





POLYMERS / COMPOSITES / 3BS MATERIALS 2023 International Joint Conferences

22-24 FEBRUARY 2023 BANGKOK, THAILAND

Book of Abstracts

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Polymers / Composites / 3Bs Materials 2023 Joint International Conferences Preliminary Program

22 - 24 Feb 2023, Bangkok - Thailand

Wed. 22 Feb. 2023				
08:00 - 12:00	08:00 - 12:00 Participants registration & welcome coffee break			
Polymers / Composites / 3Bs Materials 2023 Session I. A				
	Conference Room Sukhumvit 5&6 3rd Floor			
Session's Chairs: Prof Stanisław Kuciel, Cracow University of Technology, Poland Prof. Ana Pilipovic, University of Zagreb, Croatia Prof Tae Hyun Kim, Soonchunhyang University. Rep. of Korea				
10:00 - 10:30	Improvement of Packaging Materials Properties by Nanocoating with Plasma Technology P. Rachtanapun	Prof.PornchaiRachtanapun,ChiangMaiUniversity,Thailand		
10:30 - 11:00	Solution plasma synthesis of electrocatalytic carbon-based composite materials for oxygen reduction reaction T. Ishizaki , K. Fukushima, K. Tanaka, S. Ando, K. Sasaki and S. Chae	Prof. Takahiro Ishizaki, Shibaura Institute of Technology, Japan		
11:00 - 11:30	Electrospinning parameters: effect on the morphology of PLA/PBS fibers H. Al-Turaif and U. Saeed	Prof. Hamad Al-Turaif , King Abdulaziz University, Saudi Arabia		
11:30 - 11:45	Short Oligomeric Molecules Demonstrate Behavior of Bistable Machines A.D. Muratov , M.A.Frolkina, A.A. Markina, V.S. Petrovskii, A.F. Valov and V.A. Aveti-sov	Dr. Alexander Muratov , Russian Academy of Sciences, Russia		
11:45 - 12:00	Highly Flexible Amino Functionalized Metal Organic Frame- work/rGO Composite Film for Advanced Anodes for Li-ion Batteries R. Shah, S. Alia, S. Ali, P. Xia, F. Raziq, Adnan , F. Mabood, S. Shah, A. Zada, P.M. Ismail, A. Hayat, A.U. Rehman, X. Wu, X. An, Q. Kong, H. Xiao, X. Zua, S. Li and L. Qiao	Prof. Adnan Adnan , University of Swat, Pakistan		
12:00 - 14:00	Lunch Break – Atrium Restaurant (Lobb	y Level)		
	Polymers / Composites / 3Bs Materials 2023 Session	I. B		
	Session's Chairs: Prof. Pornchai Rachtanapun, Chiang Mai University, Thailand Prof. Hamad Al-Turaif, King Abdulaziz University, Saudi Arabia Prof. Mounsif Ech-Cherif El-Kettani, AMS- LOMC UMR- Le Havre, France			
14:00 - 14:30	Design and manufacturing of thermoplastic matrix composite panels with over-moulded stiffening grids P. Olivier , B. Castanie and F. Neveu	Prof. Philippe Olivier , University of Toulouse, France		
14:30 - 14:45	 Analysis of the e effect of adhesive aging on the efficiency of bonded composite repair of aluminum panels using elastic-plastic approach B. Bachir Bouiadjra, S.M.A.K. Mohammed, F. Benyahia and A. Albedah 	Prof. Abdulmohsen Albedah, King Saud University, Saudi Arabia		
14:45 - 15:00	Integrated design framework of 3D printed planar stainless tubular joint: modelling, optimization, manufacturing, and experiment X. Deng and S. Huang	Dr. Xiaowei Deng, University of Hong Kong, Hong Kong		
15:00 - 15:15	Fabricaion of the PHB Copolymers Drawn Films by Microcrystalline Nucleation Stretching Method with Different Soaking Solvents in Isothermal Crystallization Process K. Weng , T. Tanaka, Y. Takayama and M. Nishijo	Mr. Kai Weng , Shinshu University, Japan		
15:15 - 15:30	Carbon fiber reinforced polymer composite fin heat exchanger for Air source heat pump system under frosting and defrosting condition S. Abbas and C.W. Park	Mr. Saleem Abbas, Jeonbuk National University, Rep. of Korea		

15:30 - 15:45	Photodegradable, tough and highly stretchable hydrogels R. G. Fonseca , F. De Bon, P. Pereira, F. M. Carvalho, M. Freitas,	Dr. Rita Fonseca , University of Coimbra, Portugal
	M. Tavakoli, A. C. Serra, A. C. Fonseca and J. F. J. Coelho	J
15:45 - 16:00	Mechanical properties of glassy polymer nanocomposites via atomistic and continuum models: The role of Interphases H. Reda , T. Hazirakis, A. F. Behbahani, N. Savva and V. Harmandaris	Dr. Hilal Reda , The Cyprus Institute, Cyprus
16:00 - 16:15	Multiscale Process Modeling Analysis for the prediction of Composite Strength Allowables G.M. Odegard and M. Maiaru	Dr. Marianna Maiaru, University of Massachussetts, USA
16:15 - 16:30	Experimental assessment of evaporative cooling performance of Palm leaves pad S. Ghani and E. Mahdi	Prof. Saud Ghani , Qatar University, Qatar
16:00 - 18:00	Afternoon Coffee Break and Posters Networking & Discussions Session	

Thu. 23 Feb 2023				
Polymers / Composites / 3Bs Materials 2023 Session II. A				
	Conference Room Sukhumvit 5&6 3rd Floor			
	Session's Chairs: Prof Stanisław Kuciel, Cracow University of Technology, Poland Prof. Philippe Olivier, University of Toulouse, France Prof. Istvan Toth. The University of Queensland, Australia			
09:00 - 09:30	Influence of aging on tensile properties of agriculture films A. Pilipović , I. Tucman and M. Rujnić Havstad	Prof. Ana Pilipovic, University of Zagreb, Croatia		
09:30 - 10:00	Polymer-Surfactant Binding for Environmental Separations M. Tsianou	Prof. Marina Tsianou , University at Buffalo, USA		
10:00 - 10:30	Innovative investigation on key-structural elements of offshore wind-energy generation, Smart composite Large-size wind-blades and electric-transport cables M. Drissi-Habti	Prof. Monssef Drissi-Habti, Université Gustave Eiffel, France		
10:30 - 11:00	Morning Coffee Break (Level 3)			
Session's Chairs: Prof. Istvan Toth, The University of Queensland, Australia Prof Stanisław Kuciel, Cracow University of Technology, Poland Prof. Philippe Olivier, University of Toulouse, France				
11:00 - 11:30	Valorization of Plastic Waste: Research Advances in Molecular Recycling P. Alexandridis	Prof. Paschalis Alexandridis, University at Buffalo. USA		
11:30 - 12:00	Ultrasounds Methods for Non-Destructive Evaluation of Composite Structural Bondings Aging in Marine environment. D. Leduc, M. Ech-Cherif El-Kettani, P. Manoucherehnia and M- V. Predoi	Prof. Mounsif Ech-Cherif El- Kettani, AMS- LOMC UMR- Le Havre, France		
12:00 - 14:00	Lunch Break - Atrium Restaurant (Lobby	/ Level)		
	Group Photo at 13:45			
	Polymers / Composites / 3Bs Materials 2023 Sess	ion II. B		
	Session's Chairs: Prof. Tapas K. Mandal, Yeungnam University, Rep. of Korea Prof. Ramin Sedaghati, Concordia University, Montreal, Canada Prof. Tae Hyun Kim, Soonchunbyang University, Rep. of Korea			
14:00 - 14:30	GnRH Peptide/Adjuvant Conjugate Vaccine Candidates to Treat Cancer and for Veterinary Immunocastration I Toth	Prof. Istvan Toth, The University of Queensland, Australia		
14:30 - 15:00	Hybrid composites based on biopolypropylene modified with basalt and microcellulose fibers with the addition of antibacterial turmeric S. Kuciel , A. Banas, K. Rusin-Zurek	Prof Stanisław Kuciel, Cracow University of Technology, Poland		
15:00 - 15:30	Multi-faceted Approach for Forming Nanostructures for Surface Enhanced Spectroscopy Applied to Detection of Biologically Relevant Molecules in Agriculture and Food Industry H. Takei , T. Okamoto and A. Gölzhäuser	Prof. Hiroyuki Takei , Toyo University, Japan		
15:30 - 15:45	Basalt fibers reinforced polylactide composites modified by antibacterial nanoparticles K. Rusin-Zurek , K. Mazur and S. Kuciel	Ms. Karina Rusin-Zurek, Cracow University of Technology, Poland		
15:45 - 16:00	On Chemical Actuation of Shape Memory Polymers (SMPs) Y. Shen , G. Eggeler and K. Neuking	Ms. Yucen Shen, Ruhr University Bochum Germany		
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Session's Chairs: Prof. Monssef Drissi-Habti, Gustave Eiffel University, France Prof. Ramin Sedaghati, Concordia University, Montreal, Canada Prof. Hiroyuki Takei, Toyo University, Japan			
16:30 - 17:00	Multiplexed Nanomaterial-Based Sensor Array for Detection of Pathogenic Microbes T.K. Mandal and S.W. Joo	Prof. Tapas K. Mandal, Yeungnam University, Rep. of Korea	
17:00 - 17:15	Mesenchymal Stem Cell Adhesion on Plasma-Coated Biodegradable Nanofibers A.M. Manakhov, A.O. Solovieva and N.A. Sitnikova	Dr. Anastasiya Solovieva , RICEL- Branch of ICG SB RAS, Novosibirsk, Russia	
17:15 - 17:30	Positive Impact of composite materials with Ag modification on wound healing N.A. Sitnikova , A. O. Solovieva, A.M. Manakhov and E.S. Permyakova	Ms. Natalia Sitnikova , RICEL- Branch of ICG SB RAS, Novosibirsk, Russia	
17:30 - 17:45	Application of graphitic carbon nitride nanosheets as a multifunctional nanofiller in cryogels for wastewater treatment and quality monitoring K. Dziza , L. Vásquez, V. Binas, A. Athanassiou and D. Fragouli	Ms. Katarzyna Dziza, IIT Italian Institute of Technology, Italy	
17:45 - 18:00	Effect of Graphene Oxide Doped PEDOT: PSS as a Hole Transport Layer and Annealed Temperature on the Inverted Perovskite Solar Cell From the Waste of Electric Arc Furnace Electrode Y.R. Denny , M. Fadli, T.A. Maulana, S.D. Ramdani L.D. Assaat, R. Alfanz, M. Siswahyu and S. Hamaguchi	Dr. Yus Rama Denny , University of Sultan Ageng Tirtayasa, Indonesia	
18:00 - 18:15	Effect of Filler Concentration and Sonication Time on Graphite- ZnO Composites with Epoxy Resin Matrix as Microwave Material Absorbing Y. R. Denny, S. D. Ramdani , A. Trenggono, S. E. A. Anggraini 5, Y. Taryana and S. Ari-tonang	Dr. Sulaeman Deni Ramdani, University of Sultan Ageng Tirtayasa, Indonesia	

Fri. 24 Feb. 2023			
	Polymers / Composites / 3Bs Materials 2023 Session III		
	Conference Room Sukhumvit 5&6 3rd Floor		
	Session's Chairs: Prof Thomas Gries, RWTH Aachen University, Germany Prof. Monssef Drissi-Habti, Gustave Eiffel University, France Prof. Mounsif Ech-Cherif El-Kettani, AMS- LOMC UMR- Le Havre, France		
09:00 - 09:30	Task-Specific Design and Functionalization of Porous Poly- Calixarene for Water Purification A. Trabolsi	Prof. Ali Trabolsi , New York University Abu Dhabi, UAE	
09:30 – 10:00	Application of the SSA thermal fractionation technique to recycled polyolefin blends and thermoplastic polyurethanes A. J. Müller	Prof. Alejandro J. Müller , University of the Basque Country UPV/EHU, Spain	
10:00 - 10:30	10:00 - 10:30 Morning Coffee Break (Level 3)		
Discussion panel on Sustainability transitions with and for polymers, composites, biobased, biodegradable, and biomimetic materials			
	Chairs: Prof Thomas Gries, RWTH Aachen University, Ge Dr. Jan Vincent Jordan, RWTH Aachen University,	ermany Germany	
10:30 - 11:00	Contributions of composites to climate adaptation and water security J.V. Jordan , M. Raina, D. Granich and T. Gries	Dr. Jan Vincent Jordan, RWTH Aachen University, Germany	
11:00 - 12:00	 Workshop program Discussion of sustainability challenges in the production of polymers, composites, biobased, biodegradable and biomimetic materials Collection of best practices to address these challenges Discussion of sustainability challenges of industry and society that polymers, composites, biobased, biodegradable and biomimetic materials currently and in the future addresses Collection of best practice examples, project & funding schemes and ideas to realise the sustainability potentials of polymers, composites, biobased, biodegradable and biomimetic materials Conclusions, wrap-up and outlook on potential further steps 	 Prof. Thomas Gries, Director of the Institut für Textiltechnik of RWTH Aachen University, Germany Mr. Uday Gill, Chief Strategy Officer/Executive Director, Indorama Ventures PLC, Thailand Mr. Sunphat Pojanavaraphan, Managing Director SC Grand, Thailand 	
12:00 - 14:00	Lunch Break and Conference Closure - Atrium Resta	aurant (Lobby Level)	

Polymers / Composites / 3Bs Materials 2023 Posters

Online: during and after the conference Onsite: Posters Networking and Discussions - 22 Feb.2023 16:00 - 18:00

