vitro collection (it has more than 80 collection samples) in accordance with the needs and requirements for the size/shape of nanoparticles.

### Acknowledgment

The work was carried out with the financial support of the NAS of Ukraine (Project # 0123U101081).

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**Keywords:** *Artemisia annua*, hairy roots, “green” synthesis, gold nanoparticles, reducing activity

## INNOVATIVE SENSORS: NEW STANDARDS OF ACCURACY AND EFFICIENCY

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The paper discusses how to create a new generation sensor, as well as the improvement of existing converters.

More specifically, after finding and processing information about deformation sensors, a number of features were identified, which, on the one hand, should be taken into account when creating a new sensor, and on the other hand, it is necessary to find ways to solve the problems that prevent the use of existing sensors and obtaining accurate information from them.

The paper presents an optical transducer of deformation created by me, which will allow us to investigate the deformation of bodies, so that we are not limited in the material and size of the bodies, the measurement results are as little dependent on environmental factors as possible, and the sensor is low-budget, easy to create and convenient to install. When creating the sensor, the properties of silicon used as the main material, as a light-conducting material, were taken into account, which is expressed in both temperature stability and its optical properties, in particular, taking into account the high reflection index of the light beam. The flexibility of silicon was also taken into account, which was a problem in many considered deformation sensors.

# ADVANCED PROTECTIVE COATINGS FOR POWER GENERATION, OIL AND GAS PRODUCTION, AND MINERAL PROCESSING: MAJOR PROCESSING PRINCIPLES, PROPERTIES AND APPLICATIONS

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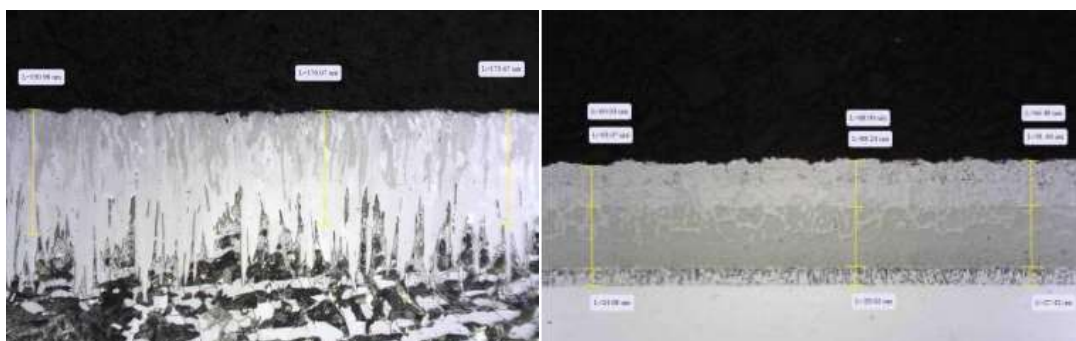
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The challenges in production and processing equipment service in power generation, including renewable technologies, downhole oil & gas production, and mining and mineral processing are outlined.

In the majority of considered application situations, tubing and components made of steels and alloys experience severe degradation due to wear and high temperature corrosion, which lead to necessity of these components' protection. Advanced ceramic protective coatings can be successfully employed to resolve these problems significantly improving the components' integrity and extending their service life. The major principles of the coatings' formation and manufacturing through Thermal Diffusion (TD) CVD-based processes are discussed and analyzed. The process is based on diffusion of certain atoms, like B, Al, Cr, Ta, to the steels' or ferrous alloys' structure with formation of borides or intermetallides' compounds with nano-crystalline structures protecting the metallic surfaces (**Figure 1**). The obtained coatings consist of 2–3 layers (i.e. with multi-layered architectures), which form simultaneously through a “single” process cycle. They also may have an additional top layer of a few-micron thickness based on selected oxides or non-oxides forming composite coatings.



**Figure 1.** Examples of microstructures of boronized (left) and aluminized (right) coatings on steels.

The TD coating architectures and total thickness (from ~20 to 250  $\mu\text{m}$  or greater) depend on the metallic substrate, selected starting batch compositions and process parameters, as well as on application requirements. The beneficial results of corrosion, erosion, abrasion and corrosion-wear resistance at room and elevated temperatures (up to 1000°C) of the produced materials will be presented. The coatings' major processing steps and features are outlined.

Complex shape components and long tubing with selected coatings were successfully produced, and these components with particular compositions and structures are successfully served in severe wear and/or high temperature corrosion conditions. They include solar and nuclear power generation involving flows of molten salts and molten metals, high temperature/high pressure steams and gases, and brines, oil & gas and mineral production involving severe wear- and wear-corrosive media impacts, geothermal processing and some other conditions. Multi-layered structure and diffusion-induced bonding between protective layers and the substrate promote the coatings' integrity and delay micro-crack propagation under stress conditions occurring in service.

**Keywords:** protective coatings, thermal diffusion, corrosion, wear, microstructure

## ADVANCEMENTS AND CHALLENGES IN INTENSITY-MODULATED RADIATION THERAPY (IMRT)

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Over the past few decades, intensity-modulated radiation therapy (IMRT) has emerged as a cornerstone in radiation oncology, revolutionizing the delivery of radiation treatment for various types of cancer. IMRT offers significant advantages in treatment efficacy and reduced toxicity by precisely shaping radiation beams to conform to the contours of tumors while sparing adjacent healthy tissues. This comprehensive review explores the advancements and applications of IMRT, examining its evolution from inception to state-of-the-art implementations. We delve into the underlying principles of IMRT, including optimization algorithms, treatment planning techniques, and delivery systems, highlighting the intricate mechanisms that enable highly conformal dose distributions.

Furthermore, we explore the broad spectrum of clinical applications of IMRT across different disease sites, ranging from head and neck cancers to prostate, breast, and central nervous system tumors. By synthesizing evidence from clinical studies and trials, we evaluate the efficacy, safety, and long-term outcomes of IMRT in various patient populations, underscoring its role as a care standard in modern radiation oncology [1 – 3].

Additionally, this review addresses ongoing research efforts and emerging trends in IMRT, such as advancements in imaging technologies, treatment adaptation strategies, and integration with other modalities like chemotherapy and immunotherapy. We discuss potential challenges and future directions, envisioning the continued evolution of IMRT as a vital tool in the fight against cancer.

By providing a comprehensive overview of the advancements and applications of IMRT, this review aims to serve as a valuable resource for radiation oncologists, medical physicists, clinicians, researchers, and healthcare professionals involved in cancer care. Through a deeper understanding of the capabilities and limitations of IMRT, we strive to optimize its utilization and further enhance outcomes for patients undergoing radiation therapy.

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**Keywords:** intensity-modulated radiation therapy (IMRT), radiation oncology, radiation therapy advancements, cancer care optimization

# DEVELOPMENT OF BIOCOMPATIBLE POLYMER NANOFIBERS FUNCTIONALIZED WITH SUPERPARAMAGNETIC IRON OXIDE NANO- PARTICLES VIA ELECTROSPINNING FOR BIOMEDICAL APPLICATIONS

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Nanotechnology is rapidly advancing and holds great promise for biomedicine and healthcare. Recent research has focused on the development of multifunctional polymeric micro/nanofibers through electrospinning – a technique that produces nano-sized fibers with diverse applications, including drug delivery, tissue engineering, and regenerative medicine. This research aims to synthesize and functionalize biocompatible SuperParamagnetic Iron Oxide Nanoparticles (SPIONs) to create polymer nanofibers with enhanced mechanical, chemical, and electrical properties, while also ensuring exceptional biocompatibility and biodegradability. By incorporating agents such as drugs, biomolecules, and nanoparticles into the polymer matrix, we aim to develop hybrid nanocomposite fibers with unique characteristics.

A relatively new category of composite materials, magneto-responsive polymer-based fibrous nanocomposites, falls under the broader category of stimuli-responsive materials. These composites feature magnetic nanoparticles embedded in a polymeric fibrous matrix. This research focuses on the synthesis and characterization of magnetically sensitive nanofiber composites using biocompatible polymers (PEG, PVA, PEI, and PLC), with superparamagnetic iron oxide ( $\text{Fe}_3\text{O}_4$ ) nanoparticles modified by small organic molecules like Citric Acid (CA) or Folic Acid (FA), and loaded with the drug DOXorubicin (DOX).

Electrospinning, a fast, economical, and versatile method, is employed to produce nano- and micro-sized nanocomposite fibers. In this technique, a strong electrostatic field applied to a polymer solution causes the formation of a Taylor cone at the droplet's tip. As the jet moves towards a collecting screen, the solvent evaporates, leaving behind the desired nanofiber product. Electrospun nanofibers exhibit a high specific surface area, strong plasticity, and customizable properties, making them ideal for biomedical applications [1 – 3].

Within this work, PVA– $\text{Fe}_3\text{O}_4$  and PVA– $\text{Fe}_3\text{O}_4$ –CA nanocomposite materials were synthesized, and their physical and chemical characteristics were assessed. Further investigations into these materials will be conducted as part of the ongoing project. The obtained materials exhibit significant potential for various biological applications.

## Acknowledgment

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**Keywords:** polymer nanocomposites, electrospinning, magnetic nanoparticles

# GRAPHENE OXIDE INCORPORATED POLYSULFONE NANOCOMPOSITE MEMBRANES FOR ENHANCED PERFORMANCE IN ULTRAFILTRATION PROCESS

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The escalating global concern regarding organic pollution demands the development of advanced water treatment strategies. Over time, organic compounds can accumulate on a membrane's surface, resulting in biofilms forming. This buildup of biological material can compromise the efficiency of the membrane and decrease its useful lifespan, requiring more frequent and expensive cleaning processes. To mitigate these issues, it is essential to modify the membrane to improve its properties and increase resilience to biofilm formation [1]. This study investigates the potential of biocidal ultrafiltration membranes that have been modified with various nanomaterials, specifically Graphene Oxide (GO) and its composites incorporating silver NanoParticles (AgNPs) and titanium dioxide (TiO<sub>2</sub> NPs). Ultrafiltration membranes were produced using polysulfone and GO and nanocomposites based on GO–AgNPs, and GO–TiO<sub>2</sub>NPs. GO was obtained by the oxidation method, while GO–AgNPs and GO–TiO<sub>2</sub>NPs nanocomposites were obtained by the gel method. The GO was prepared by the oxidation method, while the nanocomposites were synthesized via the sol–gel method [2]. Membrane films were produced from polymers homogeneous solutions (PS–1%GO, PS–3%GO, PS–5%GO, PS–1%GO–Ag/NPs, PS–1%GO–TiO<sub>2</sub>NPs) by the phase inversion method, with use of Automatic Coating Machine (Memcast TM, Porometer NV). Membrane pores sizes were determined with use of the POROLUX™ 500 (Porometer NV), an instrument based on capillary flow porometry measuring pore size distribution [3]. The obtained data have significant implications for the filtration process as well as for further modification of the biocidal ultrafiltration membranes.

The antimicrobial property of the polysulfone composites was examined by standard plate count protocols to get the number of viable colonies of each tested bacteria gram-negative (*Escherichia coli*) and gram-positive (*Staphylococcus aureus*) bacteria. The results of the experiments have demonstrated the potential of these membranes for filtering food products, while the addition of nanocomposites has been found to enhance the membranes' resistance to biofilm formation on their surfaces.

