

ICNTC E-CONFERENCE
INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

7th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY
25 - 26 SEPTEMBER 2021

7th ICNTC BOOK OF ABSTRACTS

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25 – 26 SEPTEMBER 2021

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ICNTC E- Conference 2021

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Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of “7th International Conference on New Trends in Chemistry”, to be held as based on Online Presentations dates between September 25-26, 2021

Limited number of Papers and Posters with the below mentioned topics will be accepted for our conference:

- Polymer Chemistry and Applications
- Pharmaceutical Chemistry
- Computational Chemistry
- Bio Chemistry
- Physical Chemistry
- Analytical Chemistry
- Inorganic Chemistry
- Organic Chemistry
- Material Chemistry
- Environmental Chemistry
- Food Chemistry

The selected papers which are presented as oral in the conference will be published in a international peer-reviewed journal which is scanned by SCOPUS as Q4. Each manuscript will have doi Numbers.

We kindly wait for your attendance to our online conference to be held on 25 –26th of September 2021,

All informations are available in conference web site. For more information please do not hesitate to contact us. info@icntconference.com

Respectfully Yours,

On Behalf of the Organization Committee of ICNTC Conference

Assoc. Prof. Dr. Dolunay SAKAR DASDAN
7th ICNTC 2021 | Conference Chair
Yıldız Technical University – Istanbul / Turkey
Chemistry Department

SCIENTIFIC PROGRAM

25 SEPTEMBER 2021 SATURDAY

Online access : with given username and password.

10:00 – 10:10

Welcome Speech : **Assoc. Prof. Dr. Dolunay SAKAR DASDAN** / Conference
Chair

Yildiz Technical University, Turkey

10:10 – 11:00

Keynote Speaker : **Dr. Hatem AMIN** / Cairo University, Egypt
Speech Title : **Oxygen Electrocatalysis at Metal Oxides and Sulfides:
From Fundamentals to Applications**

11:00 – 11:15	B R E A K
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SESSION A

SESSION CHAIR	Dr.Hatem AMIN	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
11:15 – 11:30	Powder Mixtures of β -Tricalcium Phosphate and Potassium Hydrosulfate Homogenized Under Mechanical Activation For Ceramics Preparation	Tatiana SAFRONOVA, Marat AKHMEDOV, Tatiana SHATALOVA, Snezhana TIKHONOVA, Gilyana KAZAKOVA, Maksim KAIMONOV, Alexander KNOTKO
11:30 – 11:45	Olive Leaf Extract and Potential of Transdermal Application	Hicran BELLUCCI, Ozlem DOGAN
11:45 – 12:00	Antioxidant Activity of <i>Rumex Patientia L.</i> Leaves and Analysis of Its Polyphenol Contents By Lc-Ms/Ms	Derya ALTINTAS, Yesim YESILOGLU
12:00 – 12:15	Theoretical and Experimental Photodegradation of Phosmet Via Oxidation Techniques in The Presence of Aqueous TiO ₂ Suspension	Bahar EREN, Yelda YALCIN GURKAN

12:15– 13:15	LUNCH BREAK
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25 SEPTEMBER 2021 SATURDAY

Online access : with given username and password

SESSION B

SESSION CHAIR	Dr.Emel AKYOL	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
13:15 – 13:30	Determination of Some Metal Levels in Exotic Fruits by ICP-OES	Ayca KARASAKAL
13:30 – 13:45	Antibacterial Surface Properties of Polyester Fibers With Cu-Based Mof	Betul YENIDOGAN, Sennur DENIZ
13:45 – 14:00	Surface Modification of Zeolite and Kaolin with Different Silanization Agents	Cem OZEL, Cansu AKAT, Rasim ALASMANOV, Muhammet U. KAHVECI, Ceren EMIR, Sevil YUCEL
14:00 – 14:15	Gas Separation Properties of Mixed Matrix Membranes Prepared With Graphene Oxide	Sevgi CANCA, Sennur DENIZ

14:15 – 14:30	B R E A K
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SESSION C

SESSION CHAIR	Dr.Sevil YÜCEL	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
14:30 – 14:45	Biodegradable Flexible PLA/PCL Films With Natamycin and Nanocellulose	Nudem KAHRAMAN, Sennur DENIZ
14:45 – 15:00	Photocatalytic Degradation of Methylene Blue By Nano-Titanium Dioxide Composites	Emel AKYOL, Guldeniz TONBUL
15:00 – 15:15	Colorimetric Method For Insulin Detection Using a New Magnetic Nanozyme	Burcu GOKCAL, Kadriye Özlem HAMALOGLU
15:15 – 15:30	Investigation of Controlled Drug Delivery of Ethyl Cellulose	Busra TURAN, Pelin DEMIRCIVI

15:30 – 15:45	Preparation of Sulfonimide Functional Proton Conducting Polymers	Elif Busra CELEBI, Ferda HACIVELIOGLU
15:45 – 16:00	Synthesis and Characterisation of a Glutathione-Stransferase (hGSTP1-1) Single Nucleotide Polymorphs (Part II)	Sadhna MATHURA
16:00 – 16:15	B R E A K	

25 SEPTEMBER 2021 SATURDAY

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POSTER SESSION A

SESSION CHAIR	Dr.Yelda YALÇIN GÜRKAN	5 min oral presentation after that questions from participants
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
16:15 16:45	Preparation of Gelatin Coated Alginate Capsules	Gulzhan YERLAN, Bakyt TYUSSYUPOVA, Sagdat TAZHIBAYEVA, Kuanyshbek MUSABEKOV
	Synthesis and Characterization of Terpyridine Functional Cyclophosphazene	Elif Büşra ÇELEBİ, Halil DUYAR, Ferda HACIVELİOĞLU
	Investigation of Trace and Major Element Concentrations of Almond Milk by Using an Inductively Coupled Plasma Optical Emission Spectrometer	Ayca KARASAKAL
	Synthesis and Characterization of LDH Materials and Their Application in Wastewater Treatment	Abderrahmane HIRI, Achour DAKHOUCHE, Kamel NOUFEL Kamel NOUFEL

26 SEPTEMBER 2021 SUNDAY

SESSION D

SESSION CHAIR	Dr.Bahar Eren	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
09:30 - 09:45	Determination of Human Papillomavirus-11 with Impedimetric CRISPR Biosensor	Zihni Onur UYGUN
09:45 – 10:00	Thermal Analysis and Isoconversional Kinetics Study of Thermal Decomposition of Polycyclohexene Oxide Polystyrene (PCHO-PSt) Comb-Shaped Polymer	Hacer DOLAS, Nasrettin GENLI
10:00 – 10:15	CRISPR-dCas9 Based Biosensor System for Detection of Sickle Cell Anemia	Hilmiye Deniz ERTUGRUL UYGUN
10:15 – 10:30	Phenol Containing Bodipy Functionalized Anderson Type Pom: Synthesis, Characterization and Photophysical Properties	Seda CETINDERE
10:30 – 10:45	Determination of Free Energy Difference Between Anomaly Solid-Liquid Phase Transitions of Silicon Using Pseudo-Supercritical Thermodynamic Path: A Molecular Dynamics Study	Chandan K DAS
10:45- 11:00	Investigation of Stability and Activity of Poly(ethylene-alt-maleic anhydride) Copolymer in Different pHs and Simulated Body Fluids	Dolunay ŞAKAR DAŞDAN
11:00– 11:15	B R E A K	

26 SEPTEMBER 2021 SUNDAY

Online access : with given username and password

SESSION E

SESSION CHAIR	Dr.Dolunay ŞAKAR DAŞDAN	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
11:15 – 11:30	Production And Characterization of Composite Scaffolds By Electrospinning Technique From Bioceramics Synthesized From Seashells	Sema Nur SAHIN , Erdi BULUS, Demet Sezgin MANSUROGLU, Bahadir BOZKURT, Aziz KORKUT, Yesim Muge SAHIN
11:30 - 11:45	New Approaches in Green Chemistry: Vaniline Based Imin Synthesis and Wound Dressing Production by Nanotechnology	Yeşim Müge SAHIN , Erdi BULUS, Demet Sezgin MANSUROGLU, Bahadir BOZKURT, Hatice Dilara SARAC, Funda OZKOK, Nihal ONUL, Tatyana TISHAKOVA, Gulru OZAY
11:45 – 12:00	Synthesis and Dielectrophoretic Alignment of Metal Oxide Nanowires for Applications in Diverse Devices	Raitis SONDORS , Davis GAVARS, Matiss RAMMA, Donats ERTS, Jana ANDZANE
12:00 - 12:15	The Biosphere Self-Organization Attractors Drive Perfect Order Homeostasis Reactions to Link Bioenergetic with Functionally Activate Oxygen and Carbon Dioxide Molecules	Aris KAKSIS
12:15 – 12:30	CLOSING CEREMONY	

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OXYGEN ELECTROCATALYSIS AT METAL OXIDES AND SULFIDES: FROM FUNDAMENTALS TO APPLICATIONS

Hatem M.A. AMIN¹

¹ Faculty of Chemistry and Biochemistry, Ruhr University Bochum, 44801 Bochum, Germany

Abstract

Developing sustainable energy devices is key part for all future socially, environmentally and economically sustainable energy systems. Among others, fuel cells, metal-air batteries and electrolyzers are the most promising concepts. However, water splitting particularly the oxygen evolution reaction (OER) is a current challenge due to its sluggish kinetics and large overpotential, and thus it is imperative to search for high performance electrocatalysts. Current OER catalysts still rely mostly on Ir and Ru, which are scarce and expensive. Alternatively, transition metal oxides such as NiFe layered hydroxide and Co₃O₄ showed high catalytic activity [1-3]. In this presentation, the bifunctional catalytic activity of a mixed Ag + Co₃O₄ catalyst will be discussed towards oxygen evolution and reduction reactions and also in gas diffusion electrodes [1, 3]. The possible origins of synergistic effect between Ag and Co₃O₄ will be addressed.

Compared to metal oxides, transition metal sulfides, namely pentlandites (FeNi)₉S₈, exhibit higher conductivity [4]. Thus, a conductive support or binder will not be needed in electrode preparation. The performance of various pentlandites towards OER will be presented [5]. The surface transformation phenomenon at pentlandite which is critical during OER and is assumed to be responsible for the OER activity, will be discussed. This approach offers insights into rational design strategies of high-performance oxygen electrocatalysts.

