



# Book of Abstracts

International UFAZ Conference, CPM's 2025 Edition  
Chemistry Process Materials

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## Contents

This book contains all abstracts submitted to the International UFAZ Conference, CPM's 2025 Edition. The abstracts represent cutting-edge research and developments in Chemistry, Process Engineering, and Materials Science. Each abstract has been carefully reviewed by the Scientific Committee and accepted for presentation at the conference. The compilation preserves the original formatting and content of each submission while providing a comprehensive overview of the diverse research topics covered at the conference.

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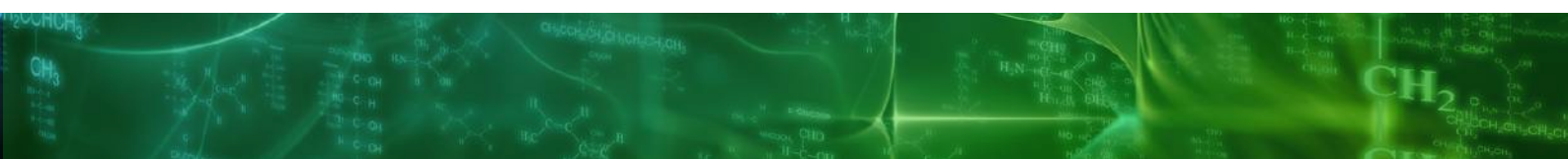
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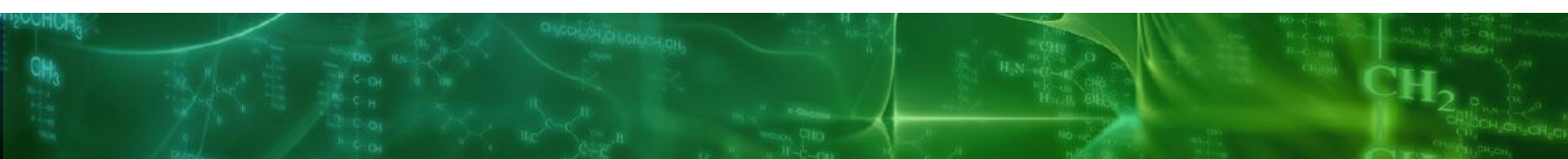
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## Abstracts



# Niobium-Based MXenes: Synthesis and Characterization as High-Performance Photothermal Agents for Cancer

Gulnaz Gahramanova<sup>1</sup>, Kailin Feng<sup>2</sup>, Laura Fusco<sup>3</sup>, Tetiana Hryhorchuk<sup>4</sup>, Benjamin Chacon<sup>4</sup>, Ahmad mirshaghagh<sup>2</sup>, Yuri Gogotsi<sup>4</sup>

<sup>1</sup> French-Azerbaijani University under Azerbaijan State Oil and Industry University, Baku, Azerbaijan

<sup>2</sup> Department of Bioengineering, University of Pennsylvania, Philadelphia, USA

<sup>3</sup> ImmuneNano-Lab, Department of Biomedical Sciences, University of Padua, Padua, Italy

<sup>4</sup> A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, USA

E-mail: [gulnaz.gahramanova@ufaz.az](mailto:gulnaz.gahramanova@ufaz.az)

## Abstract

Two-dimensional (2D) materials have garnered significant attention due to their unique properties and diverse applications. MXenes (2D carbides, nitrides, and carbonitrides of early transition metals) have rapidly grown into one of the largest and most studied families of 2D materials since their discovery in 2011 and their general formula is  $M_{n+1}X_nT_x$  ( $n = 1 - 3$ ), where M stands for transition metal carbides (like Ti, Nb, Zr, Ta, Hf, V, Sc, Cr, Mo), and X is carbon or nitrogen [1]. MXenes, synthesized by selectively etching "A" elements (Group IIIA or Group IVA element) from MAX phases ( $M_{n+1}AX_n$ ), exhibit remarkable properties such as high electrical conductivity, tunable surface functionalities, and excellent mechanical strength [2]. These characteristics make them promising candidates for a wide range of applications, including energy storage, catalysis, and biomedicine. Furthermore, MXenes demonstrate strong near-infrared (NIR) absorption, making them ideal for photothermal therapy (PTT), a cancer treatment modality that utilizes photothermal conversion agents to generate localized heat and destroy tumor cells [3].

In this study, Nb-based MXenes were synthesized by selectively removing aluminum layers from  $Nb_2AlC$  and  $Nb_4AlC_3$  MAX phases using a mixture of hydrofluoric and hydrochloric acid [4]. The resulting multilayer MXenes were then delaminated into single-layer flakes, reducing their size. The produced  $Nb_2C$  and  $Nb_4C_3$  MXenes were characterized using X-ray diffraction (XRD), energy-dispersive spectroscopy (EDS), and UV/Visible spectroscopy.

Both MXenes samples exhibited strong photothermal conversion capabilities, with a rapid temperature increase to  $45^\circ\text{C}$  observed in deionized water upon exposure to an 808 nm laser at a power density of  $0.7\text{ W/cm}^2$ . Biocompatibility was confirmed through assays using 4T1 tumor cell lines, which showed good viability across different concentrations of MXenes. Furthermore, PTT experiments demonstrated the effectiveness of these MXenes in killing 4T1 tumor cells upon laser irradiation, suggesting their potential as photothermal agents for cancer treatment.

These findings highlight the potential of  $Nb_2C$  and  $Nb_4C_3$  MXenes for PPT applications. The observed photothermal conversion, biocompatibility, and tumor cell death upon laser treatments suggest that Nb-based MXenes could be a valuable component of future cancer therapies.

**Keywords:** 2D materials, MXenes, photothermal therapy.

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## Physical-Chemical studies of $\text{Bi}_2\text{Se}_3$ thin films obtained by electrodeposition

S.P. Javadova, V.A. Majidzade, S.F. Jafarova, A.Sh. Aliyev, D.B. Tagiyev

Institute Catalysis and Inorganic Chemistry named after acad. M. Nagiyev MSE of Azerbaijan

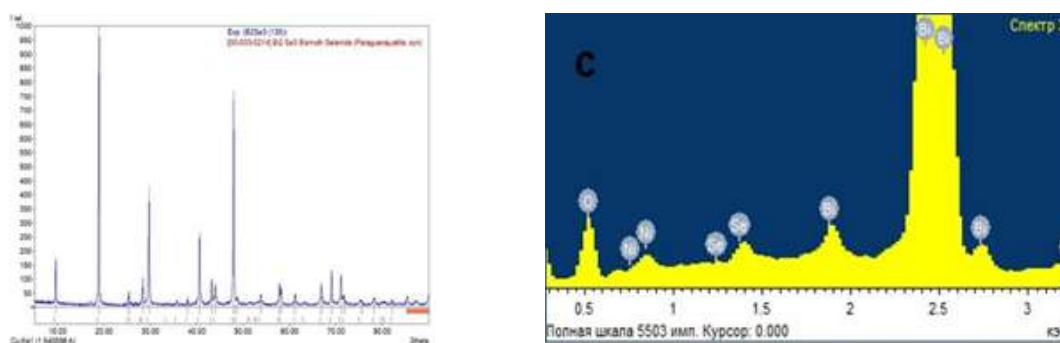
E-mail: [sevinc92.mva@gmail.com](mailto:sevinc92.mva@gmail.com); [yuska\\_80@mail.ru](mailto:yuska_80@mail.ru)

### Abstract

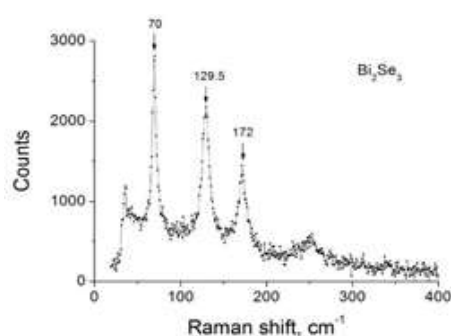
Thin films of  $\text{Bi}_2\text{Se}_3$  were obtained by electrochemical deposition from non-aqueous electrolytes. The synthesized films were characterized using modern methods of analysis (XRD, SEM, EDS, Raman spectroscopy, FTIR, etc.), their conductivity type was determined, and some semiconductor and photoelectrochemical properties were studied.

With the development of technology, the need for multifunctional new materials based on metal chalcogenides is rapidly growing.

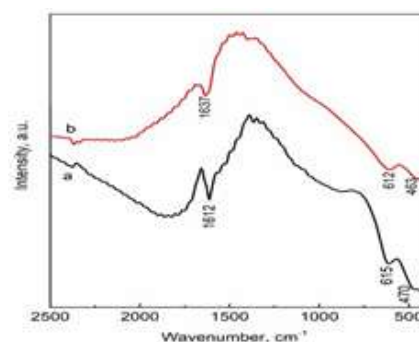
One of such interesting functional materials is  $\text{Bi}_2\text{Se}_3$  [1-3].  $\text{Bi}_2\text{Se}_3$  is one of the promising n-type semiconductor materials belonging to the VB-VIA group, with a band gap of 0.3 eV in single-crystal form and 0.9–2.3 eV in thin-film form. Photoemission studies of bismuth selenide show that it is a three-dimensional topological insulator with non-degenerate spins, which makes it an ideal option in electronics and spintronics.



**Fig. 1.** X-ray diffraction pattern (a) and elemental composition (b) of  $\text{Bi}_2\text{Se}_3$  thin films obtained from ethylene glycol. Electrolyte composition (M):  $0.07 \text{ Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O} + 0.03 \text{ H}_2\text{SeO}_3 + \text{C}_6\text{H}_8\text{O}_7$ ;  $T=298\text{K}$ .  $E_V=0.02 \text{ V/s}$ .



**Fig. 2.** Raman spectrum for  $\text{Bi}_2\text{Se}_3$  samples



**Fig. 3.** FTIR spectra of  $\text{Bi}_2\text{Se}_3$ : a) powder; b) thin film

The development of new material compositions, creation of new methods for processing and synthesizing materials, as well as the study of their structure and properties at the atomic and molecular levels are of great importance for finding the possibilities of their practical application. From this point of view, the electrodeposited thin films were investigated by some physicochemical methods.

According to the results of X-ray phase analysis, the peaks observed at  $2\theta$  angles close to  $\sim 9^\circ$ ,  $\sim 18^\circ$ ,  $\sim 25^\circ$ ,  $\sim 28^\circ$ ,  $\sim 30^\circ$ ,  $\sim 40^\circ$ ,  $\sim 43^\circ$ ,  $\sim 44^\circ$ ,  $\sim 48^\circ$ ,  $\sim 54^\circ$ ,  $\sim 58^\circ$ ,  $\sim 61.5^\circ$ ,  $\sim 65^\circ$ ,  $\sim 69^\circ$  and  $\sim 71^\circ$ , respectively, are characteristic of rhombohedral  $\text{Bi}_2\text{Se}_3$  [2]. To increase crystallinity, the resulting films were annealed in an argon atmosphere.

The results of EDS analysis also show the deposition of both components on the Ni electrodes (Fig. 1b).

Fig. 2 shows a typical Raman spectrum of  $\text{Bi}_2\text{Se}_3$  thin films. Four distinct Raman peaks can be seen at 37, 70, 129.5 and  $172\text{ cm}^{-1}$ , which correspond to  $E^1_g$ ;  $A^1_g$ ;  $E^2_g$  and  $A^2_g$  bulk modes [4]. In the spectrum, the low-frequency mode  $E^1_g$  has a very low intensity, since it was not observed in most of the results available in the literature [5]. The following  $A^1_g$ ;  $E^2_g$  and  $A^2_g$  modes confirm the good crystallinity of the structure.

Fig. 3 shows the comparative results of the FTIR analysis of the  $\text{Bi}_2\text{Se}_3$  powder (a) and thin film (b). It is noted that the peak positions on both curves are close, and the peaks in the range of  $450\text{--}700\text{ cm}^{-1}$  are related to the Bi-O stretching vibrations. The peaks at  $1612$  and  $1637\text{ cm}^{-1}$  for the  $\text{Bi}_2\text{Se}_3$  powder and thin film, respectively, are related to the C=O and OH stretching vibrations. The presence of stretching vibrations containing carbon, oxygen, and hydrogen may be related to the use of ethylene glycol in the synthesis of  $\text{Bi}_2\text{Se}_3$  powder and thin-film crystals [6, 7].