N.	Poster Title	Author, Affiliation, Country
1.	Production of 2,5-Furandicarboxylic Acid from Fructose Using dual magnetic- based Catalyst L-J. Chien, T-L. Ho, H-C. Tsui , and Y-H. Cai	Mr. Han-Chun Tsui , Ming Chi University of Technology, Taiwan
2.	The role of Al2O3 interlayer in the synthesis of ZnS/Al2O3/MoS2 core-shell nanowires E. Butanovs, A.Kuzmin, A. Zolotariovs, S. Vlassov and B. Polvakov	Dr. Boris Polyakov , University of Latvia, Latvia
3.	Aldehyde-free resins based on resorcinol and natural alkylresorcinols modified with styrene A. Jurkeviciute , L. Grigorieva, K. Tõnsuaadu and T. Yashicheva	Mrs. Ana Jurkeviciute , Tallinn University of Technology. Estonia
4.	Laser Ablation Synthesis of Semiconductor Nanocomposites with Tunable Plasmonic and Paramagnetic Properties Y.V. Ryabchikov	Dr. Yury V. Ryabchikov , Institute of Physics of the Czech Academy of Sciences, Czech Rep.
5.	Physical Treatment of Biopolymer and Its application in Elastomeric Composites Z. Mičicová , P. Skalková, I. Papučová, J. Pagáčová, A. Dubec, R. Janík, M. Janeková, D. Koštialiková and A. Prnová	Dr. Zuzana Mičicová , Alexander Dubček University of Trenčín, Slovak Rep.
6.	Effect of Surface Treated Biopolymer on Curing Behavior and Tensile Properties of Natural Rubber Composites Z. Mičicová , P. Skalková, D. Ondrušová, M. Pajtášová, J. Dobrovská	Dr. Zuzana Mičicová, Alexander Dubček University of Trenčín, Slovak Rep.
7.	Influence of maleinized rubber on the properties of elastomeric composites filled with biopolymer J. Vršková. I. Labai. P. Skalková. A. Dubec and M. Paitášová	Dr. Juliána Vrškova, Alexander Dubček University of Trenčín. Slovak Rep.
8.	Pretreatment and modification of cellulose as a filler for elastomeric composites R. Janík , I. Labaj, P . Skalková and J. Dobrovská	Dr. Róbert Janík, Alexander Dubček University of Trenčín, Slovak Rep.
9.	Effect of surface modification conditions of cellulose on final properties of elastomeric composites I. Labaj , P. Skalková, J. Vršková and D. Ondrušová	Dr. Ivan Labaj, Alexander Dubček University of Trenčín, Slovak Rep.
10.	Characterization and Thermal Stability of Surface Modified Cellulose in Polymer Composites P. Skalková , Z. Mičicová, I. Papučová, J. Pagáčová, A. Dubec, R. Janík, D. Ondrušová, M. Pajtášová and S. Božeková	Prof. Petra Skalková, Alexander Dubček University of Trenčín, Slovak Rep.
11.	Hybrid Implant with Improved Osseointegration Properties E. Aghion , N. Gabay, T. Ron and A. Shirizly	Prof. Eli Aghion , Ben- Gurion University of the Negev, Israel
12.	Radiative cooling of dark tone pigments with high near-infrared reflection properties J.S. Hwang and Y-S Kim	Dr. Young-Seok Kim, Korea Electronics Technology Institute, Rep. of Korea
13.	Prediction of Creep Behavior of Pressure-sensitive adhesives Y. Kim , H. Yun and C-J. Lee	Dr. Youngmin Kim, Korea Electronics Technology Institute, Rep. of Korea
14.	Skin Absorption Protective Silver Micro-particles as an Upcoming Nontoxic Antimicrobial Agent N. Parvin and S. W. Joo	Dr. Nargish Parvin, Yeungnam University, Rep. of Korea
15.	A novel poly(3-hydroxyoctanoate) diclofenac decorated dressings for wound healing M. Guzik , K. Haraźna, K. Kasarełło, D. Solarz-Keller, A. Cudnoch- Jędrzejewska, T. Witko, Z. Rajfur and M. Seta	Dr. Maciej Guzik , Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences- Krakow, Poland
16.	Polyhydroxyalkanoates – biodegradable and biocompatible polymers produced by environmental bacteria J.Prajsnar , R.Bugno, A. Bojarski, K. Stępień and M. Guzik	Ms. Justyna Prajsnar , Jerzy Haber Institute of Catalysis and Surface Chemistry, Poland
17.	Ultra-Sensitive Sensor based on Single-walled Carbon Nanotube Field-effect Transistor for Detection of Endocrine Disruptors Nonylphenol T. Hyun Kim and H. Cho	Ms. Hyunju Cho, Soonchunhyang University, Rep. of Korea

18.	Hydrogen Peroxide Sensing of Prussian Blue/Graphene Quantum Dots Electrodeposition Electrode Y. Cho and T. Hyun Kim	Ms.YujinCho,SoonchunhyangUniversity,Rep. of Korea
19.	Electrochemical Aptasensor for Detection of EcoRV Based on rGO/GCE H.,Kim and T. Hyun Kim	Mr. Hyunbeom kim, Soonchunhyang University, Rep. of Korea
20.	First-principle calculations of DNA/RNA on MoOS Janus layer S. Laref , X. Gao and T. Gojobori	Dr. Slimane Laref , King Abdullah University of Science and Technology (KAUST), Saudi Arabia
21.	Deep Learning Assisted Protein Entanglement Prediction based on Gauss Linking Integral Matrix P. Deng , L. Xu, Q. Ye, J. Yu, W. Zhang and H. Gao	Mr. Puqing Deng , Hong Kong University of Science and Technology, Hong Kong
22	Aaryl 1-(Methoxymethyl)Vinyl Ketone-based Corrosion Inhibitor for Mitigating Acidic Corrosion During Well Stimulation N. Aljeban	Ms. Norah Aljeban , Saudi Aramco, Saudi Arabia

Polymers / Composites / 3Bs Materials 2023 Session I. A

Improvement of Packaging Materials Properties by Nanocoating with Plasma Technology

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Abstract:

science technology Material and have dramatically changed human life over the past decades. development, two In this nanotechnology has gained keen attention. It has a high surface-to-volume ratio of 1-100 nm, producing new structures, materials, and devices. Nanocoatings are single or multilayer in the nanometer level of material deposited on the selected surface. Plasma coatings are one of the most exciting areas of plasma technology, which can significantly improve the functionality of reinforcements in polymer-matrix composites. The material accelerates due to the intense heat and impacts on a substrate material. Plasmaapplied nanocoatings provide a molecular level. The plasma is a quasi-neutral ionized gas composed of photons, ions, free electrons, and atoms in their fundamental or excited states with a net neutral charge. The surface modification of a material using a plasma process, such as reactions, alters the surface morphology of the packaging material and shows the benefits of plasma processes. Plasma does not cause environmental issues and leads to eco-friendly. The plasm-treated surfaces promoted waterresistant and improved surface roughness properties.

In our research, the key finding of plasma nanocoating technology has increased the packaging materials' water resistance properties. The sulfur hexafluoride (SF_6) plasma-treated methylcellulose (MC) film, polylactic acid (PLA) film, and Kraft paper (KP) [Figure.1] increased the hydrophobicity of water contact angle and water absorption time. However, altering pressures, powers, and treatment times leads to a better impact on the plasma nanocoating. Plasma-polymerized hexamethyldisiloxane (HMDSO) films were deposited in Ar and O2 gas. Ar contained a polymeric structure in SiO_xC_yH_z and enhanced the barrier to water vapor of PLA. Further, showed fluorine-rich carbon film better antimicrobial activity. Plasma coating modified the surface at the nano-layer range, creating super-hydrophobicity surfaces on packaging materials.

Keywords: Nanocoating, plasma treatment, fluorine-rich carbon film, contact angle, fluorine, surface roughness, water absorption; poly(lactic acid), hydrophobicity, barrier property.



Figure 1: SF₆ plasma coating on KP surfaces. F atoms replaced the O and H atoms in the cellulose structure.

- Rachtanapun, P., Boonyawan, D., Auras, R.A., Kasi, G. (2022), Effect of Water-Resistant Properties of Kraft Paper (KP) Using Sulfur Hexafluoride (SF₆) Plasma Coating. *Polymers.*, 14, 3796.
- Chaiwong, C., Rachtanapun, P., Sarapirom, S., Boonyawan, D. (2013), Plasma polymerization of hexamethyldisiloxane: Investigation of the effect of carrier gas related to the film properties. *Surf. Coat. Technol.*, 229, 12-17.
- Jinkarn, T., Thawornwiriyanan, S., Boonyawan, D., Rachtanapun, P., Sane, S. (2012), Effects of treatment time by sulfur hexafluoride (SF₆) plasma on barrier and mechanical properties of paperboard. *Packag. Technol. Sci.*, 25, 19-30.
- Chaiwong, C., Rachtanapun, P., Wongchaiya, P., Auras, R., Boonyawan, D. (2010), Effect of plasma treatment on hydrophobicity and barrier property of polylactic acid. *Surf. Coat. Technol.*, 204, 2933-2939.
- Rachtanapun, P., Wongchiaya, P., Boonyawan, D. (2010), Effect of sulphur hexafluoride (SF₆) plasma on hydrophobicity of methylcellulose film. *Adv. Mat. Res.*, 93, 214-218.

Solution plasma synthesis of electrocatalytic carbon-based composite materials for oxygen reduction reaction

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Abstract:

Theoretical calculations and experiments demonstrated that introducing nitrogen into carbon lattices could induce charge redistribution and result in the creation of the net positive charge on the adjacent carbon, which enhance the adsorption of O₂ molecules and thus become an effective ORR catalyst.¹⁻³ However, rational design of a new catalyst system based on nitrogen-doped carbon materials is still present intriguing challenges in ORR catalysis research. Herein, a new kind of nitrogen-doped carbon nanoparticle-carbon nanofiber (NCNP-CNF) composite with advanced ORR catalytic activity has been developed via solution plasma process. The carbon composite nanomaterials were synthesized bv growing nitrogen-doped nanoparticles through 2-cyanopyridine (C6H4N2) on CNFs.⁴ This integration led to a unique morphological feature and modified physicochemical properties. Firstly, the incorporation of nitrogen atoms in the carbon composite nanomaterials synthesized was confirmed by various analysis and the nitrogen content of NCNP-CNFs was found to be approximately 1.35 atom %. SEM and TEM observation revealed that most of NCNPs attach to the CNF surface throughout almost area investigated, giving rise to a unique morphology with an interconnected porous structure. From linear sweep voltammetry (LSV), CNFs demonstrated a two-step reduction process with low current density whereas NCNP-CNFs showed a single-step wide plateau of higher limiting current density. The calculated electron transfer number of NCNP-CNF composite were estimated to be 3.21-3.51. The enhancement in ORR activity of NCNP-CNF composite can be attributed to the synergistic effects of good electron transfer from highly graphitized CNFs as well as abundance of exposed catalytic active sites originated from meso/macroporosity in NCNPs.

Keywords: solution plasma, oxygen reduction reaction (ORR), carbon, carbonnanofiber (CNF), electrocatalyst, Li-air battery.



Figure 1: Synthesis of NCNP-CNF composite nanomaterials by solution plasma.

Acknowledgement

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- I. Z. Yang, Z. Yao, G. Li, G. Fang, H. Nie, Z. Liu, X. Zhou, X. Chen, S. Huang, ACS Nano, 2012, 6, 205.
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- 4. 4. G. Panomsuwan, N. Saito, T. Ishizaki, ACS Appl. Mater. Interface, 2016, 8, 6962.

Electrospinning Parameters: Effect On the Morphology Of PLA/PBS Fibers

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Abstract:

Development of nanofibers with the help of electrospinning is being prioritized as method of choice because of simplicity and efficiency of process. The parameters of electrosopinning process effectively convert the polymer solution into electropsun final product made of desired diameter of nanofiber. The aim of the study presented is to recognize and analyze the effect of proposed parameters biodegradable and biocompatible PLA/PBS nanofiber developed by electrospinning process. The morphology of the fiber is being characterized by implementing Scanning Electron Microscope. Studies were conducted to characterize the result of using different electrospinning parameters on the final diameter and orientation of fiber. It was determined that varying polymer solution concentration, feed rate and applied voltage shows different outcomes. The best results was obtained at 6% polymer solution concentration, 20 KV and 0.5 ml/h which can be applicable for biomedical application. Finally, protein adsorption and mechanical testing was conducting on the PLA/PBS fiber.

Keywords: Electrospinning, Polylactic acid (PLA), Polybutylene succinate (PBS), Morphology.

References:

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- 2. Hasan, A., et al., Electrospun scaffolds for tissue engineering of vascular grafts. Acta biomaterialia, 10(1), 2014.
- 3. S. Ramakrishna, K. Fujihara, W.-E. Teo, T.-C. Lim, and Z. Ma, An Introduction to Electrospinning and Nanofibers, World Scientific 90, 2005
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electrospinning of ultrafine poly (ethylene oxide) fibers. polymer, 45 (9), 2004.

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Short Oligomeric Molecules Demonstrate Behavior of Bistable Machines

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Abstract:

The quest of creation and construction of twostate nanoscale devices motivates the search of small molecular systems whose dynamics resemble those of bistable mechanical systems, such as Euler arch sor Duffing oscillators. Nanosystems capable of spontaneous vibrations and stochastic resonance and spontaneous vibrations are of particular interest. Through atomistic molecular dynamics simulations we explore several oligomeric molecules a few nanometers in size and identify short fragments of thermoresponsive polymers subject to external force load that demonstrate the bistable behavior similar to an Euler arch with spontaneous vibrations and stochastic resonance activated by conventional thermal noise. Moreover, reasonable shifts of the spontaneous vibrations and stochastic resonance modes were observed when the system was bound with another molecule; such shifts are sensitive to both the molecular mass and binding affinity. Also we reveal that short pyridine-furan springs exhibit the bistable dynamics of a Duffing oscillator. Our findings suggest some reasons to believe that nano-sized oligomeric structures stabilized by short-range low-energy couplings can exhibit bistability with thermally-activated spontaneous vibrations and stochastic resonance.

Keywords: Duffing oscillator; Euler arch; nanomechanics; bistability; spontaneous vibrations; stochastic resonance; thermoresponsive oligomers.



Figure 1: Pendulum-like behaviour of an internal turn of short pyridine-furan spring between two competing equilibrium states. The aromatic groups on the turn could form a stacking pair with either the right or left end of the spring, forcing the turn to swing between the ends.

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Highly Flexible Amino Functionalized Metal Organic Framework/rGO Composite Film for Advanced Anodes for Li-ion Batteries

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Abstract:

Advanced electrode design is crucial in the rapid development of flexible energy storage devices for emerging flexible electronics. Metal-organic frameworks (MOF) for lithium storage have gained intensive attention, but their key limitations are the low electronic conductivity and limited cycling stability under redox conditions. An introduction of functional group strategy to improve the cycling stabilities is explored, inspired by the study of the stability and structure of metal ions coordinated with the amino group. Herein, rational organization of redox active building block, 2-amino-1,4benzenedicarboxylic acid-based metal-organic framework (MOF) material, Ni(BDC-NH2)/rGO, was synthesized and applied as freestanding anode for the first time in lithium ion batteries. Compared with Ni(BDC)/rGO and Ni(BPDC)/rGO composite films the Ni(BDC-NH2)/rGO electrode deliver high specific discharge capacity 2145 mAh g-1 based on mass of Ni(BDC-NH2), along with superior high-rate capability and excellent cycling stability for 1000 cycles at 1 Ah g-1. Furthermore, electrochemical behaviors of Ni(BDC-NH2)/rGO anode material at different states of discharged and charged were carefully investigated through X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), and X-ray photoelectron spectroscopy (XPS). Discussing the electrochemical performances on the basis of capacity contributions from the central metal (Ni+2) and organic ligands (oxygen and nitrogen) proposes an alternative mechanism of enhanced capacity for the MOF materials used in lithium batteries. This improved understanding will shed light on the designing principle of MOF-based freestanding electrode for their practical application in battery sciences.

Keywords: Chemical Synthesis, Metal Organic Framework, Anode, Electrochemical Performance, Flexible Lithium-ion Batteries.



Figure 1: Schematic diagram of the Ni(BDC-NH2)/rGO membrane and its digital photos illustrating the flexibility (flat, rolling and bending) states.

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Polymers / Composites / 3Bs Materials 2023 Session I. B

Design and manufacturing of thermoplastic matrix composite panels with overmoulded stiffening grids

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Abstract:

Automotive industry use for several years now the stiffening of mechanical polymeric parts [1]. Usually in airframe structure, composite panel are stiffened owing to cocured stringers and ribs. There are only few examples of laminated composites, we mean long carbon fibre composites (made with unidirectional or textile reinforcements), stiffened owing to overmoulded grids. This is why it was decide to get out from usual materials encounterd in overmoulding i.e. short fibres composites overmoulded with unreinforced polymer and initiate news studies aiming to stiffening laminated composites themselves reinforced with long carbon fibres.

