



THE SECOND INTERNATIONAL CONFERENCE OF NANOTECHNOLOGY FOR
ENVIRONMENTAL PROTECTION & CLEAN ENERGY PRODUCTION



CERTIFICATE OF PARTICIPATION

THIS CERTIFICATE IS PROUDLY PRESENTED TO

Sihem Menassel

FOR ATTENDING THE SECOND INTERNATIONAL CONFERENCE OF NANOTECHNOLOGY FOR ENVIRONMENTAL
PROTECTION & CLEAN ENERGY PRODUCTION HELD AT THE FRÈRES MENTOURI UNIVERSITY-CONSTANTINE 1,
ALGERIA ON OCTOBER 09-10TH, 2023 WITH POSTER REPORT ENTITLED:
"MORPHOLOGY AND SUPERCONDUCTIVITY STUDIES OF BSGO WITH SN DOPING"
THE INCLUDED CO-AUTHORES RESPECTIVELY ARE: S. CHETIOUL, S.P.ALINTAS AND C. TERZIOGLU.

DATE
10/10/2023



SMAIL HAMAMDA
GENERAL CHAIR



Nº 080



People's Democratic Republic of Algeria
Frères Mentouri University–Constantine 1, Algeria
Faculty of Exact Sciences



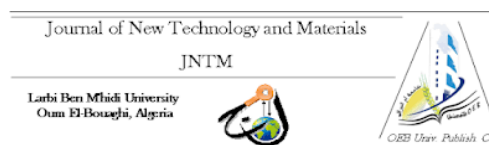
Conference Program

**The Second International Conference of Nanotechnology for
Environmental Protection and Clean Energy Production “ICNEP’2023”**

Organized by:

**Laboratory of Thermodynamics and Surface Treatments of Materials “LTTSM”, Frères
Mentouri University–Constantine 1, Algeria**

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Constantine, Algeria – October 09-10th, 2023

ICNEP'2023: The 2nd International Conference of Nanotechnology for Environmental Protection and Clean Energy Production

Frères Mentouri University–Constantine 1, Road of Ain El Bey, 25017, Algeria

Web site: <https://www.umc.edu.dz/index.php/fr/component/k2/item/3504-icnep-2023>

email : ICNEP2023@gmail.com



ICNEP'2023 Technical program

	08H30 09H00	09H00 09H30	09H30 10H00	10H00 10H45	10H45 13H00	13H00 14H00	14H00 14H45	14H45 16H30	16H30 16H45	16H45 18H00
Monday Oct. 09th, 2023	Registration	Opening	Coffee Break	PS1 : Amphi Pr. Yu. I. Sementsov	Amphi : Oral Ids : 42, 84, 98	Lunch	PS2 : Amphi Pr. S. G. Nedilko	Amphi : Oral Ids : 22, 78, 47	Coffee Break	Space-1 : Poster Ids : 1, 6, 16, 44, 45, 46, 54, 55, 72, 77, 99, 102, 103
					Amphi : Oral Ids : 93, 25, 36			Amphi : Oral Ids : 48, 86		Space-2 : Poster Ids : 4, 27, 35, 51, 52, 63, 65, 70, 74, 90, 91, 100, 116
					Amphi : Oral Ids : 7, 85, 26			Amphi : Oral Ids : 33, 12		Space-3 : Poster Ids : 2, 13, 14, 20, 61, 83, 88, 89, 96, 105, 108, 111, 113, 114, 18, 19
		09H00 09H45	09H45 10H30	10H30 10H50	10H50 12H00	12H00 12H30				
Tuesday Oct. 10th, 2023		PS3 : Amphi Pr. K. O. Ivanenko	PS4 : Amphi Dr. A. Settar	Coffee Break	Space-1 : Poster Ids : 17, 23, 24, 39, 40, 41, 79, 97, 107, 112, 115, 117	Closing	Lunch			
					Space-2 : Poster Ids : 3, 5, 21, 37, 38, 49, 50, 53, 67, 75, 76, 92, 28, 29, 30, 31					
					Space-3 : Poster Ids : 9, 10, 11, 15, 56, 57, 80, 87, 94, 95, 101, 104, 106, 58, 59, 60, 64, 68, 69, 71, 73, 81, 82, 119, 120					

- PS: Plenary session
- SO: Oral Session
- SP: Poster Session

Ids: paper's identification number

Space-1,2,3: Space's number to place Posters



PLENARY Sessions program

**The Second International Conference of Nanotechnology for
Environmental Protection and Clean Energy Production
(ICNEP'2023)**

Regular Plenary Session 01

Pr. Yu. I. SEMENTSOV

Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute, Ningbo University of Technology, Ningbo, China
Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, Ukraine

Title:

**The Carbon Nanotubes, Graphene Nanoparticles their
Oxygen Modified Forms and Composites**

Regular Plenary Session 02

Pr. S. G. NEDILKO

Taras Shevchenko National University of Kyiv, Kyiv, 01601, Ukraine

Title:

**Study of interphases in dielectric nanocomposites:
Luminescent aspect**



Regular Plenary Session 03

Prof. K. O. IVANENKO

Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, Ukraine

Title:

**Estimation of The Percolation Threshold and its
Influence on the Properties of Epoxy Resin-Based
Polymer Composite Materials Filled Carbon Fibers and
Carbon Nanotubes**

Regular Plenary Session 04

Dr. Abdelhakim Settar

INSA Centre Universite Oleans, France.