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**Keywords:** biocidal ultrafiltration membranes, antimicrobial activity, graphene oxide, nanoparticles of silver, titanium dioxide

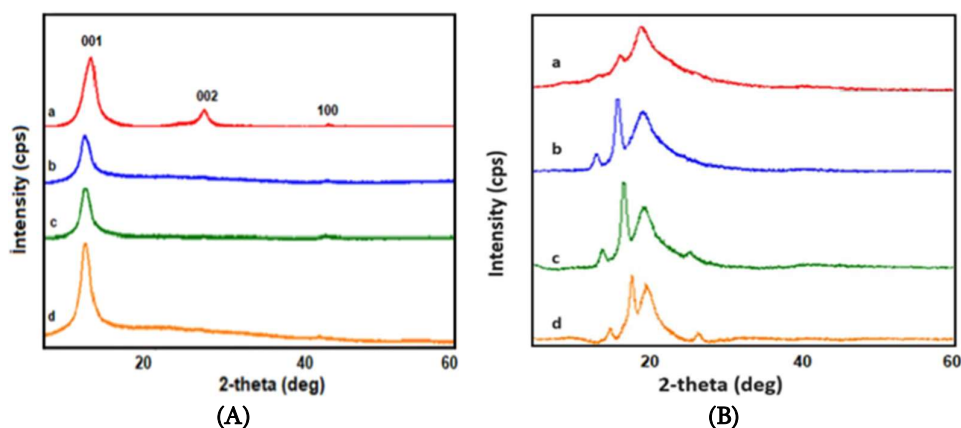


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Recent advances in polymer nanocomposites have sparked significant interest due to their controllable properties and versatile applications. Among these materials, Graphene Oxide / PolyVinyl Alcohol (GO/PVA) composites stand out for their extensive applications, including supercapacitors and memory devices [1]. While prior studies have explored the properties of these composites, the effects of gamma radiation on their physical properties have not been thoroughly investigated.

In this research, GO was synthesized using a modified Hummers method. The synthesized GO was incorporated into a PVA matrix at varying weight ratios (1 and 5%) and mixed via ultrasonication. The resulting mixtures were filtered into petri dishes and air-dried for a week, yielding thin films with 1 and 5% weight concentrations of GO/PVA composites. These films were subsequently exposed to gamma rays at doses of 1, 50, and 150 MRad. Structure analysis, shown in **Figure 1A**, revealed characteristic peaks for GO, with  $2\theta$  values at  $11.98^\circ$  and  $42.04^\circ$ , and a residual graphite peak at  $26.30^\circ$ . Post-irradiation, the disappearance of the residual graphite peak suggested its decomposition and oxidation due to gamma radiation. The interplanar distance of GO also varied with irradiation, measuring 7.38 (unirradiated), 8.03 (1), 7.94 (50), and 7.8449 Å (150 MRad). **Figure 1B** presents the XRD spectra of 1%GO/PVA nanocomposites. The spectrum for the unirradiated sample (**Figure 1B-a**) lacked characteristic GO peaks due to the dispersed distribution of GO within the polymer. Instead, it exhibited PVA peaks at  $2\theta = 19.90^\circ$ ,  $14.00^\circ$ , and  $16.77^\circ$ , indicating the complete exfoliation of GO into individual layers within the polymer matrix.



**Figure 1.** Diffractograms of (A) GO and (B) 1wt.%GO/PVA composites exposed to different doses of gamma radiation: (a) non-irradiation, (b) 1, (c) 50 and (d) 150 MRad.

Irradiated samples showed increased intensity of additional peaks, attributed to the breaking of hydrogen bonds and separation of GO particles, allowing the polymer to intercalate between layers and form new oriented structures. Furthermore, a new peak at  $2\theta = 25.40^\circ$  emerged in samples irradiated with doses of 50 and 150 MRad, indicating wrinkling and twisting of GO sheets at higher radiation doses. This was accompanied by the breaking of hydrogen bonds, polymer softening, and GO layer folding, promoting the formation of new oriented structures within the polymer matrix [2].

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**Keywords:** gamma radiation, nanocomposites, structure, supercapacitors, X-ray diffraction

ON DIRAC CONES AND BEYOND: FEATURED ELECTRONIC  
BAND STRUCTURES OF 2D MATERIALS WITH CHARGE  
CARRIERS MIMICKING MASSLESS DIRAC FERMIONS

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First discovered in graphene, Dirac cones have become the defining features of so-called “Dirac materials” two-dimensional mono- and bilayer crystalline allotropes of various elements and their compounds. Emerging as a small cone-shaped islands at the corners of the Brillouin zone of graphene, charge carriers in these Dirac cones can propagate at constant velocities, like relativistic particles with no inertia, thus imitating massless Dirac fermions despite their finite effective masses. This feature is shared by fermionic excitations in variety of different Dirac materials.

We show that in each case this effect is inevitably associated to the emergence of structures in their electronic bands in the form of so-called *ruled surfaces*, one of the representatives of which is a cone. Based on the properties of the ruled surface that forms the energy band and determines its dispersion characteristics, the appearance of charge carriers that imitate massless Dirac fermions in two-dimensional materials is consistently explained. This is in contrary to the conventional explanation, when the band dispersion is incorrectly interpreted as “linear”, which leads to an incorrect conclusion about “zero effective masses” of charge carriers.

In our discussion we fully account for the principal, though often overlooked, distinction between free massless Dirac fermions and charge carriers in solids – collective fermionic excitations – whose energy-momentum relation depends on the direction they travel within the energy band. The possibility of engineering energy bands with landscapes containing Dirac cones, as well as structures with *doubly ruled surfaces* to support charge carriers imitating massless Dirac fermions, may open new avenues for controlling and localizing high-mobility charge carriers in two-dimensional materials.

PHOTOREGULATION OF BIOSYNTHETIC ACTIVITY OF *Lentinula edodes* (Berk.) PEGLER USES COLLOIDAL SOLUTIONS OF BIOGENIC METAL NANOPARTICLES AND LOW-INTENSITY LASER RADIATION

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In this study, we present new data on the integrated use of colloidal solutions of nanoparticles and low-intensity laser radiation on the biosynthetic activity of the medicinal mushroom *Lentinula edodes in vitro*. Advances in nanotechnology open up many opportunities for their application in biology, medicine, agricultural technology, and genetic engineering [1].

In recent years, the application of nanotechnology in biological systems has led to the emergence of new fields such as nanobiotechnology and nanomedicine, which focus on the development of new therapeutics, ranging from targeted drug delivery to manipulation of individual biomolecules using laser tweezers, new bioimaging agents. The small size of NanoParticles (NPs) determines a number of features of their interaction in the cells of living organisms, including mushrooms. Due to their chemical properties, large surface-to-volume ratio, and unique quantum effects, biogenic metal NPs often exhibit properties that are qualitatively different from their macroscopic counterparts, making them valuable for numerous applications, including industrial scales [1].

Previous studies have demonstrated the effect of colloidal solutions of biogenic metal nanoparticles AgNP, FeNP and MgNP on the biosynthetic activity of the medicinal mushroom *Inonotus obliquus* (Ach.: Pers.) Pilát [2]. In addition, studies have proven that low-intensity laser radiation and Light-Emitting Diodes (LEDs) can be effectively used as environmentally friendly growth stimulators and for the biosynthetic activities of biotechnologically important species of edible and medicinal mushrooms [3]. Understanding the physiology and evaluating how nanoparticles and lasers can affect *L. edodes* biosynthetic activity in vitro can provide practical data for cultivation process intensification for this valuable mushroom species.

It was found that colloidal solutions of nanoparticles of all metals used increase the growth characteristics of *L. edodes* (65–77%), and irradiation of the fungal inoculum with laser light in a medium with nanoparticles reduces the growth activity of *L. edodes* mycelium. by 10.3–25.5%. Silver nanoparticles (AgNP) in a nutrient medium suppressed the biosynthesis of extracellular polysaccharides, and laser irradiation in the same medium increased the synthesis of intracellular polysaccharides by 13.3 times. Magnesium nanoparticles (MgNPs) and iron nanoparticles (FeNPs) inhibited the synthesis of intracellular polysaccharides in the mycelial mass of *L. edodes*.

At the same time, laser irradiation of the MgNP inoculum, on the contrary, caused a sharp increase in the amount of polysaccharides in the culture liquid (17 times). Treatment of the inoculum in a medium with nanoparticles with a laser caused an intensification of the synthesis of flavonoids in the mycelial mass. The results obtained suggest the possibility of complex use of colloidal solutions of FeNPs, AgNPs, MgNPs and low-intensity laser radiation as environmentally friendly factors for regulating biosynthetic activity in the biotechnology of cultivating the valuable medicinal mushroom *L. edodes*.

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**Keywords:** laser, metal nanoparticles, polysaccharides, mycelial biomass, flavonoids, *in vitro*

# DEVELOPMENT AND TESTING OF NANOPARTICLES FOR TREATMENT OF CANCER CELLS BY CURIE TEMPERATURE CONTROLLED MAGNETIC HYPERTHERMIA

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A vast amount of nanoparticles has been developed and proposed for the local hyperthermia of cancer during the last decades, but only a few of them correspond to the mandatory requirements of having therapeutic range Curie temperature ( $T_c = 41\text{--}45^\circ\text{C}$ ), high-rate crystallinity and “strong” magnetic properties, strictly controlled homogeneity and dispersion of the nanoparticles, good bioavailability and harmless decomposition products. Among them are the nickel–copper (Ni–Cu) and silver doped lanthanum manganite ( $\text{Ag}_x\text{La}_{1-x}\text{MnO}_3$ ) nanoparticles. The precise control of tumor temperature is especially important to avoid the tumor “overheating” or “underheating”. The developed research showed that the materials obtained at lower than usual temperatures using microwave enhanced synthesizes and annealing can be successfully used for local hyperthermia revealing high magnetic properties. Behavioral toxicity testing of the developed nanoparticles was enhanced by blood oxygen saturation measurements using noninvasive oximetry in white rats. Both of the developed nanomaterials revealed the better or similar magnetic properties and a significantly lower toxicity level than the commercially available  $\text{Fe}_2\text{O}_3$  nanoparticles. Eighty samples of silver doped lanthanum manganite nanoparticles and eighty samples of Cu–Ni nanoparticles ( $10\pm 0.05$  g each) with argentum content  $x = 0.15$  and Ni to Cu at.% ratios R from 1.9 to  $3.0\pm 0.05$  have been synthesized using a 1500 W microwave reactor OLT-CR-50. They were prepared using the synthesis methods described in [1, 2]. The microwave enhanced synthesis was conducted at two microwave power levels (700 and 1000 W) to investigate the possible dependence of the capacity of synthesis and properties of the yielded nanoparticles on the applied microwave power. The magnetic properties of nanoparticles (coercivity  $H_c$ , remnant magnetization  $M_r$  and saturation magnetization  $M_s$  have been measured to investigate their possible correlation with the microwave enhanced synthesis power and particle size, uniformity and morphology. The main result of the reported research are the data on the optimum synthesis parameters and properties of nanoparticles with Curie temperature in the therapeutic range. The above data clearly show that the developed materials can be successfully used for the Curie temperature controlled hyperthermia in the therapeutic range  $41\text{--}45^\circ\text{C}$  or, if needed, for thermal ablation of malignant tumors. Testing of the relative acute toxicity of the newly developed using the visible and infrared oscopy of chick embryos and the long term monitoring of behavioral and physiological parameters of exposed laboratory animals also shows the extremely low levels of acute and chronic toxicity of the nickel–copper (Ni–Cu) and silver doped lanthanum manganite ( $\text{Ag}_x\text{La}_{1-x}\text{MnO}_3$ ) nanoparticles.