Key Words: *Oxygen Evolution; Oxygen Reduction; Pentlandites; Cobalt spinel; Surface Transformation*

References:

- [1] Amin HMA, Bondue CJ, Eswara S, Kaiser U, Baltruschat H (2017) *Electrocatalysis* 8: 540–553
- [2] Cai Z, Bu X, Wang P, Ho JC, Yang J, Wang X (2019) *J. Mater. Chem. A* 7: 5069–5089
- [3] Amin HMA, Königshoven P, Hegemann M, Baltruschat H (2019) *Anal. Chem.* 91: 12653–12660.
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- [5] Amin HMA, Attia M, Tetzlaff D, Apfel U.-P. *Chemelectrochem* (2021) doi.org/10.1002/celec.202100713

POWDER MIXTURES OF β -TRICALCIUM PHOSPHATE AND POTASSIUM HYDROSULFATE HOMOGENIZED UNDER MECHANICAL ACTIVATION FOR CERAMICS PREPARATION

Tatiana SAFRONOVA¹, Marat AKHMEDOV², Tatiana SHATALOVA³,
Snezhana TIKHONOVA⁴, Gilyana KAZAKOVA⁵, Maksim KAIMONOV⁶, Alexander
KNOTKO⁷

¹Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, t3470641@yandex.ru

²A.N. Kosygin State University of Russia (Technology. Design. Art), 117997, Russia, Moscow, Sadovnicheskaya str., 33, p. 1, akhmedov.mm@yandex.ru

³Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, shatalovtb@gmail.com

⁴Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, kurbatova.snezhana@yandex.ru

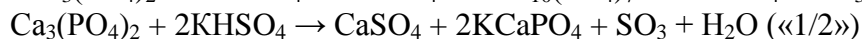
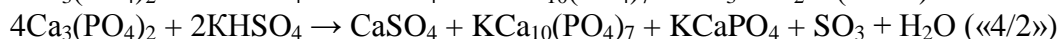
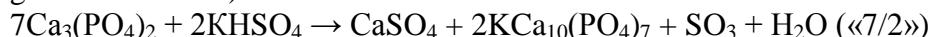
⁴Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, gilyanak@gmail.com

⁵Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, m.r.kaimonov@yandex.ru

⁶Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, alknt@mail.ru

Abstract

Powder mixtures of β -tricalcium phosphate β -Ca₃(PO₄)₂ and potassium hydrogen sulfate KHSO₄ homogenized under mechanical activation in acetone medium in planetary mill were used for producing of ceramics in K₂O-CaO-SO₃-P₂O₅ system. Powder mixtures were prepared at molar ratios of Ca₃(PO₄)₂/KHSO₄ established as 7/2, 4/2 and 1/2. The following formal reactions were used for calculation of quantities of starting components to create opportunity of preparation of ceramic composite materials containing calcium sulfate anhydrate CaSO₄ and phases of double calcium potassium phosphates such as potassium-substituted tricalcium phosphate KCa₁₀(PO₄)₇ and potassium rhenanite KCaPO₄ (labeling is given in brackets):



According to XRD analysis data β -tricalcium phosphate β -Ca₃(PO₄)₂ was the main phase in all powder mixtures after treatment in planetary mill in acetone media. Only powder mixture $\langle\langle 1/2 \rangle\rangle$ has slight quantities of additional phases. K₈H₉(SO₄)₇PO₄ and K₄H₅(SO₄)₃PO₄ were found additionally to β -tricalcium phosphate β -Ca₃(PO₄)₂ in powder mixture $\langle\langle 1/2 \rangle\rangle$. Presumably phases of syngenite K₂Ca(SO₄)₂·H₂O and/or gorgeyite K₂Ca₅(SO₄)₆·H₂O presented in powder mixtures in quasi-amorphous form after treatment in planetary mill.

Compacted (P_{specific}=100MPa) powder pre-ceramic items based on prepared mixtures were fired at temperature range of 700-900°C for producing ceramic samples. It was found that phase composition of ceramic samples considerably depends on composition of starting powder mixtures. According XRD analysis after firing at 800°C phase composition of ceramic samples $\langle\langle 7/2 \rangle\rangle$ and $\langle\langle 4/2 \rangle\rangle$ contained potassium calcium phosphate Ca₁₀K(PO₄)₇, β -calcium pyrophosphate β -Ca₂P₂O₇ and calciolangbeinite K₂Ca₂(SO₄)₃. Phase composition of ceramic samples $\langle\langle 1/2 \rangle\rangle$ contained calciolangbeinite K₂Ca₂(SO₄)₃, β -calcium pyrophosphate β -Ca₂P₂O₇ and potassium sulfate K₂SO₄. Up to our knowledge all phases of prepared ceramic samples are biocompatible. It should be noted that potassium sulfate K₂SO₄ presented in ceramics $\langle\langle 1/2 \rangle\rangle$ is water soluble salt. So additional investigations are required for creation of ceramics in the K₂O-CaO-SO₃-P₂O₅ system for different uses including biomedical purposes.

Acknowledgements: The financial support of RFBR project # 20-03-00550.

Key Words: *calciolangbeinite; potassium calcium phosphate; potassium sulfate; calcium pyrophosphate; ceramics*

OLIVE LEAF EXTRACT AND POTENTIAL OF TRANSDERMAL APPLICATION

Hicran Bellucci, Özlem Dogan

Yildiz Technical University, Chemical Engineering Department, 34210 Davutpasa – Esenler, Istanbul, Turkey,
e-mail: hicranarslan5@gmail.com

Abstract

Oleuropein is known to be the main phenolic compound in the olive tree. It is abundant in unprocessed olive fruit and leaves [1]. It has been determined to have positive effects on certain cancer diseases such as colon and breast cancer. Studies have shown that oleuropein treatment results in a significant reduction in breast cancer xenograft and melanoma tumor volumes, and prevents the development of cancer caused by Ultraviolet B [2]. In addition, research on wound healing has shown that it accelerates the wound healing process in the skin [3].

Olive leaves attract the attention of researchers and consumers because of their positive effects on health. In this study, extraction kinetics of olive leaves were examined by using water at various temperatures and ethyl alcohol at different rates. Then, the total polyphenol content of olive leaf extracts was determined. Release studies of the hydrogel films produced with the extract obtained from olive leaves were performed using Franz diffusion cell. The results indicated that release behaviour of films changed with hydrogel films combination.

Key Words: *Oleuropein, hydrogel, controlled release, polyphenol, diffusion*

References

- [1] Nediani, C., Ruzzolini, J., Romani, A., Calorini, L. (2019) Oleuropein, a bioactive compound from *olea europaea* L., as a potential preventive and therapeutic agent in noncommunicable diseases. *Antioxidants*. 8(12), 578, 1-26.
- [2] Goldsmith, C. D., Bond, D. R., Jankowski, H., Widenhofer, J., Stathopoulos, C. E., Roach, P. D., Scarlett, C. J. (2018) The olive biophenols oleuropein and hydroxytyrosol selectively reduce proliferation, influence the cell cycle, and induce apoptosis in pancreatic cancer cells. *International Journal of Molecular Sciences*, 19 (7), 1937, 1-17.
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ANTIOXIDANT ACTIVITY OF RUMEX PATIENTIA L. LEAVES AND ANALYSIS OF ITS POLYPHENOL CONTENTS BY LC-MS/MS

Derya ALTINTAS¹, Yesim YESILOGLU²,

¹ Trakya University, Arda Vocational College, Edirne, Turkey, deryaaltintas@trakya.edu.tr

² Trakya University, Faculty of Pharmacy, Edirne, Turkey, yesimyesiloglu@trakya.edu.tr

Abstract

Rumex patientia L. is generally known under the name “labada” in Turkey. It is a plant of Polygalaceae family and its leaf is a significant source of natural antioxidant of ascorbic acid [1] [2]. Furthermore, the leaves of the *Rumex* have an analgesic, anticancer, antihypertensive, antipyretic and anti-inflammatory effects [3]. The antioxidant and phytochemical properties of *Rumex patientia* L. were examined in this study.

The antioxidant and radical scavenging activities of water extract of dried leaves (WEDL), methanol extract of dried leaves (MEDL), water extract of fresh leaves (WEFL) and methanol extract of fresh leaves (MEFL) were determined using various *in vitro* methods including ferric thiocyanate (FTC) method, chelating capability on Fe⁺², ferric ions reducing capacity (FRAP) and 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS⁺) scavenging assay. LC-MS/MS was used to analyse extracts compounds. Total phenolic and flavonoid contents were determined as mg of gallic acid equivalent per g of *Rumex patientia* L. extract. The results were evaluated in comparison with antioxidants such as α -tocopherol, butylated hydroxyanisole (BHA), ascorbic acid and butylated hydroxytoluene (BHT) and data from the similar plant samples in literature. By means of this study, it was concluded that on account of its rich rutin content, the leaves of this plant could be used *in vitro* pharmacology studies. In conclusion, this study confirms that *Rumex patientia* L. leaves could be used in medicine as a natural antioxidant instead of synthetic antioxidants.

Key Words: Antioxidant; *Rumex patientia*; LC-MS/MS; Radical scavenging; Rutin.

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THEORETICAL and EXPERIMENTAL PHOTODEGRADATION of PHOSMET VIA OXIDATION TECHNIQUES IN THE PRESENCE of AQUEOUS TiO₂ SUSPENSION

Bahar EREN¹, Yelda YALCIN GURKAN²,

¹ Tekirdag Namik Kemal University, Faculty of Agriculture, 59030 Tekirdag / Turkey beren@nku.edu.tr

² Tekirdag Namik Kemal University, Department of Chemistry, 59030 Tekirdag / Turkey yyalcin@nku.edu.tr

Abstract

This study is conducted with the aim to analyse the reaction kinetics of Phosmet with the OH radical, and to determine its mechanism. Due to the lack of determination of radical midproducts occurring during the reactions experimentally, the theoretical stage has been quite informative. In this study, in order to determine all the probable reaction paths theoretically, the geometric optimization of the reactants and transition state complexes were conducted using DFT/B3LYP/6-31G(d) basic set of Quantum Mechanical Density Functional Theory (DFT). As a result of the calculations, the energy values at ground state, and rate constant and activation energies (E_a) at transition state (TS) of the probable reaction paths were determined, and finally, the primary midproducts were found out by the determination of the atom where the OH radicals attach, and the hydrogen atoms it removes. The reaction mechanism was clarified through the determination of the midproducts. Since the reaction of pesticides with the OH radical is essential in terms of water purification and the atmospheric chemistry, the calculations were done at gaseous phase and also at aqueous phase by modelling the solvent impact. In the experimental stage, the degradation reactions under light impact of the pesticide, chosen as pollutant, in aqueous TiO₂ suspensions, was analysed. The optimum photocatalysts amount and TiO₂ concentration amounts were determined. The degradation rates were determined, and the impact of the initial concentration was analysed. At the end of this research, the mechanism of the reactions of Phosmet with the OH radical in the atmosphere and water were clarified, and reaction products were also identified.

