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14-17 September, 2022 ALBANIA

6th International ISCMP

JOINT SCIENCE CONGRESS OF MATERIALS AND POLYMERS

BOOK OF ABSTRACTS & PROCEEDINGS

EDITORS

Ayhan ORAL, Ph.D.
Oğuz GÜRSOY, Ph.D.
Arianit REKA, Ph.D.

14-17 September, 2022 ALBANIA

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In loving memory of our dear colleague and friend

Dr. Hakan Bilgili

His family lost a great son, and our scientific community lost a great friend, scientist, and collaborator.

You will be missed and never forgotten

ISCMP 2022

VI. International Joint Science Congress of Materials & Polymers
September 14-17, 2022 Durres, Albania

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VI. International Joint Science Congress of Materials and Polymers
September 14 – 17, 2022, Durres, Albania

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WELCOME ADDRESS

Dear Colleagues,

The International Joint Science Congress of Materials and Polymers (ISCMP), which is organized with the aim of sharing scientific developments related to materials science and technology with a wide range of stakeholders, has been held every year since 2017. Following the first ISCMP (Ohrid, North Macedonia) in 2017, the Congress was successfully held in Durres, Albania (ISCMP 2018), Pristina, Kosovo (ISCMP 2019), Tetovo, North Macedonia (ISCMP 2020), and Burdur, Turkey (ISCMP 2021).

The sixth of the congress (ISCMP 2022), which will be organized by Canakkale Onsekiz Mart University (Turkey) in collaboration with the Chemists Society (Turkey), Burdur Mehmet Akif Ersoy University (Turkey), Turkish Cooperation and Coordination Agency (Turkey), Agriculture University of Tirana (Albania), University of Tetovo (North Macedonia), University of Prishtina (Kosovo), University of New York Tirana (Albania), Society of Chemists and Technologists of Macedonia, Tunisian Chemical Society, the Chemical Society of Pakistan, and The Turkish Maarif Foundation (Albania) will be helded in Durres, Albania.

It is our pleasure to invite you to the 6th International Joint Science Congress of Materials and Polymers, which will be held in Durres, Albania, 14-17 September 2022.

The subjects of the Congress include all the areas of materials science and technology and of different related fields (e.g., chemistry, energy, food science, and technology). The official language of the Congress is English. The abstracts and full texts will undergo double-blind peer review and will be published in the congress book of abstracts/proceedings, which will be included in EBSCO host. Optionally, the full texts could be published in different supported journals after being subjected to regular publication processes of the journals. A congress special issue will be published in Open Chemistry (SCI-Expanded, Impact Factor: 1.977, De Gruyter Open Access). The unpresented abstracts and the full texts will not be included in the congress book of abstracts/proceeding and will not be published in the journals' special issues.

Congress attendees will have the chance to benefit from scientific exchange with colleagues from different backgrounds during either the formal activities or the informal meetings. They will also be able to see Albania's natural and historical beauties. Hereby, we would like to thank everyone that has supported us by accepting our invitation to be an invited speaker and to organize workshops. We would also like to thank all the public and private sector organizations that have provided financial support for our congress.

We hope you will enjoy the meeting and we are looking forward to welcoming you to Albania!

Prof. Ayhan Oral & Prof. Oğuz Gürsoy

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ISCMP 2022 – SCIENTIFIC PROGRAM

September 15, 2022 (Thursday)

09:00-12:00	Registration	
10:00-11:00	Opening Remarks	
Session 1	**Chair: Metin Hayri Acar, Ph.D.**	
11:00-11:30	**Yusuf Ziya Menceloğlu**, *Ph.D.*	Future in plastics industry: sustainability and nanotechnology ***(INVITED SPEAKER)***
11:30-13:00	***OPENING COCKTAIL***	
13:00-13:20	Kledi Xhaxhiu	Composite photosensors of polyazulene and mixed valence inorganic solids
13:20-13:40	Ahmed Jashari	Optimization of the Hantzsch reaction and synthesis of some novel tiazolyl-hydrazinylidene-chroman-2,4-diones as highly potent anti-cancer drugs
13:40-14:00	Avni Riza Berisha	Adsorption of pesticides on 2D carbon nanomaterials. An experimental and theoretical study
14:00-15:30	Lunch	
Session 2	**Chair: Kledi Xhaxhiu, Ph.D.**	
15:30-16:00	**Metin Hayri Acar**, *Ph.D.*	Development of breast phantom ***(INVITED SPEAKER)***
16:00-16:30	**Ilaria Fratoddi**, *Ph.D.*	Thiol functionalized noble metal nanoparticles: a versatile platform for advanced applications ***(INVITED SPEAKER)***
16:30-16:50	Piotr Koczon	Spectral qualification and quantification of selected microorganisms growing on different materials
16:50-17:30	Coffee Break	
09:00-18:00	***POSTER SESSION***	

ISCMP 2022 – SCIENTIFIC PROGRAM

September 16, 2022 (Friday)

Session 3	**Chair: Yusuf Ziya Menceloğlu, Ph.D.**	
09:00-09:30	**Klaus Bente**, *Ph.D.*	Minerals (clay) for treatments of contaminated wastewater environmental protection ***(INVITED SPEAKER)***
09:30-09:50	Veprim Thaçi	A theoretical and experimental study of adsorbent dye removal from (2E, 5E)-2,5- bis[(4-dimethylamino) benzylidene] cyclopentanone using diatomaceous earth as an adsorbent
09:50-10:10	Vllaznim Mula	Development of a method for the detection and characterization of volatile organic compounds in the atmosphere using passive sampling
10:10-10:30	Ayhan Oral	Effect of phenyl ethyl alcohol on crystallinity and biodegradation of poly (lactic acid)
10:30-11:00	Coffee Break	
Session 4	**Chair: Ahmed Jashari, Ph.D.**	
11:00-11:30	**Jasmina Petreska Stanoeva**, *Ph.D.*	Risk assessment of natural toxic pyrrolizidine alkaloids in the food chain ***(INVITED SPEAKER)***
11:30-12:00	**Ilir Mazreku**, *Ph.D.*	In vivo evaluation of carboxylated graphene oxide's impact on oxidative stress and other biochemical markers in snail Helix locurum ***(INVITED SPEAKER)***
12:00-12:20	Seda Çetintaş	Evaluation of the effect of glucose fatty acid esters on thermal degradation of vegetable-based oils
12:30-14:30	Lunch	
Session 5	**Chair: Klaus Bente, Ph.D.**	
14:30-15:00	**Valentin Mirceski**, *Ph.D.*	Advanced pulse-voltammetric techniques ***(INVITED SPEAKER)***
15:00-15:20	Yusuf Dilgin	Fabrication of a novel colorimetric glucose biosensor using copper(II)-neocuproine as chromogenic oxidant and glucose dehydrogenase immobilized magnetite nanoparticles
15:20-15:40	Mustafa Akın	Determination of antimicrobial, DPPH scavenging, and tyrosinase inhibitory activities of *Thymus vulgaris*, *Helichrysum arenarium*, and *Rosa damascene* Mill. ethanol extracts
15:40-16:10	**Halil İbrahim Çiftçi,** *Ph.D.*	Development of novel strategies for eradication of HIV-1 using structural and computational analysis ***(INVITED SPEAKER)***
16:10-16:30	Coffee Break	
09:00-18:00	***POSTER SESSION***	

ISCMP 2022 – SCIENTIFIC PROGRAM

September 17, 2022 (Saturday)

Session 6	**Chair: Arianit Reka, Ph.D.**	
10:00-10:30	**Neven Duic**, *Ph.D.*	Energy transition and material needs ***(INVITED SPEAKER)***
10:30-10:50	Ertuğrul Şahmetlioğlu	Highly flexible binder-free supercapacitor electrode based on carbon material
10:50-11:10	Fatma Kılıç Dokan	Quantum dots functionalized egg viol derived carbon and strontium oxide for high performance zinc ion hybrid supercapacitor
11:10-12:00	***CLOSING REMARKS***	
12:30-14:00	Lunch	
14:30-	***SOCIAL ACTIVITY***	

ISCMP 2022 - POSTER PROGRAM

September 15, 2022

NO	PRESENTER	TITLE
1	Oğuz Gürsoy	Some physicochemical, rheological, antioxidant, microbiological and sensory properties of kefirs with propolis at different ratios
3	Gülen Türker	Green seaweed *Ulva rigida* extracts as potential antioxidant ingredients in Yoghurt
5	Vllaznim Mula	Assessment of organic contaminants in some urban locations in the Republic of Kosovo
6	Emel Atılal	Synthesis of epoxidized vegetable oils and determination to use in PVC paste as a viscosity regulator
7	Tuğba Güngör Ertuğral	Preparation and characterization of antiviral HDPE-ZnO food packaging composite material
8	Yalçın Coşkun	Some properties of black cumin volatile oil added PLA films
9	Edina Latifi	Synthesis of poly(3-hexylthiophene-2,5-diyl) and improvement of the optic and electric properties by sensibilization with thiazolyl-hydrazinylidene-chroman-2,4-dione
10	Gizem Akgün, Gülşah Konak	Initiator effect on gel for breast phantom preparation
11	Ahmet Çifci	Physical properties and electromagnetic absorption performance of Fe_2O_3 doped rigid polyurethane materials
12	Songül Şen Gürsoy Mevlit Dema	Synthesis and electrochemical characterization of polyvinylidene fluoride/polypyrrole (PVDF/PPy) composite

ISCMP 2022 - POSTER PROGRAM

September 16, 2022

NO	PRESENTER	TITLE
13	Veprim Thaçi	Evaluation of diatomaceous earth's adsorptive properties toward (2E, 5E)-2,5- bis (4-methoxybenzylidene) cyclopentanone. An experimental and theoretical study
14	Avni Riza Berisha	A theoretical investigation of anticancer drugs as potential corrosion inhibitors
15	Ardhmeri Arsim Alija	Monte Carlo and experimental studies on the adsorption of (2E, 5E)-2,5- bis (4-methoxybenzylidene) cyclopentanone molecule on the graphene oxide
16	Rilinda B. Plakaj	A theoretical and experimental study of the adsorptive removal of (2E, 5E)-2,5- bis [(4-dimethylamino) benzylidene] cyclopentanone using graphene oxide
17	Ardhmeri Arsim Alija	The interaction of (2E, 5E)-2,5- bis (4-methoxybenzylidene) cyclopentanone organic molecule onto the graphene oxide surface
18	Serkan Ateş	Examination of fatigue behaviors of Al6061 matrix SiC Al_2O_3 and blast furnace slag reinforced hybrid composites
19	Serkan Ateş	Examination of fatigue behaviors of Al6061 matrix SiC Al_2O_3 and marble powder reinforced hybrid composites
20	Makfire Sadiku	Experimental and theoretical study of methyl violet adsorption onto halloysite nanoclay
21	Ali Sungur	Determination of geochemical fractions of heavy metals in soils formed on schist and granite
22	Mentor İsmaili	Determination of heavy and toxic metals in power plants of Kosovo
23	Salih Can Suner	Grafting of polystyrene on electrospun gelatin nanofibers by photopolymerization

VI. International

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LIST OF ABSTRACTS


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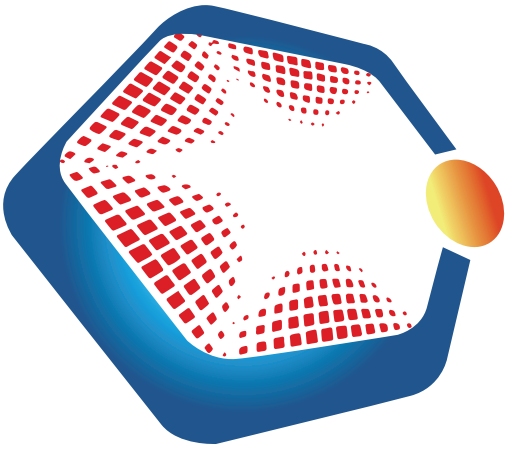

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INVITED LECTURES

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Future in Plastics Industry: Sustainability and Nanotechnology

Yusuf Ziya Menceloğlu*
Prof.
Materials Science and Nanoengineering,
Sabancı University, Turkey

Plastics are indispensable materials of modern economy due to their unrivaled functional properties, lightness and low cost. The use of plastic materials has increased 20 times in the last 50 years, and this rapid increase is expected to double in the next 20 years, given fact that the lifespan of modern polymer science has been developed in the last 100 years. In parallel, it is a fact that many plastic wastes reach the seas and oceans because of the leakages/defects in the collection systems of single-use plastics, creating pollution in nature. Green consensus and circular economy programs have been initiated in the European Union to reduce the environmental pollution caused by plastics, which are a part of our daily life and used in many sectors from health, textile, food packaging to automotive. In addition, it is obvious that the losses in the food sector and the burden of CO_2 emissions are much higher if plastic packaging is not used. It is clear that it can be produced with new technologies and multifunctional polymeric materials, both to extend the shelf life of foodstuffs and to reduce the use of plastic. In this talk we will cover plastic industry challenges due to the green deal action plan. How recycling and up-cycling will help on sustainability of the plastics and how nanotechnology can reduce the use of plastic in the green deal and circular economy approach. With this end we will explore how we can design plastic film which has multi functional properties such as good barrier properties, antimicrobial, gas absorption, oxygen scavenging as well as thermal modulation. Addition to these functionalities nanosize additives will increase the mechanical properties of the film and reduce thickness of the film, therefore while increasing functionality one can reduce the amount of polymer used during film production.

Keywords: Plastic, Sustainability, Nanotechnology

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Development of Breast Phantom

Sinem Yildiz
M.Sc. Student
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Metin Hayri Acar*
Prof.
Department of Chemistry,
Istanbul Technical University, Turkey

Tuba Yilmaz
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Department of Electronics and Communication Engineering, Istanbul Technical University, Turkey

Ibrahim Akduman
Prof.
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The Microwave Imaging Technology has been developed for the last 20 years to detect breast cancer. Microwave is the electromagnetic wave in the the frequency range of 300 MHz-30 GHz with which humans interact most and which is not strong enough to ionize tissues in the human body. These properties are relative permittivity, electrical conductivity and magnetic permeability. While relative permittivity and electrical conductivity is changing, the magnetic permeability does not change in all human tissues. Each tissue in the breast has different relative permittivity and electrical conductivity. Cancerous tissue has a much higher relative permittivity than normal tissue, and the relative permittivity of it is close to water. The aim of this study is preparing gel phantoms that able to mimic the breast tissues including cancer tissue. For this aim, firstly poly(acrylic acid) (PAA) gels were synthesized with different cs-lk ratio. It was observed that swelling ratios of gels were decreased by increasing cs-lk amounts. The relative permittivity's of the solvents/solvent mixtures were found to be close/suitable with relative permittivity's of the breast tissues (normal and cancer tissues). Swelling ratios and dielectric properties of the phantom gels in different solvents/solvent mixtures were investigated. The dielectric properties of gels swollen in these solvent/solvent mixtures were also shown very close to breast tissues (normal and cancer tissues). It is observed that PAA gels are very suitable for mimicking breast tissues (normal and cancer tissues). Beside that, the cancer tissue phantom was clearly seen within the normal tissue phantom in Microwave Breast Imaging device.

Keywords: Breast Cancer, Phantoms, Dielectric Properties,

Acknowledgement: Research Foundation of Istanbul Technical University (Project no: TYL-2021-43339) and The Scientific and Technological Research Council of Türkiye (TUBITAK, Project no: 1003-118S074) are highly acknowledged.