**Keywords:** electrodeposition,  $\text{Bi}_2\text{Se}_3$  thin films, Raman Spectroscopy.

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# Transparent Superhydrophobic Coatings Based on Carbonaceous Soot-PDMS/DTMS for Self-Cleaning, Anti-fouling and Anti-Corrosion Applications

Mohammad Irfan<sup>1</sup>, Chinthalapudi Naga Lakshmi<sup>1</sup> and Narendra Singh<sup>1\*</sup>

<sup>1</sup>Department of Chemical Engineering, Indian Institute of Technology Tirupati, India.

E-mail: [narendra@iittp.ac.in](mailto:narendra@iittp.ac.in)

## Abstract

Transparent superhydrophobic coatings with self-cleaning and anti-corrosion capabilities hold great potential for outdoor applications, including photovoltaics, solar panels/lens, automotive windshields, and protective surfaces [1]. However, their broader adoption is hindered by challenges such as limited optical transparency and reliance on fluorinated compounds [2]. To address these limitations current study presents a transparent superhydrophobic coating developed through an economical and eco-friendly two-step process. First, a polydimethylsiloxane (PDMS) polymer suspension was spin-coated onto glass slide (GS) and Inconel alloy (IN617) substrates at 2000 rpm for 30 sec. This was followed by the deposition of carbonaceous soot, after which the samples were cured at 80°C for 1 h and subsequently calcinated at 460–520°C for 10 min. During calcination, the oxidized PDMS inherited the unique structure of the carbon soot, rendering the coating transparent and superhydrophilic. The samples were then sprayed and functionalized with dodecyltrimethoxysilane (DTMS) and dried at 120°C for 2 h, resulting in a low surface energy and micro/nano hierarchical structure. The final coating exhibited a water contact angle (WCA) of 162.4° and a sliding angle (SA) of 1°. It achieved an average transmittance of ~95% in the visible light range (400–800 nm) and demonstrated excellent thermal stability up to ~200°C range. Furthermore, the coating maintained its functionality after exposure to strong acidic and alkaline solutions (pH 1–9), while exhibiting effective self-cleaning and anti-fouling properties. Additionally, the carbonaceous soot-PDMS/DTMS superhydrophobic coating on the IN617 substrate demonstrated remarkable anti-corrosion performance, with a significantly reduced corrosion rate (mm/y) when exposed to a 3.5 wt.% NaCl aqueous solution. These findings highlight a significant advancement in the development of self-cleaning, anti-fouling and anti-corrosion coatings for various outdoor applications.

**Keywords:** Carbonaceous soot, PDMS, Superhydrophobic coatings, Transmittance (%), Self-cleaning, Anti-corrosion.

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# SERS-based Approaches for the Characterisation of Micro- and Nanoplastics in Environmental Matrices

Lara Mikac<sup>1</sup>, Hrvoje Gebavi<sup>1</sup> and Mile Ivanda<sup>1</sup>

<sup>1</sup> Laboratory for Molecular Physics and Synthesis of New Materials, Ruder Boskovic Institute.

E-mail: [lmikac@irb.hr](mailto:lmikac@irb.hr)

## Abstract

Micro- and nanoplastics (MNPs) are widespread environmental pollutants produced by the degradation of plastics. Their small size, longevity and potential impact on ecosystems and human health have caused global concern.<sup>1</sup> However, their reliable detection, especially at the nanoscale, remains an analytical challenge. Advanced spectroscopic approaches are needed that enable sensitive, specific and rapid identification of plastic particles in complex environmental samples.

In this work, a combined application of surface-enhanced Raman spectroscopy (SERS) and micro-Raman mapping for the detection and characterisation of MNPs in environmental and water samples is presented. Silver nanoparticles were synthesised directly on silicon filter substrates by in situ reduction and subsequent gold sputtering to improve stability and performance. In addition, colloidal gold nanoparticles with different morphologies were synthesised and tested as SERS-active colloids. Raman mapping was used to analyse solid substrates and micro-Raman spectroscopy was used to identify polymers in bottled water and lake sediment samples.

The prepared SERS substrates enabled picomolar detection of 4-mercaptobenzoic acid and micromolar detection of melamine. Polystyrene (PS) and polyethylene (PE) nanoparticles as small as 50 nm were successfully imaged on solid substrates. Colloidal SERS showed strong signals for PS (350 nm) and weaker but detectable signals for PE (1–4  $\mu$ m). Analysis of six brands of bottled water revealed the presence of microplastics (<5  $\mu$ m), including PE, PET and PA. In particular, higher concentrations were found in bottles made from untreated PET compared to recycled PET. Microplastics were also detected in lake sediments from four urban lakes. The polymers detected included PS, PE, PET, polypropylene (PP) and nylon, with most particles in the 5–10  $\mu$ m range. The composition of the polymers varied from site to site, suggesting local environmental influences.

These results demonstrate the potential of SERS and micro-Raman spectroscopy for sensitive detection and polymer characterisation of micro- and nanoplastics in water and sediment. The approach offers tools for environmental monitoring, supports risk assessment and provides information for strategies to control plastic pollution in consumer products and natural ecosystems.

**Keywords:** Microplastics, Raman spectroscopy, SERS, Environmental monitoring, Nanomaterials.

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## Study of Thermodynamic Properties of GeTe-rich Germanium Antimony Tellurides

Elnur N. Orujlu<sup>1</sup>, Elnur R. Nabiyev<sup>2</sup>, Yusif A. Yusibov<sup>2</sup>, Mahammad B. Babanly<sup>3</sup>

<sup>1</sup> Azerbaijan State Oil and Industry University, Baku, Azerbaijan

<sup>2</sup> Ganja State University, Ganja, Azerbaijan

<sup>3</sup> Institute of Catalysis and Inorganic Chemistry, Baku, Azerbaijan

E-mail: [elnur.oruclu@yahoo.com](mailto:elnur.oruclu@yahoo.com)

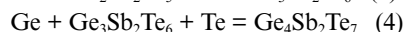
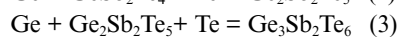
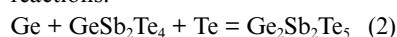
### Abstract

Tellurides of group 14 and Group 15 elements with a layered tetradymite-type structure have long attracted significant attention from researchers as thermoelectric materials [1,2]. Ge-B<sup>V</sup>-Te alloys are also widely used in optical storage devices and are considered a key class of materials with a reversible phase transition between amorphous and crystalline states [3,4]. After the discovery of topological insulators (TIs) [5], it was found that ternary compounds of the types A<sup>IV</sup>B<sup>V</sup><sub>2</sub>Te<sub>4</sub>, A<sup>IV</sup>B<sup>V</sup><sub>4</sub>Te<sub>7</sub>, A<sup>IV</sup>B<sup>V</sup><sub>6</sub>Te<sub>10</sub>, and others (where (A<sup>IV</sup>-Ge, Sn, Pb; B<sup>V</sup>-Sb, Bi) are 3D TIs and highly promising for high-tech applications.

The knowledge of phase equilibria and reliable thermodynamic data of corresponding systems are crucially important for designing and synthesizing novel complex phases. Here we studied the thermodynamic properties of germanium antimony tellurides in the GeTe-Sb<sub>2</sub>Te<sub>3</sub>-Te composition region using EMF measurements with a liquid electrolyte.

Alloys of the GeTe-Sb<sub>2</sub>Te<sub>3</sub>-Te system were prepared using pre-synthesized starting binary compounds and elemental tellurium. A mixture of components was placed in the evacuated (~10<sup>-2</sup> Pa) quartz ampules and synthesized at 950 K for 5 h followed by quenching in icy water. The resulting ingots were further annealed at 700 K for 45 days to form equilibrium phases. All alloys were examined using powder X-ray diffraction (Bruker D2 PHASER diffractometer) technique. EMF measurements were performed using a Keithley 2100 6 1/2 Digit Multimeter.

For EMF measurements, the concentration cell of (-) GeTe (solid) | glycerol + KCl | Ge-Sb-Te (solid) (+) (1) type was assembled. Measurements show that EMF temperature dependence increases linearly with temperature in the 300–450 K range. Considering a linear connection between the EMF and temperature, the experimental data were analyzed using the least squares approach. At the first stage, relative partial molar functions of germanium in the GeTe-Sb<sub>2</sub>Te<sub>3</sub>-Te composition area were calculated. According to the solid-phase diagram of the GeTe-Sb<sub>2</sub>Te<sub>3</sub>-Te system, partial molar quantities of the germanium can be considered thermodynamic functions of the following virtual cell reactions:

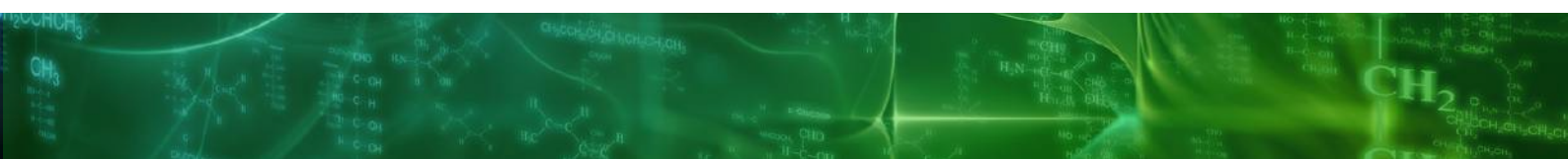


Using these data and the corresponding thermodynamic functions of GeTe and Sb<sub>2</sub>Te<sub>3</sub>, the standard thermodynamic functions of formation and standard entropies of the Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>, Ge<sub>3</sub>Sb<sub>2</sub>Te<sub>6</sub>, and Ge<sub>4</sub>Sb<sub>2</sub>Te<sub>7</sub> compounds were calculated.

**Keywords:** thermodynamic properties, layered materials, EMF measurements, thermodynamic properties, topological insulators.

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## Characterization of Toxicity, Assessment of Engineered TiO<sub>2</sub> and Ag Nanoparticles in Biological Objects

Kamala Badalova<sup>1</sup>, Antonio Moreda Piñeiro<sup>2</sup>

<sup>1</sup>Pharmaceutical toxicology and chemistry department, Azerbaijan Medical University

<sup>2</sup>Department of Analytical chemistry, Bromatology and Nutrition, Santiago de Compostela University, Spain

E-mail: [kamala.badalova@mail.ru](mailto:kamala.badalova@mail.ru)

### Abstract

The rapid advancement of nanotechnology has led to the widespread use of engineered nanoparticles (ENPs) in various fields, including medicine, electronics, and environmental applications. However, the unique properties of these nanoparticles raise concerns regarding their potential toxicity and interactions with biological systems. The toxicity of nanoparticles is influenced by several factors, including size, shape, surface charge, composition, and agglomeration state. Smaller nanoparticles tend to exhibit higher reactivity and bioavailability, leading to increased cellular uptake and potential toxicity. Mechanistically, NPs can induce oxidative stress through the generation of reactive oxygen species (ROS), disrupt cellular membranes, interfere with mitochondrial function, and trigger inflammatory responses. The environmental impact of nanoparticles is also a growing concern. Their release into ecosystems can affect aquatic organisms and terrestrial wildlife through bioaccumulation and biomagnification processes.

The increasing use of titanium dioxide (TiO<sub>2</sub>) and silver (Ag) nanoparticles in various applications, including cosmetics, pharmaceuticals, and environmental remediation, has raised concerns regarding their potential toxicity to living organisms.

The increasing use of nanoparticles in various industries has raised concerns regarding their potential toxicity and impact on living organisms. This investigation focuses on the determination and assessment of toxic nanoparticles within biological systems, aiming to elucidate their sources, mechanisms of toxicity, and effects on health. Various in vitro and in vivo models have been employed to assess nanoparticle toxicity. In vitro studies using human cell lines have demonstrated that different types of nanoparticles (e.g., silver, titanium dioxide, carbon-based materials) exhibit varying degrees of cytotoxicity depending on their physicochemical properties. In vivo studies in animal models have revealed that nanoparticles can accumulate in vital organs such as the liver, lungs, and kidneys, leading to systemic effects and long-term health implications.

Utilizing advanced characterization techniques such as transmission electron microscopy (TEM), dynamic light scattering (DLS) and atomic force microscopy (AFM), we investigate the physicochemical properties of various nanoparticles, including their size, shape, surface charge, and functionalization. We employ a multi-faceted approach that combines advanced analytical techniques, including inductively coupled plasma mass spectrometry (ICP-MS), scanning electron microscopy (SEM), and fluorescence microscopy, to identify and quantify nanoparticles in biological samples.