Here we have designed and manufactured an injection mould enabling carbon fibre textile reinforced thermoplastic laminated panels to be overmoulded with high melting temperature short carbon fibre reinforced thermoplastic. In this work, TenCate Cetex PEI 10 plies long carbon fibre (textile) / thermoplastic composites panels with the stacking following sequence $[(0,90)/(\pm 45)/(0,90)/(\pm 45)/(0,90)]_{S}$ have been stiffened owing to overmoulded grids made of short carbon fibres reinforced PEEK or short carbon fibres reinforced PPS.

Choosing such high melting temperature thermoplastic matrices (310° C for PEI) has led us to include a hot bloc inside the injection mould. The injection of short fibres composites onto the top surface of the long carbon fibre laminates (in plane dimensions 220 x 200 mm) was simulated using Moldflow® in order to determine the number and location of injection points and welding lines.

Key Findings. Series of overmoulded plates were manufactured at CETIM, and submitted to low velocity impact test in order to quantify compressive mechanical strength after impact since we are speaking about structure. Here airframe within the Composites Conference Bangkok 2023 frame, key findings will be focussed on the effects of moulding process upon the laminate microstructure and the interface Effectively, three injection strength. temperatures were tested for injecting short carbon filled PPS over laminated PEI plates interfacial and both strength and microstructures were respectively measured and analysed.

Keywords: Composites Materials, Carbon fibres, Thermoplastic matrices, Manufacturing, Overmoulding.



Figure 1: Overmoulded stiffening grids made of thermoplastic matrix renforced with short fibres(carbon/PPS ou carbon/PEEK) injected on a long carbon fibres reinforced thermoplastic panel (carbon/PEI).

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Analysis of the e effect of adhesive aging on the efficiency of bonded composite repair of aluminum panels using elastic-plastic approach

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Abstract:

The use of composite materials for the repair of damaged aeronautical structures is an effective technique because the load transfer from the damaged area to the composite patch through the adhesive layer leads to an increase in the fatigue life of the repaired structure [1]. The good mechanical strength of organic matrix composites and their low weight make them the most suitable materials for this repair technique. However, the major disadvantage of composite materials and all polymeric materials is their sensitivity to the external environment and particularly to moisture, the absorption of which leads to a degradation of the mechanical properties of the composite material and the adhesive. The design of repair patches must therefore take into account the long-term absorption of moisture by the composite and the adhesive [2].

In this study , the concept of elastic-plastic fracture mechanics was used to evaluate the performance of bonded carbon/epoxy repair on cracked plate in Al 2024 T3 after water absorption by the adhesive. The variation of the J integral around the crack head was calculated for aged Araldite 2021 epoxy adhesive. The shear and peel stresses along the adhesive layer were evaluated to estimate the strength of the adhesion after water absorption. The effect of the immersion time in water on the J in integral of repaired crack was also highlighted. The obtained results show that humidity absorption by the adhesive leads to an increase of the J integral around the crack tip and consequently the repair efficiency will be reduced (see Fig. 1). The humidity absorption increases the stresses un the adhesive layer which will have a negative effect on the durability of the repair.

Keywords: Bonded composite repair; water absorption; adhesive; J integral; adhesive stress. **Figure 1**: Figure illustrating the fundamental question that we are tempting to solve experimentally: what is the importance of silica surface modification nanoporous silica-based sol-gel



Fig. 1 Jintegral vs crack length for different time of immersion in distilled water

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Integrated design framework of 3D printed planar stainless tubular joint: modelling, optimization, manufacturing, and experiment

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Abstract:

Nowadays, tubular joints with superior structural properties have been extensively applied in constructing the complicated multi-planar steel joints that are often adopted in the grid shell structure system. However, sometimes it is challenging to maintain high-quality onsite welding joints or even difficult to assess the quality of onsite welding, especially for the overhead welding. This paper presents an integrated design framework of the 3D printed planar stainless tubular joint, and this framework is implemented by Solid Isotropic Material with Penalization Method (SIMP). Three joints with different brace to chord width ratios are optimized, and the re-engineered joints are obtained using computer-aided design software. Joints independently designed and manufactured by 3D printing methods can be riveted with other structural members to simplify the installation process and improve the construction efficiency, thus reducing the difficulty of on-site welding. Non-contact DIC (Digital Image Correlation) is used to analyze the strain distribution more intuitively for 3D printed and welding planar tubular joints. Moreover, the coupon tensile test proposed to analyze the stress-strain is relationship when considering different printing orientations. Experiments show that the orientation of material additive manufacturing affects the yield strength, ultimate strength and elongation at fracture to a certain extent but has little influence on Young's modulus. The optimized joint exhibits different failure modes than the traditional tubular joints, which can achieve strong-joint and weak-component mechanisms and avoid failure of the entire joint when local damage occurred. In addition, the plump curve according to the hysteresis loop suggests that the energy dissipation of the optimized joint is larger than the traditional welding joint, which is beneficial to enhance the seismic performance of the structures. The developed framework can also be extended to the complex spatial joints, which is subjected to multi-planar loads in the future.

Keywords: Topology optimization, Solid Isotropic Material with Penalization Method (SIMP), Additive manufacturing, Printing

*Manufacturing 1. Steel joints optimization Additive Re-engineering with the optimized results manufacturing SIMP optimization Conventional welding 2. Coupons tensile tests Different materials Coupons cut from Coupons 3D printed and High-strength steel) welded joint with different materials (SP, HP) (MW,SW) Digital image correlation . 3. Compression tests for TJs and REJs 2D-DIC for TJ Welded and 3D 3D printing reprinted tubular engineered joints joints (MW-TJ. SW 3D-DIC for REJ (SP-REJ, HP-REJ) TJ, SP-TJ, HP-TJ)

orientation, Digital image correlation (DIC), Strong-joint and weak-component mechanism

Figure 1: Diagram of topology optimization for steel joints.

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Fabricaion of the PHB Copolymers Drawn Films by Microcrystalline Nucleation Stretching Method with Different Soaking Solvents in Isothermal Crystallization Process

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Abstract:

The concept of low-carbon and environmental protection has promoted the application of biodegradable polymers ^[1]. Poly[(R)-3-hydroxybutyrate] (PHB) and its copolymer can be completely converted into CO₂ and water upon enzymatic degradation by microorganisms in the soil or ocean. However, due to its poor mechanical properties and low brittleness, its widespread application is limited ^[2]. High-strength and flexible degradable materials are currently urgently needed. Cast films of poly[(R)-3-hydroxybutyrate-co-(R)-3-

hydroxyvalerate] (PHBV) and Poly[(*R*)-3hydroxybutyrate-*co*-(*R*)-3-hydroxyhexanoate]

(PHBH) were prepared by microcrystalline nucleation stretching method which drawn after isothermal crystallization (IC) near the glass transition temperature (T_g) for constant time, simultaneous in different cold soaking solvents for IC. Different processing samples were made copolymers films that were with PHB isothermally crystallized in air (without contact with solvent), ice-water, hexane and methanol, and further studied the effects on undrawn and drawn films after IC. These results showed that the elasticity, morphology and mechanical properties of the films after IC are significantly difference between different soaking solvents. The drawn films in ice-water or hexane for IC showed white turbidity whereas the drawn films in air for IC showed transparent and necking morphology. Cross-section observed by scanning electron microscopy (SEM) of drawn films in poor solvents (ice-water or hexane) showed structure (Figure Mechanical porous 1). properties of drawn films in ice-water / hexane showed a significant increment in tensile strength up to 99 MPa, about 2 times, compared to the drawn films in air. The coagulation effect of icewater and hexane on amorphous films promoted the growth of crystals and the formation of microcrystalline nucleus during the isothermal crystallization process. The contact between methanol and PHB copolymer film inhibits the flow of molecular chains and does not have

stretchability. Only air provides an atmosphere near T_g , maintaining the amorphous state of the molecular chain. Additionally, the characteristic changes in drawn films can apply for reference as further research regarding heat retention and transparency control materials.

Keywords: Biodegradable polymer, Microcrystalline nucleation stretching, Effect of soaking solvent, White turbidity, Pores.



Figure 1: SEM images of PHBH films after isothermal crystallization in air and ice-water. The cross-section of samples shows the plane perpendicular to the stretching direction. The arrow indicates the drawing direction.

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Carbon fiber reinforced polymer composite fin heat exchanger for Air source heat pump system under frosting and defrosting condition

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Abstract:

Air source heat pumps system is one of the most energy efficient and environmental friendly system for building heating purpose. However, under extremply low ambient temperature and high humidity condition, frost forms on evaporator fins which reduce the overall thermal performance of system because of surface resistance and fin air blockage [1]. Periodic defrosting as well as delayed frost formation is crucial to enhance thermal efficiency [2]. Carbon fiber reinforced polymer composite (CFRP) has great potential to be used as evaporator fin based on resistive heating which can be utilized to increase the surface temperature for efficient defrosting. Figure 1 shows the application of resistive heating to generate surface temperature of fin which can be potentially used for derfrosting purpose. The corresponding temperature distribution on fin surface was recorded with flir as thermographical camera to show the uniform temperature distribution. To investigate the frosting and defrosting performance, a temperature and humidity controlled chamber was established to make natural convection steady state experimental setup. Brine was used as refrigerant with inlet temperature of -21 °C while 6 °C of ambient temperature of chamber with 80% relative humidity was maintained during the experiment.



Figure 1: Figure illustrating the resistive heating mechanism in a single fin as well thermographical image of surface temperature distribution in CFRP based heat exchanger under resistive heating consition.

Keywords: carbon fiber reinforced polymer compsoite, polymer composite heat exchanger, frosting and defrosting, heat pump system, resistive heating, heat transfer, thermal system, heating and cooling application.





Frost thickness was observed after every 5min interval to understand the thickness effect on heat transfer rate. Retaine drops were dried completely for 2nd frosting cycle which will be observed in detail by implementation of surface treatment and applied volatge.

Acknowledgments:

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Photodegradable, tough and highly stretchable hydrogels

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Abstract:

We present for the first time highly stretchable and tough hydrogels with controlled lighttriggered photodegradation. A double-network of alginate/polyacrylamide (PAAm) is formed by using covalently and ionically crosslinked Ca^{2+} subnetworks. The ionic alginate interpenetrates a PAAm network covalently crosslinked by a bifunctional acrylic crosslinker containing the photodegradable *o*-nitrobenzyl (ONB) core instead of the commonly used methylene bisacrylamide (MBAA). Remarkably, due to the developed protocol, the change of the crosslinker did not affect the hydrogels' mechanical properties. The incorporation of photosensitive components in hydrogels allows external temporal control of their properties and degradation. Rheological tuneable and mechanical analysis demonstrated the loss of properties of ONB-based DN hydrogels after irradiation, confirming the efficient destruction of the covalently crosslinked network, resulting in the loss of mechanical properties. SEM analyses also visually confirmed the network photodegradation. Cell viability and cell proliferation assays revealed that hydrogels and photodegradation their products are biocompatible and safe. In one example of application, we used these hydrogels for biopotential acquisition in wearable electrocardiography. Surprisingly, these hydrogels showed a lower skin-electrode impedance, compared to the common medical grade Ag/AgCl electrodes.

This work lays the foundation for the next generation of tough and highly stretchable hydrogels that are environmentally friendly and can find applications in a variety of fields such as health, electronics, and energy, as they combine excellent mechanical properties with controlled degradation.

Keywords: Hydrogel, double-network, tough hydrogel, stretchable, photodegradable, nitrobenzyl, biosensor, wearable soft electronics, green electronics.



Figure 1: Schematic representation of the alginate/poly(acrylamide) (PAAm) structure composed by covalently crosslinked PAAm through ONB-based crosslinkers, and Ca^{2+} mediated ionically crosslinked alginate network made of both short and long chains. Toughness is attributed to the synergy of two mechanisms: crack bridging by the PAAm network and hysteresis by unzipping the alginate network.¹ Photodegradation through photolabile crosslinker leads to efficient destruction of the covalently crosslinked network, resulting in the loss of mechanical properties of the hydrogel.

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Mechanical properties of glassy polymer nanocomposites via atomistic and continuum models: The role of Interphases

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Abstract:

The effect of interphases property on the mechanical behavior of silica-polybutadiene polymer Nanocomposite (PNC) is investigated via combined homogenization and molecular dynamics simulation. In the current work, we propose а multi-scale computational methodology consisting of detailed microscopic simulations and continuum modelling (homogenization) approaches for predicting the spatial distribution of the mechanical properties in polymer nanocomposites (PNC). The homogenization methodology is based on a systematic nano/micro/macro coupling between detailed atomistic molecular dynamics (MD) simulations and the variational approach based on the Hill-Mandel lemma. The model system we studied glassy-PB/silica NC's for different volume fraction of NP. Using MD simulations, the polymer/NP interphase in PNCs is directly examined by probing the distribution of the density and the stress profile at equilibration. The effective Young modulus and poison ratio of the interphases are calculated from the relation between the local stress and strain showing high rigidity in compared to the bulk material. The mechanical properties at the interphases and the polymer matrix are used, together with homogenization approach, to develop a continuum model for the prediction of mechanical properties of the PNC. A good agreement between the calculated effective mechanical properties through MD and continuum models is observed. Although using appropriate interphase model within an micromechanical model is of high importance, the high accuracy should also be considered. To address such challenge and requirements, we present a closed-form analytical model to estimate the mechanical properties of interphase zone, through the molecular dynamic simulation without the aid of any continuum model. mechanical Moreover, the properties of interphases are investigated at different position between the NP and the matrix region in order to ensure the continuously changes from the

nanosilica properties to the polymer matrix properties.

Keywords: protein folding, nanoporous sol-gel glasses, silica-based biomaterials, circular dichroism spectroscopy, surface hydration, crowding effects, micropatterning, biomedical applications.



Figure 1: Prediction of local mechanical properties in PNMs

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Multiscale Process Modeling Analysis for the prediction of Composite Strength Allowables

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Abstract:

During the processing of high-performance thermoset polymer matrix composites, chemical reactions occur during elevated pressure and temperature cycles, causing the constituent monomers to crosslink and form a molecular network that gradually can sustain stress. As the crosslinking process progresses, the material naturally experiences a gradual shrinkage due to the increase in covalent bonds in the network. Once the cured composite completes the cure cycle and is brought to room temperature, the thermal expansion mismatch of the fibers and matrix cause additional residual stresses to form. These compounded residual stresses can compromise the reliability of the composite material and affect the composite strength.

Composite process modeling is greatly complicated by the multiscale nature of the composite architecture. At the molecular level, the degree of cure controls the local shrinkage and thermal-mechanical properties of the thermoset. At the microscopic level, the local fiber architecture and packing affect the magnitudes and locations of residual stress concentrations. At the macroscopic level, the layup sequence controls the nature of crack initiation and propagation due to residual stresses.