Key Words: OPs, Phosmet, DFT, Heterogeneous catalysis, Aqueous TiO₂, TS.

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DETERMINATION OF SOME METAL LEVELS IN EXOTIC FRUITS BY ICP-OES

Ayca KARASAKAL

Namik Kemal University, Science and Letters Faculty, Department of Chemistry, Tekirdağ
akarasakal@nku.edu.tr

Abstract

Major, minor and toxic element concentrations in exotic fruits by using inductively coupled plasma optical emission spectrometry (ICP-OES) after different microwave acid digestion procedures were investigated. The efficiencies of digestion in exotic fruit samples were analyzed and compared. HNO₃ + H₂O₂, HNO₃ + HCl and HNO₃ were used for microwave acid digestion procedures. The parameters of the merit evaluated were validated according to limits of detection (LOD) and limits of quantification (LOQ), linearity, recovery, and precision. The highest results of LOD and LOQ were found for Ca, K, Na, Mg, and S. In addition, the digestion efficiency was correlated with the residual carbon content, which was determined by total organic carbon analyzer (TOC). 6 mL HNO₃ + 2 mL HCl digestion method was chosen as the effective digestion method because of the lowest residual carbon contents and the accuracy results.

Key Words: ICP-OES, Exotic fruits, Microwave digestion

ANTIBACTERIAL SURFACE PROPERTIES OF POLYESTER FIBERS WITH Cu-BASED MOF

Betül YENİDOĞAN¹, Sennur DENİZ¹

¹ Yıldız Technical University, Faculty of Chemical and Metallurgical Engineering,
Chemical Engineering Department, 34220, Esenler, Istanbul-Turkey

e-mail: f2020099@std.yildiz.edu.tr; deniz@yildiz.edu.tr

Abstract

In the fast developing world, more than 60 percent of produced polyethylene terephthalate (PET) are for fibers. PET fibers is used in many fields such as upholstery fabrics for polyester fibers, sailcloth, and sewing threads. Due to the COVID-19 pandemic, there has been a high demand for antibacterial products recently. Antibacterial products are now used in various fields such as carpets, clothes, automotive upholstery, surgical masks and aprons, and baby diapers. The aim of the study is to give antibacterial properties to PET fibers using with Cu-based metal organic frameworks.

Metal-organic frameworks (MOFs) with metal ions and organic ligands show strong antibacterial properties. Due to this feature, it has started to be used in various industrial areas such as medicine, food, textile and ventilation. Since MOFs are porous, they are used as reservoirs of nickel (Ni²⁺) silver (Ag⁺), zinc (Zn²⁺) or copper (Cu, Cu²⁺) metal ions. It is known that metal ions provide superior antibacterial properties [1]. MOFs have superior antibacterial properties than metal ions due to their crystal structure, constituents, and release of metal ions. The antibacterial properties of the MOF structures, which consists of organic ligands and metal ions, affect the ligands. Therefore, the antibacterial properties of MOFs with different metal ions were tested. First, the antibacterial properties of Ag-MOFs were tested and it was observed that the Ag-MOF structure showed superior antibacterial properties than silver nanoparticles. Studies have continued for the antibacterial activities of other MOF species and it has been proven that the Zn-MOF structure has biocidal properties against E.coli bacteria. It has been observed that it interacts with lipophilic acid or hydroxyl groups in the bacterial membrane to damage bacteria [2]. The release of metal ions by diffusion or biodegradation provides antibacterial properties. MOFs can contain multiple metal ions in the same structure. The advantage of using MOFs loaded with metal ions on natural and synthetic polymers is that the distribution and speciation of metal active surfaces in the MOF is homogeneous.

There has to be done some surface modifications in order to increase polyester's function. In this study, it is aimed to bring in antibacterial feature to polyester fibers by surface modification operation with Cu-based MOF (Cu-MOF). We examined the Cu-MOF metal organic structure since cupric metal has antibacterial feature. Positive charged Cu-MOF clings to negative charged the surface of polyester fibers. In this work, it is aimed to find the most ideal way for Cu-MOF metal organic structure to cling to the surface of polyester fibers during Cu-MOF synthesis. For this, it is worked on research the reaction conditions on surface modification studies which were done earlier, clinging to surface ways and used chemicals. Hereby, it is expected making a positive contribution for environment and nature alongside making longer life of fabrics.

Key Words: *PET fiber, surface modification, metal organic framework (MOF), Cu-MOF, antibacterial properties*

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SURFACE MODIFICATION OF ZEOLITE AND KAOLIN WITH DIFFERENT SILANIZATION AGENTS

Cem ÖZEL¹, Cansu AKAT¹, RASIM ALOSMANOV², Muhammet U. KAHVECİ³, Ceren EMİR¹, Sevil YÜCEL¹

¹Yildiz Technical University, Faculty of Chemical and Metallurgical Engineering, Department of Bioengineering, Istanbul/TURKEY, cemozel@yildiz.edu.tr, ckececi@yildiz.edu.tr, syucel@yildiz.edu.tr

²Bakü State University Faculty of Chemistry, Department of High-Molecular Compounds Chemistry, Bakü/AZARBEIJAN, r_alosmanov@rambler.ru

³Istanbul Technical University, Chemistry Department, İstanbul/TURKEY, kahvecimuh@itu.edu.tr

Abstract

Zeolites are crystalline, hydrated alumina silicates of alkali and alkaline earth cations used as cation exchangers and molecular sieves. They have also antibacterial, biocompatible and surface modification properties makes them useful in various biomedical areas such as drug delivery, hemostatic agents and soft and hard tissue applications [1]. Kaolin is an industrial clay, particularly consisting of hydrated aluminum silicate mineral named as kaolinite ($\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$). Kaolin is an important mineral in several world markets including uses in paper coating and filling, ceramics, paint, plastics, rubber, ink, fiberglass, cracking catalysts and many other uses. Kaolin functions as pharmaceutical excipient in commercial products, such as; granulating agent, film-coating additive, diluent, pelletizing agent, suspending and anti-caking agent and also accelerates blood clotting [2]. The surface modification of kaolin enables it to be used in different industries. Surface modification of inorganic materials is carried out with silanol agents. Silanization agents such as 3-aminopropyltriethoxysilane (APTES), 3-metakriloksipropiltrimetoksisilan (MAPTES), 3-aminopropyltrimethoxysilane (APTMS) are mainly used for surface modification [3-4]. The purpose of this study is the surface modification of a zeolite and kaolin with APTES and MAPTES in different ratios and different solvent medium (ethanol, toluene, DMSO) and also temperature. Zeta Potential, Fourier transform infrared analysis (FTIR), Scanning electron microscopy (SEM) were employed to investigate the structures of the samples. The surface-modified inorganic materials with promising properties have been prepared by functionalization of the natural kaolin and zeolite with alkoxysilanes. The effective surface modification of these clays was confirmed by zeta potential, SEM and FTIR spectroscopy.

Key Words: Zeolite, Kaolin, APTES, MAPTES, Silanization.

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GAS SEPARATION PROPERTIES OF MIXED MATRIX MEMBRANES PREPARED WITH GRAPHENE OXIDE

Sevgi ÇANÇA¹, Sennur DENİZ¹

¹Yıldız Technical University, Faculty of Chemical and Metallurgical Engineering,
Chemical Engineering Department, 34220, Esenler, Istanbul-Turkey

e-mail: f2020058@std.yildiz.edu.tr; deniz@yildiz.edu.tr

Abstract

Hydrogen is seen as the energy carrier of the future with its high energy density and environmentally friendly features. Hydrogen, which is not found in pure form in nature, can be separated from the gas mixture by various techniques. Gas mixtures are separated in industrial systems using cryogenic distillation, adsorption and polymeric membranes. Membrane-based separation has shown notable advantages in terms of high energy efficiency, low capital cost, large separation capacity and ease of scale-up. The most important parameters emphasized when examining the efficiency of membrane systems are selectivity and permeability. Permeability and selectivity are the key parameters for evaluating the separation performance of a membrane. Permeability reflects the rates at which components (penetrants) are transported through a membrane, and selectivity is the ratio of the permeability of the more permeable component to the less permeable one. Both high selectivity and high permeability are required for an effective gas separation system [1].

A new approach, mixed matrix membranes (MMMs), are mixed matrix materials consisting of homogeneously intertwined polymeric and inorganic particle matrices. Metal-organic frameworks (MOFs) have attracted attention due to their unique properties in terms of low density, high porosity and high surface areas, especially for their superior potential in gas storage and gas separation applications. Various types of MOFs can be synthesized by varying the combination of different organic binders and metal ions. This adaptability makes MOFs promising candidates for separation applications compared to zeolites and other inorganic fillers. The selection of suitable MOF/polymer pairs is crucial for experimental efforts to improve the performance of MMMs. The aim of this study is to develop a mixed matrix membrane with different polymeric bases of poly(ether-b-amide) (PEBA) and Polyimide (PI) containing graphene oxide (GO) as inorganic filler for hydrogen separation. Matrimid[®] 5218 is a commercially available thermoplastic PI. In this study, we used PEBA and PI as a monomer in synthesis of polymer membrane while the modification agent is GO. PEBA/GO and PI/GO mixed matrix membranes were prepared by adding graphene oxide (GO) dopant at % 0-0.1-0.2-0.3 percent by weight to PEBA and PI polymer solution. Polymer membranes prepared by solution casting method. The gas permeability and selectivity of modified polymer membranes were tested. The gas separation experiments of the membranes were performed at 35 °C and 3 bar feed pressure. The main aim of this study is to increase the selectivity and permeability of membranes in gas separation applications.