**Keywords:** Nanoparticles, Toxicity, Assessment.

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## Synthesis Of Para-[1-(3-)Methylcyclohexyl] Nonylphenols and Some of Their Derivatives

U.R.Gurbanova<sup>1</sup>, Ch.K.Rasulov<sup>1</sup>, G.Z.Heydarli<sup>1</sup>, A.H.Movsumova<sup>1</sup>, P.A.Aghayeva<sup>2</sup>

<sup>1</sup>Academician Y.H. Mammadaliyev Institute of Petrochemical Processes of the Ministry of Science and Education of the Republic of Azerbaijan, Baku

<sup>2</sup> Baku Higher Oil School of SOCAR

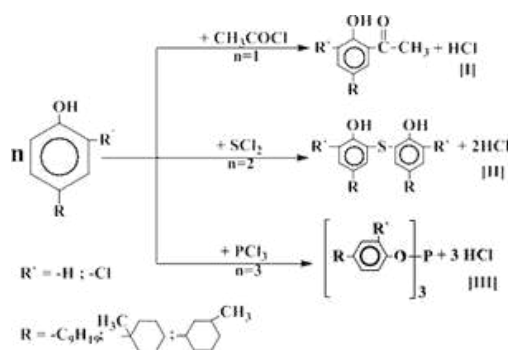
E-mail: [ulviyyagurbanova01@gmail.com](mailto:ulviyyagurbanova01@gmail.com)

### Abstract

Alkylphenols are primarily used as raw materials in producing various industrial products, including surfactants, detergents, phenolic resins, polymer additives, and lubricants. The global demand for alkylphenols is estimated at 500,000 tons per year, with nonylphenol being the most widely used, holding a market share of 80-90%. In Western Europe, the annual production of nonylphenol ranges between 75,000 and 80,000 tons[1],[2].

This study explores the preparation of phosphorus, sulfur, and carbonyl derivatives of para-(alkyl)phenols produced from the alkylation reaction of phenol with propylene trimer and 1-(3-) methylcyclohexane in the presence of hydrochloric acid-impregnated zeolite KN-30 catalyst.

In the specified reactions, the equations for the acylation, sulfonation, and phosphorylation reactions of alkylphenols, which are more commonly utilized in petrochemicals, are given:



The alkylation of phenol with propylene trimer and 1-(3-)methylcyclohexane using an HCl-impregnated KN-30 catalyst (100- 120°C, 4-6 hours, 1:1 molar ratio, 10% catalyst) yielded 76.5% of the target product with 87.8% selectivity. Further modifications included acylation with acetyl chloride (ZnCl<sub>2</sub>, KU-23, 145-150°C, 30-40 min) to obtain 2-hydroxy-5-alkyl acetophenones, sulfonation with dichlorosulfide (40-50°C, 4 hours) forming 2,2'-thiobis-(4-alkylphenols), and phosphorylation with phosphorus trichloride (50-80°C, N<sub>2</sub> atmosphere, 1-5 hours) producing tri-(para-alkylphenyl)phosphites.

As a result of the research, 2-hydroxy-5-alkyl acetophenones were tested as antioxidants in diesel fuel, 2,2'-thiobis-(para- alkylphenols) as vulcanizates in rubber mixtures, tri-[para-(alkyl)-phenyl]phosphites as antioxidants in oils and polyolefins, and positive results were obtained.

**Keywords:** phenol, para-[1(3)-methylcyclohexyl]phenols, nonylphenol, zeolite KN-30 catalyst, acylation, sulfonation, phosphorylation, antioxidant.

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# Synthesis of Carbon Microtubes at Low Pressures by CVD Method

Asgar Huseynov, Minira Aghahuseynova, Eldar Zeynalov, Dunya Babanli

Azerbaijan State Oil and Industry University

E-mail: [minira\\_baku@yahoo.com](mailto:minira_baku@yahoo.com)

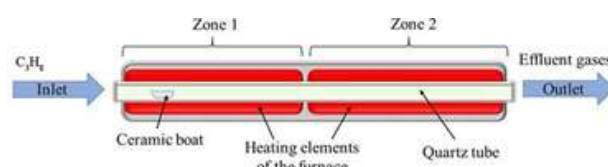
## Abstract

Over the past thirty years, since the first discovery of carbon nanotubes researchers have developed some methods to produce carbon nanotubes both economically and efficiently.

This paper summarizes the progress of conducted work which investigates synthesis of carbon structures at low pressure from various types of raw materials and can bring new insights into the synthesis of carbon nanotubes. In these experiments, we used 1 gaseous raw material and 5 liquid raw material as a carbon source, but precursor was the same for all of the experiments. For the investigation of theoretical and experimental results of the synthesized carbon nanotubes, some analysis methods has been used, such as Scanning Electron Microscopy (SEM), Electron dispersion Xray (EDX) and X-Ray Diffraction (XRD) is successful to analyze physico-chemical properties of the obtained CNTs.

CVD setup which we used in our experiment is a complex system which has several parts, and every part serves for different purposes. Every component in the CVD system used serves to control reaction conditions such as pressure, temperature, flow rate and so on. Setup provides exact control over process parameters and helps to implement highly reproducible experiments. This ensures consistent product quantity and quality. The control multiple parameters at once makes experiments to be carried out under various reaction conditions.

In this experiment, synthesis of carbon nanotubes involved some stages such as preparation of raw material, synthesis process, and purification stage. For this experiment, various kinds of feedstocks were used as a carbon source, however precursor was ferrocene which was the same for all of the experiments. For better understanding of CNTs, liquid and gaseous feedstocks was used in the experiment.



**Fig. 1.** Schematic representation of cross-section of the furnace during the synthesis of carbon nanotubes with propane feedstock.

As a gaseous raw material, propane gas was selected and for the liquid raw material 5 different liquid material was selected. In this case, introduction of the feedstock into the furnace changes based on the type of the raw material. Major parameter which makes this experiment unique is the pressure (10-15 kpa) which is lower than atmospheric pressure

## Conclusion

1. Synthesis of MWCNTs at low pressures and study peculiarities of the effect on the synthesis process have been provided.
2. The analysis of synthesis products at low pressures proved that the main product when using propane acetonitrile toluene as raw materials is a carbon mega tubes, which are much less studied.
3. As it can be seen from our results the diameter of carbon mega tubes are hundreds of time thicker than those of CNTs and amount to several microns.
4. In our experiments with using a mixture of xylene isomers as a raw material, as well as cyclohexane the formation of a large amount of coke and soot was observed, but when using ethyl alcohol clean mega tubes were formed.

**Keywords:** Carbon microtubes, CVD method, low pressure, liquid raw material, gaseous raw material.

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# Design and Catalytic Applications of a Novel Cerium Metal Organic Framework

Shabnam Feyziyeva<sup>1</sup>, Nizami Israfilov<sup>1,2</sup>, Benoît Louis<sup>1</sup>

<sup>1</sup> ICPEES UMR 7515, Université de Strasbourg, 25 rue Becquerel, F-67087 Strasbourg, France.

<sup>2</sup> CMC UMR 7140, Université de Strasbourg, 4 rue Blaise Pascal, F-67000 Strasbourg, France.

E-mail: [shabnam.feyziyeva@etu.unistra.fr](mailto:shabnam.feyziyeva@etu.unistra.fr)

## Abstract

In recent years, metal–organic frameworks (MOFs) have gained attention for their applications in separation, storage, and catalysis.<sup>1</sup> The combination of appropriate metal cations and organic linkers often results in the formation of open metal sites (OMSs), which can play diverse roles, including acting as coordination sites for guest molecules or contributing to catalytic properties [2].

In this study, we synthesized a cerium(III)-based MOF using both microwave-assisted and solvothermal methods. Cerium MOFs are particularly advantageous due to their ability to facilitate redox reactions, which enhance their catalytic activity [3]. More over, lanthanide-based MOFs are known to yield very stable MOF's, due to their high coordination number[4].The microwave-assisted synthesis produced the MOF in powder form, while the solvothermal method yielded a microcrystalline material. Both methods exhibited the same XRD patterns, confirming correlation between the two synthesis methods, while the microwave method significantly reduced the reaction time from one day to 20 min. The most characteristic feature of Ce-MOF is its 1-D zigzag chains of metal cations with Ce–Ce distances of 4.137 Å, coordinated by solvent molecules from the same direction, enabling densely aligned 1-D OMSs upon solvent removal

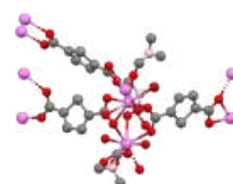
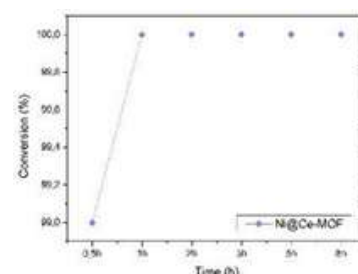


Fig. 1. The molecular structure of Ce-MOF (view from c axis)

The acidity of the material was evaluated using  $\text{NH}_3$ -TPD, which revealed the two distinct desorption peaks at approximately 290°C and 379°C, thus indicating the presence of acidic sites of varying strength. Thermogravimetric analysis (TGA) showed the MOF decomposes at 450°C, confirming its high thermal stability. Interestingly, although the MOF exhibits  $10 \times 17$  Å pores characteristic of its 3D structure, its surface area is relatively small (9 m<sup>2</sup>/g) and  $\text{CO}_2$  adsorption capacity is around 1 mmol/g at 273K, 1.2 bar. This disparity may arise from pore collapse due to breathing or other effects, yet the pore dimensions and aligned OMSs remain advantageous for catalytic applications.



The nickel-exchanged cerium-based MOF was synthesized to enhance its catalytic activity for the methanol-to-dimethyl ether (MTD) process at 280°C, with a WHSV of 1.69 h<sup>-1</sup>. Nickel was introduced to improve the MOF's ability. The material achieved 99% methanol conversion within 30 minutes and maintained complete conversion (100%) up to 8 hours of reaction time (Fig.2.) Small amounts of byproducts, such as  $\text{CH}_4$  and  $\text{CO}$ , were observed at 5 and 8 hours but did not affect the overall conversion.

In conclusion, the cerium-based MOF showed good stability and catalytic performance, with the nickel-exchanged version improving its activity and long-term stability, supported by its structure.

**Keywords:** Cerium-MOF, Catalysis, Open Metal Sites.

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## Synthesis of Binary Zn-containing Catalysts and Study of Their Properties in the Process of Acetone Production from Bioethanol

Tahmina Taghi<sup>1</sup> and Vaghif Baghiyev<sup>2</sup>

<sup>1</sup> French-Azerbaijani University

<sup>2</sup> Azerbaijan State Oil and Industry University

E-mail: [tahmina.taghi@ufaz.az](mailto:tahmina.taghi@ufaz.az)

### Abstract

Acetone is one of the most important solvents and is widely used in the synthesis of various chemical compounds and polymers. Currently, acetone is mainly produced by the cumene method, which uses benzene and propylene as raw materials. Phenol is obtained as the second main product. Other methods for obtaining acetone are dehydrogenation or oxidative dehydrogenation of isopropyl alcohol, oxidation of propylene, and steam conversion of ethanol to acetone. The synthesis of acetone from ethanol has several advantages. Firstly, bioethanol is a renewable raw material. Secondly, it does not form phenol as a by-product. Moreover, it is an ecofriendly compound and nowadays it is widely used in green chemistry.

Binary zinc-containing catalysts with different composition were synthesized by coprecipitation method. Their activity and other properties were studied in the reaction of ethanol vapor-phase conversion to acetone. BET surface area of the synthesized catalyst was studied. IR and X-ray analysis were conducted to study structural properties of the catalysts and predict a possible mechanism of the reaction. Acid-base properties of the catalytic surfaces were studied by isomerization reaction of but-1-ene to but-2-enes.

The main product of the reaction of ethanol conversion in the presence of water vapor is acetone. Acetaldehyde, ethylene and carbon dioxide are also formed as by-products. Influence of atomic ratio of metals in the catalyst on conversion of ethanol was studied. The acetone yield showed a positive correlation with the specific surface area of the catalysts. X-ray diffraction analysis of the phase composition of the synthesized catalysts was performed using an automatic powder diffractometer ("D2 Phaser" with CuK $\alpha$  radiation and a Ni filter). The influence of the degree of crystallinity of catalysts on their activity was also studied. The crystallinity of the catalysts ranged from 70.1 % to 87.3 %, and a strong correlation was found between crystallinity and catalytic activity, with higher crystallinity leading to improved acetone yields.

It is found that the catalytic sample with the atomic ratio Mg : Zn = 1 : 9 exhibited the highest activity in acetone formation at 450°C, with an acetone yield of 68.7%.