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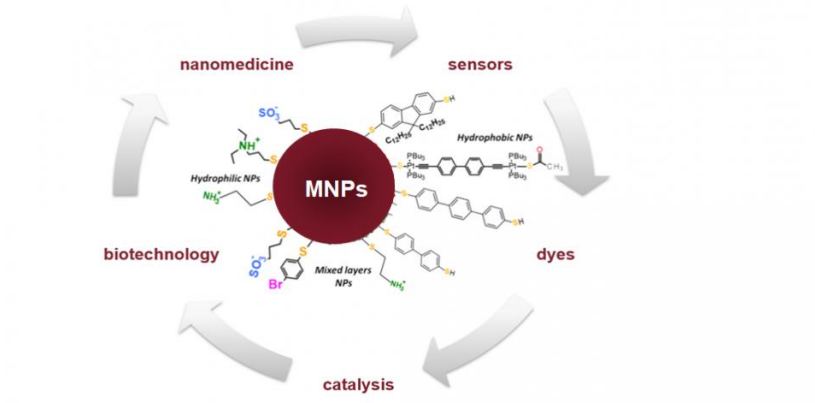
Thiol Functionalized Noble Metal Nanoparticles: A Versatile Platform for Advanced Applications

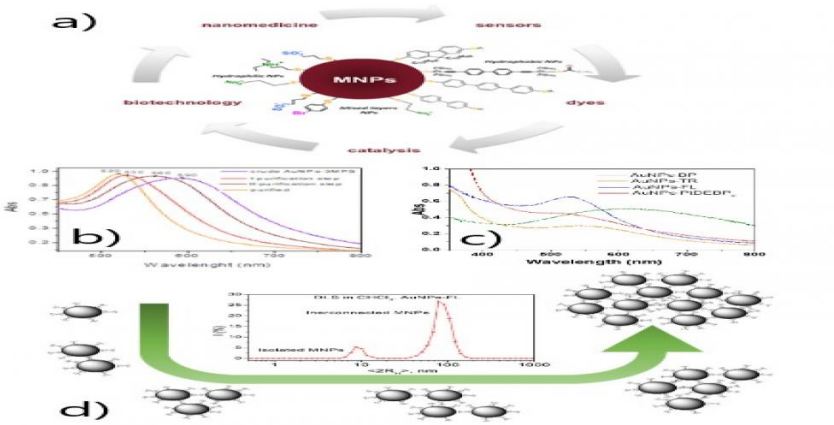
Ilaria Fratoddi*
Prof.
Department of Chemistry,
Sapienza University of Rome, Italy



Thiol-functionalized noble metals nanoparticles based on gold or silver metals (AuNPs and AgNPs, respectively) have been thoroughly investigated in recent years and due to their surface chemical versatility, optical and electronic characteristics, along with a general biocompatibility, they have been tested in several emerging fields ranging from sensing, energy, memory devices, to catalysis and nanomedicine with new synergistic and multidisciplinary perspectives. The wet chemical reduction approach from metal ions precursors in the presence of reducing agents and with the appropriate choice of functionalizing ligands, allows the formation of stable, hydrophilic, or hydrophobic colloidal nanoparticles. Isolated or interconnected systems with size in the range 5-50 nm can be obtained depending on the presence of mono- and bifunctional thiol end groups. Their use in biotechnology and nanomedicine for hydrophilic NPs has garnered considerable attention for their potential to facilitate drug loading and surface reactivity. Particularly attracting are also hydrophobic noble metals nanoparticles and their composites with polymeric materials which show promising applications in large area, flexible, and low-cost organic/hybrid electronics, sensors and memory devices. Here, an overview on the synthesis, characterization methods and applicative studies of functionalized noble metals nanoparticles will be presented.

Keywords: Metal Nanoparticles, Au Nps, Ag Nps,

References: 1. Fratoddi, I. et al, J. Phys. Chem. C, 115, 2011, 15198. 2. Fratoddi, I. et al, J Phys. Chem. C 121, 2017, 18110. 3. Li Voti, R. et al, Nanoscale Advances, 3, 2021, 4692. 4. Matassa, R, et al, Nanoscale, 8, 2016, 18161. 5. Venditti, I. et al, J. Phys. Chem. C, 121, 2017, 8002. 6. Chronopoulou, L. et al, Int. J. Biol. Macromol. 146, 2020, 790. 7. Venditti, I. et al, Part. Part. Syst. Charact. 2022, 2100282. 8. Cerra, S. et al, Materials Sci. & Eng. C, 117, 2020, 111337. 9. Fratoddi, I. et al, ACS Applied Nano Materials, 4, 2021, 2930. 10. Grigorian S. et al, Synth. Met., 283, 2022, 116973. 11. Cerra, S. et al, J. Mater. Sci.: Mat. Electr. 31, 2020, 12083. 12. Cerra, S. et al, Coll. Surf. B: Biointerfaces, 203, 2021, 111727



THIOL FUNCTIONALIZED NOBLE METAL NANOPARTICLES: A VERSATILE PLATFORM FOR ADVANCED APPLICATIONS Ilaria Fratoddi Department of Chemistry, Sapienza University, Italy ilaria.fratoddi@uniroma1.it Abstract Thiol-functionalized noble metals nanoparticles based on gold or silver metals (AuNPs and AgNPs, respectively) have been thoroughly investigated in recent years and due to their surface chemical versatility, optical and electronic characteristics, along with a general biocompatibility, they have been tested in several emerging fields ranging from sensing, energy, memory devices, to catalysis and nanomedicine with new synergistic and multidisciplinary perspectives. The wet chemical reduction approach from metal ions precursors in the presence of reducing agents and with the appropriate choice of functionalizing ligands, allows the formation of stable, hydrophilic, or hydrophobic colloidal nanoparticles. Isolated or interconnected systems with size in the range 5-50 nm can be obtained depending on the presence of mono- and bifunctional thiol end groups. Their use in biotechnology and nanomedicine for hydrophilic NPs has garnered considerable attention for their potential to facilitate drug loading and surface reactivity. Particularly attracting are also hydrophobic noble metals nanoparticles and their composites with polymeric materials which show promising applications in large area, flexible, and low-cost organic/hybrid electronics, sensors and memory devices. Here, an overview on the synthesis, characterization methods and applicative studies of functionalized noble metals nanoparticles will be presented. Introduction Noble metals hydrophilic and hydrophobic metal nanoparticles based on gold or silver metals (AuNPs and AgNPs, respectively) have been thoroughly investigated in recent years and due to their surface chemical versatility, optical and electronic characteristics, along with a general biocompatibility, they have been tested in several applicative fields. Applications ranging from sensing, energy, memory devices, to catalysis and nanomedicine have been explored with new synergistic and multidisciplinary perspectives [1,2]. One of the most popular way to obtain AuNPs and AgNPs is the two-phase Shiffrin-Brust method [3] that, due to the soft character of both S and Au, exploits thiol ligands that strongly bind to the metallic surface, in particular for gold. The size control together with the size distribution is a rather delicate process, being driven by the reactivity and passivation rate of the nanoparticles and growth of the nanoparticle. The redox reaction and growth process have been deeply investigated together with the role of thiol ligands [4,5]. One of the main properties that allows these nanoparticles to be used in different fields is the scattering and absorption of light at resonant wavelengths. This phenomenon is known as due to the excitation of plasmon oscillations (Surface Plasmon Resonance, SPR). The resonant wavelength depends on the size, shape, and geometry of the nanostructures, thus providing a variety of information and making them the model system of choice in a wide range of biomedical and optoelectronics applications. Water or organic solvent soluble colloidal systems can be isolated and studied with the aim of understanding their internal structure and surface and interface chemistry and reactivity, which in turn are fundamental to face applicative studies. In particular, their use in biotechnology and nanomedicine has garnered considerable attention for their potential to facilitate both selective recognition, drug loading and surface reactivity, through their peculiar chemical and

physical characteristics. In this field, hydrophilic ligands such as 2-diethylaminoethanethiol hydrochloride (DEA) and 6-amino-1-hexanethiol hydrochloride (6EA) alone or in combination with or Sodium 3-mercapto-1-propanesulfonate (3MPS) have been used to build up different bio-conjugated systems that favour the immobilization of hydrophobic drugs and bioactive molecules such as enzymes and antibodies [6-9]. Particularly attracting are also noble metals nanoparticles functionalized with organic or organometallic dithiols, such as 9,9-didodecyl-2,7-bis(acetylthio)fluorene (FL), p-terphenyl-4,4?-dithiol (TR), biphenyl-4,4?-dithiol (BP) or trans,trans-4,4?-diethynyl(bistributylphosphine-Pt(II)thioacetyl) biphenyl, (Pt-DEBP) and their composites with polymeric materials which show promising applications in large area, flexible, and low-cost organic/hybrid electronics, sensors and memory devices [10-13]. Here, an overview on the synthesis, characterization methods and applicative studies of functionalized noble metals nanoparticles will be presented (see figure 1a). Materials and Methods Characterization methods. UV-Vis absorption spectra were obtained on a Varian Cary 100 Scan UV-Vis spectrophotometer, FTIR and Far-IR (FIR) spectra were recorded on cast deposited films from chloroform solutions using KRS-5 cells with a Bruker Vertex 70 spectrophotometer, in the range 4000-400 cm-1 and 600-200 cm-1, respectively. NMR spectra were recorded on a Bruker Avance II 300 MHz instrument in CDCl3 solutions; chemical shifts are reported in ? values. Dynamic Light Scattering (DLS) and ?-potential measurements were carried out using Malvern Zetasizer Nano-ZS90. Materials. All reagents and analytical grade solvents were purchased from commercial sources and used as received unless otherwise stated. AuNPs and AgNPs were prepared as previously described [6-13]. Discussion The wet chemical reduction approach from [AuCl4]- gold or Ag+ precursors in the presence of sodium borohydride as inorganic reducing agent, allows the formation of stable colloidal nanoparticles with size in the range 5-50 nm. The appropriate choice of functionalizing ligands allows modification and tailoring of the surface hydrophilicity or hydrophobicity, with the use of end-groups bearing ammonium, sulfonate, carboxylic, aromatic, organic or organometallic moieties mono and dithiols, allowing to produce isolated or interconnected nanoparticles [14-16]. The optical properties of colloidal metal nanoparticles have been deeply investigated through Mie scattering theory, together with their dependence on the particle size effect and in figure 1b the UV-vis spectra of interconnected AuNPs stabilized with FL, BP and TR dithiol ligands are presented in comparison with AuNPs stabilized with the organometallic Pt-DEBP linker. The shift in the position of the SPR band could be related to the size, aggregation, and dispersity of AuNPs and can be correlated to DLS measurements and Photoacoustic spectroscopy (PAS) results, in order to better ascertain and discriminate different sizes of AuNPs from covalent interconnection between them. Looking at the behavior of hydrophilic MNPs, the surface plasmin resonance can be tuned by a proper choice of the ligands and molar ratios during synthesis approach. In the case of AuNPs-3MPS for example, the purification steps can be optimized to separate and identify different populations of MNPs (see figure 1c). PAS technique allows to experimentally measure both absorption and scattering coefficients, separately in a single measurement, allowing assess the presence of isolated and interconnected nanoparticle systems [17]. In figure 1d a schematic representation of single to interconnected nanoparticles evolution is shown, together with DLS measurement. Among biotechnology and nanomedicine applications, drug and bioactive molecules loading, and release was studied. In this case, hydrophilic nanoparticles can be selected thanks to their general biocompatibility and low size and size distribution [7897-9]. MNPs functionalized with hydrophobic thiols and dithiols were used to prepare sensing devices and MNPs/polymer blends films [12,11]. The MNPs and composite materials were investigated by electrical measurements to study their optical, structural and electrical properties. The ability to control the optical, structural and the charge transport properties by tuning the amount of the MNPs opens the way for the use of these new composite materials in organic-based devices Conclusions In conclusion, MNPs based materials show a versatile surface functionalization and depending on the hydrophilic/hydrophobic behaviour of the external layers it is possible to finely modulate the solubility and interaction properties at surface level. Here, a short overview on the synthesis and characterization methods has been presented with a glance on applicative

studies of functionalized noble metals nanoparticles.

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349389

Risk Assessment of Natural Toxic Pyrrolizidine Alkaloids in the Food Chain

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Pyrrolizidine alkaloids (PAs) and their corresponding N-oxides (PANOs) are a group of secondary metabolites produced by plants and they are considered as natural toxins which present possible risk to humans from the use of toxic plant species as herbal teas or traditional medicines or the consumption of PA-contaminated food such as grain or grain products, honey, milk, tea, beverages. In our work systematic study of extraction efficiency of PAs and PANOs in plant material and in honey samples was carried out. The optimal extraction was achieved with methanol and one clean up step using SPE C18 column or QuEChERS, which resulted in matrix effect (ME) lower than 10%. Additionally, liquid chromatography (LC) tandem mass spectrometry (MS) method utilizing electrospray ionization (ESI) for qualitative and quantitative analysis of 17 most common PA and PANOs was developed and validated. Screening the PAs in plants originally containing them has revealed the presence of twenty-two different compounds. It is noteworthy that the most abundant species in Macedonia (Echium vulgare and Symphytum officinale L.) have relatively low total contents of PAs and PANOs, which implies that the risk of their incorporation and concentration in the food chain is low. Analysis of PAs in forty-eight tea samples indicate that most of the analysed samples are safe and there is not potential health risk. The highest content of PAs was found in rooibos tea ranged from 147 to 517 µg/kg. According to obtained results for presence of PAs and PANOs in honey samples it can be concluded that in contrast to honeys purchased from local markets, samples collected from local beekeepers were less contaminated. Care should be taken with honeys harvested abroad; consumers should vary the purchased brands in order to dilute the potential intake of PAs, particularly frequent honey consumers and sensitive populations such as toddlers

Keywords: Pyrrolizidine Alkaloids, Plant Material, Honey Samples, Liquid Chromatography, Mass Spectrometry, Risk Assessment

Acknowledgement: Authors gratefully acknowledge the financial support provided by the OPCW for the project titled: "Risk Analysis of Natural Toxic Pyrrolizidine Alkaloids in the Food Chain: Development, Validation, and Application of HPLC/MSn Methods", Grant L/ICA/ICB/222477/20

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In Vivo Evaluation of Carboxylated Graphene Oxide's Impact on Oxidative Stress and Other Biochemical Markers in Snail Helix Locurum

7

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The purpose of this study was to determine whether carboxylated graphene oxide (GO-COOH) has any influence on the oxidative stress response of tissue, cell membrane necrosis, or glucose levels in the snail Helix locurum. Snails (40 animals, average weight 22g) were gathered near Prishtina (Gërmia park), Kosovo, from an unpolluted region. They were fed cabbage-Brassica oleracea for two weeks during the acclimation period. A solution of GO-COOH (1 ppm) was produced and stored at 4°C. The animals were divided into four groups, with the first serving as a control, and the remaining groups receiving 0.25 µg/g GO-COOH per os and 0.25µg/g GO-COOH in the snail foot. After 24 hours (second group), 48 hours (third group), and 72 hours (fourth group), the animals were euthanized. Enzymatic activity (catalase) was determined in centrifuged homogenates of the hepatopancreas, albumin gland, gut, and mantle. LDH and glucose levels were determined using the snail's hemolymph. Catalase activity results indicated a time-dependent increase in enzyme activity between 24h and 72h. The results of the LDH activity in hemolymph shown that while enzyme activity is significantly increased in the 24h group compared to the control group, it tends to decrease in the 48h and 72h groups. A similar pattern was observed for the glucose levels in animal hemolymph. The data indicate that GO-COOH has an influence on membrane necrosis and the oxidative stress response in several snail tissues.