The goal of this research is use molecular dynamics (MD) and finite element analysis (FEA) to predict the residual stresses in composite laminates and the corresponding effect on composite failure. MD is used to predict the polymer shrinkage and thermomechanical properties as a function of degree of cure. This information is used as input into FEA to predict the residual stresses on the microscopic level resulting from the complete cure process. Virtual testing is subsequently conducted to predict strength allowables. Experimental characterization is used to validate the modeling. An example of the results is shown in Figure 1. The Young's modulus of a bisphenol-F epoxy resin increases linearly as a function of crosslink density. Experimental values are also included in the graph to validate the modelling. Because the MD results are at a very high strain rate (1×108)

s-1), the predicted modulus is substantially higher than the experimental data points (strain rate indicated in the figure). However, it is clear that as the experimental strain rate increases, the match with modelling becomes closer. Similar results apply to other mechanical properties (1-3) and resins.

This research demonstrates that multiscale modelling can be used to accurately determine resin properties as a function of degree of cure, which can be used to inform processing modelling using FEA. The FEA analysis is subsequently used to predict the micro-scale strength of the composite, and thus the lamina strength. Once the lamina strength is determined, the laminate and structural strength can be established with further FEA modelling.



Figure 1: Figure illustrating the fundamental question that we are tempting to solve experimentally: what is the importance of silica surface modification nanoporous silica-based sol-gel glasses prepared from functionalized organosilane precursors on the parameters affecting the conformation, biological activity and functionality of encapsulated biomolecules.

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Experimental assessment of evaporative cooling performance of Palm leaves pad

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Abstract:

This paper investigates the performance of palm leaves as an evaporative cooling material that could be used as a sustainable cooling solution for farms and standalone domestic evaporative cooing units. The cooling efficiency of the proposed pad and its resistance of airflow are experimentally measured and compared to typically used cellulose-cooling pad.

Prof. Saud GhaniFirstly, the mechanical and morphology characterization of the date palm leaves fiber (DPLF) is evaluated. The Sultana palm leaves were sourced locally from Qatar University farm (Raodat Al-Faras, Qatar). The morphology examination was carried out using scanning electron microscopy (SEM). Morphological properties indicated that the Sultana lumen size is high of dimension of 39.2±19.8 µm. Tensile properties revealed that dry Sultana palm leaves fiber had tensile strength/tensile modulus of (81.10±13.12MPa/5.11±0.48GPa). Water absorption has significant effects on the mechanical properties of date palm leaf fiber reinforced epoxy composite. Accordingly, as the moisture content increases, Young's modulus, the tensile strengths of DPLF/epoxy composites in wet Sultana palm leaves fiber decreased to (60.58±9.59 MPa /3.40±0.49 GPa). On the other hand, as the moisture content increases, the toughness of DPLF/epoxy composites increases. The SEM morphology of the DPLF crosssection showed high hemicellulose content. The observed micro-scale damage characteristics from tensile test fractured specimens indicate that material experienced fiber breakage, fiber fracture, and fiber pullout. Using an air handling unit (AHU), the cooling efficiency of a cooling pad made of wet DPLF was compared to a typical Cellulose cooling pad. The results shows that DPLF cooling pad have a cooling efficiency of 66% in comparison to 78% to a typical Cellulose cooling pad. Nevertheless, the DPLF pad cooling efficiency will be greatly enhanced if the DPLF pad was manufactured with air cooling passages.

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Influence of aging on tensile properties of agriculture films

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Abstract:

It is known that the tensile properties of polymer materials exposed to atmospheric influences are significantly reduced. But when it comes to films, especially when they are used in greenhouses to protect plantations, they must retain certain mechanical properties after a long period of exposure to the sun and water. The purpose of this study was to compare the tensile properties of three different types of films: ethylene tetrafluoroethylene (ETFE), polyethylene (PE) clear, and polyethylene (PE) diffused, before and after their aging (rain, UV rays and humidity). Aging was done according to ISO-4892-2 at an irradiation of 550 W/m², a temperature of 65 °C and humidity 65% for 1000 h. Two types of PE was chosen in accordance with that in the continental part of Croatia it is recommended to use clear films and in the coastal part of Croatia diffuse films are most often used. ETFE film was tested as a potential new material that is increasingly used in all industries. Upon exposure to atmospheric aging (Figure 1), tensile properties of the ETFE film increased after aging but properties of PE films remains the same. Slightly small increase are observed in strain in diffused PE film, which is an excellent indicator that the properties do not change with aging. Although the ETFE film showed the best tensile properties its price is still too high to justify the economic profitability of its application in greenhouses.

Keywords: aging, agriculture, ethylene tetrafluoroethylene, greenhouses, plastic films, polyethylene, tensile properties



Figure 1: Comparison of the tensile properties of different plastic films during aging. Legend:

ETFE – ethylene tetrafluoroethylene film, K-ETFE – aged ETFE film, PE-P – transparent PE film, K-PE-P – aged transparent PE film, PE-D – diffused PE film, K-PE-D – aged diffused film.

Acknowledgements:

The work was created as part of the project *Development of an innovative mobile system for covering and protection of plantations* (Project code: KK.01.2.1.02.0311) financed from the Operational Program "Competitiveness and Cohesion 2014-2020" from the European Fund for Regional Development as part of the call KK.01.2.1.02 - Increasing the development of new products and services resulting from research and development activities (IRI) - phase II. The authors would like to thank the European Union for funding this project.

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Polymer-Surfactant Binding for Environmental Separations

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Abstract:

Surface active per- and polyfluoroalkyl substances (PFAS) are used in a wide range of consumer products and industrial applications owing to their high chemical and thermal stability, their incompatibility with both water and hydrocarbons, and their unique ability to render surfaces non-stick. However, several PFAS surfactants are extremely resistant to degradation, accumulate in the environment, and can have adverse effects on human health. In the context of developing materials for sequestering PFAS surfactants from aqueous media, we research how such surfactants associate with other molecules or surfaces. To this end, we utilize complementary experiments (small-angle neutron scattering, SANS) and modeling (molecular dynamics, MD), and present examples on how the structure of micelles formed in water by the notorious PFAS surfactant perfluorooctanoate (PFOA) responds to the presence of polymers (poly(ethylene oxide) (PEO), PEO-based amphiphilic block copolymers, and polymer networks) across a wide range of compositions. A detailed description emerges on how PFAS distribute around polymer segments which is used to rationalize the macroscopic properties of the mixtures. Fundamental knowledge on PFAS surfactant-polymer interactions supports the design of new materials to selectively capture and remove PFAS pollutants from aqueous media. The capability established in our studies to predict from first principles micelle formation and structure, confirms that such multiple and often competing interactions have been properly accounted for. Micelles are relevant to environment and health in that PFAS surfactants, while typically found in very low bulk solution concentrations, they tend to accumulate on surfaces in the context of separations and bio-interfaces.

Some Examples of smart composites for infractructures and offshore wind-generation

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Abstract:

In many structural applications, the drawback inevitably conjures up the question of how well metal structures resist the combined action of corrosion and mechanical stresses. Another important issue is the necessary use of nondestructive testing (NDT) techniques to prevent premature failure of key structural components, which is not an easy task in offshore. One solution is the use of composites embedded with sensors providing continuous structural health diagnostics.

For smart composite materials are accepted for structural applications, several points regarding the intrinsic and extrinsic mechanical behavior to the parent material should be finely characterized and modeled. By intrinsic problems we mean the potential areas of excess stress in the parent composite material; while by extrinsic problems, we aim those linked to the presence of the sensors inserted in the heart, for a better structural health monitoring. When one is interested in embedded sensors and before focusing on the physical aspects, some very important points should be studied, understood and modeled. These points are the mechanical compatibility, thermal and physicochemical between the sensor and the parent material and how to make these reliable and durable interactions during a cycling fatigue, for example. Finally, for a specific industrial application, the choice of sensor, its physics, its shape, its placement, are of a critical nature. Some aspects of the use of smart composites for infrastructures will be detailed in the case of offshore wind-energy. Numerical simulation was implemented to predict the stress distribution over a wind turbine blade and composite High-Voltage cables. The scope was to determine areas with high stress concentration. Finite Element Analysis (FEA) was used to find optimal material and bonding techniques to construct the structures. Appropriate SHM sensors were designed and numerically modeled to ensure the best use.

Keywords: Smart composite, durability, sensors, numerical simulation, offshore wind energy



Figure 1: Critical zone identification by finite element analysis in a wind-blade; FEM simulation of fiber optic sensor embedment in composite lay-ups; Simulation of inter-wires silding-friction and its effect on the mechanical behavior of Hi-Voltage offshore composite cables.

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Valorization of Plastic Waste: Research Advances in Molecular Recycling

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Abstract:

Polymers are highly versatile materials that constitute numerous products, ranging from the ubiquitous water bottles to personal protection equipment. 44 million tons of plastic waste were managed in the US in 2019, with 86 % of all that plastic landfilled, and only 5 % recycled. Ample room exists for improvement upon the current situation. The presentation will report on trends on plastic production, use and misuse, discuss recent disruptions affecting plastic waste management, and point to current concerns of plastics contributing to greenhouse gas emissions and littering the land and the oceans. Recent research advances will be highlighted in the identification of plastic type for mechanical recycling, and in solvent-based molecular recycling of plastic waste, whereby polymers are selectively dissolved and precipitated to achieve separation and recovery.

Because the polymer chains do not break, this presents a promising, low-greenhouse gas methodology for recycling waste plastic. Through the dissolution/precipitation method, individual polymers can be separated from mixtures or blends, purified from additives or fillers, reduced in volume, and obtained in an acceptable form without negatively affecting the properties of the original polymers.

Ultrasounds Methods for Non Destructive Evaluation of Composite Structural Bondings Aging in Marine environment.

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Abstract:

With the growing use of marine renewable energies production, it become of great interest to control the state of health of tidal and wind turbine blades as they are the first components in contact responsible of the energy conversion. Somme industries of renewable energies systems use assembled composite materials for blades manufacturing. The composite materials are used thanks to their well-known properties of lightness and robustness. One of the most used technique of assembly of composite materials is based on the gluing, as it permits a stress repartition on the hole surface of the materials and a lightness of the assembled resulting structure, by opposition to mechanical methods based on riveting or bolting which provide local stress and heaviness, and could also be responsible on the entrance of defects in the structure. Due to their function, the blades are placed in a hostile humid, saline and windy environment which can be responsible of damage and degradation. It is then crucial to have information on their state of health both to optimize energy conversion efficiency and to indicate advanced degradations requiring maintenance or replacement. This is the aim of this work: to give ultrasounds nondestructive indicators on the health state of structural composite bonding aged in marine medium.

In this work, several samples are manufactured: single layer of composite material, bilayer composite/Epoxy adhesive and trilayer composite/Epoxy adhesive/composite. Some samples are kept as reference samples, the other samples are degraded with climatic and marine in situ aging. Different ultrasounds experimental methods are used based on the propagation of bulk longitudinal waves or guided Lamb waves, which provide Cscan analysis and dispersion curves for the reference samples and the aged samples. Experimental results are compared to numerical ones obtained from a numerical model solved by Finite Elements Method (FEM). Different states of aging are quantified by driving out the acoustic tensor constants.

Keywords: Blades aging, marine environment, ultrasounds evanluation



Figure 1: Experimental dispersion curves superimposed on the numerical ones.

Aknowledgment:

This research work was supported by the European Regional Development Fund via the INTERREG TIGER project.

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Polymers / Composites / 3Bs Materials 2023 Session II. B

GnRH Peptide/Adjuvant Conjugate Vaccine Candidates to Treat Cancer and for Veterinary Immunocastration

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Abstract:

Poor oral absorption and rapid enzymatic degradation are the major hurdles in the oral delivery of peptide drugs and vaccines. We developed stable, orally available peptide drugs through the chemical addition of specifically designed lipophilic immunoadjuvants, creating amphiphilic compounds capable to reassemble to form nanoparticles. Fertility is controlled by decreasing the level of circulating Gonadotropin-Releasing Hormone (GnRH) or stimulating the downregulation of GnRH receptors on gonadotrope cells. Using an oral vaccine candidate we regulated the action of GnRH on gonadotropic cells, thereby controlling fertility in both feral and domesticated animals. We designed contraceptive vaccines for farm animals and for controlling pest animal population by immunocastration. Generally, vaccines administered via injection, the need to restrain animals for treatment limits the field applications of injectable vaccines, so oral administration would broaden vaccine applicability. We explored contraceptive vaccine candidates composed of GnRH peptide antigen, universal and species-specific T helper epitope and an adjuvanting delivery system (MAP, poly(lipoamino acid) and lipophilic poly(methylacrylate). These amphiphilic complexes self-assembled into nanoparticles and induced the production of high IgG titers after both subcutaneous and oral administration. Importantly, in mice and antibody titer was stable even after six months. In conclusion, we developed simple GnRHpolymer based contraceptive vaccine candidates. The technology is generally applicable for other antigens.

Keywords: immunocastration; GnRH; oral vaccine; lipophilic adjuvant, T helper epitopes; antibody

Figure 1: Cntrolling of gonadotropin hormone level



*similar feedback system applies for the female reproduction system

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Hybrid composites based on biopolypropylene modified with basalt and microcellulose fibers with the addition of antibacterial turmeric

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Abstract:

The aim of the study is to assess the possibility of producing hybrid polymer composites based on biopolypropylene produced from biomass with the addition of basalt fiber, cellulose fibers and turmeric as a natural antibacterial agent [1].

The matrix used was bio-based polypropylene [2] (NP BioPP 202-48 by NaturePlast). Basalt fibers (BCS17-6,4-KV 02 by Basaltex) with a length of 6.4 mm and cellulose fibers (EFC 950, 50-150 um by J. Rettenmaier & Söhne). The six types of composites were produced by injection molding with the addition of 5,10, 15% by weight basalt and cellulose fiber and additionally 2% wt. dry turmeric powder. The basic strength properties were determined in a static tensile, bending and impact tests. The low-cycle dynamic test was carried out to determine the changes in dissipation energy and the development of relaxation processes. In order to assess the effect of water absorption on the mechanical properties of the samples, a hydrolytic degradation test was carried out. SEM micrographs were also made on the gold-sputtered after tensile-test fracture surfaces of specimens. The results obtained an improvement in strength properties by the addition of basalt fibers and also by the use of EFC cellulose fibers. Materials with the addition of basalt and EFC 950 cellulose fibers have highest flexural and tensile strength than polypropylene. The addition of 10% basalt fibers caused 33% increase in strength, while the same amount of EFC caused an 18% increase in strength. The impact test shown that polypropylene has a much higher strength compared to the produced composites. Comparing the results from the bend test after hydrolytic degradation, it can be concluded that the values of the maximum stress in each of the tested composites decreased. The highest decreasing of strength properties after degradation was observed for the composite with the highest amount of fillers, i.e. PP15B15EFC, the bending strength value in this case decreased by 9.38 MPa. The SEM photos show good homogenization of both fillers and their even distribution in the polypropylene matrix. Basalt fibers crack as a result of processing to a length of about 0.5 mm, while cellulose fibers are

uniformly dispersed in the images of fractures after tensile test.

Only about 10% of the basalt fibers are pulled out of the matrix, the rest break on the cross-sections. The best reinforcement effects are achieved by hybrid composites with 10% of basalt and cellulose fibers. A further increase in the proportion of fibers leads to an increase in stiffness with a decrease in strength.