Key Words: Gas separation, Mixed matrix membranes, Poly(ether-b-amide), Polyimide, graphene oxide

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BIODEGRADABLE FLEXIBLE PLA/PCL FILMS WITH NATAMYCIN AND NANOCELLULOSE

Nudem KAHRAMAN¹, Sennur DENİZ¹,

¹Yıldız Technical University, Faculty of Chemical and Metallurgical Engineering,
Chemical Engineering Department, 34220, Esenler, İstanbul-Turkey
e-mail: f2018025@std.yildiz.edu.tr; deniz@yildiz.edu.tr

Abstract

In this period, when the industry has not yet fully transitioned to green chemistry and chemical diversity has increased, the biggest problem is the waste caused by these chemicals. Although the usage areas of chemicals that cause millions of tons of waste per day are quite wide, the biggest step to be taken is to prevent waste generation from the beginning. Based on this reason, it should be aimed that the chemical raw materials used in any sector should be environmentally friendly and should be developed according to the desired properties. Packaging materials are among the products that generate the most waste and have high usage. Sectoral needs are being evaluated for the use of biodegradable materials with a very high potential for use. Poly(lactic acid) (PLA), which can be obtained from renewable resources such as corn starch, is a biodegradable, semi-crystalline thermoplastic with great tensile strength and high modulus. However, the usage areas of PLA, which has a very fragile structure, are limited due to this feature. Therefore, mixing of PLA with biodegradable poly(caprolactone) (PCL), which is known to have flexible properties, is one of the preferred methods.

In our previous study to obtain flexible packaging material, as a result of the trial conducted at different rates; it was concluded that the optimum film mix is 20%PLA/80%PCL [1]. In order to further increase the flexibility, the material to be added to the film mixture is also intended to be environmentally friendly and to give the film a new feature. For this reason, tocopherol, which is known to extend the shelf life of foods and is also environmentally friendly, was preferred and it was concluded that the optimum addition rate was 1.5 wt.%. According to the mechanical test results after adding tocopherol to the film solution, it was observed that the flexibility of the packaging material increased. The aim of our new study is to discover materials that can improve the mechanical properties by increasing the flexibility of the packaging material and to increase the diversity in this regard, as well as to compare the mechanical properties of the added materials with the effect of tocopherol. Based on this idea, one of the materials that we think will improve additional properties to the material when added is natamycin, which is used to increase the shelf life of foods. The other is nanocellulose with high mechanical strength, which is obtained by mechanical decomposition of wood pulp obtained from wood, sugar beet, potato, hemp and flax. As a result, it was concluded that tocopherol gave PLA/PCL film a more flexible structure than natamycin and nanocellulose.

Key Words: *Biodegradable films, flexible films, poly(lactic acid), poly(caprolactone), natamycin, nanocellulose*

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PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE BY NANO-TITANIUM DIOXIDE COMPOSITES

Emel AKYOL¹, Guldeniz TONBUL¹,

¹Yildiz Technical University, Department of Chemical Engineering, Istanbul, Turkey, eakyol@yildiz.edu.tr

Abstract

Titanium dioxide (TiO₂) is important and promising catalysis in photocatalysis studies with its unique semiconductor optical and electrical properties. Among many photocatalysts, titanium dioxide is an ideal material for present and future industrial applications [1-3].

In this study, nanosized titanium dioxide nanocomposites were prepared from titanium powder by a simple flame transfer method. Hydroxyapatite and barium sulfate were used to obtain titanium dioxide nanocomposites and their characterizations were done. The effects of hydroxyapatite and barium sulphate on photocatalytic properties of TiO₂ were investigated. It was observed that the photocatalytic degradation of methylene blue with titanium dioxide nanocomposites obtained with hydroxyapatite and barium sulfate was better when it was compared to pure titanium dioxide.

Key Words: *Titanium Dioxide; Nanocomposites; Photocatalysis; Hydroxyapatite; Barium Sulphate*

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COLORIMETRIC METHOD FOR INSULIN DETECTION USING A NEW MAGNETIC NANOZYME

Burcu GÖKÇAL¹, Kadriye Özlem HAMALOĞLU²

¹Chemical Engineering Department, Hacettepe University, 06800, Ankara, Turkey,
burcugokcal@hacettepe.edu.tr

²Chemical Engineering Department, Hacettepe University, 06800, Ankara, Turkey, ozlemnaz@hacettepe.edu.tr

Abstract

Insulin is an important polypeptide hormone that regulates carbohydrate metabolism [1]. Also, it is one of the main indicators in monitoring and control of diabetes. Therefore, reliable quantification of insulin is important for treatment of diabetes [2]. In this study, magnetic nanozyme was developed for colorimetric determination of insulin. Magnetic and monodisperse-porous silica microspheres were synthesized 6.5 μm in size, by “staged sol-gel templating protocol”. Iminodiacetic acid linked-glycidoxypropyltrimethoxysilane (IDA-GPTMS) was used as the chelating ligand for immobilization of Cu (II) ions on silica shell coated magnetic silica microspheres (Cu(II)@IDA-GPTMS@SiO₂@MagSiO₂). 3,3',5,5' Tetramethylbenzidine (TMB) was used as a synthetic substrate in the presence of hydrogen peroxide (H₂O₂). The colored product (oxidized TMB) was measured by using a UV-Visible spectrophotometer. The colorimetric response (measured at 652 nm) is linear in the insulin concentration range of 0-0.7 mg/mL. The observed peroxidase-like activity exhibited a linear decrease with the increased insulin concentration. The procedure was developed based on interaction between the IDA-Cu(II) complex immobilized on the magnetic silica microspheres and histidine residues of insulin. A new and reusable magnetic nanozyme investigated in this study may be useful for the colorimetric detection of proteins.

Key Words: *Nanozyme, Colorimetric detection, Peroxidase like activity*

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PREPARATION OF SULFONIMIDE FUNCTIONAL PROTON CONDUCTING POLYMERS

Elif Büşra ÇELEBİ, Ferda HACİVELİOĞLU

Gebze Technical University Department of Chemistry, 41400, Gebze, Kocaeli, Turkey
bsracelebi@gmail.com

Abstract

Fossil fuels are the main energy sources of the world. In addition to the decrease in fossil fuel reserves, the polluting effect of atmosphere by harmful gases released during their use increases the need for environmentally friendly and sustainable energy sources. Polymer electrolyte membrane fuel cells (PEMFC) are considered as one of the most important clean energy conversion systems due to their high power and energy density. The membrane material, which is one of the most important part of the PEMFCs, should be resistant to high oxidative conditions as well as having a sufficient proton conductivity. Perfluorosulfonic acid (PFSA) membranes, e.g., Nafion, have been chosen as the standard due to their high mechanical strength, high proton conductivity, excellent chemical and thermal stability which are the requested properties to provide high performance for PEMFCs. On the other hand, environmental concerns, high fuel diffusion, loss of ionic conductivity at high temperatures and high cost due to high fluorine content are just a few of the disadvantages of PFSAs [1]. For this reason, studies on alternative membrane materials that can be recycled without releasing CFC gases, which can provide high proton conductivity at high temperatures have accelerated in recent years.

Polyphosphazenes, which contain sequential P and N atoms in their main chain, are one of the most important inorganic polymers. Sulfonic and phosphonic acid functional polyphosphazenes have similar proton conductivity to PFSA membranes, while also providing lower fuel crossover and lower water swelling properties [2]. Sulfonimid functional materials have comparable ionic conductivity to sulfonic acid derivatives whereas they can also provide additional unique features to polymer electrolyte membrane. Moreover, since the degradation products of the polyphosphazene backbone are mainly H_3PO_4 and NH_3 , they can be recycled without the release of harmful CFC gases compared to PFSA membranes [3]. Therefore, combination of the features of both polyphosphazenes and sulfonimid groups may yield better PEM materials. In the present study, we are going to report some new results from our research based on a series of sulfonimid functional polyphosphazene derivatives.

Key Words: *Conducting Polymer; Sulfonimide; Polyphosphazene*

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SYNTHESIS AND CHARACTERISATION OF A GLUTATHIONE-S-TRANSFERASE (hGSTP1-1) SINGLE NUCLEOTIDE POLYMORPHS (PART II)

Sadhna MATHURA¹

¹University of the Witwatersrand, Johannesburg, SOUTH AFRICA, sadhna.mathura@wits.ac.za

Abstract

Glutathione-S-transferases (GSTs, E.C. 2.5.1.18) comprise a superfamily of multifunctional enzymes involved in catalytic cellular **detoxification** reactions [1, 2]. Mutations in GST proteins, particularly single nucleotide **polymorphisms** (SNP), have been linked to several human diseases and ailments such as Alzheimer's- and Parkinson's disease, asthma, cancer and so on [3-5]. Understanding the intimate **structure-function** relationship of these SNP mutations (relative to wildtype) is therefore of growing interest. What are the structural implications of GST polymorphism and the subsequent influences on its detoxification function? Consequently, in this work we aim to synthesise and characterise a single nucleotide polymorph (Y80C) in the hydrophobic domain of canonical cytosolic human GST class pi (**hGSTP1-1**).

Interestingly, the Y80C residue sits at the interface of both the subunit and the domain regions, respectively (Figure 1). Our strategy is therefore to examine the structure-function significance of the Y80 residue using an interesting SNP mutation [6], Y80C. We compare the structure-function features relative to those of the wild-type (WT) to elucidate how the identity of the residue at this position influences the catalytic, structural and stability properties at the binding sites. Circular dichroism and fluorescence spectra reveal minor secondary and tertiary alterations of Y80C structure relative to WT. These preliminary findings form the basis for other SNP studies in this series.