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**Keywords:** cancer, magnetic hyperthermia, Curie temperature, super-paramagnetic nanoparticles, therapeutic window

**QUALITATIVE EXPLANATION OF IRRADIATED SILICON  
ELECTRICAL CONDUCTIVITY: FORMATION  
OF NANOSIZED CORE-SHELL STRUCTURES**

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A qualitative model of the silicon electrical conductivity of semiconductors irradiated with sufficiently high-energy particles is constructed.

At certain conditions (irradiation temperature and dose, and subsequent thermal treatment), high-energy particles fluence, in addition to primary and secondary point radiation defects, forms a number of nano-sized disordered regions, highly conductive (“metallic”) compared to the semiconductor matrix. Their high total volume fraction can lead to the charge major carriers’ effective Hall mobility significantly exceeding that of the matrix. Due to elastic stresses created by these disordered inclusions, a high concentration of point radiation defects tends to form defective shells. In certain temperature ranges, such nanosized core-shell structures act as capacitors storing the electric charge sufficient for the Coulomb blockade of the major current carriers. Transformation of high-conductive inclusions into low-conductive (“dielectric”) ones manifests in a noticeable decrease in effective Hall mobility.

The proposed model qualitatively explains all the experimental data available on single-crystalline n- and p-type silicon irradiated with high-energy electrons and protons and isochronously annealed.

## PARTICLE BEAM CONTROL POSSIBILITIES WITH FIELD PROGRAMMABLE GATE ARRAY

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Field Programmable Gate Arrays (FPGA) has been widely used for CERN CMS HGCAL upgrade. FPGA is a type of configurable integrated circuit that can be repeatedly programmed after manufacturing. FPGAs are a subset of logic devices referred to as Programmable Logic Devices (PLDs). They consist of an array of programmable logic blocks with a connecting grid, that can be configured “in the field” to interconnect with other logic blocks to perform various digital functions.

For reading out HGCAL, FPGA firmware was developed targeting the off-detector hardware. The firmware is responsible not only for the readout of the detector but also for its slow control and timing. To facilitate system maintenance, the firmware is optimized to handle all the different Front-End electronics configurations and data rates using a single – highly configurable – design.

In this paper possibilities of muon beam control is reviewed. The aim of the study is to detect cosmic muons with amplifier, record and control them with Amd Xilinx Zynq UltraScale + MPSoC board and Xilinx Vivado software. Also importance of p-n junction in the FPGA’s chip is discussed in this paper.

**Keywords:** FPGA, muon, particle beam

## ACUTE TOXICITY OF ZINC HYDROCARBONATE NANOPARTICLES AND CALCIUM HYDROPHOSPHATE NANOPARTICLES IN RAT MODEL

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The development and use of NanoParticles (NPs) with redox properties to correct stress conditions, microelement deficiencies, infertility, metabolic disorders in the body of animals, and especially the prooxidant-antioxidant system is a relevant topic. Inorganic NPs are becoming widely used in livestock farming due to their advantageous characteristics, such as low toxicity, high bioavailability, significant surface area compared to macroergs, and prolonged action [1, 2]. Various NPs have become a significant focus of research in animals. It should be noted that NPs containing zinc and calcium are characterized by small sizes and exhibit a wide range of properties due to increased digestibility in the gastrointestinal tract and the effect on target tissues of the body. However, the limitations of their widespread introduction into livestock and poultry farming are caused by the possible toxic effect, which is due to their physicochemical characteristics (route of administration, dosage, etc.) [2]. There are conflicting data on the toxicological parameters of NPs containing zinc and calcium on laboratory animals [3, 4], therefore the research of new nanostructured zinc, calcium materials are an urgent scientific task.

The purpose of this study was to assess the acute toxicities of zinc hydrocarbonate  $Zn_5(CO_3)(OH)_6$  and calcium hydrophosphate  $CaHPO_4 \cdot nH_2O$  NPs created by means of new synthetic methods in a rat model. Determination of the main parameters of acute toxicity of NPs was carried out under the conditions of intragastric administration to white rats of both sexes. Shown, that the introduction of NPs to animals of both sexes and during the entire observation period (14 days), no signs of intoxication or deviations in the state of health, behavior, or appearance of the experimental animals were recorded. Integral indicators, such as body weight in dynamics and weight coefficients of internal organs, did not undergo statistical changes.

The acute toxicity criteria indicate that hydrosols of zinc hydrocarbonate and calcium hydrophosphate NPs are virtually non-toxic substances and can be utilized in veterinary medicine as intended.

### Acknowledgment

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**Keywords:** hydrosol of nanoparticles, calcium hydrophosphate, zinc hydrocarbonate, acute toxicity



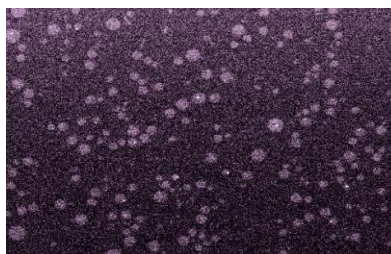
## APPLICATION OF TITANIUM DIOXIDE NANOPARTICLES AS EFFICIENT CONTRAST AGENT IN NANOMEDICINE

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Light scattering is a phenomenon where particles in its path deflect light. When light interacts with NanoParticles (NPs), the scattering behavior depends on the size, shape, and composition of the NPs and the wavelength of the light [1]. This occurrence has significant implications for the development and application of NPs in medicine. Due to their high scattering of visible and Near-Infrared (NIR) light, facile manufacturing, and chemical stability, titanium dioxide nanoparticles (TiO<sub>2</sub>NPs) have applications in tissue restoration, tissue visualization, intelligent drug delivery, and wound healing [2].



**Figure 1.** Distribution of TiO<sub>2</sub>NPs around the eukaryotic cells, resulting in enhancements of their visualization. Image was captured in the NIR spectrum.

In this work, we used TiO<sub>2</sub>NPs as a contrast agent to significantly improve the resolution of eukaryotic cells. We conducted experiments on plant and animal cells, including the mammalian healthy and cancerous cells. In the case of plant cells, the TiO<sub>2</sub>NPs were distributed around the damaged cells, and regarding the mammalian cells, the TiO<sub>2</sub>NPs were arranged around the cancer cells. This phenomenon can be explained by the circumstances in which the outer membrane of the lipid layers is destroyed for damaged cells, which leads to the emergence of free radicals and non-uniform distribution of the membrane's electrostatic field. Accordingly, the TiO<sub>2</sub>NPs, which have a plasmonic electron distribution, easily interact with cell membrane fields, leading to the arrangement of titanium nanoparticles around said cells. As a result, sharp contrast images were obtained around eukaryotic cells, caused by the appropriate arrangement of nanoparticles, **Figure 1**. Because the TiO<sub>2</sub>NPs significantly scatter light in the NIR region of the optical spectrum, having high penetration in the tissues, the experiments have been carried out in the 700–850 nm ranges. The proposed method can be used in biomedical applications as the contrast agents in tissues and as drug delivery systems to the body because they can precisely find diseased cells and carry the drugs to them.

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**Keywords:** titanium dioxide nanoparticles, light scattering, eukaryotic cells, nanomedicine

## PHOTOCATALYSIS EFFECT-BASED OPTICAL INFORMATION RECORDING ON LUMINESCENT DYE-DOPED TiO<sub>2</sub> NANOCOMPOSITE

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Photocatalysis includes reactions that take place by utilizing light and a semiconductor. Because of its unique features, TiO<sub>2</sub> can be called the best semiconductor photocatalyst [1]. TiO<sub>2</sub> NanoParticles (NPs) are widely used in photocatalysis to decompose organic pollutants. This effect can degrade the luminescent dyes, as well. In this work, we prepared a NanoComposite (NC) consisting of a polymer matrix doped with TiO<sub>2</sub> NPs, and Luminescent Dyes (LDs) and, using an effect of photocatalysis, recorded a high density of optical information. In experiments the next initial substances were utilized: PolyVinyl Alcohol (PVA), a colloidal monodispersed TiO<sub>2</sub> NPs with an average size of 40nm, and the LD Rhodamin 6G. To obtain a TiO<sub>2</sub>/RG6/PVA NC, an initial PVA was dissolved in colloidal monodispersed TiO<sub>2</sub> NPs in 5 mg/mL proportion and stirred at 600 rpm for at least 3 h at room temperature. The resulting solution was doped with a luminescent dye of Rhodamin 6G with the concentration ratio by weight: 99.98% NC+0.02%RG6. Then, the prepared NC was deposited by drop coating on the surface treated with deionized water.

The coated NC film on substrates was stored for 24 h at room temperature, and then the solvent was removed by heating in a bake oven at 70°C for 2 h. At the end of all procedures and solvent evacuation, a uniform layer of NC with 20 μm thickness has been obtained. The NC film was irradiated with a laser light source at λ = 532 nm. The light intensity of the laser beam at the sample was 50 mW/cm<sup>2</sup> and the exposure time was 2 min, respectively.

Using an inverse grayscale photomask a photo recording procedure was implemented. As a result, high-density optical information, as gratings, was recorded (**Figure 1**). The proposed NC film is promising for the production of mechanically flexible, environment-friendly, lightweight, large-area optical devices that can be fabricated by room-temperature solution processing, which has great potential for the development of high-performing optically gated photonic devices, anti-counterfeiting, identification, and traceability of goods for security, as well as light-controlled molecular and fluorescent switches.



**Figure 1.** Optically recorded grating on NC.

### Acknowledgment

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**Keywords:** titanium dioxide, nanocomposite, luminescent dye, photocatalysis, optical information

## AMBIENT TEMPERATURE-CONTROLLED CHOLESTERIC LIQUID CRYSTAL MIRROR-BASED SMART WINDOW

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Dynamic and intelligent regulation of solar radiation intensity penetrating buildings is a big challenge due to the global warming and climate change that modern civilization faces. The incoming solar radiation intensity within the visible and infrared range of the optical spectrum can be adjusted using smart windows [1].



**Figure 1.** Temperature-dependent color change of CLC-based smart window at variable ambient temperatures.

In this work, we demonstrate the prototype of a smart window, the operation principle of which is based on the thermo-optic properties of the Cholesteric Liquid Crystals (CLC). Due to the polymer-free design, the fabricated smart window is transparent, reflecting certain portions of visible or infrared light without needing an external power source, making it easier to install and exploit. Besides, it can intelligently respond to the environmental temperature to independently rearrange a light reflection, which can be adjusted to daylight time and climate regions (**Figure 1**). Unlike now existing or developing smart windows, our smart window reflects solar radiation, does not heat itself, and does not act as a heat-emitting and heat-transferring source. The proposed technology of the CLC mirror-based smart window will reduce consumed energy costs by reflecting out excessive sunlight and heat transfer, increasing the comfort for occupants within the buildings and homes.