**Keywords:** Bioethanol, Acetone, Activity.

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## Major Byproducts Of Hexachlorobenzene In Isopropanol Under Gamma Radiolysis

Samir Karimov

French-Azerbaijani University under Azerbaijan State Oil and Industry University

E-mail:[samir.karimov@ufaz.az](mailto:samir.karimov@ufaz.az)

### Abstract

This study investigates the gamma radiolysis-induced degradation of hexachlorobenzene (HCB), a persistent organic pollutant (POP), in isopropanol. By exposing HCB-isopropanol solutions to varying durations of gamma irradiation using a cobalt-60 source, we aimed to identify major byproducts and examine their formation dynamics. The experiments were performed at a dose rate of approximately 6.26 kGy/h, with total absorbed doses ranging up to 170 kGy. Gas chromatography-mass spectrometry (GC-MS) analysis enabled the separation and identification of principal byproducts, including 2,5-hexanedione, 1,1-diethoxypentan-4-one, methylpentachlorobenzoate, and 1-propoxy-2-propanol. The formation of these compounds was monitored over time, and their peak areas were used to evaluate the degradation kinetics of HCB under irradiation. Results revealed a strong correlation between irradiation dose and byproduct formation, confirming continuous decomposition of HCB with increasing gamma exposure. However, the appearance of structurally diverse and potentially toxic byproducts suggests a nonselective degradation mechanism in isopropanol. This underscores the critical importance of solvent choice in radiolytic degradation studies. Overall, this work contributes to understanding the degradation pathways of chlorinated aromatic pollutants and highlights the need for developing more selective and environmentally benign solvent systems for gamma irradiation-based remediation.

**Keywords:** Persistent Organic Pollutants, Hexachlorobenzene, Gamma radiolysis, Nuclear energy, Environmental remediation.

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## Modification Of Poliisoprene

S. Rahimova<sup>1</sup>, R. Rahimov<sup>2</sup>

<sup>1</sup> French-Azerbaijani University under Azerbaijan State Oil and Industry University

<sup>2</sup> BEU, head of chemical engineering laboratory

E-mail: [sabina.rahimova@ufaz.az](mailto:sabina.rahimova@ufaz.az)

### Abstract

In modern industry, the demand for high-performance elastomeric materials is steadily increasing. Enhancing the durability and service life of such materials is essential to conserve raw materials, energy, and labor resources. One of the most accessible and effective approaches to improve elastomer properties is their modification through blending with other reactive polymers or reactive low molecular weight compounds. In this work, polyisoprene rubber (SKI-3) was modified with various polymers—namely butadiene-nitrile rubber (SKN-40), polyvinyl chloride (PVC) and polyvinyl acetate (PVAc)—to develop heat- and adhesion-resistant materials with improved structural and mechanical performance. Binary blends of SKI-3 with SKN-40, PVC, and PVAc at different mass ratios (90:10, 80:20, and 70:30) were prepared. Vulcanization was carried out using both sulfur-based and peroxide systems, with additional use of hexachloroparaxylene (HCPX) as a structuring agent and metal oxides (ZnO, MgO, Al<sub>2</sub>O<sub>3</sub>) as activators. FTIR spectroscopy and swelling-based Zol-Gel analysis were used to study structural changes and crosslink density in SKI-3 blends with SKN-40, PVC, and PVAc under heat. Thermal decomposition of polar groups, HXPK-mediated chlorination, and polysulfide bond formation were confirmed. EPR spectroscopy revealed narrow singlet signals corresponding to free radicals, verifying a radical crosslinking mechanism during vulcanization. Mechanical properties (tensile strength, elongation, and elasticity) were also evaluated. It was shown that HXPK, in the presence of metal oxides, acts as an effective crosslinking agent under heat, forming polysulfide (C–S<sub>n</sub>–C) and carbon-carbon (C–C) bonds. The reactivity order of modifiers was found to be SKN-40 > PVC > PVA. EPR spectroscopy confirmed the formation of symmetrical singlet signals associated with free radicals during the vulcanization. ZnO was identified as the most effective activator (ZnO > MgO > Al<sub>2</sub>O<sub>3</sub>). The peroxide system, when optimized with ≥2.0 parts of dicumyl peroxide, enabled formation of sulfur-free vulcanizates with high heat resistance and elasticity at 150–200°C. Modified composites showed improved cohesion strength, thermal aging resistance, and swelling resistance compared to sulfur-vulcanized counterparts. The developed modification and vulcanization approaches enable the production of advanced elastomeric materials with enhanced thermal and mechanical stability. These materials are suitable for use in seals, gaskets, and components operating under dynamic loading and in aggressive media. The findings provide practical guidelines for the selection of optimal modifier ratios and vulcanization systems in industrial rubber formulation.

**Keywords:** polyisoprene, butadiene-nitrile rubber, polymer modification.

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## The Effect of Thiol Side Group on Release Kinetics of Thiolated Cationic Polyaspartamides

Aysel Mammadova<sup>1,2</sup> and Benjámín Sándor Gyarmati<sup>2</sup>

<sup>1</sup> Baku Higher Oil School

<sup>2</sup> Budapest University of Technology and Economics

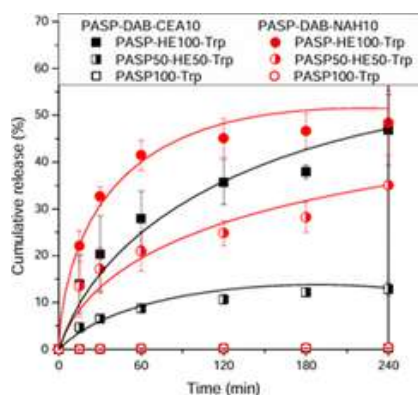
E-mail: [aysel.mammadova@bhos.edu.az](mailto:aysel.mammadova@bhos.edu.az)

### Abstract

Due to the advantages of thiolated cationic polymers in the formation of in situ gelling hydrogels for various biomedical and environmental applications, extensive research has been dedicated to developing new strategies for synthesizing thiolated polymers and improving gelation properties and stability of hydrogels. The main characteristic of these systems is that they are in the sol state before application and turn into gel under certain physiological conditions such as pH, temperature, UV irradiation, etc[1,2].

Thus, thiolated cationic polyaspartamides were prepared by thiolating the polysuccinimide with different thiolating agent (cysteamine and N-acetyl-DL-homocysteine thiolactone), which was later followed by introducing the different cationic side groups. The structure of polymers was confirmed by <sup>1</sup>H NMR spectroscopy while gelation process, and the stability of the disulfide cross-linked hydrogels were analyzed by oscillatory rheological measurements. Drug release experiments were performed to study the release profiles of fluorescent labelled PASP derivatives with different surface charge from disulfide cross-linked cationic polyaspartamide hydrogels.

Thiolated polyaspartamides synthesized with both strategies converted into stiff hydrogels under mild reaction conditions through the oxidation-induced intermolecular disulfide formation and gelation time and stiffness of hydrogels could be adjusted by the degree of thiolation (Fig. 1). However, the presence of longer side-groups (PASP-DAB-NAH) largely accelerated gelation and the stiffness of the resultant hydrogels was higher than those short thiolated side chain counterparts (PASP-DAB-CEA). PASP-based macromolecular model drug with a controlled concentration of anionic groups was entrapped in the hydrogels during the in situ gelation. Fully anionic PASP (PASP-Trp) was entrapped completely in the hydrogels, whereas the reduction in the number of anionic groups caused the partial release of PASP derivatives (PASP50-HE50-Trp), which reveal the charge density of model drug and cationic polyaspartamides controlled the release kinetics of the linear anionic polyelectrolytes from the cationic polymer hydrogel network (Figure 1). Thus, the release of anionic macromolecular drugs from cationic polyaspartamide hydrogels could be controlled by the degradation of the hydrogels in a reducing medium used for modeling the reductive environment of cells.



**Fig 1.** Cumulative release of model drugs from thiolated polyaspartamides.

**Keywords:** Thiolated polymers, Cationic polyaspartamides, Drug delivery.

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# Macromolecular Engineering to Tune Materials for Biomedical Applications

Nicolas Zydziak,<sup>1</sup> Alireza Kavand,<sup>1</sup> Amélie Augé,<sup>1</sup> Quentin Bievelot,<sup>1</sup> Tetiana Dorosh,<sup>2</sup> Philippe Laval,<sup>3</sup> Nicolas Anton,<sup>4</sup> Thierry Vandamme,<sup>4</sup> Yves Mély,<sup>5</sup> Frédéric Przybilla,<sup>5</sup> Alain Chaumont,<sup>2</sup> Fouzia Boulmedais,<sup>1</sup> Christophe Serra,<sup>1</sup> Delphine Chan-Seng<sup>1</sup>

<sup>1</sup> Université de Strasbourg, CNRS, Institut Charles Sadron UPR 22, F-67000 Strasbourg, France

<sup>2</sup> Université de Strasbourg, CNRS, Laboratoire de modélisation et simulation moléculaire UMR 7140, F-67000 Strasbourg, France

<sup>3</sup> INSERM, Biomaterials and bioengineering UMR\_S 1121, 1 rue Eugène Boekel, F-67000 Strasbourg, France

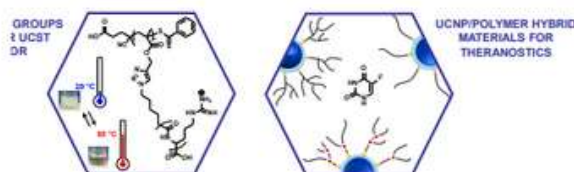
<sup>4</sup> INSERM, Université de Strasbourg, Regenerative nanomedicine UMR\_S 1260, 1 rue Eugène Boekel, F-67000 Strasbourg, France

<sup>5</sup> Université de Strasbourg, CNRS, Laboratoire de bioimagerie et pathologies UMR 7021, F-67000 Strasbourg, France

E-mail: [delphine.chan-seng@ics-cnrs.unistra.fr](mailto:delphine.chan-seng@ics-cnrs.unistra.fr)

## Abstract

Advances in the field of polymer chemistry have permitted to prepare polymers of controlled topologies, functionalities and microstructures using various strategies to access complex architectures with a variety of functional groups positioned at well-defined localizations on the polymer chain. [1] This ability to control the architecture and microstructure of polymers along with their functionalities are an asset to adjust the properties of polymers and tune their performances according to the targeted application. [2,3] This presentation will illustrate the ability of macromolecular engineering, especially the topology of polymers, to afford polymers of specific and tunable properties with a focus on biomedical applications through two examples as depicted on Fig. 1. The first part of the presentation will focus the design of comb polymers with peptide sequences as pendent grafts through the macromonomer approach. It will be illustrated through the use of macromonomers with oligoarginine pendent grafts. [4] This polymer exhibited a thermoresponsive behavior in water with a solubilization of the polymer upon increasing the temperature (upper critical solution temperature behavior). In a second part, the preparation of hybrid materials based on upconversion nanoparticles (UCNPs) and polymers will be discussed emphasizing on how the structure of the polymer covalently attached to UCNPs could be designed to fulfil the requirement of theranostics. [5,6]



**Fig. 1.** Tuning the structure of polymers towards the development of thermoresponsive polymers and hybrid materials.

**Keywords:** polymer chemistry, stimuli-responsive polymers, hybrid materials.

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# Fabrication of Hydroxyapatite Nanoparticle/Polymer Composite Microfibers using a Capillary-based Microfluidic Device

Leyla Aliyeva,<sup>a,b</sup> Afsana Guliyeva,<sup>b</sup> Christophe A. Serra,<sup>a</sup> Marc Lenertz,<sup>c</sup> Alain Carvalho,<sup>a</sup> Fabrice Vigneron,<sup>d</sup> Maxime Florent,<sup>b</sup> Ulviyya Hasanova,<sup>b</sup> Delphine Chan-Seng<sup>a</sup>

<sup>a</sup> Université de Strasbourg, CNRS, Institut Charles Sadron UPR 22, F-67000 Strasbourg, France

<sup>b</sup> CPML (UFAZ), Azerbaijan State Oil and Industry University, Azadlıq Avenue, 20, Baku AZ 1010, Azerbaijan

<sup>c</sup> Université de Strasbourg, CNRS, Institut de physique et de chimie des matériaux de Strasbourg UMR 7504, F-67000 Strasbourg, France

<sup>d</sup> Université de Strasbourg, CNRS, Institut de chimie et procédés pour l'énergie, l'environnement et la santé UMR 7515, F-67000 Strasbourg, France

E-mail: [leyla.aliyeva@ufaz.az](mailto:leyla.aliyeva@ufaz.az)

## Abstract

Drug delivery systems are designed technologies that allow medicinal drugs to be delivered with precision and/or controlled release [1]. Nanotechnology [2] is allowing new medication delivery vehicles to emerge. Hydroxyapatite (HA;  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ ) is widely used in tissue engineering, bone, and teeth repairs due to its biocompatible, biodegradable properties and analogy to natural bone [3]. HA is known as a good bone graft material with its high bioactivity offering a robust chemical bond with the native bone tissue. HA can be obtained from natural origins or by different synthesis methods. To expand the potential application of HA nanoparticles, polymer microfibers can be a good candidate. Surgical sutures, dialysis devices, wound dressings, and tissue engineering scaffolds are just a few of the medical applications for polymeric fibers. Engineered fibers for usage as drug delivery vehicles have evolved because of advances in polymer and drug delivery sciences. Over the last decade, there has been an increased development of therapeutically active fibers [4]. Microfluidic-based processes hold great potential for the synthesis of these microfibers. It is the technology of manipulating fluids in channels with diameters of tens of micrometers. Microfluidic systems have arisen as a unique new area of research in recent years because of their applicability in a wide range of domains, including chemistry, biology, medicine, and physical sciences [5]. These systems have some advantages that increase their attractiveness, like the use of a small amount of reagents, a high selectivity, being environment-friendly, and providing faster reactions by controlling flow rates [6]. In this communication, the synthesis of HA nanoparticles obtained using a capillary-based microfluidic device will be discussed, but also their incorporation into polymer microfibers using the same microfluidic device.