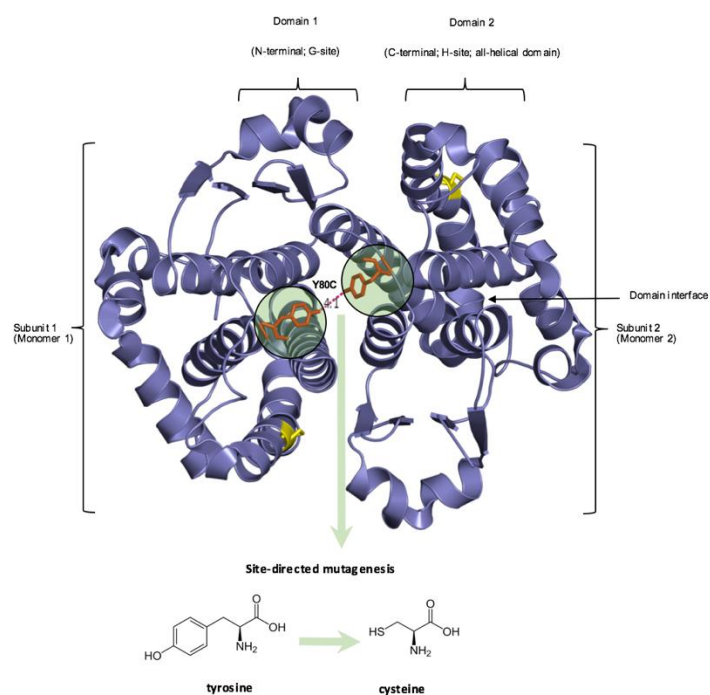


Figure 1: Quaternary structure of the homodimeric hGSTP1-1 (PDB: 2a2r). The monomer subunits, domains and interfaces are indicated. The amino acid residue highlighted in green indicates the Y80 region for site-directed mutagenesis to synthesise the Y80C SNP mutant.

Key Words: *hGSTP1-1; SNP; polymorphism; structure-function relationship; detoxification proteins.*

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PREPARATION OF GELATIN COATED ALGINATE CAPSULES

Gulzhan Yerlan*, Bakyt Tyussyupova, Sagdat Tazhibayeva, Kuanyshbek Musabekov

Al-Farabi Kazakh National University, Almaty, Kazakhstan

[*erlan.gulzhan@mail.ru](mailto:erlan.gulzhan@mail.ru)

Abstract

The prevalence of diabetes in the 21st century is approaching pandemic proportions. Diabetes is considered one of the most dangerous diseases in terms of its rate of spread and the side effects it has on the body.

It is a global disease, which frequency increases exponentially [1].

Because of its ease of administration and low healthcare costs, oral drug delivery is a more preferred mode of administration. However, due to gastrointestinal barriers that result in inconsiderable oral bioavailability of macromolecular drugs, oral protein formulations are currently commercially not accessible [2].

The aim of this study was to obtain capsules for creating an oral form of insulin based on biodegradable polymers such as alginate and gelatin. The composition of the capsule should protect insulin from aggressive environments of the stomach and provide access to the intestines.

The capsules were obtained by ionotropic gelation. Alginate capsules are prepared by adding a sodium alginate solution in the form of drops to the crosslinking agent solution [3].

In order to optimize the method of obtaining capsules by the method of ionotropic gelation, solutions of various concentrations (0.5%; 1.0%; 1.5%; 2.0%) of the CaCl₂ crosslinking agent were used. Capsules with high morphological stability were obtained using 1.5%; 2% solutions of the crosslinking agent CaCl₂.

When the drug is homogeneously dispersed in a polymer matrix, the final product can be in the form of swelling microspheres or ordinary tablets. The release of the drug from such systems occurs by diffusion through the swelling and dissolution of the matrix [4].

The degree of swelling of alginate capsules obtained by ionotropic gelation was studied in order to observe their changes in the gastrointestinal tract. Since the degree of swelling of the capsules when using 1.5% CaCl₂ solution was mainly higher when obtaining alginate capsules compared to other concentrations of the crosslinking solution, 1.5% CaCl₂ was chosen as the optimal crosslinking solution for obtaining alginate capsules.

In order to increase the stability of alginate capsules to acidic and alkaline environments, the capsules were coated with a gelatin membrane (2%; 5%; 8% gelatin solutions) and the degree of their swelling was studied.

According to the results of the study, the degree of swelling of alginate - gelatin capsules was higher by 0.52 units at pH = 1.0; 0.74 units at pH = 4.01; 1.59 units at pH = 6.86; 1.78 units at pH = 9.1 than the degree of swelling of alginate capsules.

It can be assumed that an increase in the degree of swelling of capsules before reaching a plateau indicates their ability to retain immobilized insulin.

It is important that the capsules are stable, not dissolving in an acidic environment. Since this is a guarantee that they will not release immobilized insulin in the acidic environment of the stomach at an early stage.

Consequently, gelatin coating decreases the solubility of alginate capsules in an acidic environment and increases stability to the aggressive environment of the gastrointestinal tract.

Key Words: *insulin, sodium alginate, gelatine, crosslinking agent, ionotropic gelation method*

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SYNTHESIS AND CHARACTERIZATION OF TERPYRIDINE FUNCTIONAL CYCLOPHOSPHAZENE

Elif Büşra ÇELEBİ, Halil DUYAR, Ferda HACİVELİOĞLU

Gebze Technical University Department of Chemistry, 41400, Gebze, Kocaeli, Turkey
bsracelebi@gmail.com

Abstract

Commercially available hexachlorocyclotriphosphazene ($N_3P_3Cl_6$) is a very useful (Cp) precursor and can undergo nucleophilic substitution reactions with a wide array of structurally diverse nucleophiles. Therefore, it allows to prepare a variety of cyclotriphosphazene-based dendrimers [1] and polymers [2] with desired functions. Cp has a planar nonlocalized cyclic ring structure consisting of alternating nitrogen and phosphorus atoms, which can let to prepare an interesting class of materials that offers access to solution processable dendrimeric materials. Cp cores have many advantageous properties for application in solution-processable OLEDs. Many studies have focused on the use of electron-withdrawing groups such as pyridine, pyrimidine, triazine, and other nitrogen-containing heterocycles to improve the electron-transporting capabilities of materials [3]. Pyridine is favored because of its strong electron-accepting character and the ability to adjust the electron-transporting ability of the molecule by changing the substitution site [4]. The pyridine derivatives have exhibited superior performance when incorporated in electroluminescent devices due to their excellent electron transport and electron injection capabilities [5].

In this study, Cp-based terpyridine was synthesized through simple nucleophilic substitution reaction. HCCP-TPY was characterized by FT-IR, NMR, and MALDI TOF spectral data. Thermal properties were investigated by DSC and TGA methods. In addition, it is thought that it will be a potential candidate to be used in advanced technological devices considering the results obtained by examining its photophysical and electrochemical properties.

Key Words: *Cyclophosphazene; Terpyridine*

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INVESTIGATION OF TRACE AND MAJOR ELEMENT CONCENTRATIONS OF ALMOND MILK BY USING AN INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETER

Ayca KARASAKAL

Namik Kemal University, Science and Letters Faculty, Department of Chemistry, Tekirdağ
akarasakal@nku.edu.tr

Abstract

This work aims to determine the concentrations of trace and major elements in almond milk samples that were collected from Turkish supermarkets by using inductively coupled plasma–optic emission spectroscopy (ICP- OES) and compare the accuracy and precision of digestion procedures. Microwave digestion procedure was preferred because the times required for microwave digestion procedure were less than the other digestion techniques. Na, Mg, K, Ca, P, Fe, Cu, B, Mn, Zn, Al, S, As, Bi, Cd, Co, Cr, Mo, Ni, Pb, Pt, Sb, Se, Sn, Ti, W, and Hg were investigated in almond milk. The methods were validated by linearity, limits of detection and quantification, precision, and analyzing certified reference material (NIST SRM-3235), soybean milk. The highest values of LOD were found Pb, P, and Bi, and the highest values of LOQ were found Mo, Pb, and Sb.

Key Words: ICP-OES, Almond milk, Microwave digestion

SYNTHESIS AND CHARACTERIZATION OF LDH MATERIALS AND THEIR APPLICATION IN WASTEWATER TREATMENT

Abderrahmane HIRI¹, Achour DAKHOUCHE², Kamel NOUFEL Kamel NOUFEL³

¹m'sila university inorganic materials laboratory e-mail: abderrahmane.hiri@univ-msila.dz

²m'sila university inorganic materials laboratory e-mail: achour.dakhouche@univ-msila.dz

³m'sila university inorganic materials laboratory e-mail: kamel.noufel@univ-msila.dz

Abstract

Hydrotalcites (Layered Double Hydroxides, LDH) belong to the class of inorganic lamellar compounds, and have a high anion insertion capacity[1]. The basic structure of LDH compounds is similar to that of a natural hydrotalcite $Mg_6Al_2(OH)_{16}CO_3 \cdot 4H_2O$, in this structure magnesium (divalent cation) has been substituted by aluminium (trivalent cation) with a general formula: $[(OH)_2]_x+[A^n]_{x/n} \cdot mH_2O$. In recent years, LDH compounds have received considerable attention; The anion exchange properties have been widely studied. The interest in the magnetic and electrochemical properties of LDH allows heterogeneous catalysis and applications in the treatment of polluted water[2]. LDH compounds have been used as adsorbents or catalysts in the reaction of degradation into non-biodegradable products. In this work, carbon samples of LDH of NiCuAl-CO₃ type were synthesized. The products have been used as catalysts in the degradation of paracetamol with hydrogen peroxide[3]. The carbonate samples are obtained by coprecipitation at constant pH with a molar ratio R (R = M^{II} / M^{III}) equal to 1.5. LDH compounds prepared are characterized by XRD, SEM and FTIR. certain parameters were tested such as the mass of the catalyst, the volume of H₂O₂ oxidant, the temperature and the contact time.

Key Words:

Layered Double Hydroxides; Paracetamol; Fenton; Advanced Oxidation Processes; free radicals.