Keywords: hepatopancreas, Albumin gland, Heamolymph, Glucose

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Advanced Pulse-Voltammetric Techniques

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The lecture is concerned with thedevelopment of novel and advanced electrochemical techniques for electroanalysis, electrochemical sensors and materials characterisation. Commencing from the basic features of an electrochemical experiment, the technique of square-wave voltammetry (SWV) is introduced, as one of the most advanced members in the family of pulse-voltammetric techniques, with an emphasis of experimental application for analytical, mechanistic, and kinetic characterisation of a broad range of experimental systems. In the light of the current advances in the field of pulse-voltammetry, several new electrochemical techniques are presented, all being elaborated from the perspective of SWV, including double sampled differential SWV [1], multi-sampled SWV [2], electrochemical Faradaic spectroscopy [3], and the novel hybrid technique designed by merging differential- pulse and square-wave voltammetry [4]. The new techniques are comparatively and critically evaluated in termsof expected analytical performances and capabilities for fast and in-depth kinetic and mechanisticcharacterization of electrode processes.

Keywords: Electrochemistry, Pulse Voltammetry, Square-Wave Voltammetry, Electrode Processes, Electrode Mechanisms, Electrode Kinetics

Acknowledgement: The author would would like to acknowledge with gratitude the support from the National Science Centre of Poland through the Opus Lap grant no 2020/39/I/ST4/01854.

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55b37c

Development of Novel Strategies for Eradication of HIV-1 using Structural and Computational Analysis

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Main challenge of fighting with the HIV-1 is to eliminate the latent viral reservoir from the body. This reservoir is resistant to antiretroviral drug therapy and can cause viral rebound if the treatment is stopped. The removal of the reservoir enables HIV eradication, is urgently desired in HIV-AIDS research. For this purpose, a strategy called "kick and kill" was proposed, based on the hypothesis that activation of latent HIV ("kick") leads to cell death ("kill") by physical damage and/or immune activation. However, in clinical tests "kill" process was found to be not enough to reach HIV eradication. To eradicate HIV from the body, our work has recently suggested a new strategy called "lock-in and apoptosis" instead of "kick and kill". In development of this strategy, non-natural derivative of inositol hexaphosphate (IP6) named as L-HIPPO has been developed to suppress membrane localization of HIV-1 Gag protein (Pr55gag) and to induce strong apoptosis of the host cell containing the latent viruses (1). For identification of the key interaction between L-HIPPO and MA, three high-resolution crystal structures of the MA domain in complex with IP6 molecules were revealed at cryo-temperature (2.40 Å, and 2.72 Å resolution), and ambient-temperature (3.5 Å resolution) (2,3). Then, we rationally designed 8 new anti-HIV drug candidates on the basis of the structure of two acyl groups of L-HIPPO and examined their binding affinities to HIV-1 MA by molecular docking using the crystal structure of MA in complex with IP6 (PDB IDs: 7E1I), which was enlightened by our research group (3). Benzene-inserted compounds were detected to possess the most promising docking scores, which guided us to create a library involving 213 new aromatic group-inserted L-HIPPO derivatives. According to the results, 3-methoxy-4-hydroxyphenyl carrying compound was determined as the most effectively binding L-HIPPO derivative to the MA.

Keywords: X-ray crystallography, HIV-1, Matrix protein, Inositol hexaphosphate, L-HIPPO, Molecular Modelling

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Energy Transition and Material Needs

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Mitigation of climate change and security of supply needs are forcing fast energy transition. Wind and solar are abundant nearly everywhere, and are cheap compared to other alternatives, but they ask for electrification of transport and heating, by means of heat pumps and batteries. Also, decarbonisation of high temperature processes and feedstocks for industry will need hydrogen and hydrogen-based fuels. While technoeconomically such transition is straightforward and viable, socio-politically it may cause some disturbances. Also, waste amounts of some previously rarely used materials will be needed. Lithium, the main material for batteries, will be oil of the future. While mobile batteries benefit from size, thus making lithium indispensable, batteries for stationary use may use different materials. On the other hand, used car batteries may get second life in stationary use, thus postponing recycling of lithium and increasing its demand. While lithium is quite abundant in Earth?s crust, the necessary ramp up of its production is epic. Other materials in lithium batteries, like cobalt or nickel, may be replaced by iron and phosphorus, or many other combinations. Rare earths needed for wind power and electric vehicles, neodymium, praseodymium, dysprosium and, to a lesser extent, cerium, europium, gadolinium, lanthanum, terbium and yttrium, are also reasonably abundant, but their production is currently concentrated in small number of countries. While there will be enough materials for energy transition, there will be bad bottlenecks on the way, and it is crucial to start removing them as soon as possible.

Keywords: Energy, Material, Transition

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6th International ISCMP ALBANIA 2022
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Composite Photosensors of Polyazulene and Mixed Valence Inorganic Solids

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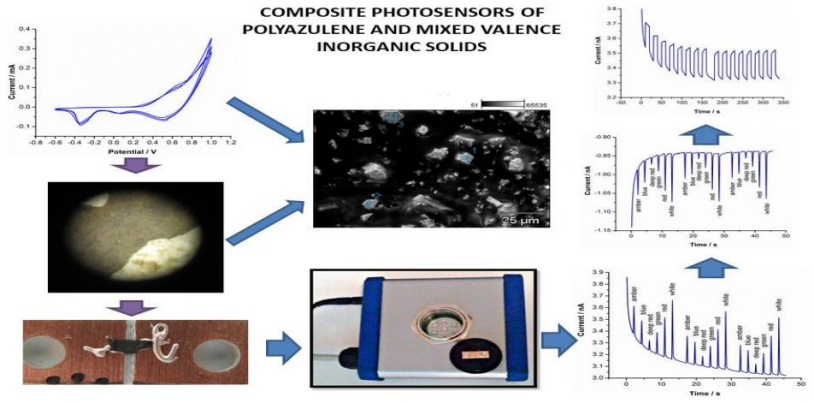

This research focuses on two types of sandwich polyazulene-composite thin films . In-situ cyclic voltammetry measurements display distinguishable changes between polyazulene and composite films. Peak shifting and the appearance of extra oxidation/reduction effects as well different current jumps involved in each polymerization process are observed for the considered composites. Post syntheses FTIR measurements show the existence of extra bands located at 772 cm^{-1}, 946 cm^{-1}, 1568 cm^{-1}, along with those belonging to the polymer and the inorganic fillers. Under a bias of 3V, polyazulene films respond better to white (5500 K) and red (623 nm) light, followed by amber (590 nm) and blue (460 nm) light, with the highest response for white light. Targeted tuning of the inorganic filler composition, substituting two sulfur positions in the structure of In5S3Se2Cl with selenium, leads to a sandwich composite polymer with reverse photo-switching response compared to polyazulene film. Polyazulene thin film displayes negative intensities upon amber light illumination and positive ones for green and red light. The sandwich composite film of polyazulene-In5S3Se2Cl display positive intensities upon these three monochromatic lights, while the sandwich composite film polyazulene-In5SSe4Cl reacted oppositely to polyazulene film toward the selected illumination wavelengths.

Keywords: Polyazulene, Composite materials, Photo-sensitivity, Photo-chromatic, Mixed-valence, Substituions

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dc82d6

Optimization of the Hantzsch Reaction and Synthesis of Some Novel Tiazolyl-hydrazinylidene-chroman-2,4-diones as Highly Potent Anti-cancer Drugs

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Large number of heterocyclic compounds containing nitrogen, oxygen and sulphur are used as medicines in different therapeutic targets. In this course, coumarins and thiazoles scaffolds are very important pharmacophores in drug discovery and development processes, and important structural units in medicinal chemistry as they have shown antitumor, antiviral (including anti-HIV), antibacterial, anti-inflammatory, antifungal and anticoagulant activity. Given the high bioactivity shown by 4-hydroxycoumarin and aminothiazole derivatives, the area of interest is to design some new structural entities containing both heterocyclic nuclei in a single molecular skeleton. Derivatives obtained by copulation of thiazole and coumarin core showed good effect against different cancer cells. Of particular interest are the indications that the increase in hydrophobicity on the thiazole ring increases the anticancer activity. For this purpose, new derivatives with alkyl and aryl substituents on the thiazole part has been synthesized, but in the beginning the well-known Hanthzsch reaction was optimised for best results in synthesis of the given 2-aminothiazoles. Those compounds afterwards were copulated via diazotization with the coumarin ring and novel thiazolyl-hydrazinylidene-chroman-2,4-diones were obtained. All of the compounds were purified by chromatography and fully characterized by the spectroscopic techniques.

Keywords: Hantzsch Reaction, 2-aminothiazoles, Coumarin, Cancer, Spectroscopy

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30bb38

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Adsorption of Pesticides on 2D Carbon Nanomaterials: An Experimental and Theoretical study

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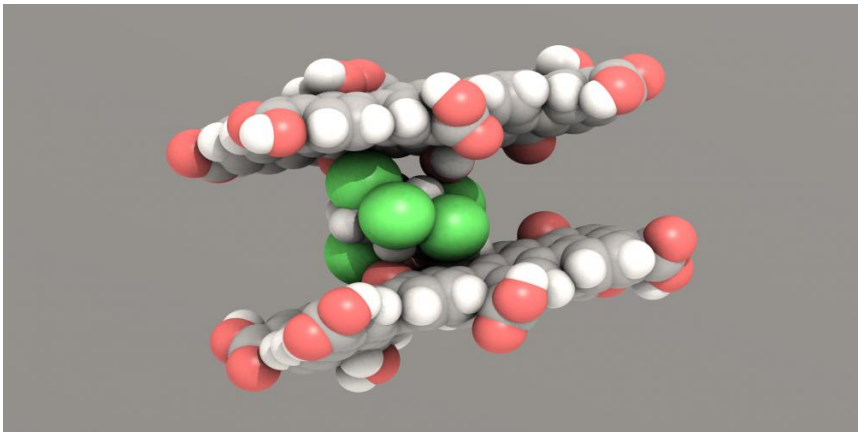

Graphene and graphene oxide are fascinating materials with diverse uses, including adsorption, composite material formulation, sensors, photovoltaics, and so on. Graphene oxide is generated in this paper by reducing graphene oxide (with ascorbic acid) using the well-known Hummers process, which may be summarized as the controlled treatment of graphite flakes with potassium permanganate in concentrated sulfuric acid. The produced materials are characterized using FTIR and UV-VIS spectroscopy [1-3].Lindane is adsorbed from hexane using a solution with a concentration range of 25 to 500 ppb and an adsorbent mass of 15 mg graphene or graphene oxide. Lindane adsorbed concentration was determined using GC-ECD. These materials have superb sorption capacity. Graphene is effective in removing up to 92.5% of Lindane from hexane solutions, whereas graphene oxide is able to eliminate up to 56.1%. Quantum and molecular mechanics-based simulations were performed to acquire a better understanding of the nature and adsorption energetics of Lindane's interaction with the two adsorbents (Figure 1).

Keywords: Graphene, Graphene oxide, Adsorption, Lindane, Pesticide, MD

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b4288d

Spectral Classification and Quantification of Selected Microorganisms Existing on Different Materials

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Different microorganisms i.e. *Escherichia coli*, *Bacillus subtilis*, *Saccharomycies cerevisiae* and *Pichia anomala* as well as their mixtures growing on different material i.e. lab coats (non-woven fabric), stones - floor or wall tiles (used to cover room floors or walls), metal - steel used for different tools in food industry were studied in terms of generating different spectral signals. Using statistical methods i.e. PLS microorganism-free surfaces of studied materials were distinguished from contaminated. Type of microorganism present were differentiated by specific statistical discriminant models. Spectra containing experimental data used for calibrating models were registered in NIR region. Beside qualitative models for distinguishing microorganism type, quantitative models were calibrated to determine the level of concentration of given microorganism. From practical point of view, differentiation of contaminated from clear surfaces of studied materials is crucial. Differentiation of different microorganisms and determination of their concentrations is crucial from scientific point of view.

Keywords: Spectral classification, Microorganism, FT-IR

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7750ca

A theoretical and experimental study of adsorbent dye removal from (2E,5E)-2,5-Bis[(4-dimethylamino)benzylidene]cyclopentanone using diatomaceous earth as an adsorbent

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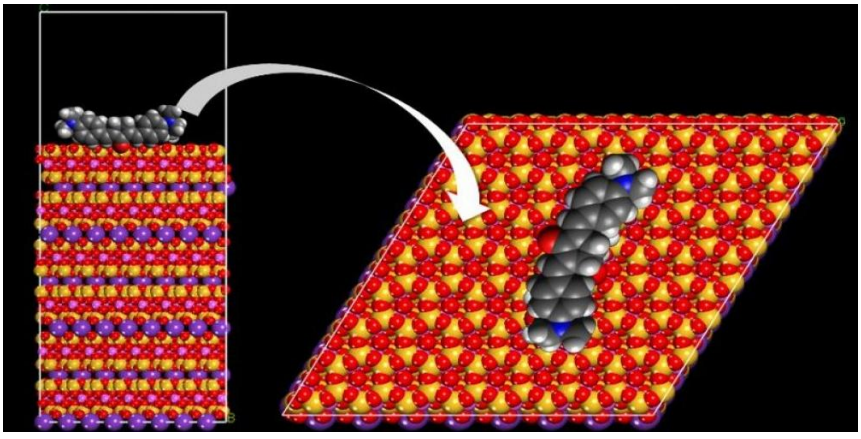

This study is focused on the adsorption of (2E,5E)-2,5-Bis[(4-dimethylamino)benzylidene]cyclopentanone using diatomaceous earth. First, the monocarbonyl compound was synthesized, then crystallized and characterized was done with IR, NMR, etc. The theoretical calculations based on Density Functional Theory (DFT) and Monte Carlo (MC) calculations were used to explore the preferable adsorption site, interaction type, and adsorption energy of the (2E,5E)-2,5-Bis[(4-dimethylamino)benzylidene]cyclopentanone onto diatomaceous earth. Figure 1: Monte Carlo lowest energy geometry obtained during the adsorption of the adsorption of the (2E,5E)-2,5-Bis[(4-dimethylamino)benzylidene]cyclopentanone using diatomaceous earth modelled using Muscovite structure (Amcsd 0000854). Diatomaceous earth soil is cleaned, homogenized and characterized by various spectroscopic methods and is used as an adsorbent. The adsorptive ability of the diatomaceous earth toward the (2E,5E)-2,5-Bis[(4-dimethylamino)benzylidene]cyclopentanone was evaluated

using UV-Vis measurements.

Keywords: MACs, adsorbent, theoretical calculation, NMR, IR, synthesis

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Development of a method for the detection and characterization of volatile organic compounds in the atmosphere using passive sampling

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The objective of this study was introduction of appropriate methods for detection and characterization of volatile organic compounds in the atmosphere of selected sites in the Republic of N. Macedonia and Kosovo. The method involves the use of Radiello® passive/diffusive samplers for outdoor air monitoring. The advantage of the Radiello® passive air samplers are that they are small, simple to use and provide practical means for atmospheric environmental monitoring. Moreover, this technique offers higher capacity and faster uptake/sampling rates compared to traditional passive sampling techniques. The Radiello® passive/diffusive samplers were placed in nine sampling sites and the organic compounds were monitored every 28 days over a period of several months. Using gas chromatography coupled to mass spectrometry we were able to detect over thirty organic compounds. Headspace gas chromatography (HS-GC) techniques was used to detect and characterize the VOCs from vaporized mixture from several different commercially available gasolines and diesel fuels consumed in these cities. In general, based on the results from the GC-MS analyses the dominant anthropogenic VOCs are from transport fuels such as gasoline (BTEX and other hydrocarbons) and diesel (n-tetradecane and other saturated hydrocarbons). The samples taken from urban areas had similar profile, with benzene and toluene being the predominant mono-aromatic compounds in all the sites investigated. Higher concentration of biogenic organic compounds was detected in one location (Dragash, Kosovo) where monoterpenes were detected and identified as alpha-pinene and limonene. They most likely come from conifer tress such as pine which are abundant in that area. Very disquieting was the aerial presence of phthalate esters which were detected in winter and which most likely originate from incomplete combustion of polymeric materials. The ultimate goal is to identify the place of origin of areal outdoor urban contamination and to devise control measures for their reduction or elimination.