Keywords: biopolypropylene, polymer composites, basalt fibers, lignocellulose fibers, turmeric powder, injection molding, strength properties



Fig.1 Micrographs of fracture after tensile test PP10B10EFC



Fig.2 Young`s modulus of tested composites

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Multi-faceted Approach for Forming Nanostructures for Surface Enhanced Spectroscopy Applied to Detection of Biologically Relevant Molecules in Agriculture and Food Industry

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Abstract:

Characterization of biomolecules will be increasingly important. А vibrational spectroscopy such as Raman spectroscopy is definitely important because it can provide structural information of molecules in the atmosphere and solution. Its principle weakness of low signal intensity has been overcome by the technique of surface-enhanced Raman spectroscopy whereby signals from molecules adsorbed on noble metal nanostructures are enhanced by many orders of magnitude. In this paper, we describe three distinct methods for fabrication of such structures, shown in Fig. 1. In one physical approach, we form a dense monolayer of 100 nm SiO₂ nanospheres, upon which silver or gold is evaporated up to 100 nm. Resulting cap-shaped nanostructure is useful for SERS.¹ In the second method, copper nanostructures are formed with the above method. Then, they are exposed to silver nitrate for displacement reaction. The resulting structure consists of fibrous silver. In the third approach, the natural three dimensional structure of butterfly scales is exploited.² Simple silver deposition turns scales into microscopic SERS substrates. We have been using these different nanostructures for detection of various molecules. ranging from model compounds such as rhodamine 6 G, BPE, food additives such as betacarotene, melamine, pesticides such as ferbam and TBZ, volatile sulfur compounds such as dimethylsulfide and methyl mercaptan, beside many others. We have also developed a number of distinctly different device configurations. The standard substrate is suitable for deposition of a liquid sample or exposure to a volatile sample. We also prepared a stamp-like SERS substrate that can be pressed directly onto a solid surface covered by the target molecules. Yet another device is optimized for detection of molecules suspended in a flowing sample. Another consideration is to combine SERS with a separation technique such as thin layer chromatography or HPLC as separation of the

target molecule is often a prerequisite for final dection. It should be mentioned that compact and low-cost Raman spectrometers are becoming available, favoring SERS as a candidate for next generation analytical techniques in the industrial setting.

Keywords: noble metal nanostructure, surfaceenhanced Raman spectroscopy (SERS), butterfly scale, pesticide, food additive, sulfur compounds.





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Basalt fibers reinforced polylactide composites modified by antibacterial nanoparticles

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Abstract:

The aim of the study was to evaluate the effect of the addition of basalt fibers and antibacterial metal nanoparticles (copper oxide CuO and zinc oxide ZnO) on the strength properties, degradation and the ability to dissipate mechanical energy of composites produced by injection molding on a matrix of biodegradable polylactide [1]. The nine compositions were produced with the proportion of 5% and 15% by weight of basalt fibers with the addition of two types of antibacterial nanoparticles and chosen polylactide compatibilizer. The basic strength properties were determined in a static tensile, bending and impact test. The low-cycle dynamic test was carried out to determine the changes in dissipation energy and the development of relaxation processes. SEM structure images were made on the gold-sputtered after tensile-test fracture surfaces of specimens. The microbial activity of the produced composites was also compared. Addition of BFs increases the tensile and bending strength and increases the stiffness of composites. After 7 weeks of hydrolytic degradation a significant 30-50% decrease in strength and stiffness and impact strength was observed. It is related to the degradation model of PLA in which water leads to plasticization and the strengthening effect of the BFs. The addition of antibacterial metal oxide nanoparticles also lowers the properties strength.

The SEM images of the ZnO composites showed larger agglomerations of nanoparticles than those with the addition of CuO. Larger amounts of crystallites concentrated around the basalt fibers were also observed. The addition of basalt fibers reduces the mechanical energy dissipation ability of composites, while significantly reducing the creep ability and stabilizing the increase in maximum displacement. The addition of CuO nano particles increased the antimicrobial activity more than ZnO nanoparticles. The authors propose the use of composites for medical equipment.

Keywords: polylactide, polymer composites, basalt fibers, antibacterial nanoparticles, injection molding, antibacterial test



Fig.1 Micrographs of fracture after tensile testPLA 5B 2Zn, x1500

Samples	Tensile	Flexural	Impact
	strength [MPa]	modulus [MPa]	strength [kJ/m ²]
PLA	42.2 ± 2.8	3997 ± 199	$\textbf{25.3} \pm 1.8$
PLA 2Cu	42.7 ± 0.3	3950 ±197	18.9 ± 2
PLA 2Zn	40.2 ± 1.5	3874 ± 193	21.2 ± 1.9
PLA 5B	49.7 ± 2.3	5790 ± 290	14.5 ± 1.4
PLA 5B 2Cu	53.8 ± 4.8	4741 ± 237	15.5 ± 1.2
PLA 5B 2Zn	47.8 ± 2.1	4185 ± 209	15.5 ± 1.8
PLA 15B	61.7 ± 1.1	6208 ± 310	17.5 ± 1.5
PLA 15B 2Cu	59.8 ± 3.7	5695 ± 284	17.4 ± 0.8
PLA 15B 2Zn	65.7 ± 5.2	5356 ± 268	20.0 ± 1.4

Tab 1: Comparison of strength propertiessamples after injection molding

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On Chemical Actuation of Shape Memory Polymers (SMPs)

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Abstract:

Polyurethane copolymers like Estane ETE 75 DT3 (abbreviation Estane-E) show a shape memory effect, which can be thermally and chemically triggered. After programming, the deformed materials return to their original shape when the external temperature exceeds the glass temperature $T_{\rm g}$ of the hard component. Alternatively, the one-way effect can be chemically triggered, when small molecules enter the polymer and weaken the bonds between macromolecules. This results in a chemically enforced decrease of the glass temperature below room temperature, and thus initiates shape recovery, driven by entropic forces. When considering chemical triggering of the shape memory effect for actuator applications, four questions must be answered: (1) How fast do the small molecules which initiate the effect enter? (2) How does the uptake of small molecules affect the glass transition temperature? (3) Which exploitable strokes can a SMP actuator provide and how are these affected by an end load? (4) Is it possible to use physical methods like Fourier transform infrared spectroscopy (FT-IR) and synchrotron wide angle X-ray scattering (WAXS) to gain insight into the elementary molecular and morphological processes which govern the shape memory effects? In the present work, we process Estane-E specimens by extrusion from granulates obtained from Lubrizol and we program the material for the one-way effect [1]. Glass transition temperatures are measured using dynamic mechanical thermal analysis [2]. We use the weight-gain technique described by Marquardt et al. [3] to determine diffusion coefficients of the three alcohols (methanol, ethanol and 1-propanol) in Estane-E. Then we determine their effects on glass transition temperatures and use the set-up described by Dumlu et al. [4] to measure the recovery kinetics of the programmed SMP-E with and without a superimposed external tensile stress. Finally, an effort was made to identify the chemical nanoscale reactions which are responsible for the decrease of the glass temperature (FT-IR work). On the mesoscale, we make an attempt to document the shape change which occurs when the elongated

macromolecules return to their randomly coiled initial state.

The results are discussed in light of previous work published in the literature, with a special focus on the possibility to technically exploit the chemical actuation of SMP actuators.

Keywords: Shape memory polymers, chemical triggering of one-way effect, actuator performance, Fourier transform infrared spectroscopy, synchrotron wide angle X-ray scattering.



Figure 1: Results from WAXS synchrotron experiment on the programmed (elongated macromolecules, left) and the recovered (recoiled macromolecules, right).

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Multiplexed Nanomaterial-Based Sensor Array for Detection of Pathogenic Microbes

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Abstract:

The difficulty to recognize corona illness immediately is the primary reason it has become a pandemic. To address this limitation, the pseudo-3D covalent organic structure nanosheets was developed, and their co-bonding type eventually transformed them into a threedimensional nanosheets. The N region of the Covid-19 pathogen genome was employed as the target DNA to detect Covid-19 illness (Figure-1). The probes and the surface of the nanonet interacted during detection. As a result, the dsDNA was isolated from the nanonet, and the target was then quantitatively analyzed of COVID-19 DNA by restoring the probe fluorescence. The Covid-19 DNA detection limit in this approach is 2 Pico moles, with no RTPCR to replicate the virus RNA. Here we tested Covid 19 as a model but in the process, we can quickly detect any pathogenic disease ...

Keywords: nanoporous, covalenent organic framework, nanosheets, RNA, diseases, biomedical application, fluorescence



Figure 1: Figure illustrating the COF nanomaterials based sensor array detecting the specific COVID-19 pathogenic virus without any other interferences.

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Mesenchymal Stem Cell Adhesion on Plasma-Coated Biodegradable Nanofibers

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Abstract:

In the field of tissue engineering, in recent years there has been a growing interest in porous structures consisting of biodegradable fibers, the structure of which is similar to the extracellular matrix (ECM). This is confirmed by a significant number of publications. The number of publications containing the keywords "Cell", & "Adhesion" and "Nanofibers" exceeded 350 per year, although until the 2000s this topic was not covered at all.Various biomedical applications of biodegradable nanofibers are a hot topic, as evidenced by the ever-increasing number of publications in this field. However, as-prepared nanofibers suffer from poor cell adhesion, so their surface is often modified. In this work, active polymeric surface layers with different densities of COOH groups from 5.1 to 14.4% were successfully prepared by Ar/CO2/C2H4 plasma polymerization. It has been shown that adhesion and proliferation of mesenchymal stem cells (MSCs) seeded onto plasma-modified PCL nanofibers are controlled by the CO2:C2H4 ratio. At a high CO2:C2H4 ratio, a well-defined network of actin microfilaments is observed in the MSCs. Nanofibers produced at a low CO2:C2H4 ratio showed poor cell adhesion and very poor survival. There were significantly fewer cells on the surface, they had a small spreading area, a poorly developed network of actin filaments, and there were almost no stress fibrils. As shown in Figure 1, the maximum percentage of proliferating cells was recorded at a CO2:C2H4 ratio of 35:15 compared with gaseous environments of 25:20 and 20:25 (24.1±1.5; 8.4±0.9 and 4.1±0.4 %, respectively). Interestingly, no differences are observed between the number of cells on the untreated surface and the plasma-polymerized surface at CO2:C2H4=20:25 $(4.9\pm 0.6 \text{ and }$ 4.1 ± 0.4 respectively). Thus, Ar/CO2/C2H4 plasma polymerization can be an excellent tool for regulating the viability of MSCs by simply adjusting the CO2:C2H4 ratio.

Keywords: Nanofibers, biocomposites, cell adhesion, plasma, XPS, ECM.



Figure 1: The percentage of proliferating cells (on top) and cell number (at the bottom) on different samples: PCL-ref (untreated nanofibers), nanofibers coated by Ar/CO2/C2H4 plasma polymers at a CO2:C2H4 ratio of 35:15, 25:20 and 20:25.

Acknowledgment:

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Positive Impact of composite materials with Ag modification on wound healing

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Abstract

Wide spectrum of natural polymers are used in nanoengineering and biomedicine due to its specific features. Chitosan provides antibacterial, anticoagulant and hemostatic properties, and curdlan is a β -glucan showing a positive effect on human immune system [2]. Combination of such polymers can give a material of various forms and morphology, that would affect their features. For biomedicine regenerative, antibacterial protective and moisture absorbent properties are in great demand. Therefore, silver integration in curdlan/chitosan (Cur/Cs) materials could possibly create protective material with desired properties. Silver is well known for its antimicrobial features, but its high concentration can have negative effect on living cells [1]. For that reason, Ag concentration and its form is important in regenerative materials. Cur/Cs foams were created from a mixture of hydrolyzed Curdlan and chitosan by lyophilization. Ag nanoparticles were incorporated by adding AgNO3 solution during the polymerization [4]. In our previous work, it was shown that silver is from different released material polycaprolactone in the cell medium, indicating the possibility of prolong delivery in the living organisms [3]. Therefore, the purpose of the work was to determine Ag-containing if Curdlan/Chitosan foams have the impact on the wound healing in the mice model. For this purpose, foam pieces were characterized both chemically and physically, then placed on the full-thickness skin wounds of diabetic mice until full regeneration of wound site. It was shown that Cur/Cs+Ag foam contain 0,4% Ag. Addition of Ag in the Cur/Cs material decrease the absorption rate. Curdlan/Chitosan foams with Ag significantly accelerated wound healing in diabetic mice with comparison to initial composite material Cur/Cs. It reduced presence of inflammatory cells and new vessels in the wound site were formed. Curdlan/Chitosan material with Ag NPs have promising features in wound healing, especially chronic wounds typical for Diabetes disease.

Keywords: Curdlan, Chitosan, Ag, Regeneration, Biomedicine, Tissue engineering

Acknowledgment.

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Application of graphitic carbon nitride nanosheets as a multifunctional nanofiller in cryogels for wastewater treatment and quality monitoring

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Abstract: Graphitic carbon nitrides (g-C₃N₄) have recently shown outstanding potential for water treatment owed to their chemical, photocatalytic. fluorescent and electronic properties, alongside their environmental friendliness and non-toxicity.^{[1],[2],[3]} Due to the industrialization and constant technological development of the world, water contamination continues to rise, and upholding the safety and quality of this primary resource of human life is a great challenge of the 21st century. Even though there is a large amount of studies on materials for water purification and quality monitoring, these are usually limited to monofunctions and the designs for energy consuming processes. The reusability of the utilized materials is often restricted by fouling, and the material's durability is negatively affected by the caustic and corrosive solutions used for its cleaning after the pollutants adsorption, which creates secondary pollution. Owing to the various intrinsic properties of g-C₃N₄, a multi-purpose self-cleaning poly(sodium acrylate) PSA composite cryogel loaded with graphitic carbon nitride nanosheets (CNNs) is synthesized in a form of a 3D filter. The obtained PSA/CNN nanocomposite is highly efficient in the simultaneous separation of oil and the removal of cationic organic dyes^[4] and heavy metal ions from water through gravity-driven filtration. The presence of CNNs improves the cationic organic dyes adsorption capacity of the cryogel and its photocatalytic self-cleaning property under visible light irradiation enables it to be cleaned from the adsorbed organic pollutants, making possible its use for various filtration cycles. Moreover, such 3D filter is proved to be applicable for the use as a heavy metal ions fluorosensor, owing to the CNNs' fluorescence quenching occurring due to the interaction with the heavy metal ions. To the best of our knowledge, this is the first report on CNN nanocomposite hydrogels simultaneously exploiting the CNNs' photocatalytic activity, adsorption and fluorescent detection properties in order to design a highly performant multifunctional material for integrated water treatment and quality monitoring process.

Keywords: Nanocomposites, carbon nitride, cryogels, photocatalysis, fluorescence, gravity-driven filtration, adsorption



Figure 1: The material's functionalities scheme.