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**Keywords:** smart windows, cholesteric liquid crystals, temperature controlled, light reflection

# MOLECULAR ASSEMBLIES OF CYANINE DYES: FLUORESCENCE ENHANCEMENT AND STABILITY IMPROVEMENT BY PLASMON NANOPARTICLES

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Molecular aggregates of cyanine dyes are essentially low-dimensional molecular crystals exhibiting unique excitonic properties. Unlike their larger counterparts, the excitonic behavior of J-aggregates can be relatively easily tuned and manipulated. These remarkable characteristics enable J-aggregates to be widely employed in diverse fields, including photonics, sensing technologies, photovoltaics, and biological applications. However, their long-term stability and suitability for real-world applications remain crucial considerations.

Typically, in polymer films, the fluorescence of J-aggregates is significantly quenched. However, this fluorescence can be enhanced through exciton-plasmon interactions, which arise from the coupling of excitons with the local electromagnetic field of nanoparticles. The extent of plasmon enhancement is influenced by several parameters, such as the chemical composition, size, and morphology of the nanostructures, as well as the spatial separation between the nanostructures and the fluorophore molecules.

In this particular study, the fluorescence of carbocyanine dye J-aggregates was amplified by strategically positioning them at a specific distance from a layer of gold nanoparticles. To further bolster the stability of the J-aggregates, the samples were coated with a thin metallic film composed of 20 nm of gold and 3 nm of titanium, deposited using a thermal and electron beam evaporation system [1]. The experimental results demonstrated that all samples maintained robust and stable fluorescence even after a period of one month, indicating a significant enhancement in the stability of the solid samples. This innovative approach holds great promise for the practical application of J-aggregates in photonic devices, particularly in thin-film configurations.

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**Keywords:** J-aggregate, exciton, plasmon, thiacyanocyanine dye, fluorescence

## ELECTROSPINNING OF PVP/PMMA NANOFIBERS WITH INCORPORATED SILVER NANOPARTICLES

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Electrospun nanofibers incorporated with various biological compounds, drugs, and nanoparticles have a broad spectrum of promising applications in nanomedicine [1]. Blending polymers formed by biopolymers, natural polymers, and synthetic polymers have improved characteristics of nanofibers such as mechanical properties and biocompatibility. In this work, a new approach of nanofiber preparation with incorporated silver NanoParticles (AgNPs) using a blend of hydrophilic PolyVinylPyrrolidone (PVP) and hydrophobic polymethyl methacrylate (PMMA) is proposed.

In obtained nanofibers, PMMA provides the mechanical strength of the nanofibers and can facilitate the gradual release of antimicrobial agents. This approach is based on using a water-soluble PVP as a capping and stabilizing agent for AgNP formation in an aqueous medium, drying, and then mixing with PMMA in an organic solvent. The PVP surrounding the AgNPs facilitates their incorporation into PMMA and then provides access to water molecules when the nanofiber mat is soaked in an aqueous solution. The absorption peak position of the plasmon resonance band in the UV-vis spectrum was used to determine the average nanoparticle diameter and estimate the influence of the polymer environment. The average nanoparticle diameter determined by the position of the absorption peak of the SPR band in the UV-vis spectrum is 35-40 nm. The diameter of the nanofibers is determined to be in the range of 2-4  $\mu\text{m}$ . The release of antimicrobial agents from nanofiber mat by soaking them in water was monitored by absorption spectroscopy.

Although the appearance of AgNPs in water from the obtained polymeric nanofibers was not detected, nevertheless, the experiments with mat soaking in the oxidative solution showed that the nanopores in PMMA incorporated with AgNPs are open. This observation indicates the possibility of a gradual release of silver ions from such nanofibers. The proposed approach allows to preparation of nanofibers with the gradual release of silver ions from the robust PMMA environment. Thus, the membrane prepared from these nanofibers can provide simultaneously the quick and gradual release of two antimicrobial agents.

Nanofibers loaded with small molecular drugs and antimicrobial nanoparticles can be used in various biomedical fields, including the fabrication of effective wound dressing materials due to their similarity to the extracellular matrix and excellent protection from microorganisms, and can be used for drug delivery.

### Acknowledgment

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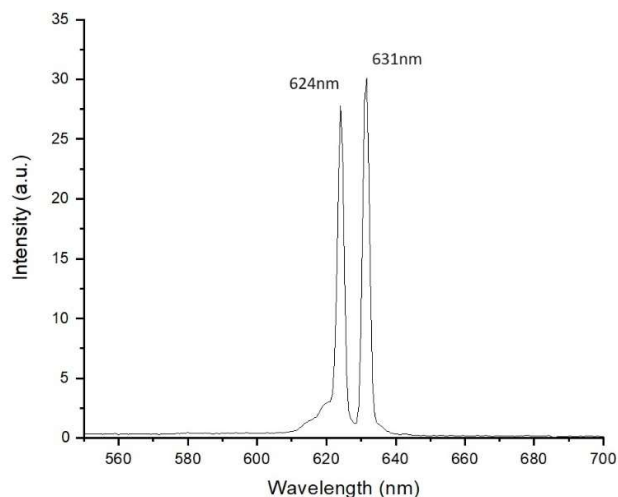
**Keywords:** electrospinning, nanofibers, polyvinylpyrrolidone, polymethyl methacrylate, antimicrobial agent

## DUAL-MODE LASING FROM POLYDOMAIN LIQUID CRYSTAL STRUCTURE

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A thin (12  $\mu\text{m}$ ) polydomain layer of a Dye-Doped Cholesteric Liquid Crystal (DD CLC) was obtained. Each domain is a periodic helical structure with the helical axis directed perpendicular to the plane of the layer. The entire layer is represented by domains of two types, which differ only in the helical pitch (period) of the structure: domains of the first type have a period of 356.3nm, and domains of the second type have a period of 353 nm, i.e. the difference between the periods is 3.3 nm and this difference is maintained over the entire area of the layer. Such high accuracy is ensured by the property of CLC structures with a nonequilibrium pitch to compress or stretch exactly half a spiral turn in order to fit between the bounding surfaces coated with an orienting polymer layer. We chose the equilibrium helical pitch of the CLC structure that could fit within the given layer thickness 12  $\mu\text{m}$  with equal probability either  $m$  times or  $m+0.5$  times, where  $m$  is an integer. Thus, two types of domains were formed with a difference of half a turn of the spiral.



**Figure 1.** Spectrum of laser emission from polydomain DD CLC structure consisting of two types of domains.

The goal of this work was to study the optical properties of such complex periodic nano-structures and, in particular, to obtain laser emission [1, 2] in them. It is shown that each domain exhibits lasing strictly in accordance with the domain period. Thus, lasing from the liquid crystal layer is observed at two wavelengths: 631nm and 624nm (Figure 1). The agreement between experimental data and theoretical calculations is shown.

### Acknowledgment

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**Keywords:** dye-doped cholesteric liquid crystals, laser emission, polydomain structure

## CHEMICAL AND THERMAL STABILITY OF InAs, InP AND THEIR ALLOYS

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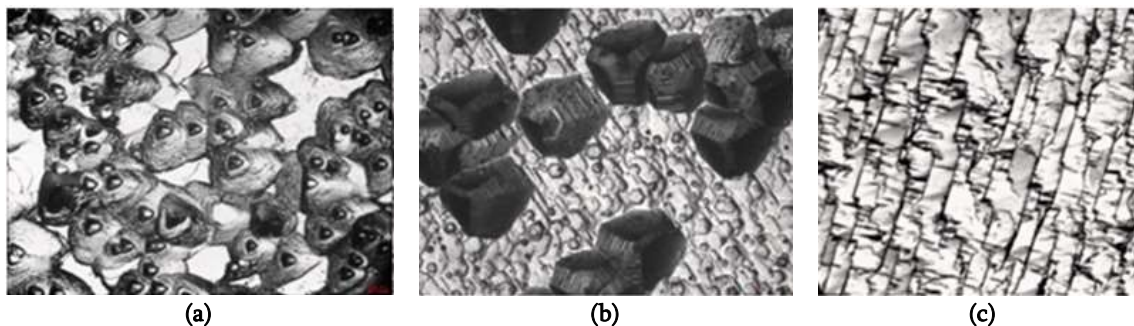
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Understanding the chemical and thermal stability of a material is an important aspect of materials' design and study, especially when it comes to decaying semiconductor materials as InAs, InP and the  $\text{InAs}_{1-x}\text{P}_x$  alloys.

In this connection powerful and robust technique of thermal-gravimetric and differential thermal analysis methods were used to explore thermal degradation reactions, phase transitions, thermal stability and suitability of these materials for determination of their application in the temperature range of 25–900°C. The presented data are also important for the development of technology of producing crystals of the InAsP alloys type. By accurately monitoring the weight of InAs, InP and  $\text{InAs}_{1-x}\text{P}_x$  solid solutions, while heating at a constant rate, it is possible to measure changes in their mass in the different stages of the heating process, and attribute the process to response of these materials to a thermal stress.

For protecting from oxidation at elevated temperatures, heating of InAs, InP and  $\text{InAs}_{1-x}\text{P}_x$  solid solutions has been carried out in air atmosphere under a protective layer of the unique flux of boron anhydride. Boron anhydride satisfies requirements of chemical stability up to the melting points of InAs, InP and  $\text{InAs}_{1-x}\text{P}_x$  (942–1062°C): the smaller density than for InAs and InP compounds, immiscibility with a melt of InAs and InP.



**Figure 1.** Dislocation structure of single crystals on (111) plane of (a) InAs, (b)  $\text{InAs}_{1-x}\text{P}_x$  and (c) InP with magnification of  $\times 250$ .

It was found that, unlike InAs and InP, InAsP alloys exhibit greater chemical and thermal stability when heated under boron anhydride. InAs-rich  $\text{InAs}_{0.70}\text{P}_{0.30}$  solid solution exhibits the highest stability. This result is all the more important, because  $\text{InAs}_{0.70}\text{P}_{0.30}$  alloy exhibits radiation stability. At the same time material retains the crystal structure without amorphous inclusions and metallic phases (Figure 1). The preservation of individuality of sublattices of InAs and InP in  $\text{InP}_x\text{As}_{1-x}$  alloys, has been revealed in other properties.

**Keywords:** alloys, semiconductor, thermal stability, single crystals, dislocation structure

## DEVELOPMENT OF GRAPHENE PRODUCTION TECHNOLOGY

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Graphene is one of the promising new materials needed for the further development of modern high technologies, the production and properties of which are still not completely clear. This is related to the peculiarities of its production technology and the unknown, unusual properties. Refining and modernizing the methods of obtaining this unique 21st century semiconductor material graphene, revealing its unknown properties and exploring new perspectives of its use are one of the most urgent problems for today's scientific community.

The purpose of the present work is to solve these problems partially and obtain mono- or multi-sheet graphene. For this, a number of tasks were worked out: development of an equipment based on the method of chemical deposition of graphite from the air phase; selection of the optimal one from hydrocarbons for pyrolysis by experiment; examining the obtained layers with an electron microscope and determining their composition. **Figure 1** shows experimental apparatus for producing typical layers of graphite on copper foil.



**Figure 1.** Experimental apparatus for producing typical layers of graphite on copper foil.

Using Energy Dispersive Spectroscopy (EDS) method of investigation of samples it has been established that:

- copper, carbon and oxygen, with a certain percentage composition, have been absorbed in all the experimentally obtained layers;
- carbon content in the investigated layers ranges from 10 to 12at.%, while the oxygen content varies in 1–3at.% range; and
- oxygen signal is caused by the copper oxide on the coating surface and partially the oxygen molecules adsorbed on the coated graphene surface.