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DETERMINATION OF HUMAN PAPILLOMAVIRUS-11 WITH IMPEDIMETRIC CRISPR BIOSENSOR

Zihni Onur UYGUN¹

¹Kafkas University Faculty of Medicine Department of Medical Biochemistry Kars Turkey
e-mail: onur_uygun@hotmail.com

Abstract

Human papillomaviruses (HPVs) are small double-stranded DNA viruses containing more than 200 genotypes. Based on the differences in their pathogenicity, the HPV family can be further divided into low-risk HPV (LR-HPV) types and high-risk HPV (HR-HPV) types. LR-HPVs are etiologically associated with genital warts, particularly condylomata acuminata (CA), which has a global widespread incidence of 160 to 289 cases per HPV-11 year. Due to the infectious and proliferative nature of HPV, CA has become a serious threat to public health, and affected patients are prone to frequent relapses and undergo multiple surgical procedures. For the diagnosis of these diseases, the diagnosis can be made by taking cervical fluid and scanning the HPV-11 genome with polymerase chain reaction (PCR). Being able to diagnose the bedside rapid test is extremely important. In this study, an electrochemical biosensor system was developed to determine the DNA sequence specific to HPV-6 only, 20 base pairs. Target HPV-11 DNA Sequence 5'ACGTGGCCTTGTGCGGTACA'3; https://blast.ncbi.nlm.nih.gov/Blast.cgi?PROGRAM=blastn&PAGE_TYPE=BlastSearch&LINK_LOC=blasthome. Those what did not show similarities in this genomic sequence were screened by tine blast. Accordingly, 20 base pairs of DNA sequences selected from regions outside of this similarity were screened for similarity using blasts, respectively, and it was observed that the ACGTGGCCTTGTGCGGTACA sequence did not show similarity except for HPV-11. Accordingly, sgRNA design was made by targeting this sequence in sgRNA design as CRISPR-dCas9 technology. Screen-printed gold nanoparticle electrodes were used as the basic electrode to be used as the sensor system. PalmSens 3 potentiostat was used as the measuring system, namely the potentiostat. Electrochemical impedance spectroscopy (EIS) measurements were performed with this device. EIS measurements redox probe solution: 5mM Fe(CN)₆^{3-/4-}, 50mM pH=7 phosphate buffer solution containing 100mM KCl. EIS Parameters: In the redox probe solution, 180 mV DC, 10 mV AC was applied and the spectrum was taken in the frequency range of 2.000-0.05 Hz.). Accordingly, the impedance data approved that GPHOXE/PAMAM/dCas9/sgRNA modification for HPV-11 DNA detection. Thus, a faster HPV-11 biosensor than PCR was developed. Accordingly, the biosensor is able to detect DNA between 50 pM and 1000 pM with good linearity and sensitivity. Chronoimpedimetric detection was also approved that the biosensor has ability to detect HPV-11 DNA in 3 minutes

Keywords: biosensor, CRISPR, HPV-11, impedance

THERMAL ANALYSIS AND ISOCONVERSIONAL KINETICS STUDY OF THERMAL DECOMPOSITION OF POLYCYCLOHEXENE OXIDE POLYSTYRENE (PCHO-PST) COMB-SHAPED POLYMER

Hacer DOLAS¹, Nasrettin GENLI²,

¹Harran University, Hilvan Vocational School, Program of Occupational Health and Safety, Sanliurfa
63900, Turkey

hacerdolas@hotmail.com, and hacerdolas@harran.edu.tr

²Dicle University, Diyarbakir Vocational School of Technical Sciences, Chemical and Chemical
Processing Technologies, Diyarbakir, 21280, Turkey
nasrettin.genli@dicle.edu.tr

Abstract

The polymers bearing end-functional group is important because of its using as precursor of block and graft polymers. Also, the polymers have been used for coating and adhesives, in medical and environmental fields.

The reaction kinetics gives the information about the durability and decomposition temperature of a polymer under various thermal conditions [1]. For this reason the thermal decomposition kinetics of the materials have been investigated [2]

In this study we aimed to investigate the thermal and the kinetics parameters of the thermal decomposition reaction of poly cyclohexene oxide polystyrene (PCHO-PSt) comb-shaped polymer that the polymer of epoxy end-functionalized polystyrene and to determine the glass transition of polystyrene presented as a unit in the polymer. Firstly, the cyclohexene oxide end-functional macro monomer of polystyrene (CHO-PSt) and its polymer, (PCHO-PSt comb-shaped polymer) by atom transfer radical polymerization were synthesized in according to literature [3]. The thermal characteristics of the polymer was evaluated through the Thermal analysis methods, differential thermal analysis (DTA), thermogravimetric analysis-derivative thermogravimetry (TG-DTG) under nitrogen atmosphere at 3, 5, 7 and 10 °C min⁻¹ from 30 °C to 600 °C. According to obtained results, the polymer decomposition exhibited a distinct mass loss step. The initial mass loss temperatures were shifted to the higher temperature region as the increasing of temperature heating rate, as well as the maximum value of the mass loss rate. To see the temperature ranges of the glass transition, crystallization and melting of the polymer, it was used DTA curves. So, the glassy transition region was seen at the range of 70-80 °C. At the range of 150-250 °C endothermic and exothermic physical transitions were observed in the history of the polymer. For the determination of the net values of these transitions the DSC cooling curve was evaluated. The cooling process was performed from 280 to -100 °C, in nitrogen media at 10 °C/min cooling rate by using liquefied N₂. So, the polymer was started freezing at 245 °C (melting region during heating) and crystallized at 149-132 °C. The glass transition was shifted to 67-70 °C due to cooling. These results were conformed with TG, DTA curves. From DSC graph an exothermic change was observed from 173.62 °C to at 199.73 °C. From TG curve this change was identified as crystallization because of lack of mass loss in the temperature range. So, the area under this range, that is crystallization enthalpy was calculated 9.7 J g⁻¹ and DSC peak was read as 184.95 °C. The melting was started at 217 °C and ended at 250.62 °C. The area under this range, that is fusion enthalpy was calculated 16.29 J g⁻¹ by DSC software. And the polymer was decomposed at 321.65 °C. During this phenomenon the absorbed heat from media was calculated as 532,86 J g⁻¹. The activation energy was calculated by OFW method being model free approach as 140.81 kJ mol⁻¹. The maximum activation energy was found as 160,82 kJmol⁻¹ at 30% conversion.

Key Words: Comb-shaped polymer, TGA-DTA, DSC, Pyrolysis, Activation energy.

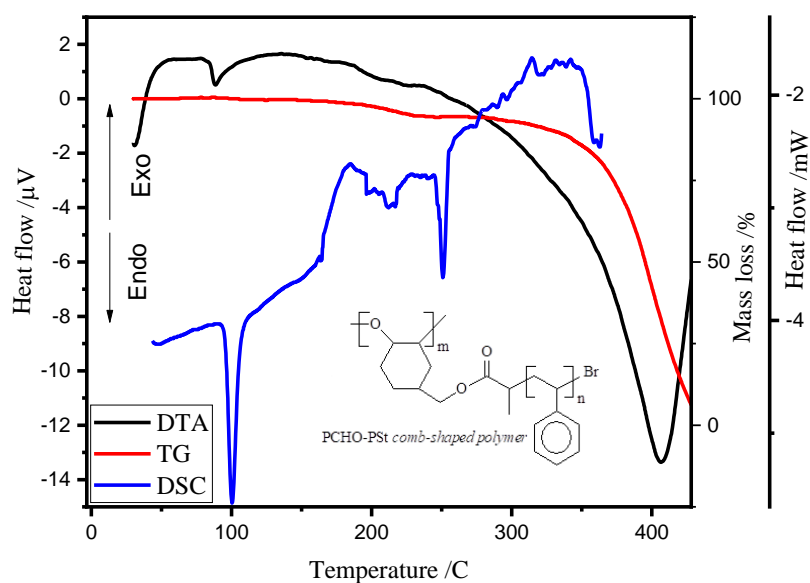


FIGURE 1. THE COMPARISON OF GRAPHS DTA, TG AND DSC CURVES.

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CRISPR-DCAS9 BASED BIOSENSOR SYSTEM FOR DETECTION OF SICKLE CELL ANEMIA

Hilmiye Deniz ERTUĞRUL UYGUN¹

¹ Dokuz Eylül University, Center for Fabrication and Application of Electronic Materials, Izmir 35390, Turkey
e-mail: deniz.uygun@deu.edu.tr

Abstract

Sickle cell anemia is one of the single point mutation diseases with symptoms such as stroke, lethargy, chronic anemia and increased mortality, and causes red blood cells to become sickle-shaped [1]. Diagnosis of this mutation, which occurs with the conversion of the GAG codon to the GTC codon as a single nucleotide mutation, is made by conventional techniques such as polymerase chain reaction [2], liquid chromatography [3] and electrophoresis [4]. Although these methods show high sensitivity, they are time-consuming and costly methods [5]. In the study, a biosensor system was developed to detect this mutation quickly and cost-effectively. This biosensor system was prepared by forming a SAM layer with 4-Aminothiophenol (4-ATP) on the gold electrode, and then amino graphene coated on it, and then modified with SG-RNA with the sequence of the target mutation after CRISPR-dCas9 immobilization. The biosensor system prepared in this way was optimized and made to perform DNA analysis. Electrochemical impedance spectroscopy (EIS) was used as the measurement method. In the electrode preparation steps, EIS and cyclic voltammetry (CV) methods were used for surface characterization. Electrochemical measurements were carried out in 50 mM pH 7.0 phosphate buffer solution, which includes 5 mM $\text{Fe}(\text{CN})_6^{3-/4-}$ and 10 mM KCl, as redox probe solution by CV and EIS in this redox probe solution. EIS parameters were 10000–0.05 Hz frequency, 10 mV AC and 180 mV DC potential, CV parameters were between - 0.2 to 0.5 V potential, 100 mV/s scan rate for 5 cycles. The DNA measurement time of the biosensor system was determined by the chronoimpedance measurements taken by applying a frequency of 500 Hz under 200 mV DC current. Measurement time of the biosensor was found to be 600 seconds. With the CRISPR-Cas9 based electrochemical biosensor system, which gives faster results compared to the measurement methods in the literature, linear measurement between 50 pM and 400 pM with a length of 200 base pairs was taken.

Key Words: Sickle cell anemia, CRISPR-dCas9; Biosensor; Electrochemical impedance spectroscopy

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PHENOL CONTAINING BODIPY FUNCTIONALIZED ANDERSON TYPE POM: SYNTHESIS, CHARACTERIZATION AND PHOTOPHYSICAL PROPERTIES

Seda CETINDERE¹

¹Gebze Technical University Department of Chemistry Gebze, Kocaeli, TURKEY
sdemirer@gtu.edu.tr

Abstract

Polyoxometalates (POMs) are inorganic metal-oxo cluster anions of the general formula $[M_xO_y]^{n-}$ consisting of two or more high-valent transition metals (M) such as W, V, Mo, Nb, Ta, which are linked via bridging μ -oxo-ligands [1]. Anderson type POMs are among the most known oxo compounds [2]. Functionalization of POMs with organic groups, provides a strategy to achieve POM-based hybrid materials. They combine the advantages of organic molecules such as good solubility and easy functionalization together with chemical stability and high redox activity of inorganic POM clusters [3]. Boron dipyrromethene (BODIPY) dyes are fluorescent organic dyes which have interesting spectral properties such as high quantum yield, large extinction coefficient and narrow emission bands. On the other hand, absorption and emission properties of these dyes can be adjustable by substitution of different groups into the BODIPY core [4].