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Effect of Graphene Oxide Doped PEDOT:PSS as a Hole Transport Layer and Annealed Temperature on the Inverted Perovskite Solar Cell From the Waste of Electric Arc Furnace Electrode

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Abstract:

Poly (3,4-ethylene dioxythiophene) polystyrene sulfonate (PEDOT:PSS) is a widely used hole transport material in inverted perovskite solar cells. However, PEDOT:PSS usually limits the ef-ficiency of perovskite solar cells (PSCs) due to its hygroscopic nature. Therefore, in this study, inverted perovskite solar cells were fabricated by modifying the PEDOT:PSS layer using graphene oxide (GO) synthesized from electric arc furnace graphite electrode waste. PSCs fabricated on a GO-doped PEDOT:PSS layer by spin-coating exhibited a power conversion efficiency (PCE) of 0.8011%, which is higher than 0.0236% of PSCs with the PEDOT:PSS layer. Furthermore, the annealing temperature of the perovskite layer is varied and exhibited a higher PCE at 100°C. However, The XRD pattern and SEM images on the sample with an annealing temperature of 130°C confirmed that there had been a degradation of the perovskite layer to PbI₂, which caused a decrease in the PCE

Keywords: Inverted perovskite solar cells, graphene oxide, PEDOT:PSS, annealing temperature, power con-version efficiency (PCE)



Figure 1: Schematic of Perovskite Solar Cell Structure, SEM Images of Perovskite Layer with Annealing Temperature, and I-V Curve of PSCs with Different HTM.

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Effect of Filler Concentration and Sonication Time on Graphite-ZnO Composites with Epoxy Resin Matrix as Microwave Material Absorbing

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Abstract:

The crystal structure, surface morphology, microwave reflection loss, and electromagnetic ab-sorption of graphite and graphite-zinc oxide (G-ZnO) have been investigated utilizing X-ray Scanning dif-fraction (XRD), Electron Microscopy (SEM), and Vector Network Analyzer (VNA). Graphite–ZnO composites with an epoxy resin matrix were synthesized using graphite powder and ZnO with a mass composition ratio of 1:1 and epoxy resin and hardener with a ratio of 2:1. The filler concentration and sonication time were varied. The XRD pattern shows that the crystal structure of graphite, G-ZnO composite, and epoxy resin is different for all composites, and the crystallite size is also discussed. VNA analysis provides the microwave reflection loss and ab-sorption percentage values (Figure 1). The microwave reflection loss and the absorption percentage are -11.04 dB and 23.07 % for graphite with epoxy, -9.978 dB, and 14.77% for pure resin epoxy without the filler. The optimum microwave reflection loss is -17.458 dB for the G-ZnO with a filler concentration of 20 wt% and 60 minutes of sonication time. The highest microwave absorption percentage is 20.42% for the G-ZnO with the filler of 20 wt% and 30 minutes of sonication time. Absorption percentage relates to the bond length, crystalline size, and lattice parameter. Our results indicate that graphite and G-ZnO composite are promising as a wideband electromagnetic wave absorption material.

Keywords: Microwave Absorbing Material, Graphite-ZnO Composite, Crystal Structure, Reflection Loss, Vector Network Analyzer.



Figure 1: Schematic of absorbing materials, XRD of graphite-zinc oxide (G-ZnO), and VNA graphite-zinc oxide (G-ZnO) with different different filler concentration and sonication time.

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Polymers / Composites / 3Bs Materials 2023 Session III

Task-Specific Design and Functionalization of Porous Poly-Calixarene For Water Purification

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Abstract:

Several modern technologies have benefited from novel multi-functional materials. In this regard, porous organic polymers (POPs) are a promising class because of their ultrahigh hydrothermal stabilities, light weight, and high yielding synthetic polymer chemistry.1 Calix[n]arenes (n = 4, 6, 8) have long been recognized as versatile supramolecular scaffolds, however, we are the first to report a calixa[n]arene based porous polymers.2 Building on these findings, we synthesized library of calixarene based porous materials with BET surface areas ranged from 500 to 1000 m2 g-1. Our design strategy has been ranging from amorphous 3D-polymers to 2D-nanosheets, and evolved toward ordered polymeric then materials. Lately, we have been working on the development of porous materials with specific application in mind. So far, these materials have been tested for multiple applications including 1) oil spill recovery,2 2) toxic dyes2,3 and micropollutants removal,4 iodine 3) enrichment, 5, 64) paraquat and mercury removal, 7 and 5) drug-delivery.8 My talk will highlight the development of this fascinating series of polymers and their superior efficiency over existing materials.

Keywords: Water, Water Purification, Calixarenes, Polymers, Porous Materials



Figure 1: Figure illustrating the use of polycalixarenes as efficient adsorbents for water purification.

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Application of the SSA thermal fractionation technique to recycled polyolefin blends and thermoplastic polyurethanes

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Abstract:

Successive Self-Nucleation and Annealing (SSA) is a powerful thermal fractionation technique designed and implemented by Müller et al.¹⁻³ that can efficiently characterize the distributions of defects (branches, comonomers, tacticity, among others) along crystallizable chains. SSA applies a series of successive cooling and heating runs to a self-nucleated sample that promotes the creation of a series of thermal fractions with a specific lamellar thicknesses and melting point distribution thanks to the presence of defects along the chains.

Recently, we applied SSA to characterize thermoplastic polyurethanes (TPUs)⁴ and polyethylene/polypropylene blends⁵⁻⁶. The changes in structure and morphology of TPUs before and after SSA fractionation were monitored by Differential Scanning Calorimetry (DSC), in situ real-time Small and Wide-angle Xsynchrotron experiments scattering ray (SAXS/WAXS) and Atomic Force Microscopy The SSA fractionated samples (AFM). experienced a general increase in lamellar thickness that has been revealed by both AFM and SAXS and a distribution of lamellar thickness estimated by DSC and AFM, see Figure 1. The refined crystalline structure obtained after SSA produced a number of clear WAXS reflections, as compared to the unfractionated materials. facilitating the determination of the TPUs crystallinity degree by WAXS.

On the other hand, a new tailor-made SSA protocol, able to fractionate both PE and PP in the same experiment, was designed and implemented. The fractionation of model blends with known composition allowed the assessment the temperature ranges of where cocrystallization among the blend components did not occur, enabling the development of a method for the quantitative evaluation of the amount of the high melting PE component and of the PP phase in a blend. Finally, the composition of two recycled blends was successfully assessed by means of the novel quantitative method and the

results were compared with those achieved by a solution-based fractionation technique on the same materials. **Keywords**: Thermal fractionation; Successive Self-Nucleation and Annealing (SSA); molecular segregation; Differential Scanning Calorimetry.



Figure 1: Figure illustrating a typical nonisothermal DSC protocol (top) and the SSA fractionation protocol (Bottom). The much larger lamellar sizes makes the morphology easier to visualize by AFM after SSA (bottom). The DSC scans after cooling from the melt or after applying the SSA protocol can be observed in the last panel on the right⁴.

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Polymers / Composites / 3Bs Materials 2023 Discussion Panel on Sustainability Transitions with and for Polymers, Composites, Biobased, Biodegradable, and Biomimetic Materials

Contributions of composites to climate adaptation and water security

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Abstract:

The EU Green Deal initiative is focusing on the products climate-neutral circular & manufacturing, with an ultimate target of reaching the carbon neutrality in Europe at 2050. In addition, the circular economy action plan includes a 'sustainable products' policy that will prioritise reducing and reusing materials before recycling them¹. Apart from that, the EU Ecodesign Directive establishes a framework under which manufacturers of energy-using products are obliged to reduce the energy consumption and other negative environmental impacts occurring throughout the product life cycle which is complemented by the Energy Labelling Directive. In this context, composite materials, in comparison with conventional materials, are used to reduce the product environmental footprints (PEF) in their using phase. New industrial sectors, such as wind and hydrogen² energy industry, are increasingly adopting composites, and the composite materials reaching their Endof-Life (EoL) are bringing new challenges to develop economically and environmentally sustainable recycling routes for these EoL composites which currently tend to not be economically attractive. ecologically or Therefore, composite material waste and secondary material sorting will be a major task not only for leading European industries and SMEs. ITA's activities on circularity in composites are poised to identify the optimal recycling and upcycling (reusing a resource for a higher value application), collection, separation methods, tools, and materials, for building a framework and novel business models for different types of fibre reinforced composites and secondary materials used in different industrial sectors, with the "design from recycle" and the "design for recycle" principle. Such framework contributes its share towards climate change mitigation in the materials and manufacturing perspective, in line with the EU Green Deal's zero pollution strategy. Furthermore as the built environment accounts to a major share of greenhouse gas emissions, sustainability in civil engineering is a guiding principle for the construction sector and textile reinforced concrete has been introduced as a promising composite structure for the built environment. In

the project "Cleanwater" funded in the frame of the Indo-German Science and Technology Centere (IGSTC) modular lightweight wastewater treatment units made with TRC for rural and periurban dwellings were developed.

Keywords: composites, textile-reinforced concrete, circularity, climate adaptation, water security, hydrogen, renewable carbon



Figure 1: Machine vision systems for the detection of defects in composite structures for hydrogen storage

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Polymers / Composites /3Bs Materials 2023

Posters Abstracts

Production of 2,5-Furandicarboxylic Acid from Fructose Using dual magnetic-based Catalyst

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Abstract:

2,5-Furandicarboxylic acid (FDCA) is the critical monomer in polyethylene 2,5-furandicarboxylate (PEF) production.PEF is the centre of the spotlight due to its greener production process, higher glass transition temperature (Tg), good mechanical performance and excellent barrier properties, which has been considered the new generation of packaging material to replace polyethylene terephthalate (PET. In this study, two magnetic particles were prepared by chemical precipitation and modification methods, Mag-SO3H and Mag-CoOx. Fructose was used as raw material, and dimethyl sulfoxide (DMSO) was used as a solvent to generate 5-hydroxymethylfurfural (HMF), which was subsequently converted into FDCA with Mag-CoOx catalyst and tert-Butyl Hydroperoxide (TBHP) as oxidant. In this dual magnetic-based catalyst system, the highest FDCA yield rate obtained was $640.5\pm 17 \text{ mg/L*h}$ via tert-Butyl Hydroperoxide as the oxidant.

Keywords: 2,5-Furandicarboxylic acid, magnetic-based catalyst, 5-hydroxymethylfurfural, 2,5-furandicarboxylate.

The role of Al₂O₃ interlayer in the synthesis of ZnS/Al₂O₃/MoS₂ coreshell nanowires

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Abstract:

Layered 2D van der Waals (vdW) materials such as transition metal dichalcogenides have recently gained a scientific attention due to their unique properties and prospective applications in various fields such as electronics and optoelectronics, nanomechanics, sensors and energy.

During the synthesis of heterostructured nanomaterials, unwanted structural and morphological changes in nanostructures may occur, especially when multiple sequential growth steps are involved. In this study, we describe a synthesis strategy of heterostructured ZnS/Al₂O₃/MoS₂ core-shell nanowires (NWs), and explore the role of the Al₂O₃ interlayer during synthesis.

Core-shell NWs were produced via a four-step route:

(1) synthesis of ZnO NWs on a silicon wafer,

(2) deposition of thin Al₂O₃ layer by ALD,

(3) magnetron deposition of MoO₃ layer,

(4) annealing of the sample in the sulphur atmosphere at 750 $^{\circ}$ C.

During sulphurization, ZnO is converted into ZnS, and MoO_3 into MoS_2 [1], while the Al₂O₃ interlayer preserves the smooth surface of an NW required for the growth of a continuous MoS_2 shell [2].

The resulting ZnS/Al₂O₃/MoS₂ core-shell NWs were characterized by transmission electron microscopy, X-ray diffraction and photoelectron spectroscopy, Raman spectroscopy, and optical photoluminescence spectroscopy.

A reported strategy can be used for the synthesis of other core-shell NWs with a transition metal dichalcogenides (TMDs) shell to protect the NW core material that may otherwise be altered or damaged by the reactive chalcogenides at high temperatures.

Keywords: composite nanomaterials, heterostructures, core-shell nanowires, layred 2D materials, transition metal dichalcogenides, X-ray diffraction, electron microscopy, micro-Raman and XPS spectroscopy, photoluminiscence.



Figure 1: TEM images of ZnS/MoS2 (a,b), and ZnS/Al2O3/MoS2 (c,d) NWs annealed in sulphur atmosphere at 750 °C.

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Aldehyde-free resins based on resorcinol and natural alkylresorcinols modified with styrene

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Abstract:

Phenol-formaldehyde resins obtained by the condensation reaction of phenol with formaldehyde are used in many fields of industry (tire, rubber and electrical products, construction, and varnish, medical paint supplies, woodworking, airgel production). At the same time the requirements for their exploitation and characteristics become more strict and accordingly the new formulations are searched. They should have improved properties as increased thermal stability, mechanical strength, good dielectric and adhesive characteristics. In addition, at the moment, environmentally friendly technologies for the production and processing of polymers, as well as composite materials, are becoming a priority.

Resins obtained by the condensation of phenol formaldehyde have a series with of disadvantages. They are characterized by a high content of volatile substances, are unstable, hygroscopic, and have a limited life-time. The reducion of the emission of formaldehyde and phenol, used in their production, into the environment is an urgent problem [1,2]. At present, attempts to obtain formaldehyde-free resins are considered the most promising solution. Syntetic resorcinol (R) [3] and oil shale alkylresorcinols (ARs) can be used as less toxic phenolic compounds. The use of ARs makes also possible to reduce the cost of resins.

The purpose of this work was to study the possibility of obtaining aldehyde-free resins using pre-modified styrene (S), R, individual ARs, their mixtures, as well as oil shale ARs.

Resins obtained are solid colored substances of orange, red, raspberry or brown color (Figure 1). Depending on the molar ratio of the initial components, resins with different final characteristics (softening point, ash content, content of volatile and unreacted components, etc.) can be obtained. It was found that the time of aralkylation of mixtures of ARs is twice as long as that of individual ones. Resorcinol-alkylresorcinol-dicyclopentadienestyrene resins contain less than <1 wt% free R, are well compatible with styrene-butadiene polymers, and are stable longer than one year. The content of volatility components is less than 1.2 %. The use of dicyclopentadiene makes it possible to obtain low ash resins (≤ 0.4 wt%) with a low content of free ARs (in R₇₀ARs₃₀DS resin - 0.5 wt%), softening point 75 – 97 °C. The resins obtained have an uniform composition and the introduction of S into the formulation leads to significant decrease in the content of unreacted R and ARs in the final product.

Keywords: resorcinol, natural alkylresorcinols, dicyclopentadiene, styrene, polycondensation, aldehyde-free resins



Figure 1: Resorcinol-dicyclopentadiene resin modified with styrene

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Laser Ablation Synthesis of Semiconductor Nanocomposites with Tunable Plasmonic and Paramagnetic Properties

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Abstract:

Facile formation of nanocomposites combining different materials with finely tunable properties is an important task for many applications in biosensing, bioimaging or cancer theranostics. Besides already developed and widely used synthesis technologies, a method of pulsed laser ablation (PLAL) attracts by its ease of the synthesis, extreme chemical purity conditions as well as simple variation of nanocomposite properties. It was shown recently that PLAL approach allows easy merging of semiconductor and plasmonic metallic elements into one nanoparticle (NP) [1]. Moreover, adapting experimental conditions, one can easily achieve changing of their chemical composition reflecting on their functional properties.