**Keywords:** graphene, layers, copper, chemical deposition, hydrocarbon



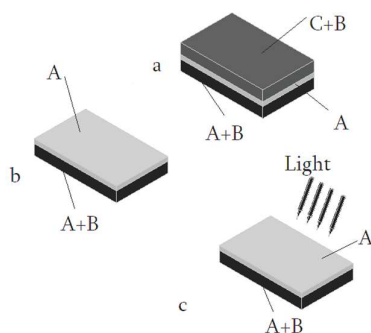
## NEW POSSIBILITIES FOR OBTAINING THIN FILMS

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Thin films are layers of any material that are deposited on a substrate or on already deposited layers and their thickness ranges from nanometers (monolayer) to several micrometers. The fantastic properties of thin films, which are not achieved, or unattainable for the material in bulk form, are directly related to the geometry of these films – nano-thickness and their two-dimensional structural forms. Due to the wide range of applications, it is difficult to find a field of activity where thin films are not presented. There are many ways (physical and chemical processes) to obtain thin films, but the main technological problems due to complexity of process remain unsolved: quality of the structure, incompatibility with the substrate, high cost, provision of an ultra-vacuum environment, low deposition rate, limitation of instant production, damage of the substrate, low efficiency of the yield product and others. Due to the increasing demands by modern technologies, it is necessary to develop such new technological principles of obtaining thin films, which are distinguished by easy practical use, price efficiency and high quality of layers. For this purpose, a new innovative technology of obtaining thin films was developed based on different solubility, density, atomic weight of atoms (gravity) of different elements. The periodic system of elements provides a wide choice of such substances. The essence of the idea is as follows. For obtaining of thin film of substance A, another material B have to be chosen in such a way, that these substances may form a two-component A–B solid solution. Then substance C have to be selected in which B dissolves well, but substance A does not dissolve.

First under optimal temperature conditions C will be deposited (**Figure 1a**) on the surface of the A–B solid solution. Then, by selecting the temperature regime, component B of the solid solution will diffuse into the molten substance C, while the other component A will not dissolve in it and will be located between the surface of the solid solution A–B and the layer of C.



**Figure 1.** Principle scheme for thin films obtaining route: (a) initial and (b) final steps, and (c) application in semiconductor technologies

The selection of the composition and conditions of the chemical etching solution ensure the removal of the C with dissolved in it component B from the surface of the remaining substance A placed on it (**Figure 1b**). The method ensures implementation of both low and high temperature processes. The presented new method of obtaining thin films is particularly attractive to electronics, whose devices' continuous miniaturization and cost reduction with maintaining high reliability are provided by this principle.

**Keywords:** micrometer, thin films, substrate, solid solution, etching

## PRODUCING OF SILICON FROM RACHA (GEORGIA) QUARTZ DEPOSITION

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Silicon technology has had a huge impact on the world economy, as it is the driving force for the development of electronics and accordingly the economy of any country. Currently, silicon has no competitor in electronics technology, and it will remain dominant in future technologies for a long time. Silicon is the unique material that follows closely to the new requirements of electronics, which are: the continuous reduction of the size of the elements, the increase of their switching speed and the reduction of the consumed energy, etc. An exponential increase in chip memory density and processor speed, and a decrease in cost are closely connected with the advances in silicon technology. Silicon is also non-competitive for application in many other industries (98% of total silicon goes mainly to producing metallurgical silicon). Therefore, the refinement of silicon production technology is still an urgent issue for the development of the country's economy.

In the multi-stage long process of obtaining different grades of silicon, the purity of the primary source of silicon, a fundamental material silicon dioxide ( $\text{SiO}_2$ ) and its special properties are of decisive importance for obtaining the final product – electronic silicon. High level of purity of electronic silicon is necessary for various applications in the electronics industry and other high-tech sectors, because even minute levels of impurities can drastically affect performance [1].

As is known not all silicon dioxide ores are suitable for electronic purity silicon production [2]. High purity silicon dioxide requires specialized processing and is an invisible cornerstone of modern silicon technology. High purity silicon dioxide is  $\text{SiO}_2$ , in its purest form with minimal contamination in crystalline or amorphous form that does not contain other substances at the microscopic level. The highest level of purity is desired to obtain ultra-high-purity silicon for the electronics industry and other high-tech industries.

We started our research by selecting high purity  $\text{SiO}_2$  and studying its properties. The quartz veins developed in the geological structure of the terrain of Georgia play an important role. Most of them are alpine type quartz veins. From the well-known alpine type quartz veins, quartzite from the Shoda–Kedela range (Oni–Ghebi district) was used in the presented work. Silica extraction processes included crushing, grinding, chemical and physical properties, namely chemical composition, thermal analysis, density and others.  $\text{MGSi}$  was obtained by reducing  $\text{SiO}_2$  in the form of sand or quartz by reaction with carbon (coke) in electric arc furnaces at a temperature of  $\sim 1800^\circ\text{C}$ . The chemical and physical properties of the obtained samples have been studied and the advantage of using Racha silicon dioxide in silicon technology compared to other ores has been determined.

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**Keywords:** electronics, silicon dioxide, reduction, thermal analysis, purity

## REPULSION DRIVEN METALLIC PHASES IN ONE-DIMENSIONAL HALF-FILLED FERMION SYSTEMS

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An unusual metallic phase is argued to develop in the one-dimensional ionic Hubbard model, at half-filling and zero magnetization, at intermediate electron–electron repulsion  $U$  when second-neighbors hopping is allowed and tuned close to a topological Lifshitz transition (connected with a change of the Fermi surface in the noninteracting system). The metallic state lies between a band insulator phase at low repulsion and a correlated (Mott-like) insulator phase at high repulsion.

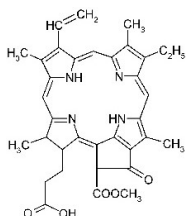
In approaching the latter, the model supports short-range antiferromagnetic order and spontaneous dimerization of both bond charge and nearest-neighbor antiferromagnetic correlations. A combination of mean-field and effective-field theory (bosonization) provides an analytical understanding of the physical processes underlying the argued phase transitions. The ground and low-energy excited states of finite-length chains are explored by Density-Matrix Renormalization-Group (DMRG) calculations, providing numerical evidence for the intermediate gapless phase. Such finite systems are attainable by cold atoms in optical lattices for a wide range of the parameter  $U$ .

## BINDING OF PHEOPHORBIDE-*a* AND ITS DERIVATIVES TO BIOPOLYMERS

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Pheophorbide-*a* (Pheo-*a*, **Figure 1**) is a natural anionic chlorophyll *a* catabolite characterized by the chlorine-type visible absorption spectrum with high molar extinction coefficient in the red region where the transparency of the tissues to the light increases considerably. It is selectively accumulated in the tumor cells and actively generates singlet oxygen when irradiated with red light that determines its strong PhotoDynamic Therapy (PDT) effect on the cancer cells *in vitro* and *in vivo*. Pheo-*a* also can be also applied for the molecular recognition of G-quadruplexes. Since the dimerization and aggregation of the dye in aqueous solutions substantially reduce its photodynamic activity, the peculiarities of the structure and physical properties of complexes formed by Pheo-*a* and its derivatives with different biological macromolecules found in the blood and body tissue cells are of great interest being subject of intensive study for last many years.



**Figure 1.** Molecular structure of pheophorbide-*a*.

Results of a comprehensive spectroscopic study on binding of Pheo-*a*, its cationic (CatPheo-*a*) and neutral (MePheo-*a*) derivatives, as well as Pheo-*a* conjugate with cationic intercalative aminophenazinium dye linked via polymethylene chain (Pheo-Pzn) to inorganic polyphosphate (poly(P)), poly-L-lysine (PLL) and nucleic acids of various primary and secondary structures (*ds*-poly(A)·poly(U), *ds*-poly(G)·poly(C), *fs*-poly(G), antiparallel telomeric DNA quadruplex Tel22) in solutions of low (1 mM Na<sup>+</sup>) and near-physiological (0.15 M Na<sup>+</sup>) ionic strengths [1 – 6] are summarized. Investigations were carried out in a wide range of P/D ratios using techniques of absorption, polarized fluorescence, fluorimetric titration, absorption and fluorescence melting, and resonance light scattering. Types of the dyes binding to the biopolymers and the features of their aggregation were established. As much as Pheo-Pzn discriminates between duplex and quadruplex polynucleotides exhibiting 50-fold emission increase upon binding to quadruplex poly(G) and quenched fluorescence in the case of *ds*-polymers, it is proposed as efficient fluorescent probe for the recognition of G-quadruplex structures.

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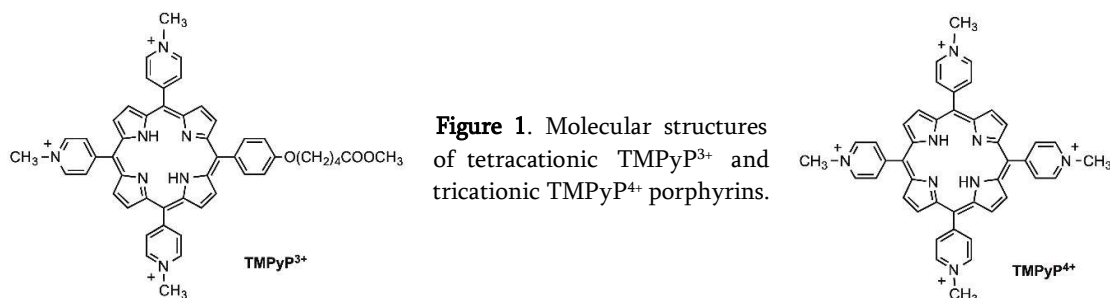
**Keywords:** pheophorbide-*a*, polynucleotide, binding, fluorescence, absorption, melting, light scattering

# BINDING OF TWO CATIONIC PORPHYRINS TO *DS*-POLYNUCLEOTIDES

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The porphyrins are macrocyclic compounds with unique spectroscopic and photophysical properties and a high biological activity. They are widely used as probes for the structure and dynamics of nucleic acids, as photosensitizers in anticancer photodynamic therapy, anti-viral and antimicrobial agents, as a carrier of antisense oligonucleotides for their delivery, stabilizers of G-quadruplexes. Dependence of the spectroscopic changes in the absorption and fluorescence spectra of TMPyP<sup>4+</sup> and TMPyP<sup>3+</sup> porphyrins (**Figure 1** and **Table 1**) resulting from their binding to double-stranded DNA (B-form) and RNA (A-form) polynucleotides, as well as to DNA-RNA hybrids (A-form) on the biopolymer base composition and spatial structure are summarized by comparing our [1, 2] and literature data.



**Table 1.** Fluorescence intensity changes upon binding of TMPyP<sup>3+</sup> and TMPyP<sup>4+</sup> porphyrins to *ds*-polynucleotides at near-stoichiometric on charge binding ratio.