Keywords: volatile organic compounds, gasoline, environmental pollution, gas chromatography, Radiello® passive sampling,

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6th International ISCMP ALBANIA 2022
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Effect of Phenyl Ethyl Alcohol on Crystallinity and Biodegradation of Poly (Lactic acid)

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The increasing interest in biopolymers has progressively increased the interest in the development and utilization of more environmentally friendly polymeric materials. Consequently, applications of biopolymers, especially Poly (Lactic acid) (PLA) have increased in recent years. The crystallinity of the polymer matrices is one of the most important parameters that could be able to affect some properties such as degradation and mechanical performance. PLA is one of the most promising bio-based, compostable polymers able to be an alternative to petro-derived polymers both in single-use applications and also for durable equipment with sufficient technical properties. Hydrolytic biodegradation describes usage areas for this kind of polymers. Manipulating this hydrolytic degradation process also affects the usage potential of polymeric materials. Crystallinity is one of the parameters that affect the degradation process on polymer matrices. In order to control the crystallinity and biodegradation of the PLA matrix, the natural product Phenyl ethyl alcohol (PEA) was inserted into the polymeric matrices at different percentages. An increase in the crystallinity was observed depending on the PEA percentage. The biodegradation was also affected thanks to the PEA insertion into the matrix. Consequently, the insertion of PEA into the PLA matrices resulted to increase in crystallinity and biodegradation.

Keywords: Phenyl Ethyl alcohol, Poly (Lactic acid), Crystallinity, Biodegradation

Acknowledgement: This work was supported by Çanakkale Onsekiz Mart University Scientific Research Coordination Unit. Project number: FBA-2018-1368

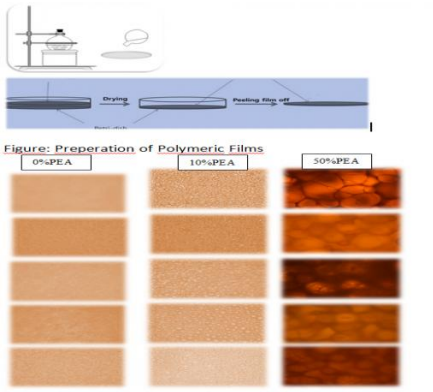

Figure 2. Microscope photographs of PLA / PEA films containing different rates of PEA (after 7 days).

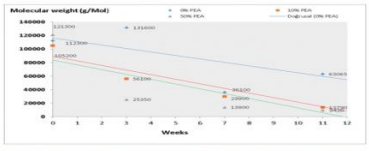

Figure. PLA / PEA films with pure PLA, 10% PEA and 50% PEA.

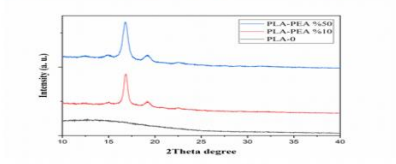

Figure. XRD Diagrams of PLA / PEA Films.

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1.Introduction

Lately, biodegradable and biocompatible polymers have become a major concern of research studies and sectoral stakeholders, especially from an ecological perspective. Recently bio-based or biodegradable polymers have been getting more importance in the polymer industry because of environmental concerns as well as their various applicability for different aims especially, biomedical products . Mechanical, thermal, and biodegradation properties of polymeric materials designate usage areas . Poly (lactic acid) (PLA) is a commercially available bio-based polymer used in a variety of applications because of its high strength, modulus, compostability, biodegradability, semicrystalline, and thermoplastic properties. PLA has rapidly evolved into a competitive commodity material over the last decade, because of these properties. A considerable number of scientists have been carrying out studies to proliferate application areas of PLA. The control of crystallinity is among the ways to increase the number of application areas . The crystallization kinetic is affected by several factors, such as nucleating agents, temperature, molecular weight, etc. It is important to control the crystallinity grade in PLA and for this purpose different kinds of nucleating agents, such as organic and inorganic chemicals, were used . Phenylethyl alcohol (PEA) is a natural volatile oil which is isolated from a rose. In the present study, the effects of temperature on the crystallinity of PLA - PEA were investigated. The polymer films were prepared by the solution casting method. PLA - PEA films, containing 0% of PEA, 10% of PEA, and 50% of PEA (w/w), were placed in tubes containing 10 ml of Phosphate buffer (pH 7.4) and incubated at 37 0C. The changes in crystallinity were investigated.

2.Materials and Methods

2.1. Materials Poly (Lactic acid) (PLA 4043-D, Natureworks LLC), Phenethyl alcohol (Merk), Dichloromethane (DCM, Merck), Tetrahydrofuron (THF, Merck), Ethyl alcohol (Merk), PO4 Buffer solution, NaOH (Merck) were used. Radwag brand AS 2020 / C / 2 Model ± 0.001 g was used for weighing chemicals. In order to prepare a suitable medium for samples, Incubator and pH meter (Hanna) were used for pH adjustment of the solution medium. 2.2. Methods Polymeric films were prepared by the solution casting method with Ika brand magnetic heater mixer. Prepared films were dried at room temperature and after this step, whole samples were kept in a vacuum oven to remove the solvent. PLA films were prepared with different weight percent content Phenyl ethyl alcohol (PEA) (w / w), as 0% PEA, 10% PEA and, 50% PEA depending on the PLA. After the, 1g of PLA and the required amount of PEA were dissolved in dichloromethane (20 ml), it was poured into the Petri dish and left to dry for 24 hours at room temperature (24-26 ºC). The films were peeled off from Petri dishes. 2.3. Hydrolytic Degradation: The films were cut into 6 mm diameter discs and placed in two test tubes in each test tube and weighed on a sensitive scale to determine the starting weight. 10 ml of Phosphate buffer (pH 7.4) was added to the tubes and placed in the incubator at 37 0C. Thus, the hydrolytic biodegradability study was initiated. The tubes were taken from the incubator at certain time intervals and films were taken out of them. After washing with ethyl alcohol and drying, it was weighed and then analyzed. 2.4. Optical Microscopy Imaging: The prepared PLA and PLA / PEA films were initially imaged with an optical microscope and their photos were recorded to determine the morphological properties of the matrix. Leica EP model Polarized Optical Microscope device and camera were used for imaging of the films. 2.5. Molecular Weight Analyses: Gel Permeation chromatography (GPC), Waters styragel column (HR series 2, 3, 5E) Tetrahydrofuran (THF) solvent at 1 mL/min injection rate and Waters 410 differential refractometer detector (UK), was used for molecular weights analysis. 2.6. X-ray diffraction Analysis: X-ray diffraction analyses were performed by using PANalytical Empyrean (Netherlands) with Cu K K? radiation (? = 1.5406 A°). The current and voltage were adjusted to 40 mA and 45 kV.

3.Result and Discussion

3.1. Optical Microscopy Imaging Samples (0% PEA, 10% PEA and, 50% PEA) were removed from the tubes, cleaned and dried. The dried samples were imagined by using optical microscopy. The increasing dimensions of divided areas in polymer matrices could be seen in the figure. Diameters of divided areas increased depending on PEA contents as proportional. PLA and porosity of the polymer films were observed depending on PEA content. 3.2. Molecular weight It is seen from the GPC graph that the molar mass of all samples decreased depending on both time and PEA content. This reduction is more common in films containing more PEA. Molecular weights of 0%PEA, 10% PEA and 50% PEA containing PLA films decreased from initial weights to 63065, 13790 and 9420 respectively, at the end of 11 weeks. PEA content affected the degradation. 3.3. XRD analyses PLA has both crystalline and amorphous areas. It can be seen from the figure that neat PLA has reflections which belong to amorphous structures. The incorporation of 10%PEA resulted in the shifting of some of the reflections. In the case of increasing PEA content to 50%, the intensities of these reflections increased. As it was expected, the diffractograms of the films showed characteristic peaks. The peaks at 12.4°, 14.9°, 16.8°, 19.3°, 22.5°and, 24.6° belong to PLA . The PLA exhibits strong reflection at 16.8° because of the diffraction from (200) and/or(110) planes and another reflection peak at 19.3° arising from (203) plane . The small diffraction peaks at 2? = 12.4?, 14.9?, 20.8? and, 24.6°represent (004)/(103), (204), (115), (016), and (206) planes of ?-crystals. And more, a reflection at 2? = 24.6?, which is characteristic of ??crystals, can be seen. These results suggest that both ? and ?? crystals exist in the polymer matrix. Insertion of PEA increased the crystal structures in the PLA matrix and the amount of PEA affects these crystal structures.

4.Conclusion

The main purpose of the research is to investigate the effect of PEA on crystallinity and hydrolytic biodegradation on PLA. Pheniletyl alcohol, natural essential oil in different proportions, was added to PLA, a biodegradable polymer. It is concluded that this added natural component increased crystallinity and accelerated the biodegradability of PLA. It was found that this acceleration increased in direct proportion to the amount of natural component added. The natural essential oil PEA affected the crystallinity and biodegradability of PLA as a biodegradable polymer. The crystallinity and biodegradation of PLA could be controlled by using PEA as a natural material. Acknowledgements This work was funded by Çanakkale Onsekiz Mart Univesity, Unit of Scientific Research Projects as project number FBA-2018-1368.

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Evaluation of the Effect of Glucose Fatty Acid Esters on Thermal Degradation of Vegetable-Based Oils

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Edible oil quality and stability are the main factors affecting oil acceptability and market value. Oxidative stability is one of the most important indicators for maintaining the quality of edible oils. The concentration of non-lipid radicals and the amount of natural antioxidants in lipids are important factors in predicting the stability of edible oils against oxidative stress [1,2]. Heat treatments of vegetable oils may lead to undesirable modifications in some components of protein fraction mainly due to lipid oxidation. Oxidation of unsaturated fatty acids is one of the main causes of the development of non-flavor compounds and reduction of the nutritional value of food products [3]. In order to delay the thermo-oxidative degradation of vegetable oils, synthetic antioxidants such as butyl hydroxytoluene (BHT), butylated hydroxyanisole (BHA), butyl hydroquinone (TBHQ) are used in refining processes. However, studies on the risk of these compounds on human health increase the interest in the use of natural antioxidants [4,5,6]. In this study, it was aimed to investigate the effect of glucose fatty acid esters on the thermal stability of vegetable oils. For this purpose, firstly, the synthesis and characterization of glucose fatty acid esters such as glucose oleate and glucose laurate were carried out. Then, the effect of these glucose fatty acid esters on the thermal stability of vegetable oils such as sunflower, corn and olive oil was carried out under an accelerated storage test at 60°C for 15 days. Studies were also conducted using commercial antioxidants and the results were compared. It has been observed that high oleic acid content increases thermal degradation in edible oils. The results showed that glucose oleate and glucose laurate are effective in preventing the thermal oxidation of vegetable oils. In addition, glucose oleate showed better antioxidant properties compared to glucose laurate [7].

Keywords: Antioxidant, Glucose esters, Oxidative degradation, Edible oils, Thermal stability

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6th International ISCMP ALBANIA 2022
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Fabrication of a Novel Colorimetric Glucose Biosensor Using Copper(II)-Neocuproine as Chromogenic Oxidant and Glucose Dehydrogenase Immobilized Magnetite Nanoparticles

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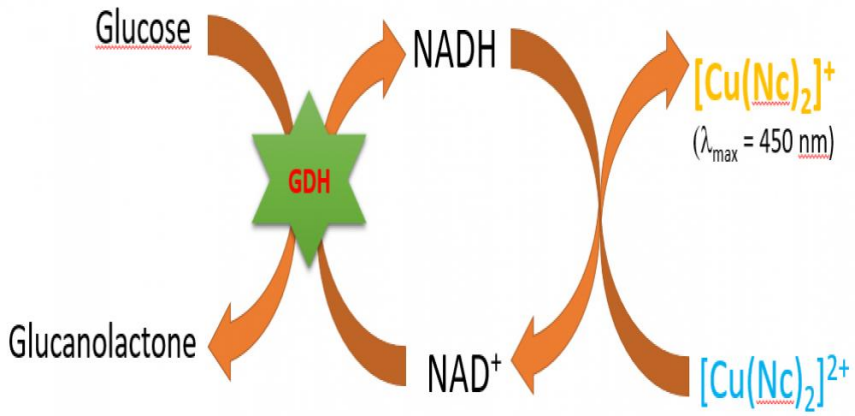

Apak et al. introduced the CUPRAC (CUPric Reduction Antioxidant Capacity) method to the world literature for the determination of total antioxidant capacity (TAC) in 2004 (1). The developed method is based on measuring the absorption at 455-460 nm of the yellow-colored Cu(I)-Neocuproin complex ([Cu(Nc)2]+) formed as a result of the reaction of pale blue Cu(II)-bis-neocuproin complex ([Cu(Nc)2]2+) with phenolic compounds. Many spectrophotometric and chromatographic methods have been developed for the determination of various analytes using this reaction and mechanism. Although glucose dehydrogenase-based optical biosensors were reported using different types of chromogenic oxidant, the integration of the CUPRAC method into biosensors based on using dehydrogenase enzymes has not been reported yet. In this study, a glucose biosensor is developed for the first time based on using glucose dehydrogenase (GDH) immobilized magnetite nanoparticles and CUPRAC reagent. In the first step, an enzymatic reaction takes place between glucose and GDH on Fe_3O_4 in the presence of NAD+. At the end of this reaction, NAD+ is reduced to NADH while glucose oxidizes to gluconic acid. After GDH immobilized Fe_3O_4 nanoparticles are separated with a magnet, a second reaction takes place between the CUPRAC reagent and enzymatically produced NADH. After this reaction, the glucose biosensor is constructed based on the measurement of the absorbance of the formed yellow-orange [Cu(Nc)2]+ complex at 450 nm. The mechanism of the constructed biosensor is shown in the graphical abstract. In the first step of the study, Fe_3O_4 magnetic nanoparticles were synthesized in the presence of a surfactant (1-hexadecyl) trimethylammonium bromide (CTAB) according to the literature and then silanized with tetraethyl orthosilicate (TEOS) and (3-Aminopropyl)triethoxysilane (APTES), respectively (2). In the following step, GDH is immobilized onto the Fe_3O_4@SiO_2 magnetic nanoparticles (GDH- Fe_3O_4@SiO_2) via a glutaraldehyde cross-linking procedure. The absorbances of yellow-orange solutions formed by increasing the concentration of glucose are measured

Keywords: Glucose, Optic biosensor, Glucose dehydrogenase, Magnetite nanoparticles, Cu(II)bisneocuproine,

Acknowledgement: The authors thank The Scientific and Technological Research Council of TURKEY (TÜBİTAK) for financial support (Project number: 120Z963).