Semiconductor-metallic nanocomposites constitute a promising nanotool with multimodal functionality able to solve various tasks simultaneously that is especially important in the field of biomedicine. Their chemical purity ensured by environment-friendly laser synthesis allows improving nanocomposite safety by reducing different toxic effects. Easily variable nanocomposite chemical content allows managing their efficiency, e.g., for molecule detection using surface-enhanced Raman scattering (SERS) [2].

In this research, the laser-ablative synthesis, characterization and applications of nanocomposites based on IV group semiconductors with tunable plasmonic properties is reported. Succesful combination of semiconductor and metallic elements in one nanoparticles is demonstrated. For this purpose, dfferent metallic targets of high purity (99,99+ %) were ablated in colloidal solutions of semiconductor (silicon or carbon) nanoparticles. Their structural and optoelectronis properties are investigated by electronic microscopy, X-ray techniques, optical and magnetic resonance spectroscopies. The formed semiconductor-metallic nanocomposites can be promising for their simultaneous applications in different fields such as molecule detection, nonlinear/linear optical bioimaging, nanothermometry.

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Keywords: nanocomposites, silicon nanoparticles, carbon nanoparticles, plasmonic nanomaterials, laser ablation, biomedical applications.



Figure 1: Tuning of plasmonic properties of semiconductor-metallic nanocomposites based on silicon (on the top) and carbon (on the bottom) nanoparticles formed by different duration of pulsed laser ablation.

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Physical Treatment of Biopolymer and Its Aplication in Elastomeric Composites

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Abstract:

Currently, a number of studies focus on different methods of chemical and physical treatment of cellulose in order to improve the interfacial adhesion between the filler/cellulose and the polymer matrix in the preparation of composites. Polymer composites containing of biopolymers as filler are interesting today mainly because of biodegradability and environmental their friendliness. One of the physical treatments is the use of ultrasound [1]. Ultrasonic waves from ultrasound facilitate the processing of cellulose in aqueous solution through the formation, growth and collision of gas bubbles. The hydrodynamic action of ultrasound could disrupt the van der Waals forces between the surface of cellulose in an aqueous solution [2, 3]. In this work, cellulose was physically treated by means of ultrasound in an aqueous environment. The time and temperature of the aqueous solution of cellulose under the influence of ultrasound were monitored, which could increase the possibility of the reaction of cellulose with microbubbles generated by the ultrasound process. Cellulose treated in this way was mixed with a matrix of natural rubber. Morphology, vulcanization physical-mechanical characteristics and properties were studied on the prepared composites. The use of ultrasound could lead to a reduction in the costs associated with the chemical treatment of cellulose (solvent, modifying agent). This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for "Centre for diagnostics and quality testing of materials" in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014+ code 313011W442.

Keywords: physical treatment, cellulose, elastomeric composites, morphology, ultrasound

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Effect of Surface Treated Biopolymer on Curing Behavior and Tensile Properties of Natural Rubber Composites

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Abstract:

The growing demand for environmentally friendly materials has prompted several researchers to explore naturally occurring biopolymers for potential applications in a variety of fields [1]. Cellulose is a biopolymer formed by the repeated joining of D-glucose building blocks and is characterized by its hydrophilicity, broad chemical modification capacity, biodegradability, and the formation of versatile morphologies of semicrystalline fibers [2]. However, the interactions between the cellulose and the polymer matrix are limited due to the fact that the cellulose is hydrophilic while the matrix is hydrophobic. The surfaces are thus not sufficiently compatible, leading to a reduction in mechanical properties. In this study, cellulose was surface treated with two types of silanes. Modified cellulose was used as filler in natural rubber composites. The influence of treated and untreated cellulose on the curing characteristics, rheological properties, mechanical properties and crosslinking density of natural rubber composites was examined. The curing characteristics of the natural rubber composites, the scorch time and cure times, decreased for natural rubber composites filled with modified cellulose compared with natural rubber composite filled with unmodified cellulose. The measured values of tensile strength and crosslinking density showed higher values for natural rubber composites filled with modified cellulose compared with natural rubber composite filled with unmodified cellulose. This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for "Centre for diagnostics and quality testing of materials" in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014+ code 313011W442.

Keywords: cellulose, natural rubber composites, surface treatment, curing behavior, tensile properties, biomaterials, silane, biopolymers

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Influence of maleinized rubber on the properties of elastomeric composites filled with biopolymer

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Abstract:

Cellulose as a biopolymer belongs to an effective filler for elastomeric composites. Its uniform dispersion in hydrophobic matrix of natural rubber, it is very difficult to achieve due to its hydrophilic character. Maleinized natural rubber is used to improve the interfacial adhesion between hydrophilic filler and a polymer matrix with a hydrophobic character. This work deals with the modification of the matrix of natural rubber with maleic anhydride and the preparation of elastomeric composites with partial substitution of natural rubber for maleinized rubber filled with cellulose. The influence of chemically modified natural rubber on the properties of elastomeric composite based on natural rubber (NR) filled with cellulose (CEL) was studied. Natural rubber was replaced by its modified form in contents of 2, 4, 6, 8 and 10 phr. Vulcanization characteristics, hardness, tensile strength, elongation at break, cross-linked density and degree of swelling, morphology were studied on the prepared composites. This research work has been supported by the Operational Program Integrated Infrastructure, cofinanced by the European Regional Development Fund by the project: Advancement and support of R&D for "Center for diagnostics and quality testing of materials" in the domains of the RIS3 SK specialization, Acronvm: CEDITEK II., ITMS2014 + code 313011W442.

Keywords: natural rubber, cellulose, modification, maleic anhydride, elastomeric composite.

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Pretreatment and modification of cellulose as a filler for elastomeric composites

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Abstract:

This study evaluates the changes in the properties of the prepared elastomeric composites. The vulcanization characteristics (minimum and maximum torque of the blends, processing safety of the blends, vulcanization speed coefficient and optimal vulcanization time) and physicomechanical characteristics (static tensile test change in strength and ductility and dynamic tensile test – using the DMA thermal method) were studied and evaluated. Natural rubber was filled by cellulose. The study of the properties of the filler-cellulose, was carried out on cellulose pretreated with ozone and cellulose modified by DCSBD plasma discharge. The mentioned pretreatment and modification are well feasible both in laboratory and industrial conditions. In addition, both represent a combination of environmentally, economically, and partly also technologically acceptable processes. The ideal setting/implementation of the pretreatment and modification of the filler, cellulose as filler, is crucial for achieving the best dispersion effect of the filler in the matrix – and thus for ensuring adequate adhesion between the filler and the matrix. At the same time, when vulcanizing rubber compounds, it is important that the blends effectively fill the mold cavities before the vulcanization itself begins. The increasing demand for materials with tailor-made properties, which must also meet multifunctional use, thus leads to the development of commercial elastomeric composites with fillers that mediate these properties. This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for "Centre for diagnostics and quality testing of materials" in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014+ code 313011W442.

Keywords: pretreatment, ozone, surface modification, DCSBD plasma, cellulose, natural rubber, composites, dynamic-mechanical analysis

Effect of surface modification conditions of cellulose on final properties of elastomeric composites

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Abstract:

Modification of fillers is used to improve the function of fillers in elastomeric composites. In the case of bio-fillers, this is often the only way to modify their properties for use in polymer blends and composites. Compared to commonly used inorganic fillers and carbon blacks, biofillers have several disadvantages, starting with their hydrophilic character and continuing with poor interfacial adhesion, which leads to lower values of physical-mechanical properties. With the help of modification, it is possible to affect the effect of bio-fillers in elastomeric blends or composites for the desired effect of improving properties. The effect of pH of individual raw materials forming elastomeric blends and composites is well described. In the case of biofillers, there is the possibility of influencing the dispersion of the filler in the matrix, as well as the resulting properties of the elastomeric blends and composites, due to the change of the fillers pH. In this work, cellulose as a bio-filler for natural rubber was modified using acetic acid and zinc oxide. Cellulose treated at different pH with zinc acetate content was added as a filler to the composite with natural rubber. The pH values of the modified cellulose affected the vulcanization process as well as the physicalmechanical properties of the prepared elastomeric composites. The result of the study is the possibility of using the modification of cellulose bio-filler for the preparation of elastomeric composites with improved properties compared to elastomeric composites prepared without filler modification. This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for "Center for diagnostics and quality testing of materials" in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014 + code 313011W442.

Keywords: natural rubber, cellulose, zinc acetate, surface modification, elastomeric composites.

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Characterization and Thermal Stability of Surface Modified Cellulose in Polymer Composites

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Abstract:

In recent years, cellulose has taken center stage of an increasing number of research papers devoted to understanding this material and its applications. Cellulose is an effective and environmental alternative material, which reduces the dependence on the conventional materials and protect our environment. From a chemical point of view, cellulose is biopolymer, which composed of polymer chains consisting of unbranched β-(1,4)-glycosidic linked D-glucopyranosyl building blocks, characterized by its hydrophilicity, biodegradability and its formation of versatile semicrystalline fiber morphologies [1, 2]. The main disadvantage of this biopolymer is poor water resistance, compatibility within the hydrophobic matrix and low mechanical strength. The free of hydroxyl groups on the cellulose surface allows for a wide range of surface modifications [3]. This work deals with the characterization and thermal stability of surface modified cellulose as filler in polymer composites. Two different silanes have been used for surface modification of cellulose due to their ability to react with the low number of free hydroxyl groups on the cellulose surface. The natural rubber (NR) composite filled with surface modified cellulose were characterized by TG/DSC, IR spectroscopy and scanning electron microscopy. This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for "Centre for diagnostics and quality testing of materials" in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014+ code 313011W442.

Keywords: thermal stability, cellulose, polymer composites, surface modification, silane, scanning electron microscopy

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Hybrid Implant with Improved Osseointegration Properties

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Abstract:

Osseointegrated implant usually relates to structural material with open spaces that enable osteoblasts and connecting tissue to migrate during natural bone growth. Subsequently, the bonding properties between the implant and natural bone can be significantly improved as illustrated in Figure 1. This in-vitro study aims to evaluate the potential of a Ti-6Al-4V lattice produced by selective laser melting (SLM) and infiltrated with biodegradable Zn-2%Fe alloy, as a hybrid Ti-Zn implant. The hybrid material was evaluated in terms of microstructure using scanning and transmission electron microscopy (SEM) and X-ray diffraction (XRD) analysis. The mechanical properties were exammined by compression strength while corrosion performance was evaluated in terms of immersion tests and electrochemical analysis (open circuit potential, potentiodynamic polarization and electrochemical impedance spectroscopy) in simulated physiological environment (phosphate buffered saline (PBS) solution). Cytotoxicity was evaluated by indirect and direct cell viability tests. The obtained results demonstrate the adequate performance of the hybrid Ti-Zn system as a non-cytotoxic structural material with acceptable mechanical integrity and corrosion rate degradation.

Keywords: osseointegration implants, additive manufacturing (AM), SLM, Ti-base lattice, bio-degradable implants, Zinc, orthopedic applications



Figure 1: Schematic illustration of the proposed osseointegrated implant.

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Radiative cooling of dark tone pigments with high near-infrared reflection properties

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Abstract:

Urban heat islands are receiving increasing attention in cities, resulting in detrimental ecological and environmental impacts, threatening the livability of cities. An important part of a building, paint absorbs and stores solar radiation and then favorably releases sensible heat into the atmosphere. This significantly alters the original surface energy balance and local microclimate, leading to different problems in different regions.

Radiant cooling emits infrared radiant heat into an atmospheric transparent window (8 to 13 μ m), which can lower the ambient temperature without polluting energy and the environment. In general, white coatings are the most effective countermeasure against daytime radiative cooling, as they strongly scatter visible light as well as nearinfrared light. However, in practical applications (such as cooling roofs and automotive coatings), dark-toned coatings are more commonly used because white coatings are prone to contamination and can cause glare problems. YInO3-based pigments can express various colors such as blue, green, and red by substituting various transition metals in the indium lattice and have high nearinfrared reflection properties. In this study, YInO3 (green and blue pigments) and FeO2 (red pigments) were mixed to prepare dark-tone pigments with high NIR reflectance. The optical and morphological properties of the resulting pigments were investigated by varying the weight ratio and calcination temperature. A dark tone pigment was coated on a transparent film and an aluminum substrate, and cooling properties were evaluated with commercially available pigments. The manufactured dark tone pigment has higher reflectance and higher heat shielding properties than commercially available pigments, so it can be used commercially.

Keywords: Radiative cooling, Pigment, Near Infra Red, Paints, Nanocomposites, Urban heat islands



Figure 1: Heat shielding properties of YInO3-based dark tone pigments.

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Prediction of Creep Behavior of Pressure-sensitive adhesives

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Abstract:

Because of the viscoelastic properties, pressuresensitive adhesives (PSAs) wet various adherends within a short contact time and feature high peel strength by dissipating the applied energy via plastic deformation accompanying fibrillation. In addition, high tack force, re-workability and excellent optical properties lead PSAs to be widely used for fabricating mobile devices such as smartphone and tablets. Given that the electronics are getting become lightweight and flexible, the demand for high-performance PSAs is increasing nowadays. Long-term stability is such a property of PSAs. Creep is a tendency of polymers to deform permanently over time when they are subject to a constant load. Therefore, the prediction of creep behavior of PSAs is crucial to judge the long-term stability of deformable multilayer films attached via PSAs. In this poster, a PSA film fabricated was subjected to a creep test under shear stress using a rheometer. The creep test results obtained were plotted as a form of deformation vs. time and then the kinetic parameters such as pre-exponential factor, apparent activation energy and exponents were attained. The effect of temperature on the creep strain rate of the PSA was evaluated using an equation including Arrhenius law [1]. The effect of stress on the rate was studied as well. The simulation curve plotted using the obtained kinetic parameters showed good fitting with the experimental data. In conclusion, the creep strain rate of the PSA increased with increasing temperature and applied stress. This study provides a useful method to predict long-term creep behavior of PSAs.

Keywords: Pressure-sensitive adhesive, Creep behavior, Simulation, Kinetic parameters

Reference:

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Skin Absorption Protective Silver Micro-particles as an Upcoming Nontoxic Antimicrobial Agent

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Abstract:

Many reports mentioned that the micro-sized Ag particles have less toxic effects than nano-sized Ag particles. Stable Hollow porous Ag microparticles (HOPO) were prepared and their shape and size distribution were characterized by TEM, SEM, and BET. The antimicrobial activity of HOPO was investigated against gram-positive and gram-negative bacteria compared with commercial silver nanoparticles (<10 nm) and with a conventional antimicrobial drug-like gentamycin. In this study, HOPO, Ag nanoparticles of the same concentrations were supplemented. As a result, both gram-positive and negative were the highest zone inhibited for HOPO than Ag nanoparticles and gentamycin. These results revealed that the HOPO can be used in diverse medical devices and antimicrobial control systems.

Keywords: nanoporous, covalenent organic framework, nanosheets, RNA, diseases, biomedical application, fluorescence



Figure 1: The figure illustrates, the hollow porous Ag microparticles give more antibacterial effects for both types of bacteria, compare to conventional Ag nanoparticles.