This study aims to functionalization of Anderson type POM with phenol containing BODIPY dye (Figure 1) and investigation of its photophysical properties to see its usability as a photosensitizer in solar energy conversion processes.

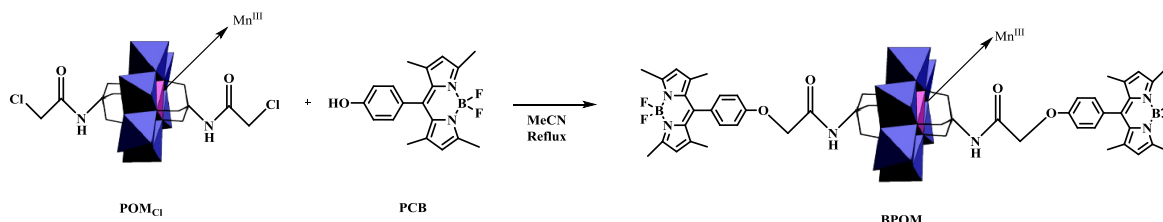


Figure 1. Synthetic pathway of BPOM

Key Words: BODIPY, POM, Anderson, phenol, photophysical properties.

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DETERMINATION OF FREE ENERGY DIFFERENCE BETWEEN ANOMALY SOLID-LIQUID PHASE TRANSITIONS OF SILICON USING PSEUDO- SUPERCRITICAL THERMODYNAMIC PATH: A MOLECULAR DYNAMICS STUDY

Chandan K Das*

*Department of Chemical Engineering, National Institute of Technology Rourkela
Rourkela, India-769008. E-mail: dasck@nitrkl.ac.in*

Abstract: Silicon shows a very different trend while melting. Melting has remained a challenging subject from a long time. Especially, predicting the melting temperature of any solid substance still exists as a problem in many cases. Also, there are certain anomalies in silicon, which makes its melting and phase transition mechanism more difficult to understand and predict. In order to understand the phenomenon, it is important to know the interaction potential governing the silicon system. Stillinger-Weber potential[1] is a good model for Si atoms which takes into account two and three particle interactions. Melting of Silicon atoms is studied using Molecular Dynamics Simulation with the help of LAMMPS software[2]. Free energy difference between phases is estimated with the help pseudo supercritical path[3,4]. The only extensive property that remains constant during phase transformation. Using this beautiful property one can estimate true thermodynamics melting temperature. Estimation of Gibbs free energy is performed with the help of pseudo-supercritical reversible thermodynamic cycle along the help of multiple histogram reweighting diagrams. Supercritical path is constructed with the help of more than one reversible thermodynamic path. Thermodynamic integration is performed using Gauss-Quadrature integration scheme.

This work is mainly focusing on determination of free energy difference between two phases during Phase transitions. Melting temperature can be predicted using Gibbs free energy. Gibbs free energy calculation involves with thermodynamics integration and multiple histogram reweighting(MHR) method[4].

In this work, I evaluate free energy gap connecting solid-liquid transitions. I present briefly the technique. (a) The liquid state is transformed into a poorly interacting liquid with the help of slowly decreasing the interatomic attractions. (b) Gaussian wells are located to the corresponding particles; simultaneously the volume is enlarged to obtain a poorly interacting oriented state. (c) Gaussian wells are removed gradually and simultaneously interatomic attractions are slowly brought back to its whole strength to obtain a crystalline state. Estimated Gibbs free energy difference is around $-4.8463 \times 10^{-15} \text{J}$.

The estimation of phase transition point from free energy analysis is combination of four stages. First step is evaluation of an approximate transition point from quenching and heating method[5,6]. Second is estimation of equation of state for the solid phase with respect

solid reference state[4]. Similarly for liquid phase is also determined with respect to liquid reference state. Equations of states are generated using multiple histogram reweighting technique. Third step is the evaluation of difference in free energy between two phases at an estimated transition point. Free energy computation is performed with the help of pseudo-supercritical transformation path. Then ultimately with the help of second and third steps evaluation of the transition point is done at zero energy difference. That point is considered as true thermodynamic transition point. The estimated melting temperature of silicon is around $1883\pm 4^\circ\text{K}$.

Keywords: Molecular Dynamics; LAMMPS; Hysteresis loop; Pseudo-super-critical Path; Thermodynamic Integration

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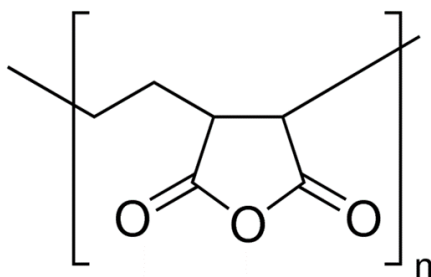
INVESTIGATION OF STABILITY AND ACTIVITY OF POLY(ETHYLENE-ALT-MALEIC ANHYDRIDE) COPOLYMER IN DIFFERENT pHs and SIMULATED BODY FLUIDS

Dolunay Şakar Daşdan¹,

¹Yildiz Technical University, Department of Chemistry, 34220, Esenler, İstanbul, Turkey
Email: dolunaykar@yahoo.com

Abstract

Poly(ethylene-alt-maleic anhydride) (Scheme 1) copolymer are used in various applications as emulsion stabilisers, detergent compositions, viscosity modifiers and drug delivery systems[1-2]. In this work, it is aimed to determine the stability and activity of poly(ethylene-alt-maleic anhydride) copolymer (PEAMA) in different pHs and various artificial body fluid mediums such as 5% dextrose solution, PBS solution and 0.9% isotonic NaCl solution. To determine the stability of PEAMA, it was measured the polydispersity, particle size, mobility and zeta potential of PEAMA at different pH values and various artificial body fluid mediums via zetasizer. The activity of PEAMA were investigated at different pH values and various artificial body fluid mediums based on the time effect by UV/VIS measurements. According to the obtained results, the optimum conditions of stability and activity of PEAMA copolymer was determined.



Scheme 1 Chemical structure of Poly(ethylene-alt-maleic anhydride)

Key Words: *Poly(ethylene-alt-maleic anhydride); stability; activity; particle size; zeta potential*

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PRODUCTION AND CHARACTERIZATION OF COMPOSITE SCAFFOLDS BY ELECTROSPINNING TECHNIQUE FROM BIOCERAMICS SYNTHESIZED FROM SEASHELLS

Sema Nur SAHIN^{1,*}, Erdi BULUS^{2,3}, Demet Sezgin MANSUROGLU^{2,4}, Bahadir BOZKURT^{2,5}, Aziz KORKUT¹, Yesim Muge SAHIN^{1,2}

^{1,*}Istanbul Arel University, Faculty of Engineering and Architecture, Department of Biomedical Engineering
Istanbul, Turkey

semanuursahin@gmail.com

azizkrkt98@gmail.com

ymugesahin@arel.edu.tr

²Istanbul Arel University, ArelPOTKAM (Polymer Technology and Composite Application and Research Center), Istanbul, Turkey

erdibulus@arel.edu.tr

³Çanakkale Onsekiz Mart University, Graduate School of Education, Department of Bioengineering and Materials Engineering (Interdisciplinary), Çanakkale, Turkey

buluserdi@gmail.com

⁴Istanbul Cerrahpasa University, Institute of Science, Chemistry Program, Istanbul, Turkey

sezgindemet82@gmail.com

⁵Istanbul Cerrahpasa University, Graduate School of Education, Department of Mechanical Engineering,
Istanbul, Turkey

bahadirbozkurt@arel.edu.tr

Abstract

The need for tissue scaffolds to support and heal damaged tissues and organs after illness or accident is increasing. Tissue scaffolds produced by electrospinning technique stand out in tissue engineering applications due to their micro to nanoscale porosity and high surface-to-volume ratio [1]. In this study, bioceramic was synthesized from sea snail shells by chemical precipitation method in order to be used to provide enhanced mechanical strength to tissue scaffolds. By using electrospinning aqueous solutions prepared by adding, polyvinyl alcohol (PVA), a biocompatible and biodegradable polymer, gelatin (GEL) with suitable binding sites for cell adhesion and differentiation, and synthesized bioceramics, it is aimed to produce tissue scaffolds with appropriate cell adhesion, biodegradability and tensile strength [2,3]. Structural, morphological, mechanical and thermal characterizations of synthesized bioceramics and fabricated scaffolds were made. As a result of the analyzes, a potential biomaterial with ideal properties that can appeal to tissue engineering applications has been produced. In addition, it is predicted that composite scaffolds, which create a suitable environment for cell adhesion and provide good mechanical properties, can be used as an intermediate layer to support bone and connective tissue formations. In this study, structural (FTIR, Fourier Exchange Infrared Spectrophotometer) and morphological (FEGSEM, Field Emission Gun Scanning Electron Microscope) of these nano biocomposites were studied.

Key Words: *Seashells, bioceramics, polyvinyl alcohol, gelatin, electrospinning, tissue scaffolds*

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NEW APPROACHES IN GREEN CHEMISTRY: VANILINE BASED IMIN SYNTHESIS AND WOUND DRESSING PRODUCTION BY NANOTECHNOLOGY

Yesim Muge SAHIN^{1,2*}, Erdi BULUS², Demet Sezgin MANSUROGLU^{2,3}, Bahadir BOZKURT^{2,4},
Hatice Dilara SARAC¹, Funda OZKOK⁵, Nihal ONUL⁵, Tatyana TISHAKOVA⁶, Gulru OZAY⁷

¹Istanbul Arel University, Faculty of Engineering and Architecture, Department of Biomedical Engineering
Istanbul, Turkey, ymugesahin@arel.edu.tr

^{2*}Istanbul Arel University, ArelPOTKAM (Polymer Technology and Composite Application and Research
Center), Istanbul, Turkey, erdibulus@arel.edu.tr

³Istanbul Cerrahpasa University, Institute of Science, Chemistry Program, Istanbul, Turkey,
sezgindemet82@gmail.com

⁴Istanbul Cerrahpasa University, Institute of Science, Department of Mechanical Engineering, Istanbul, Turkey,
bahadirbozkurt@arel.edu.tr

⁵Istanbul University, Faculty of Engineering, Department of Chemistry, Istanbul, Turkey,
ozkok@iuc.edu.tr, nihalonul@iuc.edu.tr

⁶Kharkiv National Medical University, 4 Nauky Avenue, Kharkiv, Ukraine,
ttishakova@ukr.net

⁷Yildiz Technical University, Faculty of Arts and Sciences, Department of Chemistry, Istanbul, Turkey,
gulruozay@gmail.com

Abstract

Wound dressings provide quick healing of wounds. Commercially wound dressings have several different types such as transparent film covers, hydrocolloid covers, polymer foam covers, hydrogels, hydrophilic covers, alginate covers, antibacterial covers, honey covers and biological dressings equivalent to skin structure.