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Determination of Antimicrobial, DPPH Scavenging, and Tyrosinase Inhibitory Activities of *Thymus vulgaris*, *Helichrysum arenarium*, and *Rosa damascena* Mill. Ethanol Extracts

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Antimicrobial, DPPH scavenging and tyrosinase inhibitory activities of *Thymus vulgaris*, *Helichrysum arenarium* and *Rosa damascena* Mill. ethanol extracts by using TLC bioautography and chemical screening methods. The ethanol extracts of *Thymus vulgaris* (Tv), *Helichrysum arenarium* (Ha) and *Rosa damascena* Mill. (Rm) (red) were screened for their antimicrobial, 2,2-Diphenyl-1-picrylhydra zyl (DPPH) radical scavenging and tyrosinase inhibitory activities. The test microorganisms included bacteria of *Escherichia coli* (ATCC 25922) and *Staphylococcus aureus* (ATCC 25923). Thin Layer Chromatog raphy (TLC) - bioautography, disk diffusion and well diffusion methods were used for the antimicrobial activity assays. *Rosa damascena* Mill. extract was effective against *E. coli* and all plant extracts showed antimicrobial activity against *S. aureus*. The phenolic acids in the structure of the extracts were also identified by LC-MS analysis. Humanblood agar well diffusion method and TLC-DPPH assays were used to identify the hemolytic and antioxidant activity of plant extracts, respectively, along with 10 compounds including phenolic acids as a standard. Among these compounds, caffeic acid (Rf ¼ 0.68) was detected in all extracts while vanillic acid (Rf ¼ 0.75), and gallic acid (Rf ¼ 0.51) were found in Tv extract. Kojic acid (Rf ¼ 0.36), on the other hand, was detected in Rm extract as a tyrosinase inhibitor. All plant extracts presented tyrosinase inhibitory activities on TLC-bioautography assay.

Keywords: TLC, Bioautography, Antimicrobial, DPPH, Tyrosinase inhibitors, Hemolytic activity

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Highly Flexible Binder-Free Supercapacitor Electrode Based on Carbon Material

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The increasing energy demand with the growing global population makes it necessary efficient energy storage systems. Supercapacitors are substantial energy storage devices with the capability of supplying large amounts of power unlike, batteries. On the other hand, energy storage systems are sensitive to mechanical deformation, resulting in unavoidable damage and performance loss. Recently, flexible energy storage devices are studied more extensively together with the advancements in wearable electronics. Carbon nanomaterials are ideal electrode materials for flexible supercapacitors due to their large surface area and high electrical conductivity characteristics. Herein, we report a highly flexible supercapacitor electrode which is prepared via facile and efficient way. We mostly focused on the structural design for electrode configuration to enhance the conductivity and promote the electron pathway. Cotton-textile are chosen as the flexible substrate for the construction of energy storage device due to the flexibility, and breathable structure. The strong interface bond of the carbon material onto the flexible substrate allows the mechanical stability under bending conditions and demonstrates as a promising electrode material. FESEM analysis revealed the morphological structures of the electrode material. Excellent stability was reported for the system at 1A g^{-1} with capacitance retention over 5000 cycles. The results show that the good interaction between materials, and electrical conductivity are attributed to the well electrochemical performance of the electrode material. This study showed the extremely flexible binder free electrode for next-generation supercapacitor applications. Furthermore, this research could guide the development of flexible, high-performance, and low-cost electrodes which will be useful in energy storage devices.

Keywords: Flexible supercapacitor, Low cost electrode, Binder free

REGISTER NO
8ebda5

Quantum Dots Functionalized Egg Viol Derived Carbon and Strontium Oxide for High Performance Zinc Ion Hybrid Supercapacitor

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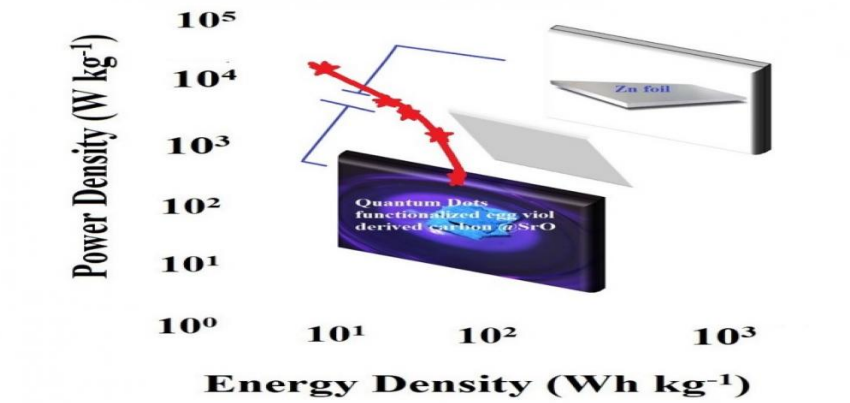
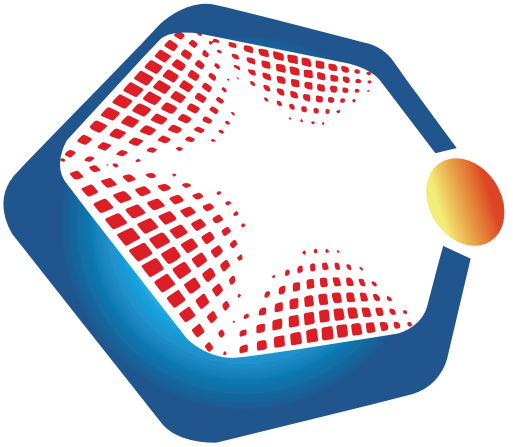


The destruction of environmental wastes or, more importantly, their reuse in different areas by providing more functionality through recycling is one of the most pivotal issue that need to be considered. For so long, some kind of bio wastes, plastic contaminants, or paper-based expended materials have drawn attention as a carbon source to produce activated carbon (AC) for energy storage (ES) applications. Among ES devices recently developed Zinc-ion hybrid supercapacitors (ZHSC) gain traction due to the prosperous unification of batteries, and supercapacitors. Herein, we developed a novel approach to reuse egg viol as a template to produce activated carbon. Unlike some previous studies, the carbonization process was carried out in Argon atmosphere using quantum dots without the requirement of CO_2 gas. Thereby, with an innovative, environmental, and cost-effective approach we ably impart electrical conductivity to egg viol. Thereafter, this carbon quantum dots functionalized material was used as a carbon source for ZHSC application when strontium oxide (SrO) was the essence material. The device achieved the potential window of 1.2 volts with a high specific capacitance of 375 F g^{-1} at a current density of 1 A g^{-1}. When,the highest energy and power densities were 75 Wh kg^{-1} and 12.1 kW kg^{-1}, respectively. These outstanding results indicate that quantum dot functionalized egg carton box-derived carbons synergistic effect with SrO can be used to gain high performance cathode material for ZHSC.

Keywords: Egg viol, Quantum dots, Zinc-ion hybrid supercapacitors



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POSTER PRESENTATIONS

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14-17 September 2022 Albania

Some Physicochemical, Rheological, Antioxidant, Microbiological and Sensory Properties of Kefirs with Propolis at Different Ratios

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In this study, kefir samples containing 5% (w/v) sugar, 0.15% (v/v) strawberry flavor and propolis extract at different ratios [0.150, 0.225 and 0.300% (v/v)] were produced, and they were stored in a refrigerator at 4±1°C for 8 days. Some physicochemical, antioxidant, rheological, microbiological and sensory properties of kefir samples were determined on the 1st, 4th and 8th days of storage. The addition of propolis extract and storage had no effect on dry matter, protein, fat contents, L* and a* values, rheological properties (apparent viscosity, consistency coefficient and flow behavior index) and total lactobacilli, lactococci and yeast numbers of kefir samples ($p>0.05$). The addition of propolis extract did not influence the pH and acidity (lactic acid) values of kefir samples ($p>0.05$) but the pH values of samples decreased ($p<0.05$) while acidity values increased during storage ($p<0.05$). Addition of propolis extract to kefir drinks increased the b* (yellowness) values of samples ($p<0.05$). All kefir samples showed pseudoplastic flow behavior. It was determined that the total antioxidant capacity and phenolic content of samples increased by an increase in the ratio of propolis extract added to kefir samples, and these values decreased during storage. It was found that the addition of propolis extract did not affect the sensory color and taste scores of kefir samples adversely. Kefir samples containing 0.225% and 0.300% propolis extract received sensory scores similar to the control group in terms of odor, and the overall liking scores of kefir samples were similar to those of control group for kefir drinks containing 0.150 and 0.225% propolis extract. Results indicated that it was possible to produce kefir drinks with 0.225% propolis extract, which was acceptable in terms of both sensory and increased functional properties, and that this product could be stored up to 8 days.

Keywords: Kefir, Propolis, Antioxidant, Phenolic, Functional food, Health

Acknowledgement: We thank Aromsa Besin Aroma ve Katkı Maddeleri Sanayi ve Ticaret A.Ş. (Kocaeli, Turkey) for providing the fruit flavors used in the study and Süt Ofis Gıda A.Ş. (Burdur, Turkey) for their assistance in chemical analyses.

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f29c21

Green Seaweed *Ulva rigida* Extracts as Potential Antioxidant Ingredients in Yoghurt

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Green seaweeds (*Ulvophyceae*) are eukaryotic organisms that produce sulfated polysaccharides that possess essential pharmacological activities such as antioxidant, anticoagulant, anti-inflammatory, antitumoral and antiviral. Ulva sp., a green seaweed, is common on the coast of the Mediterranean. It is a good candidate for culture due to its nutritional value and high antioxidant properties. Supplementing dairy products with seaweeds can contribute to extending shelf life and attaining a balanced diet, but it may affect their antioxidant activity. This study evaluated antioxidant activity contents and the reducing power of yoghurt mixtures containing four *Ulva rigida* powders (5%, 10%, 15% and 20% (w/w)) and control (0%). DPPH (1,1-diphenyl-2-picrylhydrazyl) radical scavenging activity and the reducing power were determined in ethanolic extracts of yoghurts. As a result of the study, it was determined that all experimental groups showed weak antioxidant activity. Among the experimental groups, the highest antioxidant activity was found with 20% *U. rigida* powder added. In the reducing power assay, the presence of reductants (antioxidants) in the samples could reduce the Fe^{3+}/ ferricyanide complex to its ferrous form. The amount of Fe^{2+} complex can then be monitored by measuring the formation of Perl's Prussian blue at 700 nm. A compound's reducing capacity may be a significant indicator of its potential antioxidant activity. Reducing power of extracts decreased by 0%<5% =10%<15%<20%. These results revealed that the group containing 20% *U. rigida* powder was electron donor and could react with freeradicals, converting them to more stable products. Our results show that the green seaweed *U. rigida* powder-enriched yoghurts did not exhibit high antioxidant activity and reducing power when added to yoghurt. Further research is needed to evaluate the potential of other seaweed-derived ingredients as functional components in fermented dairy products.

Keywords: *Ulva rigida*, Antioxidants, Reducing power, Green seaweeds, Yoghurt

Acknowledgement: The authors thank the Çanakkale Onsekiz Mart University Science and Technology Application and Research Center for providing laboratory facilities for our experiments.

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44c4c1

Assessment of Organic Contaminants in Some Urban Locations in the Republic of Kosovo

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Organic contaminants are not only hazardous to human health, but also key precursors of ozone and PM2.5, which cause serious air pollution. Therefore, it is essential to monitor these compounds by developing reliable and effective techniques. The method involves the use of Radiello® passive air sampler for urban air monitoring. The advantage of the Radiello® passive/diffusive samplers are that they offer higher capacity and faster uptake/sampling rates compared to other passive samplers. The Radiello® passive/diffusive samplers were placed in several municipalities in Kosovo (Dragash, Elez Han, Obiliq, Rahovec) and the organic compounds were monitored every 28 days over the period from October 2021 to January 2022. Using gas chromatography coupled to mass spectrometry (GC-MS) we were able to detect several organic compounds. The composition was complex but the most abundant organic contaminants originate from transport fuels and related derivatives such as BTEX (benzene, toluene, ethylbenzene and xylenes) and tetradecane. Additionally, in these samples, naturally occurring monoterpenes were detected (alpha-pinene and limonene). The goal of the study was to develop an efficient method for extraction of the adsorbed sample with appropriate organic solvents, as well as cleaning and conditioning of the adsorbing surface of Radiello® for subsequent use. The long term goal is to control organic contaminants and to monitor their concentrations throughout the year in the Republic of Kosovo.

Keywords: Environmental pollution, Organic contaminants, Gas chromatography, Radiello® passive sampling

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996a7f

6th International ISCMP ALBANIA 2022
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Synthesis of Epoxidized Vegetable Oils and Determination to Use In PVC Paste as a Viscosity Regulator

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Plasticizers are non-volatile organic liquid compounds that add flexibility to polymers and increase the range of application. Most of plasticizers are used in the use of polyvinylchloride (PVC) because it shows fake flow properties.Products obtained with PVC pastes formulated with various additives vary from very hard pipes and exterior coatings to flexible flooring and adhesives. [1] Due to its thermoplastic property, PVC contains two structures, amorphous and crystalline.Plasticizer is embedded in polymer matrices upon addition and bonding, lowering glass transition temperature, thus making polymers more flexible. PVC paste formulation contains multifunctional additives that determine, change, and improve the properties of the products. In general, formulations contain other specific property enhancers such as polymer (resin), fillers, plasticizers and fire-resistant materials. Thus, plasticizer increases flexibility, softness, workability of the polymer[2]. A primary plasticizer enhances elongation, softness and flexibility of polymer. They are highly compatible with polymers and can be added in large quantities. A secondary plasticizer is one that typically cannot be used as the sole plasticizer in a plasticized polymer. They are often used in mixtures with primary plasticizers. This group includes aliphatic and aromatic chlorinated hydrocarbons as well as epoxy esters of unsaturated fatty acids obtained from plants [3].They are used to give the mixture special properties: flexibility at low temperatures. The most common bio-based secondary plasticizer is epoxidized soybean oil [4]. In this study,synthesis of soybean oil in epoxy, which is used as a secondary plasticizer, was successfully carried out by peracid method. Fatty acid composition of it to be used were determined by using GC-FID and peroxide value, iodine number, saponification value, total acid number were determined. Characterization was carried out using 1H NMR and FTIR after epoxidation. Different formulations were prepared using epoxy soybean oil and its performance in PVC paste was studied.

Keywords: Plasticizer, Epoxized soybean oil, PVC, Secondary plasticizer, Glass transition temperature

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REGISTER NO

42e77b

Preparation and Characterization of Antiviral HDPE-ZnO Food Packaging Composite Material

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Epidemic diseases such as leprosy, plague, cholera, malaria, especially Covid-19 (SARS-CoV2 infection) have caused death of thousands people. Development of antiviral food packaging materials to be used in food package service systems that can active role in slowing Covid-19 epidemic rate especially. One of the food packaging material high density polyethylene (HDPE) raw material is light and cheap and Zinc oxide (ZnO) is antiviral nanoparticle. In this study, HDPE; a PE-based food packaging material was combined with antiviral ZnO nanoparticles at different concentrations (5%, 10%, 15%, 20% and 25%) in two stages that thermal homogenization and hot-press method. HDPE-ZnO composite packaging material is prepared and characterized by thermogravimetric analysis (TGA), X-Ray diffractometry (XRD) and fouirer transform infrared spectrophotometer (FTIR).

Keywords: Antiviral, Composite,, ZnO, HDPE, Food safety, Packaging

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daca41

Some Properties of Black Cumin Volatile Oil Added PLA Films

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Black cumin (*Nigella sativa*) volatile oil has been use in public treatments for a long time. *Nigella sativa* seeds have wide therapeutic effects and have been reported to have significant effects against many ailments such as skin diseases, jaundice, gastrointestinal problems, anorexia, conjunctivitis, dyspepsia, rheumatism, diabetes, hypertension, intrinsic hemorrhage, paralysis, amenorrhea, anorexia, asthma, cough, bronchitis, headache, fever, influenza and eczema. One of the most active constituent is thymoquinone and has different beneficial properties. Poly lactice acid (PLA) is natural biodegradable material. It is widely used medical applications. Due to their biodegradability, they are well suited for the preparation of disposable devices. One of the key properties of the PLA matrix is its ease of degradation by the enzymatic or hydrolytic pathway. It is very suitable material for drug carrier and delivery. In this study different percentages of black cumin volatile oil were added to PLA film matrices. It was found that thermal stability and crystalinity of the PLA film were affected by add to black cumin volatile oil. We concluded that black cumin volatile oil added PLA films can be use as natural and biodegredable material for medical applications.