**Keywords:** Microfluidic, Hydroxyapatite, Nanoparticles, Microfibers

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# Thermal Properties of Polymers Obtained by Copolymerisation of o-, p-, m-carboxyphenylmaleimides and Styrene

Shahana Guliyeva<sup>1</sup>, Aygun Alikhanova<sup>2</sup>, Eldar Garayev<sup>1</sup>, Baxtiyar Mammadov<sup>2</sup>

<sup>1</sup>Azerbaijan Medical University, A.Gasimzadeh, 14, AZ1022, Baku, Azerbaijan

<sup>2</sup>Institute of Polymer Materials of the Ministry of Science and Education of the Republic of Azerbaijan, Sumgait, Azerbaijan, Az5004, S.Vurgun St.,124

E-mail:[guliyevashahana86@mail.ru](mailto:guliyevashahana86@mail.ru)

## Abstract

In this work, the thermal properties of polymers obtained by copolymerization of styrene with derivatives of ortho-, meta-, and para-carboxyphenylmaleimides were investigated. The thermal stability of the copolymers was evaluated using thermogravimetric analysis (TGA), differential thermal analysis (DTA), and other thermal analysis methods. The results show that the presence of carboxyl functional groups has a significant effect on the thermal stability of the polymers. These copolymers exhibit notable heat-resistant properties and are considered promising materials for high-temperature applications.

In recent years, the synthesis of polymeric materials with high thermal and chemical resistance has become one of the most important directions in scientific and industrial terms. In this regard, copolymerisation of maleimide derivatives with various monomers, especially with aromatic styrene, is an important research topic [1]. Carboxyphenylmaleimides are characterized by the presence of carboxyl functional groups and aromatic rings, which positively affect the thermal properties.

O-, p-, m-carboxyphenylmaleimides were synthesized and purified in vitro [2]. The radical copolymerisation process was carried out at 70°C using azobisisobutyronitrile catalyst. O-, p-, m-carboxyphenylmaleimides and styrene were mixed and copolymerized in different molar ratios. After completion of the reaction, the obtained copolymers were precipitated with methanol and dried. Thermogravimetric analysis (TGA) was carried out in the temperature range of 25-600°C, and the mass loss and decomposition temperature were determined. For instance, while polystyrene begins to degrade at around 330 °C, copolymers with 30 mol% CPMI showed initial degradation above 370 °C. According to the results of TGA, the decomposition temperature of copolymers containing o-, p-, m-carboxyphenylmaleimide is significantly higher than that of pure polystyrene. This is explained by the stabilizing effect of carboxyl and imide groups. Increasing the amount of carboxyphenylmaleimide increases the Tg value of the copolymers. This allows the materials to retain their shape and mechanical properties at high temperatures. This improvement is attributed to the presence of rigid imide and aromatic structures which resist thermal decomposition. Additionally, the carboxyl groups may contribute to hydrogen bonding or cross-linking under thermal stress.

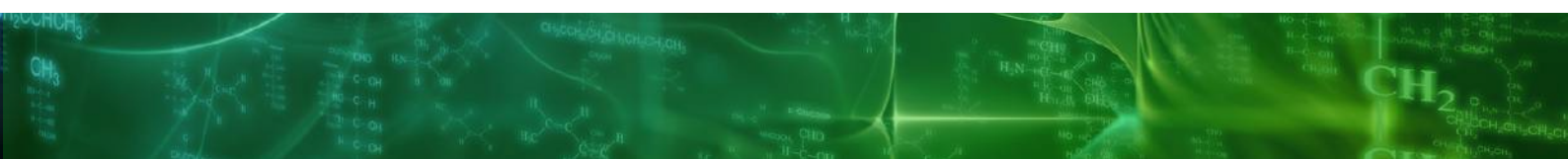
Polymers formed by styrene polymerization are stable at high temperatures. On the other hand, carboxyphenylimides can enter into certain reactions at high temperatures, but higher thermal stability can be achieved by copolymerization. The bonding between the polymers changes their properties to provide higher thermal stability. Polymers obtained by copolymerization of carboxyphenylmaleimides and styrene are widely used in various industries. High thermal and chemical stability allows these materials to be used in the electronic, automotive, pharmaceutical and building materials industries. At the same time, these polymers can be used in the production of high-quality varnishes, sheet materials, and household goods.

The study showed that copolymers synthesized on the basis of o-, p-, m-carboxyphenylmaleimides and styrene have high thermal stability. These materials can be evaluated as potential structural polymers for electronic, automotive and aerospace applications, especially those operating at high temperatures. The enhanced thermal stability and higher glass transition temperatures make these copolymers promising candidates for advanced engineering plastics and heat-resistant coatings. Further work may include exploring mechanical properties and post-functionalisation of the copolymers for specific applications.

**Keywords:** o-, p-, m-carboxyphenylmaleimides, styrene, copolymerisation, thermal properties.

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# Surface Modification of Upconversion Nanoparticles with Oligosarcosine for Bioimaging

Sakina Mammadova

2<sup>nd</sup> year PhD student CNRS – Institut Charles Sadron

Delphine CHAN-SENG; Christophe SERRA

E-mail: [sakina.mammadova@ics-cnrs.unistra.fr](mailto:sakina.mammadova@ics-cnrs.unistra.fr)

## Abstract

The encapsulation of inorganic nanoparticles in polymer particles and the attachment of polymers to the surface of inorganic nanoparticles have been studied in the development of hybrid materials based on polymers and inorganic nanoparticle.[1] A recently discovered type of luminescent nanoparticles called lanthanide-doped upconversion nanoparticles (UCNPs) is a good example of nanomaterials for the development of hybrid materials for bioimaging. UCNPs are able to convert near-infrared excitation into visible and ultraviolet emission and exhibit low phototoxicity, no conflict with the autofluorescence of biological systems, and high penetration depth of light in biological tissues. They present advantages as compared to organic dyes and quantum dots due to their sharp emission bandwidth, no photobleaching, and no photoblinking making them interesting nanomaterials for bioimaging.[2] However, the surface of UCNPs is hydrophobic limiting their use for biomedical applications. Surface modification of nanoparticles can be achieved by ligand exchange, encapsulation in a polymer shell, and surface-initiated polymerization.

While poly (ethylene glycol) is widely used in the field of biomedical applications, concerns have been raised due to the formation of antiPEG antibodies after multiple exposures. We proposed herein to introduce oligosarcosine[3], a hydrophilic polymer, as an alternative at the surface of UCNPs to render them suitable for bioimaging. In this communication, the synthesis of NaYF<sub>4</sub>:Yb<sup>3+</sup>, Er<sup>3+</sup> UCNPs by the co-precipitation method followed by a heat treatment step along with a strategy to introduce oligosarcosine chains at their surface will be discussed.

**Keywords:** upconversion nanoparticles; oligosarcosine; crystalline phase; co-precipitation; solid-phase synthesis.

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# Chitosan and Poly-N-vinylpyrrolidone-based Enterosorbents for Heavy Metals Removal

S. Fatullayeva<sup>1</sup>, N. Zeynalov<sup>1</sup>, D. Tagiyev<sup>1</sup>, D. Babayeva<sup>1</sup>, E. Nasiyyati<sup>1</sup>, L. Gulubayova<sup>1</sup>

<sup>1</sup>Catalysis and Inorganic Chemistry Institute named after acad. M. Nagiyev of Ministry of Science and Education of the Republic of Azerbaijan, Baku, Azerbaijan

E-mail: [sevafatullayeva@hotmail.com](mailto:sevafatullayeva@hotmail.com)

## Abstract

Heavy metals are considered persistent pollutants of the environment, which cause intoxication and various diseases, when accumulated in human organism [1]. Research is needed to develop methods of protection and treatment of their adverse effects. For this purpose, enterosorption was proposed as method of binding and removing various exogenous and endogenous toxic substances from the organism in the digestive tract using enterosorbents (oral sorbents). Polymer-based compounds are of great interest among enterosorbents aimed at purifying the internal environment of the organism from toxins. The aim of our research was to obtain and study new effective “smart” polymer enterosorbents with biospecific properties based on chitosan, poly-N-vinylpyrrolidone and their derivatives with “memory effect” for selective sorption of excess amounts of heavy metal ions from the human organism.

Analytical methods of analysis including FTIR, XRD, SEM, and TGA/DSC were used to determine the functional groups in the composition, crystallinity, structural changes on the surface, elemental content, and thermal stability of the synthesized samples of chitosan and poly-N-vinylpyrrolidone. In order to increase the solubility of chitosan, its quaternized sample was obtained by modifying it with 2-hydroxybenzaldehyde. Chitosan modification was carried out successfully, as evidenced by the data of FTIR, XRD, NMR, and thermal analyses. Then pure and modified chitosan, poly-N-vinylpyrrolidone samples were crosslinked using N,N'-methylenebisacrylamide (MBA) as a crosslinker [2, 3]. The crosslinked samples were analyzed using the above methods of analysis. The swelling behaviour of the obtained chitosan and poly-N-vinylpyrrolidone samples was also studied.

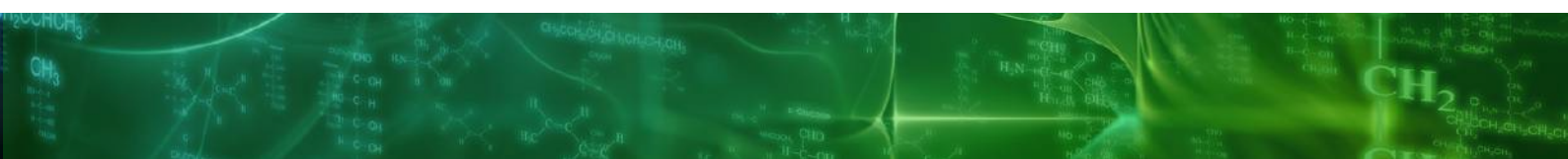
Due to non-toxicity, high biological activity, biocompatibility, and biodegradability, it is proposed to use chitosan, poly-N-vinylpyrrolidone and their derivatives as enterosorbents for the selective sorption of some heavy metal ions. Chitosan was modified to improve some properties; pure and resulting samples of chitosan were studied by FTIR, NMR, XRD, SEM, DSC and TGA. Thus, the FTIR spectra of pure and modified chitosan samples showed that reaction occurs via amino groups, and the intensified peak at  $1460\text{ cm}^{-1}$  pointed to the formation of quaternized chitosan, which was also confirmed by NMR data. Elemental composition showed increase in percentage of carbon in the quaternized sample, indicating modification of chitosan with new functional groups. TGA/DSC analysis showed a decrease in thermal stability of quaternized sample compared to pure chitosan one, and decrease in strength of intrachain interactions and crystallinity of the modified sample was also demonstrated. Crosslinked samples of chitosan and poly-N-vinylpyrrolidone were analyzed using the abovementioned methods and it has been established that crosslinking and swelling data of the synthesized samples were consistent with the literature data.

Current environmental situation in the world is cause of intoxication of living organisms. A method of cleansing the organism of toxic compounds using enterosorbents has been proposed as a promising way to solve this problem. It is proposed to use modified chitosan and poly-N-vinylpyrrolidone samples as enterosorbents for the heavy metal ions sorption. The sorption properties of the synthesized samples toward certain heavy metal ions and various factors affecting the sorption process will be studied.