In order to produce such nanotechnological membranes, electrospinning method have been utilized and polycaprolactone (PCL) is used as a composite matrix. The synthetic polymer PCL, can find applications in biological and medical fields due to their biocompatible and biodegradable properties unlike other polyesters Vanillin is a fragrant substance known as 4-hydroxy-3-methoxybenzaldehyde and naturally found as glycosylated forms of the fruit of vanilla. This aromatic compound is in the form of needle crystals, colorless, soluble in alcohol and in oily solvents even in cold. This will provide an easy and efficient production of polymeric solutions for electrospinning method. On the other hand, vaniline and its derivatives present different biological properties such as antibacterial, antifungal and anticancer. In the present study owing to these valuable properties of vaniline, a novel imine molecule have been synthesized from N-(2-Hydroxy ethylene diamine). Subsequently, the synthesized imine and PCL have been used to form nanocomposite membranes for biomedical applications [1,2]. Process optimization have been conducted during electrospinning method. The obtained imine molecule evaluated thermally by DSC (Differential Scanning Calorimeter), structurally by FTIR (Fourier Exchange Infrared Spectrophotometer) while nanocomposite membranes have been evaluated morphologically by FEGSEM (Field Emission Gun Scanning Electron Microscope) and structurally by FTIR. These study is valuable not only for the synthesized novel imine molecule but also its nanocomposite forms for biomedical applications.

Key Words: *Biomaterials, wound healing material, vanilline, amine, nanocomposite*

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SYNTHESIS AND DIELECTROPHORETIC ALIGNMENT OF METAL OXIDE NANOWIRES FOR APPLICATIONS IN DIVERSE DEVICES

RAITIS SONDORS, DAVIS GAVARS, MATISS RAMMA, DONATS ERTS, JANA ANDZANE

Institute of Chemical Physics, University of Latvia, Jelgavas str. 1, Riga, Latvia, LV-1004

Abstract

Nanomaterials have attracted great interest of researchers due to their unique properties that can be employed in different areas as electronics, optics, energy harvesting and storage, sensors, etc. Metal oxide as zinc oxide (ZnO) and copper oxide (CuO), which are abundant, cheap, non-toxic and environmentally friendly, are considered to have a significant potential for variety of applications in solar cells, materials for battery electrodes, gas sensors, photodetectors, photocatalysts, light- and field emission emitters, as well as in rapidly developing field of energy harvesting from the waste heat (thermoelectrics) [1,2]. Nanostructuring these materials results in enhancement of their unique optical, electrical, mechanical, thermoelectrical etc properties due to the increased surface area, reduced volume and decrease of number of structural defects. For practical applications of metal oxide nanowires, it is extremely important to develop high yield and high reproducibility synthesis methods, as well as reliable and scalable methods for the nanowires alignment to required positions, for example, between the electrodes.

In this work, high-yield synthesis and approach for dielectrophoretic alignment of ZnO and CuO nanowires between the electrodes for further application in diverse devices is presented. The nanowires were synthesized using cost-effective thermal oxidation technique, using Cu and Zn foil or pellets as source materials [3], and dielectrically aligned between the electrodes, prefabricated using lithography techniques. Morphology, chemical composition, mechanical properties of the nanowires and nanowire networks were characterized using scanning electron microscopy (SEM), atomic force microscopy (AFM), energy-dispersive X-ray spectroscopy (EDX). Electrical properties of the nanowire networks were measured in two-point configuration using Keithley 6430 multimeter. Influence of the synthesis parameters on the yield and morphology of the nanowires is discussed.

Key Words: *nanowires; copper oxide; zinc oxide; thermal oxidation; dielectrophoresis*

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THE BIOSPHERE SELF-ORGANIZATION ATTRACTORS DRIVE PERFECT ORDER HOMEOSTASIS REACTIONS TO LINK BIOENERGETIC WITH FUNCTIONALLY ACTIVE OXYGEN AND CARBON DIOXIDE MOLECULES

Aris Kaksis,
Riga Stradin's University,
dep. Human Physiology and Biochemistry aris.kaksis@rsu.lv,

Abstract. The quantitative studies for oxygen and carbon dioxide functional activity reveal multiply generated Self-Organization Attractors which create and maintain order the homeostasis: water concentration $[\text{H}_2\text{O}]=55.346 \text{ mol/Liter}$, $\text{pH}=7.36$, enzyme Carbonic Anhydrase CA reactivity, air oxygen level 20.95 % O_2 ^[2], osmolar concentration 0.305 M, ionic strength 0.25 M, temperature 310.15 K degree etc. that make oxygen fire safe and $\text{CO}_{2\text{aqua}}$ functional active for Life Biochemistry.

Air oxygen level 20.95 % O_2 ^[1] dissolute in organism forming [arterial concentration](#) $[\text{O}_{2\text{aqua}}]$ safe for Bioenergetic as Self-Organization Attractor ^[3] sustaining isooxia.

Thermodynamic indicate Biosphere indispensability to reach Self-Organization Attractor values. Destiny is trend to minimum of free energy change in homeostasis. Attractors made functionally active molecules Self-Organize the perfect reactions order in homeostasis. ^[2,3,4] Deviation from Attractor values disorder the homeostasis. Chaos stop the homeostasis which disappears as extinct from Biosphere.

Summary Self-Organization Attractors create perfect order of homeostasis.

Self-Organization Attractors create functional active molecules reactivity order for homeostasis and Bioenergetics. The order of functionally active molecules drives homeostasis under rule Attractors. Reaching of Attractor values create homeostasis order out of disorder. Disorder is regarding chaos for Life Biosphere. The molecules functional activation of oxygen $\text{O}_{2\text{aqua}}$ and of carbon dioxide $\text{CO}_{2\text{aqua}}$ initiates as **Self-Organization** Attractors. Attractors are two types and multipurpose: the primary Attractors common for Biosphere, the secondary Attractors for individual organisms and multipurpose $\text{pH}=7.36$, water, air oxygen.

Oxygen $\text{O}_{2\text{aqua}}$ decreased power for functional active isooxia Norma solution in blood so in cytosol too driven with four Attractors: water triplet state of oxygen, water concentration $[\text{H}_2\text{O}]=55.346 \text{ mol/Liter}$, air oxygen level 20.95 % for five hundred million Years, $\text{pH}=7.36$ for the concentration $[\text{H}_3\text{O}^+]=10^{-7.36} \text{ M}$.

CA Carbonic Anhydrase work as primary Attractor for Biosphere which forms dominate bicarbonate buffer of $\text{CO}_{2\text{aqua}}$ acid protolysis constant $\text{pK}_a=7.0512$. Henderson

Haselbalh expression calculates Attractor value 7.36, which corresponds to concentration $[\text{H}_3\text{O}^+]$. Attractor 7.36 creates functional activity of molecules with charged groups negative and positive: HPO_4^{2-} , HCO_3^- , R-COO^- , R-NH_3^+ , R-PO_4^{2-} as free and linked in amino acids, proteins, nucleic acids, carbohydrates, coenzymes, **R** molecules. Carbonic Anhydrase synthesis solve perfect order of homeostasis and bioenergetic as Self-Organization Attractor. [4,5]

The Attractors values in organism compartments dissipative structures drive the perfect homeostasis order with enzymes clusters on five type complex reactions. Order is key for surviving of organism. Deviation from Attractor values cause loss the homeostasis order of functional activity. Chaotic reactions waste the resources and stop the homeostasis, the non-equilibrium complex processes. The homeostasis becomes extinct from Biosphere.

Attractors are indispensable to form functionally active molecules for perfect order homeostasis and bioenergetic reactions. Attractors destiny are irreversible free energy change $\Delta G_{\text{Homeostasis}}$ transduction between functional active molecules.

Note: Homeostasis trend to equilibrium but never reaching because it is non-equilibrium state.

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INVESTIGATION OF CONTROLLED DRUG DELIVERY OF ETHYL CELLULOSE

Büşra TURAN¹, Pelin DEMİRÇİVİ²

¹Author's contact address and e-mail: bsrturn94@gmail.com

²Author's contact address and e-mail: pelin.demircivi@yalova.edu.tr

Abstract

Biopolymers based on chitosan and ethyl cellulose (EC) were inspected as controlled drug release system for oral administration of curcumin (CUR), which has anticancer effect. In order to specify the ethyl cellulose amount used in drug release process, adsorption of curcumin on ethyl cellulose was performed. 0.1 g ethyl cellulose was found enough to adsorb 100 mg curcumin with 79% adsorption efficiency. Curcumin adsorption was best described by Freundlich isotherm model ($R^2 = 0.90$) among the other models, which indicated that the multilayer adsorption process takes place on the adsorbent. Different ratios (1:1-1:2-1:3) of CUR/EC nanocomposites were synthesized and curcumin release in simulated gastric and intestinal fluid was investigated. The release studies were completed in 102 hours and the studies were continued with the CUR/EC ratio, which reached the slowest release. The 1:1 CUR/EC nanocomposite reached 3.78% and 26.24% in 102 hours in simulated gastric and intestinal fluid. The synthesized CUR/EC were coated with different amount of Cht (10-30% wt%) to obtain CUR/EC/Cht structure. CUR/EC/Cht nanocomposite reached 2.26% and 5.22% release in 102 h in simulated gastric and intestinal fluid. Electrostatic attractions between curcumin molecule and the structure were the main reason affecting the drug delivery mechanism. According to the results obtained, it was possible to prolong the release time of curcumin% in simulated gastric and intestinal fluid with ethyl cellulose and chitosan biopolymers.

Key Words: *controller drug delivery, ethyl cellulose, curcumin*