Keywords: *Nigella sativa*, X-Ray Diffraction, Thermo Gravimetric Analysis, Black cumin, Poly lactice acide

REGISTER NO

abd815

Synthesis of Poly(3-hexylthiophene-2,5-diyl) and Improvement of the Optic and Electric Properties by Sensibilization with Thiazolyl-hydrazinylidene-chroman-2,4-dione

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Solar energy represents an important part of renewable energies for the future. An ideal solar cell requires high optical absorption strength combined with large charge-carrier diffusion lengths and efficient collection of electrons and holes at the respective electrode. Optical solar cells have advantage of being operable under ambient conditions at low temperatures, which allows for flexible substrates. However, they still suffer from poor excision, charge carrier diffusion lengths, and low mobility. In this attempt first 3-hexylthiophene was polymerized in inert conditions and then characterized by UV/Vis and IR spectroscopy. Afterwards, a stock solution was prepared in chloroform and sensibilisation was attempted by adding different amounts of the novel organic dye (E)-3-[2-(thiazol-2-yl)hydrazinylidene]chroman-2,4-dione. This latter compound has a lot of chromophores, thus it has abroad absorption spectrum (with five maximum wavelengths), so it improves the absorption abilities. The mixture composed of polymer and dye compound was applied as a thin film on indium-thin oxide plate (ITO) and electrochemical features were studied by means of cyclic voltammetry.

Keywords: Organic solar cells, Poly(hexylthiophene), Thin films, Cyclic voltammetry

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dbe272

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Initiator Effect on Gel for Breast Phantom Preparation

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Breast cancer appears to be the most common disease among women in the world, and cancer is the first cause of death among women. Microwave imaging systems have been considered as a new more harmless technique for breast cancer detection based on dielectric contrast between healthy and cancerous tissues. In order to develop microwave imaging systems and to test the performance of the developed systems before they are used in clinical tests, it is extremely important to test these systems on phantoms that can mimic tissues in terms of electrical properties. The aim of this project is that the developed breast phantoms are suitable for the real breast structure in terms of dielectric & mechanical properties. Considering such situations, acrylic acid was used as monomer during the preparation of the gel phantom. N,N'-Methylenebisacrylamide (BAAm) as used as cross-linker and potassium persulfate (KPS) as initiator in certain ratio. After synthesis, gel phantoms were purified in different solvents. After the purification and drying procedure, synthesized gels were swelled in distilled water (DW) for 10 days. The swelling ratios of the gels were calculated and their dielectric properties were examined. It is observed that, the relative permittivities of the gels were close to the relative permittivity of DW.

Keywords: Breast cancer, Phantom, Dielectric properties, Gel phantom

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051e4e

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Physical Properties and Electromagnetic Absorption Performance of Fe_2O_3 Doped Rigid Polyurethane Materials

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The use of electrical and electronic devices is increasing rapidly. These devices generate serious electromagnetic interference that can degrade the performance of nearby devices and threaten human health. It can cause cancer and its derivatives in living organisms due to changes in cell structure as a result of long-term exposure. As seen in electromagnetic studies, it can cause irreversible damage to living organisms exposed to electromagnetic waves. Therefore, there is a need to absorb electromagnetic interference in order to prevent the negative effects of electromagnetic interference on human health and electronic devices. In this thesis, rigid polyurethane materials with 5%, 10% and 15% Fe_2O_3 by weight were produced. The physical properties and electromagnetic interference absorption performances of the produced materials were investigated. The prepared materials were characterized by Scanning Electron Microscopy/Energy Dispersive Spectrometer, X-Ray Diffraction, Fourier Transform Infrared Spectroscopy, Differential Scanning Calorimetry and Thermogravimetric Analysis. The results showed that 15 wt% Fe_2O_3 doped rigid polyurethane in the S-band provided a reflection loss below -20 dB.

Keywords: Electromagnetic interference, Electromagnetic absorption, Fe_2O_3, Physical properties, Rigid polyurethane

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26408f

Synthesis and Electrochemical Characterization of Polyvinylidene Fluoride/Polypyrrole (PVDF/PPy) Composite

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Poly(vinylidene fluoride) (PVDF) has better mechanical properties than fluorinated polymers such as poly(tetrafluoroethylene). They can be used as films, membranes and nanofibers in several fields such as electrical energy, microelectronics and biomedical field. Besides, intrinsic conducting polymers are a relatively new group of polymeric materials. Conducting polymers respond sensitively to even the slightest change in the polymer chain environment. Among these, polypyrrole (PPy) and its composites have some superior properties such as high conductivity values, ease of synthesis, excellent environmental stability and low toxicity. However, the weak mechanical properties of PPy impose restrictions for some application areas. In order to overcome the limitations of PPy, its composites are being prepared with some materials to add interesting features (electrical and mechanical). In this study, we synthesized PVDF/PPy composites with chemical oxidation method. And we characterized the PVDF/PPy composite with electrochemical method. PVDF/PPy composite was used as working electrode directly. PVDF/PPy composite material will be used as a working electrode in a sensor system in our future study. Therefore, cyclic voltammetric (CV) measurement of PVDF/PPy composite was studied in pH 7.4 phosphate buffer solution. The cyclic voltammetry study of PVDF fiber membran was gave an error because of the insulator nature of PVDF fiber membran. As a result, CV voltammograms of PPy and PVDF/PPy were compared. PVDF/PPy composite responded electrochemically due to the conductive polypyrrole layer. This result shows that the PVDF fiber layer was covered by polypyrrole smoothly.

Keywords: Poly(vinylidene fluoride), Polypyrrole, Composite, Conducting polymer, Electrochemistry, Chemical Polymerization

Acknowledgement: This study was supported by Burdur Mehmet Akif Ersoy University, Scientific Research Project Coordinatorship Under the Project number of 0855-YL-22.

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5d44ee

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Evaluation of Diatomaceous Earth's Adsorptive Properties toward (2E,5E)-2,5-Bis(4-methoxybenzylidene)cyclopentanone. An Experimental and Theoretical Study

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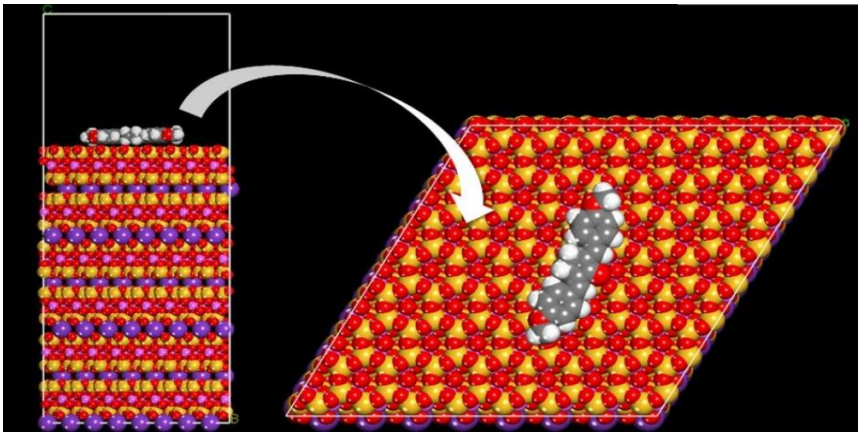

The purpose of this research is to investigate the adsorption of (2E,5E)-2,5-Bis (4-methoxybenzylidene) cyclopentanone using diatomaceous earth. The monocarbonyl compound was first synthesized, then crystallized and characterized using IR, NMR, and other techniques. The preferred adsorption site, interaction type, and adsorption energy of the (2E,5E)-2,5-Bis(4-methoxybenzylidene) cyclopentanone onto diatomaceous earth were investigated using theoretical calculations based on Density Functional Theory (DFT) and Monte Carlo (MC) calculations. Figure 1: Monte Carlo lowest energy geometry obtained during the adsorption of the adsorption of the 2E, 5E)-2,5-Bis (4-methoxybenzylidene) cyclopentanone using diatomaceous earth modelled using Muscovite structure (Amcsd 0000854). Diatomaceous earth soil is cleaned, homogenized, and characterized spectroscopically before being used as an adsorbent. UV-Vis measurements were used to assess the diatomaceous earth's adsorptive ability toward the (2E, 5E)-2,5-Bis(4-methoxybenzylidene)cyclopentanone.

Keywords: MACs, Adsorbent, Synthesis, Theoretical calculation, IR, NMR

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A Theoretical Investigation of Anticancer Drugs as Potential Corrosion Inhibitors

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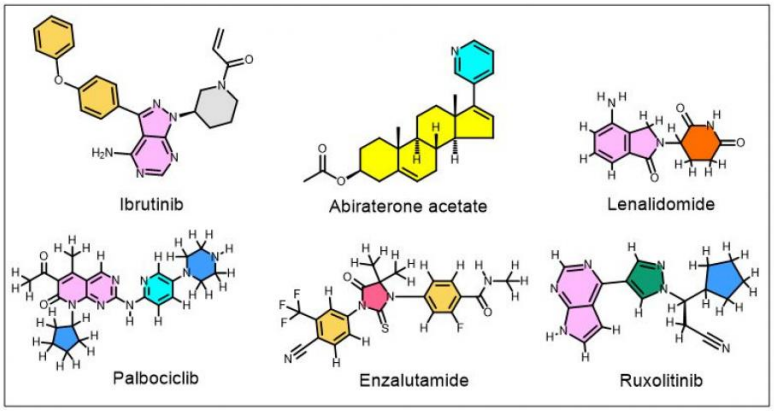

A number of anticancer drugs that contain intriguing moieties that are prone to corrosion inhibition (heterocycles and various heteroatoms) are being investigated as prospective corrosion inhibitors as part of an overall quest for novel inhibitors that have not been explored previously. The examined drugs include (Figure 1): Ibrutinib, Abiraterone acetate, Lenalidomide, Palbociclib, Enzalutamide and Ruxolitinib. Density Functional Theory (DFT), Monte Carlo simulation (MC), and Molecular Dynamics simulation [1] were utilized in order to evaluate the adsorption of the anticancer drug onto the surface of Fe (1 1 0). The data that were gathered provided information down to the molecular level on the adsorption ability, adsorption centers, shape, and adsorption energetics of anticancer onto the Fe(1 1 0) surface.

Keywords: Anticancer drugs, Corroson, Density functional theory, Monte Carlo, Molecular dynamics, Adsorption

References: A. Berisha, Ab inito exploration of nanocars as potential corrosion inhibitors, Comput. Theor. Chem. 1201 (2021) 113258.

REGISTER NO

3871bd

Monte Carlo and Experimental Studies on the Adsorption of (2E, 5E)-2,5- Bis (4-methoxybenzylidene) Cyclopentanone Molecule on the Graphene Oxide

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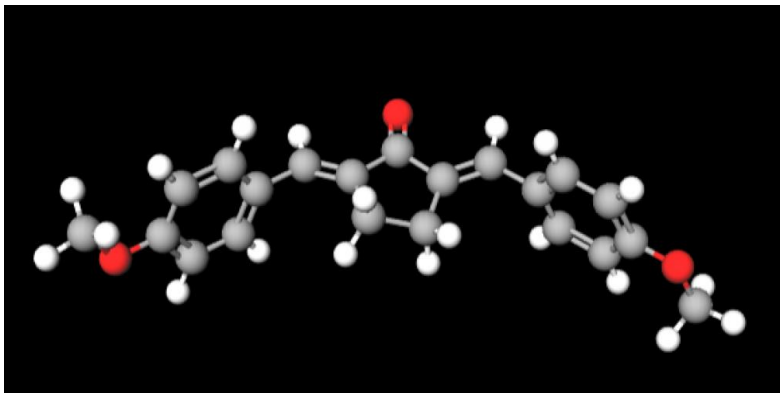

The high adsorption capacities of graphene oxide are mainly determined by its unique nanostructure, high specific surface area and suitable surface properties, which make it suitable for the storage or capture of various organic molecules . Graphene oxide is evaluated as an adsorbent for the organic molecule such as (2E, 5E) -2,5-bis (4-methoxybenzylidene) cyclopentanone dissolved in organic solvent such as acetonitrile. The functional groups in GO were characterized by using an IR spectrometer. The concentration of the organic molecule after adsorption is analyzed using ultraviolet-visible spectroscopy. Theoretical studies (Monte Carlo calculations) were also performed and showed good compatibility with experimental calculations.

Keywords: Monte Carlo, (2e, 5e) -2,5-bis (4-methoxybenzylidene) Cyclopentanone, Graphene oxide, Acetonitrile, IR spectrometer, Organic molecule

References: [1]Veprim Thaçi, Ramiz Hoti, Avni Berisha*, Jane Bogdanov*, Corrosion study of copper in aqueous sulfuric acid solution in the presence of (2E,5E)-2,5-dibenzylidenecyclopentanone and (2E,5E)-bis[(4-dimethylamino)benzylidene]cyclopentanone: Experimental and theoretical study , Open Chemistry 2020; 18: 1412?1420. [2] Ardhmeri Alija, Drinisa Gashi, Rilinda Plakaj, Admir Omaj, Veprim Thaçi, Arianit Reka, Sefer Avdiaj and Avni Berisha. A theoretical and experimental study of the adsorptive removal of hexavalent chromium ions using graphene oxide as an adsorbent. Open Chemistry, 2020: chem-2020-0148

REGISTER NO

a733fa

A Theoretical and Experimental Study of the Adsorptive Removal of (2E, 5E)-2,5 Bis [(4-dimethylamino) benzylidene] Cyclopentanone using Graphene Oxide

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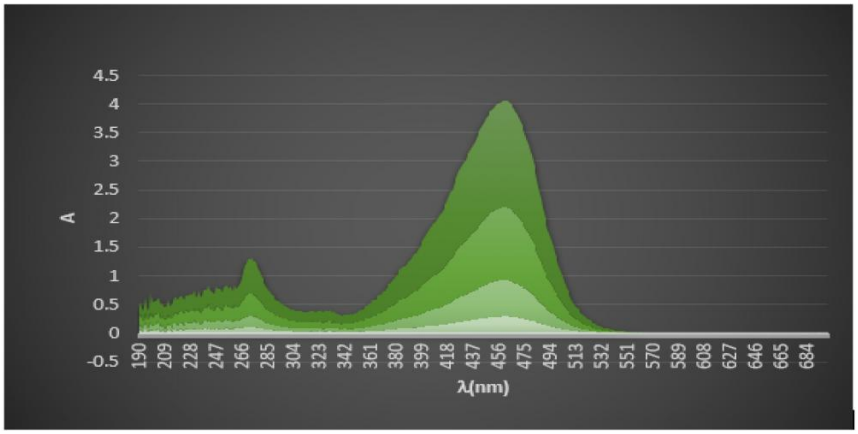

This study is focused on the adsorption of (2E, 5E)-2,5 Bis [(4-dimethylamino) benzylidene] cyclopentanone using graphene oxide (GO). The GO was prepared by chemical oxidation (Hummers method) of graphite particles. The synthesized GO adsorbent was characterized by Fourier transform infrared spectroscopy and UV-Vis spectroscopy. It was used for the adsorption of (2E, 5E)-2,5 Bis [(4-dimethylamino) benzylidene] cyclopentanone. The theoretical calculations were used to explore the preferable adsorption site, interaction type, and adsorption energy of GO toward the (2E, 5E)-2,5 Bis [(4-dimethylamino) benzylidene] cyclopentanone. Moreover, the most stable adsorption sites were used to calculate and plot noncovalent interactions. Adsorbat (pre-synthesized) is characterized by some powerful spectroscopic techniques as well.The data generated through theoretical techniques are consistent with the experimental results.