Fluorescence enhancement	Fluorescence quenching
TMPyP <sup>3+</sup> + poly(A)·poly(U)	TMPyP <sup>3+</sup> + poly(G)·poly(C)
TMPyP <sup>4+</sup> + poly(A)·poly(U)	–
TMPyP <sup>4+</sup> + poly(dA)·poly(dT)	TMPyP <sup>4+</sup> + poly(dG)·poly(dC)

The porphyrins bind effectively to the biopolymers via two binding modes, which manifest themselves at low and high *P/D* ratios correspondingly. It was established that TMPyP<sup>4+</sup> and TMPyP<sup>3+</sup> discriminate between polynucleotide duplexes containing A·U (A·T) and G·C base pairs at low *P/D* ratios resulting in the porphyrin emission enhancement in the first case, and its quenching in the last case. It was shown that in contrast to TMPyP<sup>4+</sup>, large bathochromic shift of the TMPyP<sup>3+</sup> Soret band at high *P/D* is observed for all these polynucleotides regardless of their base composition and type of the helical structure. The features of the porphyrin aggregation at a near-stoichiometric in charge phosphate-to-dye ratio were analyzed.

## Acknowledgments

Author acknowledges National Academy of Sciences of Ukraine for the financial support (Grant # 0123U100628); Wolfgang Pauli Institute (Vienna, Austria) for Pauli Postdoc research training scholarships “Data analysis in molecular biophysics” 2021/2022 and 2023/2024; and *Nanophotonics* journal, De Gruyter, Sciencewise Publishing, and the Optica Foundation for Ukraine Optics & Photonics Researcher Grant 2023.

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**Keywords:** cationic porphyrin, polynucleotide, binding, fluorescence, absorption, light scattering, aggregation

# DIRECT PRODUCTION OF CAST MULTICOMPONENT ALLOYS FROM OXIDE RAW MATERIALS BY CENTRIFUGAL SHS METALLURGY TECHNIQUE. CURRENT RESULTS AND PROSPECTIVE RESEARCH

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Starting from the first publications in 2004 and up to now, more and more attentions have been attracted by the topic of multicomponent alloys, which is also called High-Entropy Alloys (HEAs). Initially, HEAs were defined as alloys with an equiatomic composition consisting of at least 5 constituent elements. Later, the determination criteria for HEA were expanded and formulated as multicomponent alloys with component concentrations from 5 to 35at.%. It was assumed that, due to the high configurational entropy of mixing, the formation of disordered substitutional solid solutions in HEA would be more preferable than the formation of ordered phases (intermetallic) and, thus, the formed high-entropy solid solutions would have both high strength and sufficient plasticity. However, studies carried out somewhat later showed the absence of a clear correlation between the calculated values of the configurational entropy and the phase composition of the obtained experimental multicomponent alloys. It was found that the HEA phase composition is primarily determined not by the number of elements included in the composition, but by the characteristics of the atoms of these elements.

Extensive studies have shown and confirmed the outstanding mechanical properties of HEAs [1], such as high strength and toughness in a wide temperature range; great fatigue, irradiation, and corrosion resistance, which all make them potentially serve as structural materials with many applications [2].

Initially, traditional electrometallurgy methods melting and solidification were widely used to obtain HEAs: Vacuum Arc Melting (VAM), vacuum induction remelting (VIR), etc. In addition, in recent years begun to apply Powder Metallurgy (P/M), Mechanical Alloying (MA), laser cladding, electrochemical deposition and many other methods have been employed to prepare HEAs.

In this presentation, a general report will be made on the results of previously performed and currently ongoing research on the production of cast HEAs using centrifugal SHS metallurgy technique from oxide raw materials.

Systems based on transition metals, refractory metals, intermetallic alloys and the possibility of producing metal composites directly (in-situ) SHS (in combustion wave) will be considered. This method has previously proven its effectiveness in the production of high-temperature alloys based on Co, Ni, Nb and intermetallic alloys, and for the first time in world practice, the author used it in 2016 to produce cast HEAs [3].

## Acknowledgment

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**Keywords:** self-propagating high-temperature synthesis (SHS), cast alloys, multicomponent alloys, high-entropy alloys (HEA), high-temperature composite materials, SHS metallurgy, oxide fiber/HEA composites

**CENTRIFUGAL SHS-METALLURGY OF CAST HIGH-ENTROPY  
ALLOYS STRENGTHENED BY STRUCTURAL PRECIPITATIONS  
BASED ON BORIDES AND SILICIDES Mo AND Nb**

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A promising approach to the development of advanced metallic materials is based on a fundamentally new concept of avoiding the use of the main component but mixing several metal elements simultaneously. Such multicomponent alloys are called High-Entropy Alloys (HEAs) [1, 2], the most studied of which is the Co–Cr–Fe–Ni–Mn alloy with attractive mechanical properties. The single-phase fcc structure is stable in this alloy, which allows it to be used as a “model” high-entropy alloy or a single-phase multicomponent solid solution.

This paper is the first to experimentally evaluate the possibility of synthesizing strengthened high-entropy alloys with the basic system (Co–Cr–Fe–Ni–Mn) and strengthening precipitates based on borides and silicides of refractory metals (Mo and Nb), formed in situ during the combustion of thermite-type SHS systems [3, 4]. The microstructural analysis of the synthesized Ni–Cr–Co–Fe–Mn alloys with the complex modifying Mo(Nb)–Si–B additive showed that, at a higher content of the additive, the microstructure of the synthesis products exhibits the high-entropy alloy matrix and precipitates of new structural elements based on borides and silicides of refractory metals (Mo and Nb). The morphology and concentration of such precipitates depends on the concentration of the additive in the green mixture. The strengthening precipitates are of endogenous origin as they are formed in situ during SHS and are the result of chemical reactions occurring both directly in the combustion wave and during cooling of the high-temperature melt of the synthesis products. Control of SHS processes opens up new possibilities for the formation of metal-matrix composites based on high-entropy alloys.

#### **Acknowledgment**

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**Keywords:** high-entropy alloys (HEAs), cast high-entropy alloys, self-propagating high-temperature synthesis (SHS), SHS metallurgy, thermite-type SHS systems, synthesis of multicomponent alloys, modifying additives, HEA-based materials

## EPR SPECTROSCOPIC STUDIES OF HEXAGONAL BORON NITRIDE

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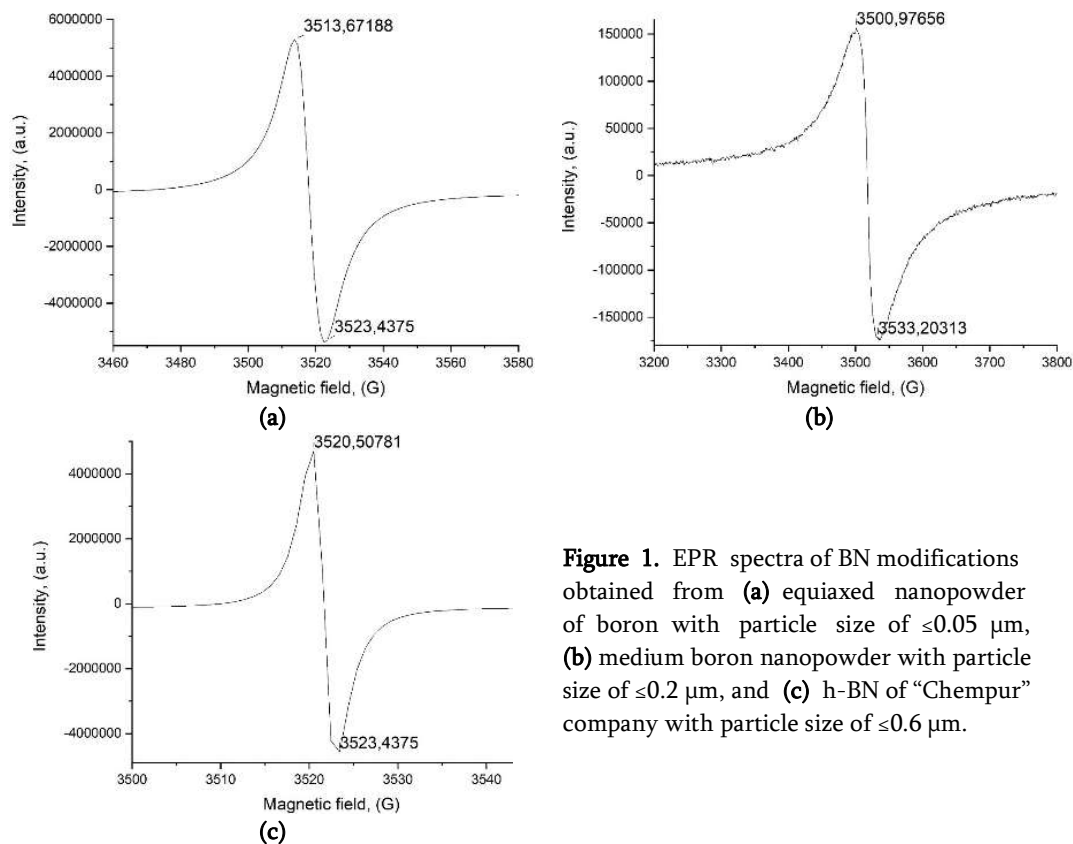
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Hexagonal boron nitride (h-BN) nanopowders prepared in a high-flux optical furnace under effect of concentrated light in a flow of nitrogen were comparatively studied with commercial nanopowder. The resulting powders were of high purity. The methods of X-ray diffraction study, TEM, SEM, FTIR spectrometer and Raman scattering were applied to investigate the complicated structure and phase diversity of the nano powder's composition.



**Figure 1.** EPR spectra of BN modifications obtained from (a) equiaxed nanopowder of boron with particle size of  $\leq 0.05 \mu\text{m}$ , (b) medium boron nanopowder with particle size of  $\leq 0.2 \mu\text{m}$ , and (c) h-BN of “Chempur” company with particle size of  $\leq 0.6 \mu\text{m}$ .

EPR has also been used to investigate h-BN nanopowders. Paramagnetic centers in h-BN have been studied, providing insights on the material's defect structure transformation. The EPR spectra of BN have been measured at room temperature. EPR spectra of BN nanopowders obtained from different synthesis methods have been



compared. The spectra show a common feature of a resonance with  $g = 2.003 \pm 0.001$ . The EPR spectra of boron nitride modifications obtained from equiaxed nanopowder of boron of a particle size  $\leq 0.05 \mu\text{m}$ , medium boron nanopowder of a particle size  $\leq 0.2 \mu\text{m}$ , and boron nitride from the “Chempur” company of a particles size  $\leq 0.6 \mu\text{m}$  do not exhibit hyperfine structure (**Figure 1**). All studied samples demonstrate a single Gaussian resonance line with  $g$ -values of 2.0058, 2.0047, and 2.0075, respectively. The deviation of the  $g$ -factor from the pure spin value ( $g = 2.0023$ ) is a result of spin-orbit interaction or structural defects. The orbital moment creates a certain local magnetic field at the location of unpaired electrons, thereby changing the magnitude of the resonance field.

EPR studies have provided valuable insights into the defects and paramagnetic centers in boron nitride (BN) materials, which are crucial for understanding their physical properties and potential technological applications.

### **Acknowledgments**

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**Keywords:** hexagonal boron nitride, nanopowders, electron paramagnetic resonance, structure, phase composition

## OPTIMIZATION OF PROPERTIES OF GEOPOLYMER MATERIALS USING ACTIVATED FLY ASH

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Concrete production is associated with high energy costs and greenhouse gas emissions, which have a negative impact on the planet's ecosystem [1, 2]. Replacing ordinary Portland cement (OPC) with geopolymer materials (GPM) makes it possible to significantly reduce this impact. Geopolymers are inorganic materials of polymer structure formed as a result of alkaline or acid activation of thermally treated aluminosilicates (kaolins, clays, ashes and slags). Another advantage of geopolymer materials over Portland cement is that various production wastes are mainly utilized in the production of geopolymers.