**Keywords:** Chitosan, Poly-N-vinylpyrrolidone, Enterosorbent, Heavy metal ions.

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# Rambutan Leaf Extract Mediated Green Synthesis of Metal Nanoparticles for Antibacterial Applications

Nikitha Joy<sup>1</sup> and Mukunthan KS<sup>1</sup>

<sup>1</sup> Department of Biotechnology, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India  
E-mail: [Mukunthan.ks@manipal.edu](mailto:Mukunthan.ks@manipal.edu)

## Abstract

Nanotechnology, which deals with nanoparticles (1-100 nm), has become a prominent area of research in material science, with applications spanning from medicine to electronics. Metal nanoparticles, in particular, are gaining interest due to their unique properties, including high surface area, catalytic activity, and antimicrobial effects. Traditional chemical synthesis methods, while efficient, often involve toxic chemicals and non-eco-friendly by-products. This has led to increased interest in biological approaches, or "green nanotechnology," utilizing microorganisms and plants for nanoparticle synthesis. This study explores the use of Rambutan (*Nephelium lappaceum* L.) leaf extract for the green synthesis of silver, iron, and silver-iron bimetallic nanoparticles, aiming for an environmentally benign and potentially valuable route for nanoparticle production.

The leaves of Rambutan plant were dried, crushed, and extracted in distilled water. The resulting extract was used for qualitative phytochemical analysis to identify various compounds present. Silver nanoparticles were synthesized by mixing the extract with silver nitrate solution, while iron nanoparticles were synthesized using iron(II) sulfate heptahydrate solution. Bimetallic nanoparticles were synthesized by a similar method, combining both metal solutions. The synthesized nanoparticles were characterized using UV-Vis spectrophotometry, X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX). Antibacterial activity of the plant extract and nanoparticles was tested against several bacterial strains using the agar well diffusion method.

The phytochemical analysis of the Rambutan leaf extract revealed the presence of tannins, phlobatannins, saponins, flavonoids, terpenoids, carbohydrates, glycosides, and fats. UV-Vis spectroscopy confirmed the formation of silver nanoparticles (SPR peak at 450nm), iron nanoparticles (SPR peak at 250nm), and silver-iron bimetallic nanoparticles (SPR peaks at 225nm and 400nm). XRD analysis indicated the crystalline nature of silver and silver-iron bimetallic nanoparticles, with a face-centered cubic structure. SEM images showed the morphology of the synthesized silver and iron nanoparticles. EDX spectroscopy confirmed the presence of silver in the synthesized nanoparticles. Antibacterial activity testing demonstrated that the plant extract and synthesized nanoparticles exhibited inhibitory effects against *Staphylococcus*, *Bacillus*, *E. coli*, *Serratia*, and *Salmonella*.

This study successfully demonstrated the green synthesis of silver, iron, and silver-iron bimetallic nanoparticles using Rambutan leaf extract. The synthesized nanoparticles showed antibacterial activity, suggesting their potential application in developing novel antimicrobial agents. This environmentally benign approach offers a promising alternative to traditional nanoparticle synthesis methods.

**Keywords:** Nanoparticles, Green Synthesis, Antibacterial activity

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## C-glycosylflavones from the Aerial Part of *Silene Schafta* Growing in Azerbaijan

Khuraman Mustafayeva<sup>1</sup>

<sup>1</sup> Azerbaijan Medical University, Department of Pharmacognosy

E-mail: [xuraman\\_mustafayeva@yahoo.com](mailto:xuraman_mustafayeva@yahoo.com)

### Abstract

The aerial parts of *Silene schafta* Gmel. ex Hohen. (Caryophyllaceae), a perennial plant endemic to the Talysh mountainous region in the South of Azerbaijan, were investigated for their C-glycosylflavone content. The plant material was collected from Gunashly village in the Lerik district, air-dried, pulverized, and subjected to ethanolic extraction, followed by successive chromatographic purification steps including polyamide and silica gel column chromatography. A major flavone-rich fraction was isolated and analyzed by UV spectrophotometry, oxidative acid hydrolysis, and HPLC. The UV spectra showed characteristic absorption peaks for C-glycosylflavones; total flavonoid content was quantified as 2.9% in the  $\text{AlCl}_3$  colorimetric method with rutin as a reference standard. The HPLC analysis of flavonoids was carried out by comparison with the relevant standards of schaftoside, vitexin, isovitexin and rutin, utilizing a calibration curve generated with LC Postrun Calibration software. The analysis was executed in three repetitions, and statistical calculations were carried out. The HPLC analysis allowed us to measure the content of schaftoside, which was found to be the major compound in the extract. This study highlights the presence of biologically significant C-glycosylflavones in *S. schafta*, contributing to the chemotaxonomic profiling of the Caryophyllaceae family and supporting the phytochemical potential of this underexplored species.

**Keywords:** *Silene schafta*, C-glycosylflavones, HPLC, schaftoside.

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# Graphene Oxide-Based Composites for the Removal of Organic Pollutants from Water

Narinj Taghiyeva <sup>1,2</sup>, Maurice Millet <sup>2</sup>, Ulviyya Hasanova <sup>3</sup>

<sup>1</sup> CPML (UFAZ) -Azerbaijan State Industrial and Oil University - Azadliq Avenue, 20 – Baku; narinj.taghiyeva@etu.unistra.fr

<sup>2</sup> ICPEES (UMR 7515 CNRS) – CNRS and University of Strasbourg – 25 rue Becquerel – 67087 Strasbourg Cedex 8 – France; mmillet@unistra.fr

<sup>3</sup> BSU (ICESCO Biomedical Materials Chair)- Baku State University -Z.Khalilov Str. 23 AZ1148, AZ1073/1;

E-mail: [u.alimammad@gmail.com](mailto:u.alimammad@gmail.com) [narinj.taghiyeva@ufaz.az](mailto:narinj.taghiyeva@ufaz.az)

## Abstract

A cost-effective and uncomplicated adsorption approach can effectively remove pollutants and hazardous compounds. Carbon-based nanomaterials, including carbon nanotubes, fullerenes, graphene, and graphene-based composites, have garnered considerable interest because of their extensive potential in various applications [1].

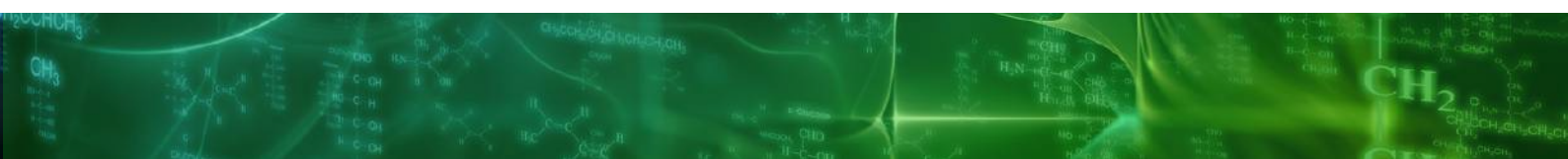
This study aimed to examine the effectiveness of functionalized graphene oxide (GO) nanosheets with Schiff Base and decreased Schiff Base in removing pesticides from aqueous solutions. The researchers used covalent functionalization techniques to modify the nanostructures. The modified nanostructures were then analyzed using solid-state nuclear magnetic resonance (SSNMR), Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and transmission electron microscopy (TEM) [2].

A selection of pesticides, including Trifluralin, Acetochlor, Chlorothalonil, Cyprodinil, Dimethomorph, and Epoxiconazole, were chosen as representative pollutants to analyze their adsorption on graphene oxide (GO) and its covalently functionalized derivatives. The study successfully demonstrated the covalent grafting of Schiff Base and decreased Schiff Base moieties onto GO, resulting in functionalization. Effective three-dimensional adsorbents were demonstrated for the nanostructures produced by covalent functionalization, which involved ester and perhaps amide bond creation, epoxy ring opening, and other processes. These materials offer a hopeful approach for eliminating pesticides from water-based treatments.

**Keywords:** Graphene oxide-based adsorbents, Covalent functionalization, Organic pollutants.

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## Hybrid Chiral Plasmonic Assemblies for Sensing

Sevil Veysalova, Olivier Felix, Matthias Pauly

Université de Strasbourg, CNRS, Institut Charles Sadron, Strasbourg, France

E-mail: [sevil.veysalova@etu.unistra.fr](mailto:sevil.veysalova@etu.unistra.fr); [olivier.felix@ics-cnrs.unistra.fr](mailto:olivier.felix@ics-cnrs.unistra.fr); [matthias.pauly@ics-cnrs.unistra.fr](mailto:matthias.pauly@ics-cnrs.unistra.fr)

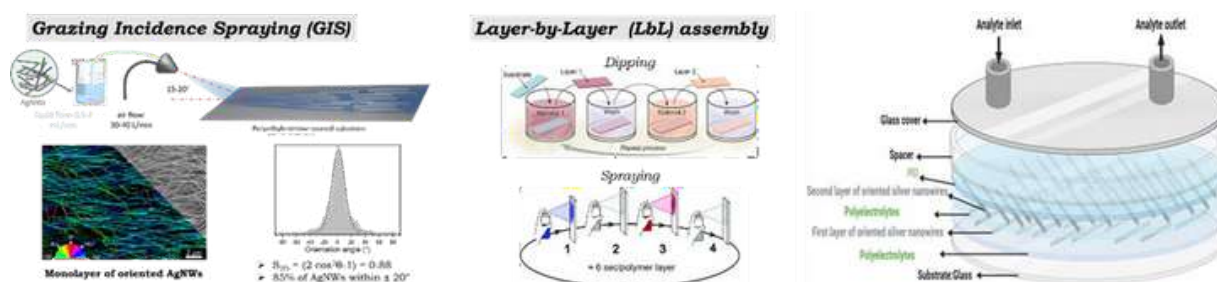
### Abstract

Chirality[1] is a long-standing area of research in the fields of biology and chemistry because it determines important aspects of a molecule's interaction and reactivity with other chiral molecules. Enantiomer discrimination[2] is important in drug development because one enantiomer can be therapeutic while the other can be harmful. Additionally, it is being discussed that chirality is fundamental to the origin of life, and without it, there would probably be no life[3,4].

Circular dichroism spectroscopy is widely used to detect chiral molecules. However, conventional CD spectroscopy suffers from weak signals at the molecular level and limited sensitivity. In addition, conventional CD measurements often require high concentrations of (bio)molecules, which limits practical applications. Recent theoretical and experimental studies have shown that the chiral properties of (bio)molecules can be determined using plasmonic chiral metasurfaces (PCM)[5-9] consisting of noble metal nanoparticles.

PCM are good candidates for biosensors due to their low cost, adaptability, faster fabrication and miniaturized form. In fact, recent studies have reported the design and fabrication of various plasmonic chiral metamaterials, mainly for the detection of enantiospecific interactions, based on plasmonic-driven amplification of naturally occurring CD signals. There is limited work on chiral plasmonic elements, mostly with chiral nanoparticles dispersed in solution, that detect changes in the surrounding medium resulting from the presence of the target analyte. However, instead of dispersing chiral nanoparticles in solution, chip-based sensing of chiral nanoparticles organized in long-range order that can be integrated into photonic circuits is more suitable for point-of-care devices. It will offer great advantages in terms of repeatability, miniaturization, integration with microfluidic components, selective binding, improved optical properties, enhanced sensitivity, real-time monitoring, better control and stability against different solvent and salt concentrations, that can cause precipitation when colloidal nanoparticles are used instead. In addition, the chipbased format would allow for simple washing steps during analytical procedures, even with complex biological samples, rather than simpler protein solutions.

Silver and gold are commonly preferred plasmonic nanoparticles due to their biocompatibility and stability. In our research, we use silver nanowires to construct plasmonic chiral metasurfaces. To achieve precise alignment of the silver nanowires, we use Grazing Incidence Spraying (GIS)[10,11]. In addition, we use Layer-by-Layer (LbL) assembly to build multilayer structures. Recently, we have integrated a flow cell on our plasmonic chiral metasurface (PCM). Using microfluidics, we have performed tests to evaluate the stability, sensitivity and repeatability of our system. As a result, we have achieved a highly sensitive, reusable and stable system. We have a sensitivity of up to 20 000 mdeg/RIU.