Keywords: Graphene oxide, Cyclopentanone derivatives, Adsorption, Interactions

References: [1] V. Thaçi, A. Berisha, R. Hoti, Experimental and Theoretical Study of Some 2,5-Diarylidenecyclopentanone Derivatives. Joint Science Congress of Materials and Polymers - ISCMP 2019. Open Chemistry [2] A. Alija, D. Gashi, R. Plakaj, A. Omaj, V. Thaçi, A. Reka, S. Avdiaj, A. Berisha . A

theoretical and experimental study of the adsorptive removal of hexavalent chromium ions using grapheneoxide as an adsorbent. Open Chemistry. https://doi.org/10.1515/chem-2020-0148 [3] Dideikin AT, Vul AY. Graphene oxide and derivatives: the place in graphene family. Front Phys. 2019;6:149. [4] Veprim Thaçi, Ramiz Hoti, Avni Berisha*, Jane Bogdanov*, Corrosion study of copper in aqueous sulfuric acid solution in the presence of (2E,5E)-2,5-dibenzylidenecyclopentanone and (2E,5E)-bis[(4-dimethylamino)benzylidene] cyclopentanone: Experimental and theoretical study, Open Chemistry 2020; 18: 1412-1420.

REGISTER NO
48ab2f

The Interaction of (2E, 5E)-2,5- Bis (4-methoxybenzylidene) Cyclopentanone Organic Molecule onto the Graphene Oxide Surface

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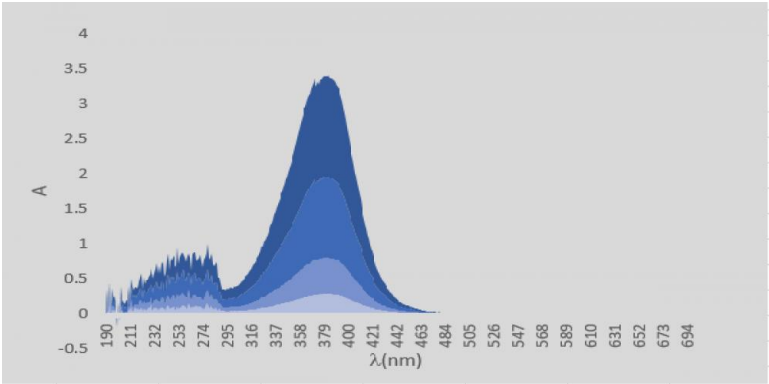

(2E, 5E)-2,5-bis (4-methoxybenzylidene) cyclopentanone as an organic molecule dissolves in organic solvents such as acetonitrile and gives a very intense yellow color .The synthesized Graphene oxide by using the Hummers method is evaluated as adsorbent toward to this organic molecule and gives satisfactory adsorption results. Hummers? method is the most common method used for preparing graphene oxide, method in which graphite powder was oxidized in the presence of concentrated H2SO4 and KMnO4. Infrared spectroscopy characterization tests were used to investigate the adsorbent structure. The adsorption performance of the material was evaluated using UV-VIS spectroscopy.

Keywords: (2E, 5E)-2,5-bis (4-methoxybenzylidene) cyclopentanone, organic solvents, Graphene oxide, UV-VIS spectroscopy, IR spectrometer, Hummers? method

References: [1]Veprim Thaçi, Ramiz Hoti, Avni Berisha*, Jane Bogdanov*, Corrosion study of copper in aqueous sulfuric acid solution in the presence of (2E,5E)-2,5-dibenzylidenecyclopentanone and (2E,5E)-bis[(4-dimethylamino)benzylidene]cyclopentanone: Experimental and theoretical study , Open Chemistry 2020; 18: 1412?1420. [2] Ardhmeri Alija, Drinisa Gashi, Rilinda Plakaj, Admir Omaj, Veprim Thaçi, Arianit Reka, Sefer Avdiaj and Avni Berisha. A theoretical and experimental study of the adsorptive removal of hexavalent chromium ions using graphene oxide as an adsorbent. Open Chemistry, 2020: chem-2020-0148.

REGISTER NO

233509

Examination of Fatigue Behaviors of Al6061 Matrix SiC Al_2O_3 and Blast Furnace Slag Reinforced Hybrid Composites

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In this study, Al6061 alloy was used as matrix material, SiC and Al_2O_3 ceramics with a powder size of 22-59µm were used as conventional reinforcement members, and blast furnace slag as waste reinforcement material. Blast furnace slag was procured from the KARDEMIR iron and steel factory operating in Karabük. The slags were pulverized in a ball mill and after getting separated according to their powder size, those with a powder size of 22-59µm were used as reinforcement members in the production of metal matrix composites. Single, binary, and tertiary hybrid composites were produced using conventional and waste reinforcement materials. The composites were produced using the two-stage mixed casting method. Al6061 alloy was heated up to 700ºC in a graphite crucible, and then the temperature of the alloy was reduced to 600ºC. The temperature of the alloy was measured using a thermocouple. Reinforcing members preheated to 250ºC were added to the alloy, which was semi-solid at this temperature, and mixed by hand. Afterwards, the temperature of the alloy was increased to 800ºC and using a mechanical mixer, mixed for 10 minutes at 250rpm. During the mixing process, nitrogen gas was introduced into the furnace to remove the oxygen in the environment, and unwanted oxide formations were tried to be prevented.

Keywords: Aluminium matrix composite, Double stir casting, Blast furnace slag, Fatigue behaviour

REGISTER NO

45645a

Examination of Fatigue Behaviors of Al6061 Matrix SiC Al_2O_3 and Marble Powder Reinforced Hybrid Composites

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In this study, Al6061 alloy was used as matrix material, SiC and Al_2O_3 ceramics, which are frequently used in the automotive industry, were used as traditional reinforcement elements, and marble powder obtained by pulverizing the marble pieces in a ball mill collected from the waste areas of the enterprises producing marble in the Afyon region was used as a waste reinforcement material. Single composites and binary and triple hybrid composites were produced using conventional and waste reinforcement materials. By making a sieve analysis of our marble dust, powders with a powder size of 22-59µm, which we will use in the study, were obtained, and SiC and Al_2O_3 supplements, with a powder size of 22-59µm, were supplied from the market. Single composites were produced at 1%, 3%, and 5%, binary hybrid composites at 4%, 6%, and triple hybrid composites at 7%, 9%, and 11% reinforcement volume ratios. The two-stage mixed casting method, which is one of the liquid state production methods, was used when creating composites. In this method, firstly, the Al6061 alloy was heated to 700ºC, the temperature of the alloy was then reduced to 600ºC, and reinforcing elements preheated to 250ºC were added to the semi-solid alloy at this temperature and mixed by hand. Afterwards, the alloy was subjected to superheating, its temperature increased to 800ºC and mixed mechanically at 250 rev/min for 10 minutes. Nitrogen gas was used as inert gas during the mixing process, thus removing the oxygen in the environment

Keywords: Aluminium matrix composite, Double stir casting, Marble powder, Fatigue behaviour

REGISTER NO
4c27ce

6th International ISCMP ALBANIA 2022
Joint Science Congress of Materials and Polymers
14-17 September 2022 Albania

Experimental and Theoretical study of Methyl Violet Adsorption onto Halloysite Nanoclay

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Halloysite nanoclay (HNC) was investigated as Methyl Violet dye adsorbent material. A batch adsorption study was performed to examine various parameters including contact time, solution pH, temperature, adsorbent dose, and initial dye concentration Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich (D-R) isotherm models were used to describe the interaction between the adsorbate and adsorbent. The sorption mechanism was described using Lagergren 1st order, pseudo 2nd order, and Weber-Morris intraparticle diffusion models. It was found that the Langmuir equation fits the equilibrium data better than the other models whereas kinetic data were better described by pseudo-second-order model and the thermodynamic studies elucidated that adsorption process was spontaneous, endothermic and occurred by physisorption. This research focuses on two different theoretical methodologies (MC and MD) based on molecular mechanics. These methods enabled a molecular understanding on how the MV molecule interacts with the halloysite surface. The theoretical results were in agreement with the experimental ones. The results demonstrated that HNC is an effective adsorbent for dyes removal from industrial effluents.

Keywords: Halloysite, Methyl violet, Adsorption, Isotherms, Molecular modelling, Monte Carlo

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0f9661

6th International ISCMP ALBANIA 2022
Joint Science Congress of Materials and Polymers
14-17 September 2022 Albania

Determination of Geochemical Fractions of Heavy Metals in Soils Formed on Schist and Granite

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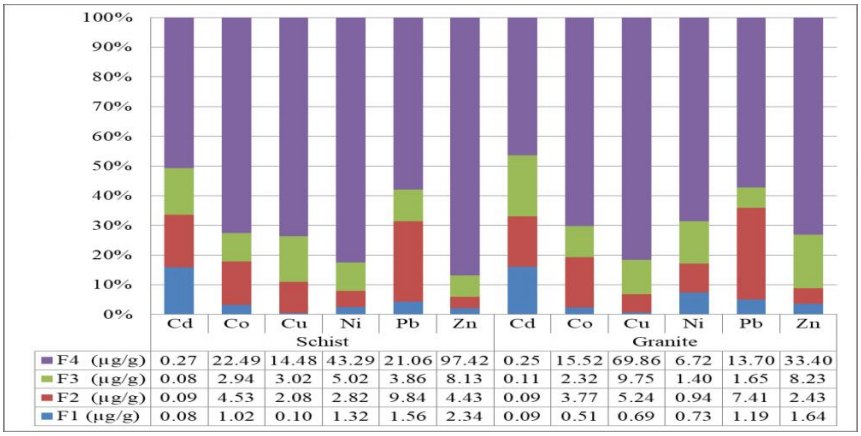

	Schist						Granite					
F4 (µg/g)	0.27	22.49	14.48	43.29	21.06	97.42	0.25	15.52	69.86	6.72	13.70	33.40
F3 (µg/g)	0.08	2.94	3.02	5.02	3.86	8.13	0.11	2.32	9.75	1.40	1.65	8.23
F2 (µg/g)	0.09	4.53	2.08	2.82	9.84	4.43	0.09	3.77	5.24	0.94	7.41	2.43
F1 (µg/g)	0.08	1.02	0.10	1.32	1.56	2.34	0.09	0.51	0.69	0.73	1.19	1.64

Heavy metals reach the soil system as a result of the decomposition of rocks in natural environments. In this study, it was aimed to determine the geochemical fractions of heavy metals (Cd, Co, Cu, Ni, Pb and Zn) in soils formed under different parent materials (schist and granite) and similar vegetation-climate effect. For this purpose, a total of 10 soil samples, five on each parent material, were taken. A sequential extraction method (The European Community Bureau of Reference-BCR) was used to determine the geochemical fractions (acid soluble, reducible, oxidizable, and residual) of metals in the soil samples. All metal concentrations were determined by flame atomic absorption spectrophotometer. The accuracy of the method was confirmed by using BCR-701 certified reference material. The mean values and percentage distribution of heavy metal fractions obtained from the sequential extraction procedure are presented in Figure 1 (graphical abstract). The total concentrations of the first three fractions (acid soluble + reducible + oxidizable) of heavy metals extracted by the BCR sequential extraction procedure are considered as the potential mobile fraction. Based on the sum of the first three fractions that do not include the residue fraction, the potential mobility of heavy metals was found in the following orderings as percentages: Cd > Pb > Co > Cu > Ni > Zn (soils formed on schist) and Cd > Pb > Ni > Co > Zn > Cu (soils formed on granite). It was concluded that the fact that Cd and Pb elements have more mobile fractions than other elements may be related to the transport of atmospheric emissions.

Keywords: Schist, granite, Soil, Geochemical fraction, Heavy metals

REGISTER NO
67e103

Determination of Heavy and Toxic Metals in Power Plants of Kosovo

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Contamination with high levels of arsenic is of concern because arsenic can cause a number of human health effects. Several epidemiological studies have reported a strong association between arsenic exposure and increased risks of both carcinogenic and systemic health effects. Environmental pollution by toxic metals is of great concern as the effect of these metals has a negative impact on when they enter the human body through the food chain. These metals often accumulate in the liver, intestines and gallbladder. Heavy toxic metals become dangerous if they start oxidation. They undergo changes and damage all cells. The problem is that they serve as the main food for bad bacteria, viruses, worms, parasites and fungi. This means that these metals can serve as a breeding ground for Streptococci A and B, *E. coli*, *H. pylori* and viruses. In our study we analyzed the concentration of heavy metals such as As, Cd, Cr, Cu, Fe, Hg, As, Zn and Pb.

Keywords: Heavy metals, Diary products, Power plants of Kosova, Arsenic, Health effects, Lead

References: 1.Khan N, Jeong IS, Hwang IM, et al. Analysis of minor and trace elements in milk and yogurts by inductively coupled plasma-mass spectrometry (ICP-MS). Food Chem 2014; 147: 220-224. 2.Bilandzic N, Dokic M, Sedak et al. Trace element levels in raw milk from northern and southern regions of Croatia. Food Chem 2011; 127: 63-66. 3.Ali H, Khan E. Trophic transfer, bioaccumulation, and biomagnification of non-essential hazardous heavy metals and metalloids in food chains/webs?Concepts and implications for wildlife and human health. Human and Ecological Risk Assessment: An International Journal 2019;25:1353-76.

REGISTER NO
0ff39b

6th International ISCMP ALBANIA 2022
Joint Science Congress of Materials and Polymers
14-17 September 2022 Albania

Grafting of Polystyrene on Electrospun Gelatin Nanofibers by Photopolymerization

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Hybrid materials are undoubtedly the ideal choice to meet the demands bioapplication because strength and durability of the synthetic component can be combined with the biocompatibility of the biologic materials (1). The increase in demand for natural fibers in development of the composites has grown rapidly due to the cost-effectiveness, low density, biodegradability, and renewability (2). Gelatin is a natural biopolymer which commonly produced from hydrolysis of collagen and its biodegradability, biocom- patibility, and cell-binding properties (3). PS is widely used in bioapplication applications because of its strength, nontoxicity, heat stability, and slow degradation (1). In this work, Gelatin-polystyrene based hybrid material was synthesized through photopolymerization type II. Fort his purpose, firstly gelatin nanofiber (GNF) was produced by electrospinning process. Then, by adding styrene monomer on the gelatin nanofiber, it was bonded to the gelatin nanofiber simultaneously with styrene polymerization by the photopolymerization type II. Chemical structure was characterized through infrared spectrum and wettability properties were investigated.

Keywords: Polystyrene, Gelatin, Electrospining, Photopolymerization

References: (1) Ge L., Li Q., Jiang J., You X. Integration of nondegradable polystyrene and degradable gelatin in a core-sheath nanofibrous patch for pelvic reconstruction, International Journal of Nanomedicine, 2015:10 3193-3201. (2) Saeed U., Dawood U., Ali A.M., Cellulose triacetate fiber-reinforced polystyrenecomposite, Journal of Thermoplastic Composite Materials 2021, Vol. 34(5) 707-720. (3) Başaran, I and Oral, A. Grafting of poly(epsilon-caprolactone) on electrospun gelatin nanofiber through surface-initiated ring-opening polymerization. International Journal of Polymeric Materials and Polymeric Biomaterials. 2018/12/12.