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A novel poly(3-hydroxyoctanoate) diclofenac decorated dressings for wound healing

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Abstract:

Human skin provides a peculiar protection against the external environment, making it vulnerable to damage. The resulting defects in the continuity of the skin sometimes require such restorations, which would be able not only to regenerate the resulting defect, but also to deliberately deliver the desired drug at the site of implantation. Our solution involves the use of a bacterial polymer - polyhydroxyoctanoate (P(3HO)) - a flexible polyester for skin regeneration¹. Polymers of this group are fully biocompatible and do not undergo rejection after transplantation. We have modified the bacterially produced P(3HO) polymer so that it is possible to controllably release the anti-inflammatory drug from a dressing created based on it. Here we used oligomers derived from the P(3HO) polymer covalently linked to diclofenac and bonded to the P(3HO) polymer matrix. The dressings thus prepared were thoroughly characterized in terms of physicochemical properties and then tested in in vitro and in vivo models. First, their safety - i.e. lack of cytotoxicity against fibroblast cells - was confirmed. Next, their effectiveness in wound healing in mice was tested. We showed that diclofenac-decorated dressings with P(3HO) help tissue integration and accelerate skin regeneration time. By integrating into the skin at the site of implantation, they create a natural architecture for tissue regeneration, which will be an asset in situations where large areas of skin have been damaged.

Keywords: wound healing; poly(3-hydroxyoctanoate); P(3HO); polyhydroxyalkanoates; porous patches; dressing materials; bioresorption; angiogenesis; CD68* macrophages.



Figure 1: Confocal microscope images showing cells growing inside dressings – cell nuclei (Hochest (blue)) – marked with white arrows, as well as fibronectin deposition (red) present in the healed tissue and P(3HO) / oli-dicP(3HO) dressing. Scale bars - 50µm.

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Polyhydroxyalkanoates – biodegradable and biocompatible polymers produced by environmental bacteria

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Abstract:

Polyhydroxyalkanoates (PHA) are polymers produced by various bacteria naturally found in soil, sediments and marine environment. PHAs are a large and diverse family of biodegradable and biocompatible polyesters that have been widely used in medicine, pharmaceutical industry and agriculture. They usually consist of (R)-3-hydroxy acids, which also makes them a valuable source of optically active and chirally pure compounds. So far, more than 150 different PHA monomers have been discovered, which contain various functional groups in their molecule. The type of polymer produced depends on a carbon source to which the bacteria have access during PHA biosynthesis, and the microbial strain itself. Based on the number of carbon atoms in their chain PHA polymers can be divided into three classes: short-chain length (up to five carbons into the chain, scl-PHA), medium-chain length (from 6 to 14 carbon atoms into the chain mcl-PHA) and long-chain length (more than 14 carbon atoms into the chain, lcl-PHA). Scl-PHA have been commercially used as food packaging, and materials in tissue engineering and implantology. Mcl-PHAs are the broadest group in the family of these polymers. These elastomers are most often used in the bioengineering of soft tissues and also as drug carriers. In the presented studies, two different PHA polymers were obtained: polyhydroxynonanoate (PHN) made of aliphatic 3-hydroxy acids, and polyhydroxyphenylvalerate (PHPV), the monomers of which have an omega-aromatic ring. Two culture strategies were used in the biosynthesis of these polymers. PHN was produced in a fed-batch reactor using Pseudomonas putida KT2440 strain. The carbon source was a mixture of nonanoic and butyric acid, and phosphate deficiency was the limiting factor in the medium. The strain used in the biosynthesis of PHPV was P. putida CA3, and the culture was carried out in a pulse-fed flask reactor. The carbon source used was the sodium salt of 5-phenylvaleric acid, and the culture medium had a limited amount of nitrates. The final cell dry weight (CDW) in the fed-batch reactor obtained 84,9 g L⁻¹, in which PHN content was

54,2%. The productivity of the culture was 1.43 g L⁻¹ h⁻¹. The content of aromatic PHA in *P. putida* CA3 bacterial cells was 2.8% higher than the amount of PHN polymer in CDW in *P. putida KT2440*. However, the amount of CDW in the pulse-fed flask reactor culture was significantly lower than that in the fed-batch reactor, which was 2.43 g L⁻¹.

Keywords: polyhydroxyalkanoates, PHA, biopolymers, polyhydroxynonanoate, PHN, polyhydroxyphenylvalerate, PHPV



Figure 1: Figure illustrating polyhydroxynonanoate obtained in 5 L bioreactor (Sartorius, Biostat B), extracted from CDW of *P. putida* KT2440 after 31 h of fermentation.

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Ultra Sensitive Sensor based on Single-walled Carbon Nanotube Field-effect Transistor for Detection of Endocrine Disruptors Nonylphenol

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Abstract:

Endocrine disruptors (EDs) are contaminants that may mimic or interfere with the body's hormones, hampering the normal functions of the endocrine system in humans and animals. For humans, these compounds may cause cancerous tumors and infertility. The traditional detection method such as enzyme linked immunosorbent assay (ELISA) and chromatography are currently the best technique for EDs detection due to their high sensitivity, robustness, and accuracy. Nevertheless, they have the disadvantage of being expensive and time-consuming, requiring bulky equipment or skilled personnel. Therefore, we proposed a simple, rapid, and sensitive electric sensor to detect one of the endocrine disruptors, Nonylphenol using peptide-modified singlewalled carbon nanotube field-effect transistor (swCNT-FET). The swCNTs were functionalized by noncovalent immobilization of the peptide aptamer using 1-pyrenebutanoic acid succinimidyl ester (PBASE) linker. The resulting FET sensors exhibited capable of label-free, rapid, highly selective, and ultrasensitive detection of nonylphenol. Moreover, our results show that the proposed sensor has the potential to measure endocrine disruptors in the aquatic environment.

Keywords: field-effect transistor (FET), singlewalled carbon nanotube, endocrine disruptors, peptide, biosensor



Figure 1: Figure is a schematic of the experimental method. The PBASE can bind by noncovalent π -stacking with the sidewall of swCNTs via its aromatic ring. The peptide aptamer probe molecule covalently binds to the linkers via its succinimidyl ester functional group. The reation between peptide and nonylphenol in swCNT-FET enables the swCNT-FET to detect nonylphenol selectively through the change of charge distribution on the CNT surface arising frome the chemical transformation.

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Hydrogen Peroxide Sensing of Prussian Blue/Graphene Quantum Dots Electrodeposition Electrode

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Abstract:

Herein, we proposed a novel sensor for the detection of hydrogen peroxide based on graphene quantum dots doped-Prussian blue by electrochemical deposition. Prussian blue (PB), which is composed of Fe²⁺, Fe3⁺, and cyanide coordinated and has a lattice structure, and graphene quantum dots were used as a dopant and supporting electrolyte to increase the stability of the PB lattice structure. Prussian blue nanoparticles and their analogs have a metal-organic framework (MOF), which scavenges reactive oxygen species through multiple enzyme-like activities such as catalase (CAT), peroxidase (POD), and superoxide dismutase (SOD). In this experiment, catalase (CAT) activity was mainly dealt with, because electron exchange between Fe²⁺ and H₂O₂ in PB is possible, which exhibits a Fentone reaction effect and enables electrochemical deposition. However, when the existing PB is used alone in the sensor, there are problems in that the electrodeposited thin film is unstable and the electrochemically deposited thick film deteriorates the electrochemical properties. Graphene quantum dots (GQDs) are nanometer-sized pieces of graphene that exhibit unique properties and are considered a new kind of quantum dots (ODs) because they are chemically and physically stable due to their intrinsic inert carbon properties. In addition, since GQDs can be doped with various elemental dopants such as nitrogen, sulfur, chlorine, fluorine, and potassium, the function of the material can be diversified. Therefore, we attached Li⁺ ions and K⁺ ions to the GQDs to preserve the electrochemical activity of PB, improve the stability of the lattice structure, and further optimize H₂O₂ sensing.

Keywords: Prussian Blue, Graphene quantum dots, crystal structure, Hydrogen Peroxide



Figure 1: This figure shows a Prussian Blue lattice structure coordinated with Fe^{2+} , $Fe3^+$, and cyanide, showing that ions attached to GQDs are used as dopant materials in the lattice structure.

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Electrochemical Aptasensor for Detection of EcoRV Based on rGO/GCE

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Abstract:

Herein, we reported a new electrochemical assay EcoRV an for the activity using electrochemically reduced graphene oxide (ERGO). EcoRV is a type II restriction endonuclease isolated from certain strains of Escherichia coli. Endonucleases are a family of hydrolyze enzymes that the internal phosphodiester in deoxyribonucleic acid (DNA) or ribonucleic acid (RNA). Therefore, EcoRV is crucial for DNA repair and replication. We carried out this investigation for this purpose. In this research, we used the electrochemical aptasensor ERGO/GCE (glassy carbon electrode) for the detection of EcoRV. The reason why using ERGO is eco-friendliness, high efficiency, energy-saving, and good controllability. We utilized methylene blue (MB) tagged doublestranded (ds) DNA with a single-stranded (ss) segment at the end for anchoring on graphene through π - π stacking for detection of EcoRV. Reduces the electrochemical current signal, after the EcoRV cleave dsDNA-MB. The EcoRV loosely binds DNA and scans for its recognition sequence. Once found, EcoRV kinks the DNA in a 50° angle and cleaves dsDNA-MB. EcoRV cleaves the sequence which is GAT^ATC. This method can detect qualitative assay, quantitative assay, and real-time.

Keywords: aptasensor, reduced graphene oxide, EcoRV, endonucleases



Figure 1: Schematic representation of ds-DNA with methylene blue target is attached by π - π stacking on the ERGO/GCE, and the target DNA is cleaved by EcoRV.

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First-principle calculations of DNA/RNA on MoOS Janus layer

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Abstract:

Sensing nucleobases through contact with the Janus MoOS monolayer is a novel concept in the field of biomaterials. Selective recognition of diverse types and sequences of deoxyribonucleic and ribonucleic acids (DNA and RNA) present in the human body is crucial and efficient in nanosensors for daily applications and is of vital importance. However, due to their dissimilar typical sandwich properties, two-dimensional (2D) layers such as MoOS single layer have displayed the interest of many researchers. In the current study, we investigated interaction energies and DNA sequencing properties at vacuum level. Additionally, we have extended these studies to solvated systems that present a different ionic energy and therefore a different bonding scheme compared to vacuum. In these cases, we have studied and compared the adsorption energy, interaction energy, and van der Waals energy as functions of the nucleobase affinity, involving van der Waals interactions driven by molybdenum d-orbitals to the actual MoOS monolayer. The exchange of weak electronic charges between the MoOS monolayer and the nucleobase molecules has been studied by means of Hirshfeld-I charge analysis. We found that the introduction of DNA/RNA nucleobase molecules alters the electronic properties of both oxygen and sulfur atomic-layers of the Janus MoOS complex systems as determined by plotting the 3D Kohn-Sham frontier orbitals. A good correlation has been found between the interaction energy, van der Waals energy, Hirshfeld-I, and dband center as functions of the nucleobase affinity and the interaction energy, suggesting an adsorption dominated by van der Waals interactions driven by molybdenum d-orbitals. Moreover, the lower adsorption energy leads to an active interaction with the dissimilar 1H-MoOS surfaces, accordingly its conduct to a shorter recovery time. Finally, the sulfur and oxygen layers on both sides of the MoOS monolayer displayed high level of selectivity for nucleobases in the biosensor modulation device. This study suggests that, in addition to graphene, dichalcogenides-Janus transition metals may also be suitable for detecting DNA/RNA bases in applied biotechnology.

Keywords: Janus material, 2D layer, DFT, molecular states, nucleobases, DNA/RNA.



Figure 1. The sensitivity of the nucleobases molecules on the Janus MoOS monolayer facets at T = 298 K, (a) on O layer, (b) on S layer, respectively.

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Deep Learning Assisted Protein Entanglement Prediction based on Gauss Linking Integral Matrix

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Abstract:

Topology and geometry play an important role in determining the functional properties of proteins. Natural proteins with nontrivial topologies like lassos, knots, and links have exhibited unique functional benefits including enhanced stability, controlled quaternary structure, and dynamic switching properties. Based on the fact that most natural proteins exist as linear chains and the artificial synthesis of proteins with certain topologies is largely constrained by the limited number of entangled structure motifs as precursors, it is essential to develop more entangled protein structures. Recently, the great success AlphaFold2 achieved in protein structure prediction has drawn wide attention to the use of deep learning algorithms in the protein science field which allows high-throughput analysis. In this work, we develop a deep-learning model to predict a homogenous dimer's entanglement features based solely on its amino acid sequence (Figure 1). We adjust AlphaFold-Multimer's model framework and transfer its prediction target from structures to entanglement properties. Since Gauss linking integral (GLN) method is a commonly used approach to studying the geometry and topology of proteins, we design our label in the form of a GLN matrix, which provides entanglement information of not only two whole chains, but also any subchains of this dimer. The model will allow us to effectively detect entanglement in protein dimers, which helps explore more entangled protein structures and boosts the synthesis of novel topological proteins.

Keywords: topological proteins, entanglement properties, deep learning algorithm, AlphFold-Multimer, Gauss linking integral, homogenous dimer.



Figure 1: Figure illustrating the idea of developing a neural network to predict entanglement properties from the protein sequence with the aim of discovering novel entangled structures.

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Aaryl 1-(Methoxymethyl)Vinyl Ketone-based Corrosion Inhibitor for Mitigating Acidic Corrosion During Well Stimulatio

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Abstract:

Acid stimulation fluids such as hydrochloric (HCl) acid and organic acids have been widely used to stimulate carbonate reservoirs. Due to the high corrosion rate of these acids, it is indispensable to add a corrosion inhibitor (CI) to minimize the corrosion rate, thereby protecting the tubular. The objective of this study is to evaluate new corrosion inhibitors over a wide range of parameters, including the CI concentration, temperature, and type of acid. The performance of Aaryl 1-(methoxymethyl) vinvl ketones-based corrosion inhibitor chemistries was investigated using the gravimetric method in different HCl acid concentrations i.e. 3.5 wt%, 15 wt% and 20 wt%. Besides, the corrosion efficiency was investigated in organic acids (acetic acid, methanesulfonic acid) and mixtures of HCl and organic acids at temperatures of (60°C to 90°C). The progress of the reaction was monitored based on the weight loss at different times. The inhibition efficiency (IE%) was calculated by the weight loss at the end of the experiments.

The weight loss revealed that some corrosion inhibitors showed promising inhibition results at high temperatures and high HCl acid concentrations. As expected, increasing the HCl acid concentration resulted in severe corrosion and had a negative impact on the performance of some corrosion inhibitors. On the other hand, the inhibition efficiency was significantly improved as a result of increasing the corrosion inhibitor concentration from 200 to 500 ppm. Some tested corrosion inhibitors managed to provide around 97 % inhibition efficiency. The performance of the CI in the organic acids were better than that in HCl acid as expected due to the difference in the corrosivity of the tested acids, apart from methanesolfonic acid where the corrosion rate was high regardless of presence or absence of corrosion inhibitors.

The synthesized CIs showed high inhibition efficiency and was thermally stable at the tested conditions. The characterization of these CIs and the detailed inhibition results would lead to further development of CIs for high temperature applications.