Fly ash is a by-product of the coal combustion process in coal-fired power plants, consisting of small particles emitted from the boiler with flue gases. The main hydration products of geopolymer materials are tobermorite-like low-basic calcium hydrosilicates and alkaline calcium hydroaluminosilicates in the form of C-S-H and N-A-S-H gels, which determines their high mechanical strength. N-A-S-H is a cementitious geopolymer product of alkaline activation of ash. Fly ash is successfully used in the production of geopolymer materials.

**Table 1.** Chemical composition of fly ash (wt.%).

LOI	SiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	TiO <sub>2</sub>	P <sub>2</sub> O <sub>5</sub>	Fe <sub>2</sub> O <sub>3</sub>	Mn <sub>2</sub> O <sub>3</sub>	CaO	MgO	SO <sub>3</sub>	Na <sub>2</sub> O	K <sub>2</sub> O
1.47	52.14	31.59	1.32	0.05	5.17	0.04	0.69	0.74	0.07	0.99	0.29

In Georgia, there are large accumulations of fly ash, which pollute the environment and are still practically not used anywhere. Work has been carried out to study the possibility of using Georgian ashes in the production of geopolymer materials using fly ash from the Kutaisi Thermal Power Plant [3]. The chemical composition of fly ash from the Kutaisi Thermal Power Plant is presented in **Table 1**.

This ash is characterized by low activity, as it was buried in the ground for several decades, due to which it became wet, aggregated and the glassy (active) component partially crystallized.

The aim of this work is to optimize the properties of GPM using different fly ash activation approaches, which will make it possible to improve the technological parameters of the binder.

### Acknowledgments

The authors are grateful to Mr. Gia Natcvlishvili and Mr. Zurab Chinchaladze for providing materials and assistance in research.

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**Keywords:** geopolymer material (GPM), ordinary Portland cement (OPC), fly ash

# STUDY OF POSSIBILITY OF REGULATING PARAMETERS OF METAKAOLIN SYNTHESIS USING CLAY ROCKS OF GEORGIA

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Metakaolin is in great demand worldwide as a highly active pozzolanic additive to Portland cement. The use of metakaolin helps to increase the density, water resistance and mechanical strength of Portland cement, which makes it possible to reduce the consumption of clinker – the most energy-intensive and expensive component of cement/concrete.

Metakaolin is usually obtained by thermal processing of kaolin clays at a temperature of 650–850°C [1]. Kaolin clay reserves in the world are strictly limited. Kaolin clays have not been identified in Georgia. However, there are kaolinized clays, which are distinguished by a lower  $Al_2O_3$  content compared to kaolin clays.

The main minerals of kaolinized clay are: kaolinite –  $2SiO \cdot Al_2O_3 \cdot 2H_2O$ , the rest is quartz, mica and feldspars. At a temperature of 500–800°C it loses 14% of water and turns into metakaolin:  $2SiO_2 \cdot Al_2O_3$  [2]. In the process of cement hydration, new phases are formed during the interaction of clinker minerals and metakaolin: calcium hydrosilicates (C–S–H), calcium hydroaluminates ( $C_2AH_8$ ,  $C_4AH_{13}$ ,  $C_3AH_6$ ), calcium hydrogarnets ( $C_3ASH_4$ ) and a highly active mineral – stratlingite  $C_2ASH_8$ , which give the cement additional strength.

Previously conducted studies have proven the feasibility of thermal modification of Georgian polymineral clays and pozzolanic additives have been obtained based on them [3].

**Table 1.** Chemical compositions of kaolinized clays of Georgia.

#	LOI	SiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	TiO <sub>2</sub>	Fe <sub>2</sub> O <sub>3</sub>	CaO	MgO	SO <sub>3</sub>	Na <sub>2</sub> O	K <sub>2</sub> O
1	8.88	58.10	22.63	0.17	3.23	2.57	0.86	0.20	1.46	1.00
2	7.99	58.33	23.27	0.11	4.57	1.43	0.97	0.32	0.51	2.00
3	8.14	56.50	27.80	0.71	1.14	0.50	0.21	0.70	2.00	2.10

The aim of this work is to study the possibility of obtaining a highly active pozzolanic additive – metakaolin based on kaolinized clays of Georgia and to regulate the parameters of their synthesis. **Table 1** presents the chemical compositions of kaolinized clays of Georgia.

Based on the results of the research, it was found that thermal treatment of kaolinized clay makes it possible to obtain an effective pozzolanic additive to cement.

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**Keywords:** metakaolin, pozzolanic additive, kaolinized clay, fly ash

## STUDY OF THERMAL CONDUCTIVITY OF EPOXY COMPOSITES MODIFIED WITH NANOFILLER

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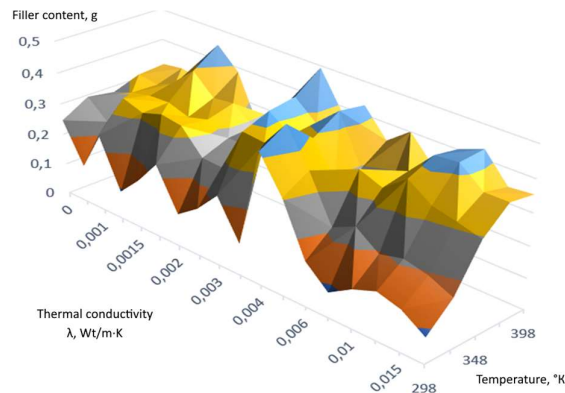
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Composite materials based on thermosetting polymers are widely used in all industries to protect equipment from environmental influences due to a set of physical, mechanical, and operational characteristics. The development of coatings for thermophysical applications using composites based on cold-curing epoxy binders for flat heating elements is relevant. This class of materials is technologically feasible for the formation of coatings on long-dimensional surfaces of complex profiles at room temperatures without the use of complex equipment. An example is the formation of electric heaters on the back side of large-diameter parabolic antennas. Their use will enable reliable operation under various climatic conditions, especially when the working surfaces of the product are iced over during long-term idle operation.



**Figure 1.** Dependence of thermal conductivity of nanoepoxy composite on filler content and temperature.

The paper investigates the effect of modifying an epoxy oligomer with nanoparticles on the thermal conductivity and heat resistance of materials. A mixture of nanopowders in the following ratio was used as a filler: 80%Si<sub>3</sub>N<sub>4</sub>+5%Y<sub>2</sub>O<sub>3</sub>+5%Al<sub>2</sub>O<sub>3</sub>+10%B<sub>4</sub>C. The powders were synthesized at the Institute for Problems of Materials Science of the National Academy of Sciences of Ukraine. The analysis of the experimental studies (**Figure 1**) has shown that filling the epoxy oligomer with nanoparticles at concentrations of 0.001–0.020% allows for a wide range of control over the thermal conductivity of materials. The results of thermal conductivity studies have proved the influence of nanoparticles on the thermal properties of epoxy composites. It was found that at a ratio of components in the range of 0.003–0.004 g of nanofiller per 100 g of binder, the thermal conductivity ( $\lambda$ ) of materials increases by 1.3–1.7 times in the temperature range of 298–398 K compared to the unfilled matrix. This parameter is  $\lambda = 0.306\text{--}0.416$  W/m·K. For materials with an optimal ratio of components, the Martens heat resistance is  $T = 398\text{--}399$  K (for an unfilled matrix,  $T = 384$  K). It should be noted that at concentrations of 0.0005–0.02 g of nanofiller per 100 g of binder, the thermal conductivity (except for the optimal ratio of 0.003–0.004 g) is lower than for the unfilled binder. Studies of the complex effect of nanofillers and force fields on the properties of epoxy composites are promising.

**Keywords:** polymers, thermoset, heat resistance, thermophysical properties, binder, nanoparticles

## INELASTIC ELECTRON INTERACTION WITH MOLECULAR COMPONENTS OF NUCLEIC ACIDS

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Paper presents the results of a complex study of the physical processes and corresponding structural changes initiated in the molecular components of nucleic acids by slow electrons with energies from 0.1 eV to tens of eV. A new approach to the study of the influence of low-impact factors on biological systems is proposed. It is based on the development of methods for obtaining biomolecules in an isolated (gaseous) state, the formation of molecular beams, and the implementation of the method of crossed electron-molecular beams.

The experiments were performed under the following conditions: the electron beam current was  $7 \cdot 10^{-5}$  A and the electron energy and an FWHM energy spread of  $E_{1/2}$  was  $\sim 0.4$  eV. The pressure of the residual gases in the chamber was equal to  $\sim 1 \cdot 10^{-5}$  Pa. The cell was heated up to the temperature of 430 K in order to avoid the condensation of vapors on the windows and electrodes of the electron gun. The methods of experiments are described in detail in [1, 2].

The physical processes in nucleic acid bases under electron impact are investigated. The radiation spectra of cytosine, thymine, uracil, adenine and guanine in the wavelength region from 200 to 500 nm for the different energies of incident electrons are obtained. Complicated nature of the spectra shows the simultaneous passage of several physical processes, including dissociative excitation and excitation of the ionized fragments of the nucleobase molecules.

To identification of spectral bands the excitation functions of biomolecules are investigated, mass spectrometry analysis of the bases are performed, semi-empirical quantum-chemical calculations of parameters of structure are conducted. It is also reasonable to compare the optical spectrum of molecules with its mass-spectrum.

Mass-spectra of molecules are investigated at electron energy 95 eV. It has been experimentally studied out that considerable amount of molecular fragments formed in biostructures under the influence of slow electrons. For example guanine,  $C_5H_5N_5O$ ,  $C_5H_3N_5O$ ,  $C_5H_4N_5O$ ,  $C_4H_3N_3O$ , CHO,  $CH_2N_2$ , CHNO,  $C_2H_3N_3$  and  $CH_2N_2$ . The most intensive lines of mass spectra correspond to molecular ions and also for products of purine fragmentation.

The absolute values of the total cross sections of production of negative ions of these molecules from a threshold to 200 eV are determined. For cytosine, the maximum of ionization cross section value of ion production makes  $(4.2 \pm 0.4) \cdot 10^{-18}$  cm<sup>2</sup> (at energy 1.5 eV). It is shown that process of negative ion production has resonant character and is accompanied with dissociation of molecules.

Information about physical structure of molecules is necessary for understanding the roles of primary physical processes for functioning the biosystems and the influence of different environmental factors upon them.