REGISTER NO
cdc0d6

6th International ISCMP ALBANIA 2022
Joint Science Congress of Materials and Polymers
14-17 September 2022 Albania

Production of Agarose Nanofibers using the Electrospinning Method

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Electrospinning has been widely used as a nanofiber fabrication technique. This method implies the application of a high voltage electric field aiming to extract very thin fibres from a polymeric fluid stream (solution or melt) potentially deliverable through a millimetre-scale needle. The electrospinning parameters such as the applied electric field, the distance between the needle and collector, flow rate, polymer concentration, viscosity and solution conductivity and needle diameter affect the properties of final materials. The environmental parameters include relativity humidity and temperature may also affect. Until now, it has been possible to determine the parameters of the distance between the needle and the collector, as well as the flow rate. Efforts are also being made to determine the applied voltage. In this work, the effects of polymer concentration and distance on the nanofiber production process were investigated. We report the successful fabrication of agarose-based nanofibers by electrospinning technique, using N,N-dimethylformamide (DMF) as solvent media. it was determined that the optimal concentration of agarose with weight average molecular weight of about (Mw) 120,000 g/mol is 12 wt %. This concentration produces fibers with no beading or film formation. The optimum distance between the needle and collector was found as 16.5 cm. Besides these parameters, the better collector material was investigated for easy peel-off from the collector surface. For this aim, aluminium foil and stretch film were used to cover the collector surface. it was found that in the case of using stretch film, the peeling off of the fibers from the collector surface is easy. The morphology of the fibers was characterized by Scanning Electron Microscope (SEM).

Keywords: Agarose, Nanofiber, Electrospinning, Scanning electron microscope

REGISTER NO

b2eeb7

Production of Exopolysaccharides by Rhodotorula Yeasts

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Due to the potential industrial and therapeutic applications of the exopolysaccharides (EPSs), there has been an increasing demand to obtain these biopolymers. This study aimed to investigate the EPS production by a number of Rhodotorula species. *Rhodotorula babjevae* DVBPG 8058, *Rhodotorula glutinis* CBS2889, *Rhodotorula glutinis* CBS5805, *Rhodotorula mucilaginosa* J350 were grown in medium containing 70 g/L glucose for 7 days at 25°C. The yeasts were grown at an initial pH of 6.0 which during fermentations decreased naturally to ~2. The supernatants of cultivations were isolated and purified from proteins by precipitation with trichloroacetic acid, then EPSs were precipitated with cold ethanol and freeze dried. *R. babjevae* DVBPG 8058 produced 2.09 g/L, *R. glutinis* CBS2889 1.82 g/L, *R. glutinis* CBS5805 0.5 g/L and *R. mucilaginosa* J350 0.57 g/L EPS. The EPSs were analyzed by H-NMR for structural determination.

Keywords: Yeast, Exopolysaccharides, Rhodotorula, Fermentation

Acknowledgement: We wish to acknowledge the COST organization for the research grant

References: 1. Ma W et al (2018) Carbohydr Polym 181:768-777. 2. Silambarasan S, Logeswari P, Cornejo P, Kannan VR (2019) Int J Biol Macromol 121:55-62. 3. Yadav KL, Rahi DK, Soni SK (2014) Appl Biochem Biotechnol 172:1898-1908. 4. Poli A, Anzelmo G, Tommonaro G, Pavlova K, Casaburi A, Nicolaus B (2010) Folia Microbiol 55:576-581. 5. Seveiri Mirzaei R, Hamidi M, Delattre C, Rahmani B, Darzi S, Pierre G, Sedighian H (2019) Medical Science 23:381-389. 6. Gientka I, Bzducha-Wróbel A, Stasiak-Róaska L, Bednarska AA, Baejak S (2016) Electron J Biotechnol 22:31-37. 7. Han M, Du C, Xu Z-Y, Qian H, Zhang W- G (2016) Int J Biol Macromol 88:603-613. 8. Parolis LA, Duus JØ, Parolis H, Meldal M, Bock K (1996) Carbohydr Res 293:101-117. 9. Ragavan ML, Das N (2019) Annal Microbiol 69:515-530.

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55743c

6th International ISCMP ALBANIA 2022
Joint Science Congress of Materials and Polymers
14-17 September 2022 Albania

Chemical and Mineralogical Characterization of Fly-Ash from North Macedonica

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North Macedonia is rich in industrial minerals like limestone, clays, diatomite, bentonite, gypsum etc. A great number of studies have been performed to determine their best possible use and application. Industrial minerals are used either in their natural state or after beneficiation/modification, either as raw materials or as additives in a wide range of applications. North Macedonia roughly produces around 900 000 - 1 100 000 t of coal fly ash. The aim of this research is to determine the chemical and mineralogical composition of fly-ash from REK Bitola. XRF results show the following composition: SiO_2 (51.812 wt%), Al_2O_3 (15.671 wt%), CaO (15.073 wt%), MgO (2.588 wt%), K_2O (1.597 wt%), TiO_2 (0.611 wt%); while the XRPD results show presence of quartz, anorthite and albite.

Keywords: Characterization, Fly-ash, ICP-MS, XRPD

REGISTER NO

eaae33

The Adsorptive Removal of Curcumin Derivative from Acetonitrile Solution using GrapheneOxide(GOx)

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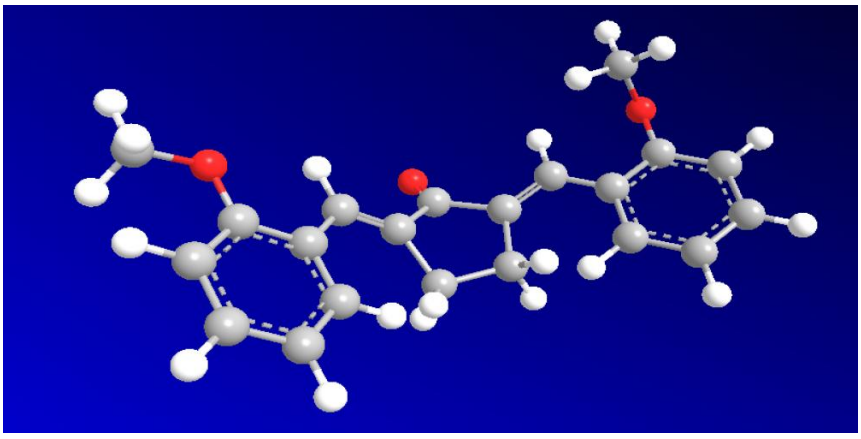

Curcumin is a bright yellow chemical produced by plants of the Curcuma longa species[1] and its derivatives give colored solutions in acetonitrile as solvent, which makes it a good specimen to be analyzed using UV-VIS spectrometry analyzing method. The adsorptive agent is Graphene Oxide (GOx) (synthesized using modified Hummers method)[2]. In further analysis we can come to conclusions of GOx capacity to remove (2E,5E)-2,5-bis(2-methoxybenzylidene)cyclopentanone from the solution. This experiment is backed up with theoretical calculations.

Keywords: Graphene Oxide, Hummers method, (2E,5E)-2,5-bis(2-methoxybenzylidene)cyclopentanone , UV-VIS spectrometry, Theoretical calculations, Colored solutions

References: [1] Majed S., 2015, Natural Products Insider [2] N.I. Zaaba, K.L. Foo, U. Hashim, S.J. Tan, Wei-Wen Liu, C.H. Voon, 2017, Elsevier.

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30ef30

Graphen Oxide as a Adsorbing Agent used to Remove(2E,5E)-2,5-bis(2-(trifluoromethyl)benzylidene)cyclopentanone

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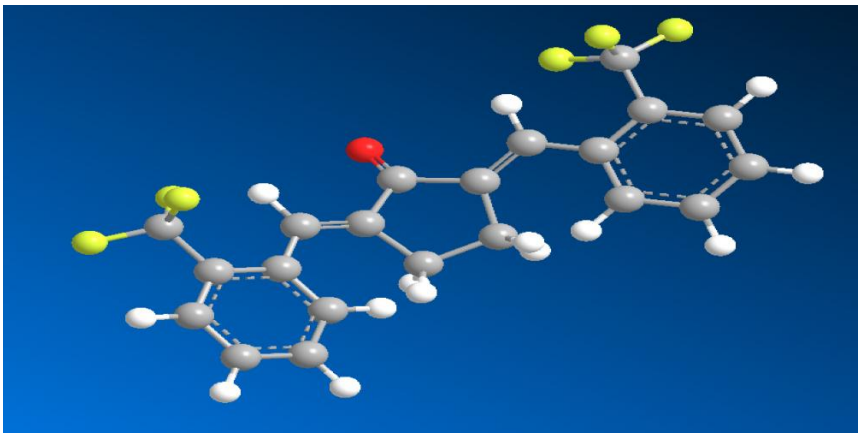

(2E,5E)-2,5-bis(2-(trifluoromethyl)benzylidene)cyclopentanone is a curcumin derivative, which in acetonitrile gives a colored solution. Graphene Oxide (GOx) was used to remove this analyte from the solution and the analysis is performed using UV-VIS spectrometry analysis technique[1]. The experimental data are further supported by theoretical data calculations and simulations.

Keywords: Graphene Oxide (GOx), (2E,5E)-2,5-bis(2-(trifluoromethyl)benzylidene)cyclopentanone, UV-VIS spectrometry, Acetonitrile, Theoretical calculations, Adsorption

References: [1] Heinz-Helmut Perkampus, Springer, 1992.

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076a0c

Adsorptive Removal of (2E, 5E)-2,5 Bis [(4-dimethylamino) benzylidene] Cyclopentanone using Graphene Oxide

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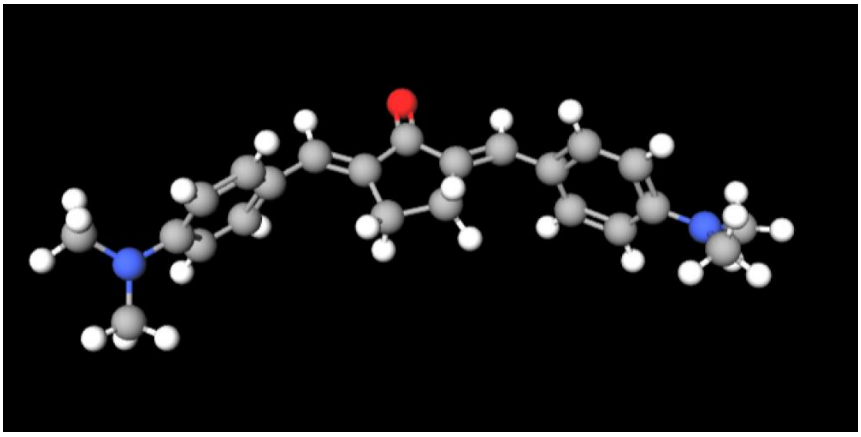

Graphene oxide (GO) obtained from graphite (using the Hummers method) was used to adsorb (2E, 5E) -2,5 Bis [(4-dimethylamino) benzylidene] cyclopentanone from organic solutions. The initial concentration of organic matter in the solution was kept constant, while the amount of adsorbent (GO) was changed, in which case the amount of adsorbed substance was followed. Assessment of the absorbency of this material is performed using UV-VIS spectrophotometry. Moreover, the use of Monte Carlo calculations shows that the strong adsorption interaction is responsible for the excellent ability of these materials to be absorbed into these organic compounds.

Keywords: (2e, 5e) -2,5 Bis [(4-dimethylamino) Benzylidene] Cyclopentanone, Monte Carlo, Spectroscopic tecnichues, Hummers method

References: [1] A. Alija, D. Gashi, R. Plakaj, A. Omaj, V. Thaçi, A. Reka, S. Avdiaj, A. Berisha . A theoretical and experimental study of the adsorptive removal of hexavalent chromium ions using graphene oxide as an adsorbent. Open Chemistry. https://doi.org/10.1515/chem-2020-0148 [2] V. Thaçi, A. Berisha, R. Hoti, Experimental and Theoretical Study of Some 2,5- Diarylidenecyclopentanone Derivatives. Joint Science

Congress of Materials and Polymers - ISCMP 2019. Open Chemistry [3] Berisha A. Interactions between the aryldiazonium cations and graphene oxide: a DFT study. J Chem. 2019;2019:5.10.1155/2019/5126071

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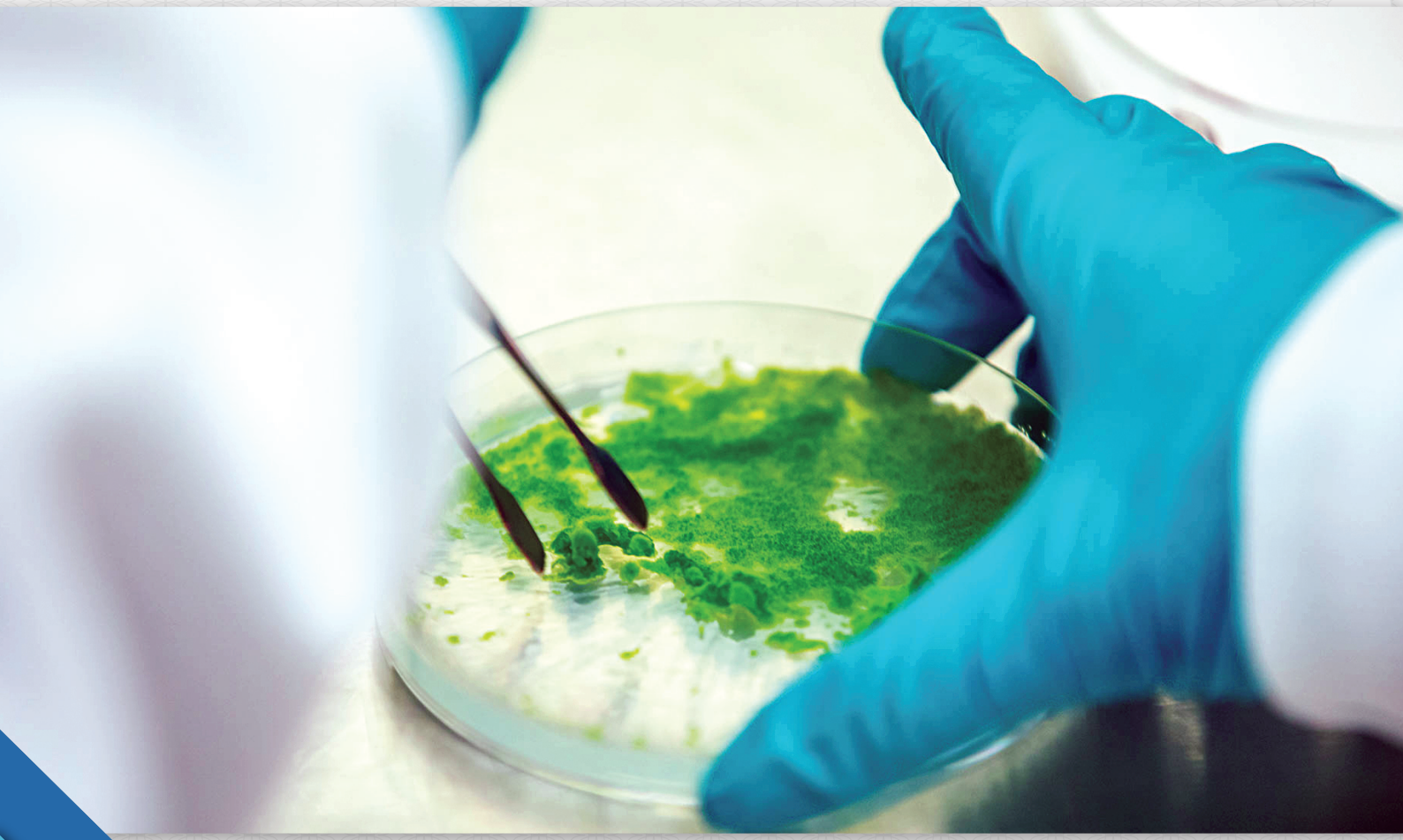

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