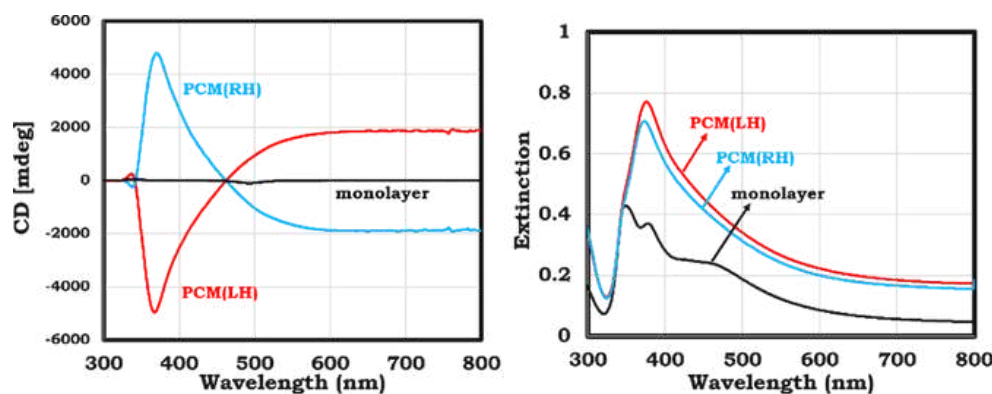


Figure 1. Grazing Incidence Spraying, Layer by Layer Assembly, Integrated flow cell, Circular dichroism and extinction spectra of plasmonic chiral metasurface (PCM)

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## Analysis of Trap Parameters Associated with Intermediate Luminescence Peaks of Quartz

A. Ahadov<sup>a</sup>, S. Mammadov<sup>a</sup>, M. Gurbanov<sup>a</sup>, A. Abishov<sup>a</sup>, A. Ahadova<sup>a</sup>

<sup>a</sup> Institute of Radiation Problems, Ministry of Science and Education, Azerbaijan, 9, B. Vahabzade str.

E-mail: [a.ahadov@irp.science.az](mailto:a.ahadov@irp.science.az)

### Abstract

Quartz, a ubiquitous mineral formed across diverse geological environments (igneous, metamorphic, and sedimentary), serves as a critical tool for probing the properties of quartz-bearing materials in geological and mineralogical studies [1][2]. The initial rise (IR) method plays a crucial role in determining the activation energies of electron levels in thermoluminescence (TL) glow curves.

This research focuses on the thermoluminescence parameters associated with intermediate luminescence peaks in quartz. By employing isothermal decay analysis, TL difference curves, and the initial rise method, we aim to identify and characterize the trap structures contributing to the TL signal. The results indicate that the TL glow peaks do not conform strictly to first- or second-order kinetics, suggesting a more complex trapping and recombination mechanism.

TL measurements were performed using a Harshaw 3500 manual reader, where the samples were heated to  $T_{stop}$  and held at that temperature for 100 seconds to observe isothermal decay. Initially, the samples were irradiated at ambient temperature with a  $^{60}\text{Co}$  source at a dose rate of 1.6 Gy/s, to a dose of 3kGy, followed by heating at 500°C for a duration of two hours. This procedure was repeated three times, with the hypothesis that the deep traps would be filled, thereby preventing them from competing with the intermediate level of traps for free electrons.

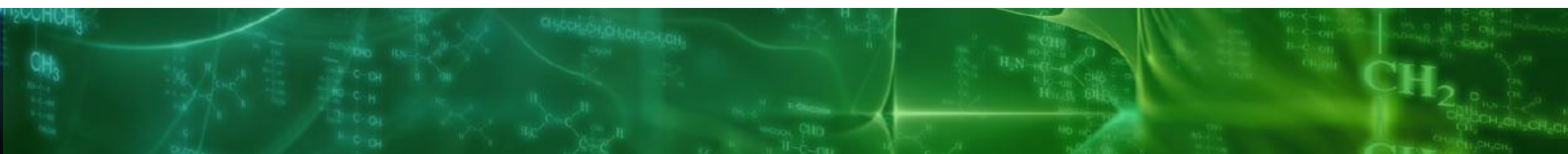
Analysis of TL difference curves with different  $T_{stop}$  temperatures, obtained by digitally subtracting the residual TL signal, facilitates the identification of three stable  $T_m$  stability regions at 145°C, 170°C, and 235°C. The glow curve obtained following isothermal cleaning at ten different temperatures, ranging from 90°C to 170°C, was analyzed to calculate the activation energy using the initial-rise method. The results indicate that the apparent activation energy decreases as the segments of the glow curve are cleaned at increasing  $T_{stop}$  temperature.

The study also highlights the impact of deep electron traps and retrapping effects on the determination of activation energy. The findings contribute to a more accurate understanding of TL kinetics in quartz, with implications for dosimetric applications.

**Keywords:** isothermal decay, quartz, activation energy, frequency factor, thermoluminescence

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## Online Production of Polyelectrolytes Microfibers

Vugar Khalilov<sup>1</sup>, Christophe Serra<sup>1</sup>, Madeline Vauthier<sup>1</sup>

<sup>1</sup> Institut Charles Sadron

E-mail: [vugar.khalilov@ics-cnrs.unistra.fr](mailto:vugar.khalilov@ics-cnrs.unistra.fr)

### Abstract

Polyelectrolyte complexes (PECs) are formed by electrostatic interaction of two oppositely charged polyelectrolytes, in our case poly(sodium 4-styrenesulfonate) (PSS) and poly(diallyldimethylammonium chloride) (PDADMAC). The physical state of PECs can be solid aggregates, liquid coacervates or dissolved solutions. The former occurs at low ionic strengths or in solution with a defined ionic strength, while the second undergoes phase separation at intermediate salt concentrations[1]. Enhancement of strong electrostatic interactions will induce the formation of solid PEC aggregates. These aggregates will respond to re-dissolution in highly ionic environments. Microfluidic systems allow precise manipulation of PECs, allowing the control of the formation of particles and fibers that can be used in drug delivery devices, wastewater treatment and tissue engineering.

For this particular work, we designed a single-capillary microfluidic method for the controlled fabrication of PEC microparticles and microfibers. In our approach, we use a “backward” formation method where a flow of polyelectrolyte solution (PSS/PDADMAC in NaCl) is injected into a continuous water flow. A wide range of flow rates and capillary sizes were studied. The polyelectrolyte dispersed phase was a solution containing 20% w/w of polyelectrolyte in 4.75M NaCl.

The shear forces resulting from the flow rate of the continuous phase and NaCl content were found to be important factors regarding PEC morphology. With high shear rate, microfibers with a diameter around 20 to 100 +/- 5µm were produced. For high dilution conditions, where the salt concentration between the two phases was quite large, the formation of fibers was favored despite the high degree of shear. On the other hand, introducing the salt into the continuous phase enabled the shift from fiber to microparticles. Under moderate shear, irregularly shaped microparticles were formed, and salt exclusion results in the formation of distinct "head-tail" particles. These morphological changes were confirmed by digital microscopy

This study showed that PECs of different morphologies could be obtained with a single microfluidic setup, by changing phases' flow rates and composition of the continuous phase. Microfibers' formation was favored under low-shear conditions, whereas high-shear yielded to the production of microparticles. These findings illustrate the promise and versatility of microfluidic synthesis in the design of PEC materials for use in medicine, environmental monitoring and food.

**Keywords:** Polyelectrolyte complexes, PSS, PDADMAC, Microfluidics

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# Usage of Modified $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Catalysts for the Conversion of Alcohols to Hydrocarbons

Farid Mammadov, Nushaba Aliyeva

Named after academician Y.H. Mammadaliyev of the Ministry of Science and Education Institute Of Petrochemical Processes

E-mail: [mammadovfarid43@gmail.com](mailto:mammadovfarid43@gmail.com)

## Abstract

The catalytic transformation of alcohols into hydrocarbons is a promising route for sustainable fuel and chemical production. In this study,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> was modified with transition metal species including MnO, ZrO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> + CoO, Co(NO<sub>3</sub>)<sub>2</sub>, and FeCl<sub>3</sub> to improve its catalytic performance for alcohol-to-hydrocarbon conversion. Catalysts were synthesized using wet impregnation methods and characterized using X-ray diffraction (XRD), differential thermal analysis (DTA), and X-ray fluorescence (XRF). Catalytic activity tests using ethanol and isopropanol revealed enhanced conversion and product selectivity in the C<sub>4</sub>-C<sub>10</sub> hydrocarbon range. Co- and Mn-based modifications led to the most significant improvements in yield and selectivity, while FeCl<sub>3</sub> and ZrO<sub>2</sub>-containing systems exhibited unique cracking and chain-growth behavior. These findings demonstrate the versatility of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> as a support and the critical influence of transition metal dopants in designing selective and robust alcohol-to-hydrocarbon catalysts.

With increasing demand for renewable and sustainable energy sources, the conversion of biomass-derived alcohols into hydrocarbons has gained significant attention [1]. Among various catalyst supports,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> remains a widely used material due to its high surface area, thermal stability, and acidic properties [2]. However, its intrinsic catalytic activity in alcohol conversion processes is limited. Modification with transition metals offers a pathway to enhance its performance by introducing redox functionality, altering acidity, and tuning product selectivity [3].

This work investigates the effect of incorporating MnO, Co(NO<sub>3</sub>)<sub>2</sub>, FeCl<sub>3</sub>, and ZrO<sub>2</sub>-CoO mixtures into the  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> framework. These modifications were chosen based on their known catalytic roles in deoxygenation, cracking, and chain-growth processes in hydrocarbon synthesis [4,5].

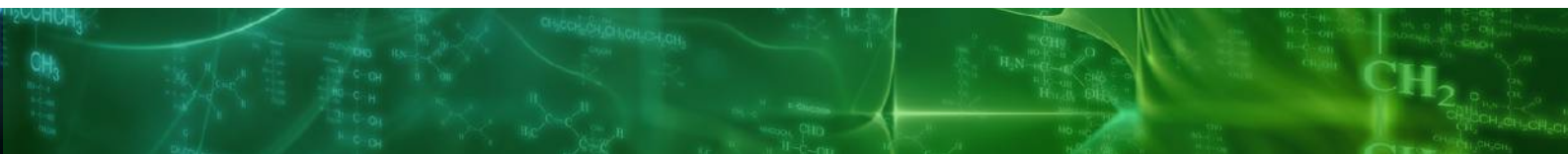
**2.1 Catalyst Preparation**  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> was modified by wet impregnation with aqueous solutions of Mn(NO<sub>3</sub>)<sub>2</sub>, Co(NO<sub>3</sub>)<sub>2</sub>, FeCl<sub>3</sub>, and a combination of ZrO(NO<sub>3</sub>)<sub>2</sub> with Co(NO<sub>3</sub>)<sub>2</sub>. After impregnation, the catalysts were dried at 110 °C for 12 hours and calcined in air at 500 °C for 4 hours.

**2.2 Characterization Techniques** XRD analysis was conducted using Cu K $\alpha$  radiation to identify crystal phases. DTA was used to study thermal behavior and transformation temperatures. XRF analysis determined the elemental composition and dispersion of the active metals.

**2.3 Catalytic Testing** Catalytic performance was evaluated in a fixed-bed flow reactor at temperatures ranging from 300 to 400 °C. Ethanol and isopropanol were used as model alcohol feedstocks. Conversion and product selectivity were measured by gas chromatography (GC).

**3.1 Catalyst Characterization** XRD confirmed the formation of highly dispersed metal oxides on the alumina surface. Co- and Mn-containing catalysts showed no bulk crystalline phases, indicating strong metal-support interaction. DTA revealed exothermic peaks associated with metal nitrate decomposition and formation of stable oxide phases. XRF analysis confirmed the successful incorporation of metal species in the desired ratios.

**3.2 Catalytic Performance** All modified catalysts showed higher alcohol conversion compared to unmodified  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>. MnO- and Co-based catalysts exhibited superior performance, with ethanol conversions >95% and hydrocarbon selectivity in the C<sub>3</sub>-C<sub>7</sub> range exceeding 70%. The FeCl<sub>3</sub>-modified catalyst promoted deeper cracking, resulting in lighter hydrocarbons and CO formation. ZrO<sub>2</sub>-CoO systems favored longer-chain hydrocarbons, likely due to enhanced acidity and cooperative redox behavior.



**3.3 Effect of Transition Metals** The role of each metal in modulating the catalytic behavior was evident. Co promoted dehydrogenation and olefin formation, Mn facilitated oxygen removal and selectivity control, while Fe and Zr enhanced cracking and chain propagation, respectively. These results align with previous reports highlighting the role of transition metals in hydrocarbon reforming and deoxygenation reactions [3,5].