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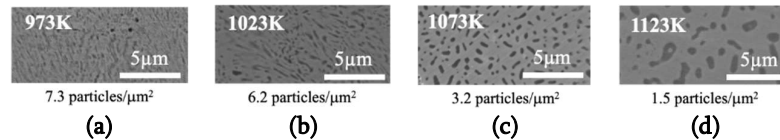
**Keywords:** electron beam, nucleic acid bases, excitation, dissociative excitation, cross section, ionization

# NANOSTRUCTURE CONTROL OF SILICIDE AND BORIDE FOR THERMAL-TO-ELECTRIC ENERGY CONVERSION

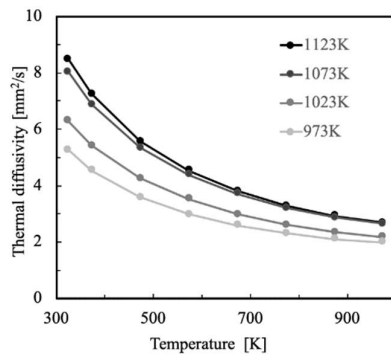
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ThermoElectric (TE) energy conversion has received renewed attention in recent years, because it has a potential to be utilized for electric power generation from waste heat. Efficiency of the energy conversion is fundamentally limited by the properties of TE materials. The inherent efficiency of any TE materials is determined by a dimensionless parameter (figure of merit)  $ZT$  given by  $ZT = S^2\sigma T/\kappa$ , where  $S$ ,  $\sigma$ ,  $T$  and  $\kappa$  are the Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively. The definition of  $ZT$  indicates that materials having lower  $\kappa$  and higher  $S$  and  $\sigma$  are desirable for TE application.



**Figure 1.** Microstructure of Si dispersed  $\beta$ -FeSi<sub>2</sub> heat treated at (a) 973, (b) 1023, (c) 1073, and (d) 1123 K, where gray matrix and dark particles are  $\beta$ -FeSi<sub>2</sub> and Si, respectively. Si particle number densities obtained from SEM micrographs are shown below each micrograph.



**Figure 2.** Thermal diffusivity of Si/ $\beta$ -FeSi<sub>2</sub>.

Semiconducting iron silicide,  $\beta$ -FeSi<sub>2</sub>, is a promising TE material, because it possesses high Seebeck coefficient and it is one of environmentally-friendly materials, while its thermal conductivity is rather high as compared with conventional TE materials. Reduction of its thermal conductivity is necessary to improve the TE performance. We are focusing on the synthesis of TE materials with fine microstructure, because smaller grain increases phonon scattering at grain boundaries. We synthesized Si dispersed  $\beta$ -FeSi<sub>2</sub> (Si/ $\beta$ -FeSi<sub>2</sub>) by heat treatment of  $\alpha$ -Fe<sub>2</sub>Si<sub>5</sub> phase. The  $\alpha$ -Fe<sub>2</sub>Si<sub>5</sub> is a high-temperature phase and decomposes into Si and  $\beta$ -FeSi<sub>2</sub> through eutectoid reaction below 1210 K [1]. **Figure 1** shows SEM micrographs of Si/ $\beta$ -FeSi<sub>2</sub> obtained at heat treatment temperatures 973–1123 K. Size of the precipitated Si decreases with decreasing heat treatment temperature, reaching as small as approximately 200 nm. As shown in **Figure 2**, thermal diffusivity of the Si/ $\beta$ -FeSi<sub>2</sub> was successfully decreased with increasing the number density of Si particle. The results suggest that the microstructure control in nanoscale is effective to improve TE properties of silicide. We are also studying microstructure control of metal-borides for improving their TE properties. Those results will be presented at the conference.

## Acknowledgment

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**Keywords:** thermoelectrics, iron silicide, metal-boride, thermal conductivity, eutectoid reaction

## ELECTRONIC STRUCTURE OF GALLIUM NITRIDE DURING SODIUM ADSORPTION

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Gallium nitride has unique electrical and optical properties. GaN is the most promising material for power and microwave electronics [1]. To successfully solve current scientific and technological problems of modern nitride microwave electronics, knowledge of the structural and electronic properties of the bulk and surface of the material is required. The most complete information about the electronic structure is provided by the results of photoemission studies using photoelectron spectroscopy. We recently studied the electronic and photoemission properties of the Cs/GaN and Li/GaN interfaces [2, 3].

In this work, we present detailed studies of the changes in electronic and photoemission properties due to the influence of sodium adsorption on the GaN surface in a range of submonolayer coatings.

The epitaxial growth of GaN sample was carried out on a Veeco GEN200 installation using plasma assisted molecular beam epitaxy. The layers were synthesized on 2-inch GaN/c-Al<sub>2</sub>O<sub>3</sub> templates 2 μm thick. Photoemission studies were carried out at the BESSY II synchrotron (Berlin, Germany) using photoelectron spectroscopy with synchrotron radiation. The experiments were carried out *in situ* in an ultra-high vacuum of 5·10<sup>-10</sup> Torr at room temperature. The spectra of normal photoemission of electrons from the valence band and the spectra of the Ga 3*d*, N 1*s* and Na 2*p* core levels were recorded.

The electronic structure of the GaN surface and the ultrathin Na/GaN interface was studied for the first time with various submonolayer Na coverages. The evolution of the spectra with the increase of the Na coverage demonstrates the adsorption activity of Ga dangling bonds on the GaN surface. It was found that sodium adsorption causes a decrease in the intensity of the core states and some changes in the spectrum in the valence band region due to charge transfer between the adsorbed Na layer and the surface GaN atoms. The position of hybridized states of Ga 4*p* – N 2*p* and Ga 4*s* – N 2*p* has been established. The Na/GaN interface is semiconductor character.

### Acknowledgments

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**Keywords:** GaN, adsorption, interface, molecular beam epitaxy, photoelectron spectroscopy



**PROSPECTS OF MANUFACTURING NANOCOMPOSITES (ANTI-CORROSION  
PROTECTIVE COATINGS) BY MEANS OF BORON AND ITS COMPOUNDS  
OBTAINED FROM PRODUCTION WASTE AND NATURAL BORATES**

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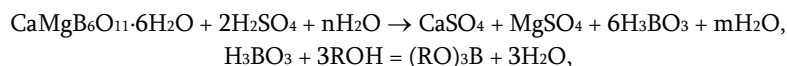
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Boron and its compounds have significant potential to play crucial roles in the metallurgical, chemical, electrochemical, nuclear, and space industries. High-purity crystalline boron is essential for manufacturing semiconductor systems, electronic and optical devices, as well as for producing special steels and alloys in metallurgy [1]. Borax and boric acid find applications in the production of leather, starch, glazes, and enamel paints. They also play a vital role in nuclear technology, slowing down thermal neutrons in nuclear reactors and serving as converters of isotope energy sources, among other uses.

Shortcomings in modern industrial methods for obtaining boric acid significantly affect the yield of the target product. When borate ores are processed using the sulfuric acid method, the output of boric acid typically ranges from 65 to 78%. A portion of the boric acid is lost in the mother solution, accounting for 18 to 30% of the total loss due to the co-solubility of boric acid and magnesium sulfate. The higher the ratio of MgO to B<sub>2</sub>O<sub>3</sub> in the starting ore, the greater the loss of boric acid. During the sulfuric acid treatment of borate ores, the yield of boric acid is negatively affected by the formation of insoluble calcium sulfate and hydrated silicic acid, taking the form of a gel. Both of these factors complicate the filtering process [2, 3].

We have developed a highly efficient laboratory method for extracting boric acid from boron production waste, where boron is in the form of boric acid, and from natural borates, transforming it into various products [4]. This method is based on the property of boric acid, which, when interacting with aliphatic alcohols, forms the corresponding alkyl borates. The hydrolysis of these alkyl borates yields boric acid in nearly quantitative yield. Boron exists in the form of boric acid in all production residues or can be easily converted from natural compounds into boric acid through the action of mineral acids:



where R = n-C<sub>5</sub>H<sub>11</sub>, iso-C<sub>5</sub>H<sub>11</sub>, or C<sub>6</sub>H<sub>13</sub>. According to this method, the output of boric acid from natural minerals, industrial wastes, as well as from artificial fertilizers is 87–97%.

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## DISTINCTIVE TECHNOLOGICAL APPROACH FOR PREPARATION OF DISPERSED AND FIBROUS NANO-STRUCTURED MANGANESE DIOXIDE USING SHS METHOD

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Production of nanoscale catalytic materials is an urgent technological problem. Catalysts have a wide range of applications and can be used, e. g., for neutralization of nuclear waste, decontamination of water polluted with mercury, purification of atmosphere of various micro-particles, in molecular sieves, as well as for chemical synthesis, oil refining, etc. Another important area of the application of nanostructured materials are the rechargeable batteries and fuel cells, where the high specific surface of nanostructured materials is needed to provide the high speed and effectiveness the interacting materials.

Active nanostructured materials having sufficiently high density of controlled surface defects meet well these requirements and, thereby, provide good possibilities to optimize the high-energy consumption of batteries.

Nowadays, the particle size of natural and industrially synthesized manganese oxide materials is in the range of microns and more. From our point of view, the most developed and promising currently used methods of manganese dioxide synthesis [1] are the ion exchange [2], hydrothermal synthesis [3], electrolytic synthesis [4] and chemical synthesis [5]. In the present work, a distinctive method of synthesizing of the nanostructured manganese dioxide is proposed, described and analyzed. Experiments were carried out to find the optimal ways of synthesis using the Self-propagating High-temperature Synthesis (SHS) method [6] as a quite distinctive technological approach using manganese ore enrichment waste as raw material and ammonium chloride as pretreatment chemical agent.

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**Keywords:** nanostructures, self-propagating high-temperature synthesis, manganese dioxide

## BIOLOGICALLY ACTIVE NANOPARTICLES USING LEUCINE BASED PSEUDO-PROTEINS

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PseudoProteins (PPs) [1 – 3] represent a family of artificial  $\alpha$ -Amino Acid (AA) based polymers – biomimetics of proteins [4]. The PPs consist of ester bonds, along with other chemical linkages, including amide, urea and urethane, within their backbones. The ester moieties facilitate hydrolytic (nonspecific chemical or an enzyme-catalyzed specific) degradation while the other linkages impart desirable thermal and mechanical properties to the PPs [1 – 3].

Recent studies have demonstrated that PPs actively support cell proliferation [5] making them a highly promising candidate for a wide range of biomedical applications [1 – 4]. Most of the PPs obtained by step-growth polymerization are generally hydrophobic and water-insoluble. Therefore, the imparting of hydrophilic properties could substantially expand the material properties of PPs rendering them multi-functional, e.g. they can be used as micellar drug delivery systems, as surface-active compounds, or as a protecting coating for NanoParticles (NPs) providing stealthy properties *in vivo*.

One of the most effective ways to render PPs hydrophilic is the grafting of PolyEthylene Glycol (PEG) molecules onto their backbones, thereby transforming the PPs into amphiphilic copolymers [6].

The novel biodegradable multipurpose amphiphilic polymers – PEG grafted PPs (PEG–PPs) promising as micellar drug delivery vehicles, surfactants, and protecting coatings for NPs were successfully synthesized using a cost-effective method – Michael conjugation reaction of methoxy-PEG-thiol and methoxy-PEG-amine with leucine based unsaturated co-poly(ester amide) (FuL6)<sub>0.5n</sub>–(8L6)<sub>0.5n</sub>.

The PEG–PPs stabilize pseudo-protein NPs were prepared from the poly(ester amide) 8L6 as well by the nanoprecipitation method, simultaneously coating them with a protective PEG cloud. The fabricated nanoparticles of size range 20.4–176.0 nm<sup>-1</sup> are suitable for applications of nanoparticles as drug delivery vehicles. Biologically active NPs loaded with two different non-proteinogenic amino acid-based dipeptides were also prepared and the main physical-chemical parameters were determined using DLS technique.

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**Keywords:** pseudo-proteins, nanoparticles, biodegradable surfactants, PEGylating agents, micelles

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