**4. Conclusion** Transition metal-modified  $\gamma\text{-Al}_2\text{O}_3$  catalysts demonstrate significant improvements in alcohol-to-hydrocarbon conversion. The nature and loading of the metal dopant critically influence product distribution, selectivity, and catalyst stability. This study confirms that tailored metal modifications on  $\gamma\text{-Al}_2\text{O}_3$  provide a versatile platform for designing efficient catalysts for renewable hydrocarbon production.

**Keywords:**  $\gamma\text{-Al}_2\text{O}_3$ , TGA, Hydrocarbons

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## Oxidative Desulfurisation of Vacuum Gas Oil in the Presence of Ozone

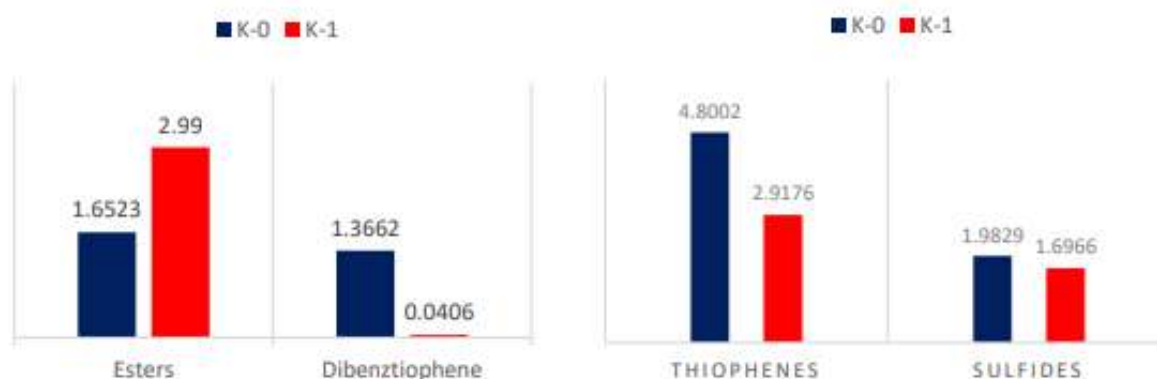
Khamis Abiyev<sup>1</sup> and Elvira Guseinova<sup>1</sup>

<sup>1</sup> Azerbaijan State Oil and Industry University

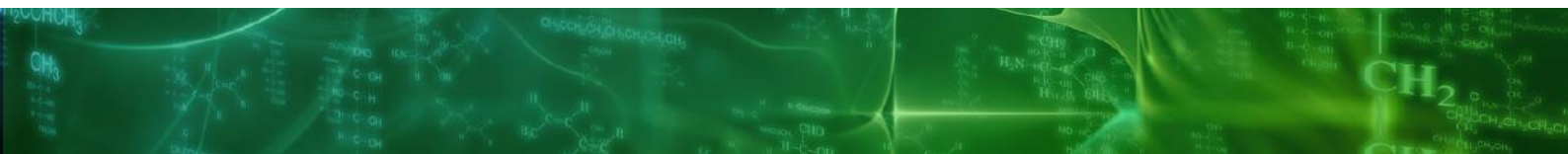
E-mail: [xamisabiyev123@gmail.com](mailto:xamisabiyev123@gmail.com)

### Abstract

In recent years, environmental protection has emerged as one of the most pressing global priorities. Within the oil refining industry, however, this issue remained largely neglected for many decades. As a result, the harmful substances released into the environment from petroleum products produced at refineries have caused significant and well-documented damage to ecosystems and public health. It is well-known that crude oil, used as the primary raw material in refining, contains sulfur and sulfur-containing compounds. These compounds play a significant role in both the corrosion of processing equipment and in causing environmental and biological harm. To mitigate such irreversible damage, crude oil must undergo preliminary treatment stages prior to processing. Nonetheless, conventional purification techniques are often insufficient to reduce the sulfur content in raw materials to the desired levels. Consequently, petroleum products obtained through these processes must undergo additional, more costly, post-treatment steps to meet environmental standards. This study investigates a novel method for desulfurising vacuum gas oil (VGO), which serves as a key feedstock in the capital-intensive catalytic cracking process. The proposed method involves ozone-assisted desulfurisation, offering a lower-cost alternative to traditional techniques. Using this approach, it was observed that sulfur-containing compounds in VGO can be transformed, via atomic oxygen, into intermediates that are more readily separable in subsequent processing stages. As noted, the separation of thiophenic and sulfide compounds in VGO typically requires extreme operating conditions and significant financial expenditure. In contrast, the ozonation method has demonstrated a substantial reduction in the concentration of these compounds. In the untreated VGO sample (referred to as K-0), the concentrations of thiophenes and sulfides were approximately 4.9% and 2%, respectively. Additionally, the sample contained about 1.7% of ether compounds and 1.4% of dibenzothiophenes. Following just 15 minutes of direct ozonation using an ozone generator, the processed VGO sample (referred to as K-1) exhibited a decrease in thiophenic compounds to approximately 2.9%, representing a 41% reduction. The concentration of sulfides in the K-1 sample also decreased to 1.7%, corresponding to a 14% reduction compared to K-0. Due to the active participation of atomic oxygen in the ozonolysis process, the concentration of oxygen-containing ether compounds in the K-1 sample increased to nearly 3%—a significant rise compared to K-0. Meanwhile, the concentration of dibenzothiophenes dropped dramatically, showing a 98% reduction to just 0.04%.



**Keywords:** Oxidative Desulfurisation, Ozone, Vacuum Gas Oil.





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## Modification Of Waste Thermoplastics With Amide Group Functionalized Co-Oligomers

Tamerlan Shirinov<sup>1</sup> and Tamilla Naibova<sup>2</sup>

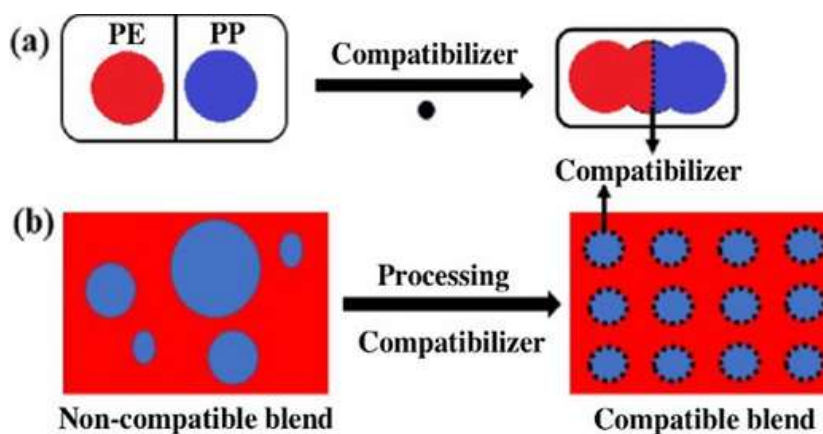
<sup>1,2</sup> Azerbaijan State Oil and Industry University

E-mail: [Tshirinov61@gmail.com](mailto:Tshirinov61@gmail.com) [Ntamilla51@gmail.com](mailto:Ntamilla51@gmail.com)

### Abstract

Polyethylene (PE) and polypropylene (PP) are widely used thermoplastics, but their extensive use creates significant recycling challenges. Found together in mixed waste streams, PE and PP are immiscible due to their differing chemical structures, preventing homogeneous blending [1-2]. Separating them before recycling is complex, energy-intensive, and often impractical [3]. Conventional methods like density-based sorting or solvent extraction are inefficient for large-scale processing, leading to significant waste ending up in landfills or incineration, exacerbating environmental pollution [4]. In this work, we address this challenge by exploring the use of compatibilizers—chemical additives designed to improve the interfacial adhesion between immiscible polymers. Compatibilizers function by reducing interfacial tension and promoting the formation of stable blends with enhanced physicochemical and mechanical properties. Specifically, we synthesized co-oligomers and functionalized them with amide-containing groups to create a tailored compatibilizer for polyethylene (PE) and polypropylene (PP) blends. The effectiveness of these amide group-functionalized co-oligomers was evaluated using a range of analytical techniques, including Fourier transform infrared (FTIR) spectroscopy, differential scanning calorimetry (DSC), melt flow index measurements, swelling tests, and scanning electron microscopy (SEM). FTIR spectroscopy confirmed the successful functionalization of the co-oligomers, while DSC analysis indicated improvements in thermal stability and crystallinity. Melt flow index measurements revealed increased viscosity, suggesting enhanced mechanical strength, and swelling tests demonstrated greater resistance to solvents. SEM analysis provided direct visual evidence of improved interfacial adhesion, showing a more homogeneous morphology with reduced phase separation in the compatibilized blends. These findings collectively demonstrate that the compatibilized blends exhibit superior mechanical, thermal, and chemical performance, making them suitable for high-value applications. A graphical representation of this compatibilization process and its effects on the PE/PP blend is provided in the graphical abstract.

**Graphical Abstract** - A visual representation of the compatibilization process for polyethylene (PE)/polypropylene (PP) blends using amide group-functionalized co-oligomers, highlighting improved interfacial adhesion and compatibility.



As illustrated in the graphical abstract the amide group-functionalized oligomers act as compatibilizers by interacting with both the polyethylene (PE) and polypropylene (PP) phases, reducing interfacial tension and promoting stronger adhesion between the immiscible polymers.

**Keywords:** Polyethylene, polypropylene, oligomer, modification, recycling.

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## Research of Antioxidant and Biological Activity of the Flavonoids from *limonium Caspiu*

E.A.Garayev\*, S.A.Pashayeva, L.A.Ahmadova, Sh.B. Aliyeva

Azerbaijan Medical University

E-mail:eldargar@mail.ru

### Abstract

Flavonoids are natural compounds widely found throughout the plant world. These substances have strong antioxidant properties. Therefore, they are of great importance for health. Flavonoids strengthen defense mechanisms by reducing oxidative stress and play an important and indispensable role in the prevention of many diseases. From this perspective, the reason why flavonoids have anti-inflammatory, anti-cancer, antibacterial, antiviral, etc. effects is clear. Currently, the study of the pharmacological effects of these substances has gained wide scope due to their importance for new therapeutic approaches. The fact that flavonoids have various biological effects makes their use both as natural food additives and as medicines relevant.

Flavonoid containing plants are widespread in the flora of Azerbaijan. *Limonium caspium* (Willd.) P.Fourn. (Plumbaginaceae) is also one of the flavonoid containing plants widely distributed in our republic. In our study, the antioxidant properties of myricetin, myricitrin, myricetin-3'-O-sulfate flavonoids obtained from the roots of this plant (which is a natural source of flavonoids) were studied in vitro and their biological activities were studied in silico. Myricetin has been widely distributed in nature. Myricetin-3'-O-sulfate is less common than myricetin flavonoid, but its semi-synthetic obtaining from myricetin can be carried out in a simple way.

First, flavonoids were individually obtained from the plant raw. For this, the roots of the plant were extracted by maceration with 80% ethanol. After concentration, the obtained extract was purified with chloroform. Myricetin, myricitrin and myricetin-3'-O-sulfate were obtained from the purified extract by sequentially treating with ethyl acetate-hexane (1:1.4) mixture, ethyl acetate and n-butanol. The DPPH method was used to determine the antioxidant activity of flavonoids. As a result of the studies, it was determined that all three substances have a strong antioxidant effect. During the DPPH analysis of the substances, IC<sub>50</sub> antioxidant activity indicators were calculated using the formula  $Y=C \cdot X^2+B \cdot X+A$  (where  $Y=50$ ). It was determined that the antioxidant index was 7.81 µg/ml for myricetin, 6.34 µg/ml for myricitrin and 6.2 µg/ml for myricetin-3'-O-sulfate. The antioxidant index of gallic acid, which was taken as a positive control, was 3.48 µg/ml.

PASS Online program was used to investigate the biological activity expectations of the substances. Myricetin has high antineoplastic (92.4%), anti prostate cancer (86.8%), antimutagenic (78.3%), myricitrin (99.0%) and myricetin-3'-O-sulfate (99.1%) have high hemostatic activities. The toxicity properties of the substances were predicted using ProTox 3.0 program and it was determined that they belong to the weak toxicity classes. Predicted Toxicity Class of myricetin is 3, myricitrin and myricetin-3'-O-sulphate are 5.

Physicochemical Properties, Water Solubility, Pharmacokinetics, Lipophilicity, Druglikeness, Medicinal Chemistry parameters were comparatively studied for all three substances using SwissADME and ADMETlab 3.0 software. According to druglikeness indicators, myricetin, myricitrin and myricetin-3'-O-sulfate fully comply with the Ghose and Pfizer rule. As a result of the conducted studies, it can be concluded that these substances have the prospect of being used as medicinal substances in the future. Research continues in this direction.