Title:

**Experimental Investigation of Conductive Heat Transfer
and Fire Protection in a Polymer-Based Plate Heat
Exchanger**



Monday 09th, October 2023

Conference Room-500 Places

09h00 - 09h30

OPENING

Plenary Session 01

Chairs: Pr. Hamamda Smail and Pr. Kara Ali Ahcene

09h30-10h15	The Carbon Nanotubes, Graphene Nanoparticles their Oxygen Modified Forms and Composites Pr. Yu. I. SEMENTSOV	ICNEP'2023 SP1
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Coffee Break: 10h15 - 10h45

Monday 09th, October 2023

Conference Room – 500 Places

Session 01: Oral Presentation

Chairs: Pr. Smail Hamamda and Pr. Ahcene Kara Ali

10h45- 11h00	Effect of dip-coating Seed Layer on the Morphological and Optical Properties of ZnO Nanorods Growth by Hydrothermal Method <i>Aldhehabi, Samer Abdulsalam*; Belkerk, Boubakeur Essedik</i>	ICNEP'2023 ID_42
11h00- 11h15	HMDSO/ZnO-graphene heterostructure coated quartz crystal microbalance transducer for VOCs Sensing <i>Grine, Leila*; BELLEL, Azzedine; Boutamine, Meriem Meriem; Sahli, Salah</i>	ICNEP'2023 ID_84
11h15- 11h30	Synthesis and Characterization of doped and c-doped ZnAl₂O₄ Nanoparticles using Sol-Gel Method <i>Nada Belmokhi, Ahcene Kara Ali</i>	ICNEP'2023 ID_98
11h30- 11h45	Impact of High temperature and Germanium rate on the electrical performance of the SiGe Heterojunction Bi-polar Transistor with DPSA-SEG architecture <i>Chems El Ghizlane, Lachkhab*; Maya, Lakhdara; Boulgheb, Abdelaaziz; Latreche, Saida</i>	ICNEP'2023 ID_93
11h45- 12h00	Study of interphases in dielectric nanocomposites: Luminescent aspect <i>Nedilko, Serhii G.*</i>	ICNEP'2023 ID_25
12h00- 12h15	Effect of Fe₂O₄ Nanoparticle on Electronic Cooling: Numerical Investigation of nanofluid Flow Through a Heat Sink <i>Bouacida, Touba T.*; Bessaih, Rachid</i>	ICNEP'2023 ID_36



12h15- 12h30	Deposition of Copper Oxide Thin Films by Spray Polaris Technique and by Copper Chloride Solution for Different Spray Number <i>Nour Elhouda, Ketita*</i>	ICNEP'2023 ID_07
12h30- 12h45	Numerical investigation of Laminar Forced Convection Heat Transfer Nanofluids Flow Using Different Base Fluids <i>Laichi, Ammar*</i>	ICNEP'2023 ID_85
12h45- 13h00	Estimation of The Percolation Threshold and Its Influence on the Properties of Epoxy Resin-Based Polymer Composite Materials Filled Carbon Fibers and Carbon Nanotubes <i>Makhno, Stanislav; Lisova, Oksana; Gorbyk, Petro; Shi, Yuli; Ivanenko, Kateryna*; Sementsov, Yurii</i>	ICNEP'2023 ID_26

LUNCH: 13h00 - 14h00

Monday 09th, October 2023

Conference Room – 500 Places

Plenary Session 02:

Chairs: Pr. Hamamda Smail and Pr. Kara Ali Ahcene

14h00-14h45	Study of Interphases in Dielectric Nanocomposites: Luminescent Aspect Pr. S. G. NEDILKO	ICNEP'2023 SP2
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Monday 09th, October 2023

Conference Room – 500 Place

Session 02: Oral Presentation

Chairs: Pr. Smail Hamamda and Pr. Ahcene Kara Ali

14h45- 15h00	Elaboration of a Reduced Graphene Oxide–Chitosan Biocomposite <i>Abdallah, Cheraitia*; Maroua, Mezrag; Roquiya , Laghrib</i>	ICNEP'2023 ID_22
15h00- 15h15	Development of Tubular Membranes from Local Terracotta Clays – Guelma <i>Abdallah, Cheraitia*; Roquiya , Laghrib ; Manal, Bouhdjar; Roumayssa , Gaoua</i>	ICNEP'2023 ID_78
15h15- 15h30	Enhanced Photocatalytic Degradation of an organic Dye Using Novel Heterojunction p-n: Experimental and Theoretical Investigations <i>Ahmia, Nada*</i>	ICNEP'2023 ID_47
15h30- 15h45	Heat Transfer Enhancement in a Parabolic Trough Solar Collector Using Inner wall Fins and Nanofluids	ICNEP'2023 ID_48

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email : ICNEP2023@gmail.com



	<i>Diafi, Halla H*</i>	
15h45- 16h00	Finite-Control-Set Model Predictive Control (FCS-MPC) and Fuzzy Self-Adaptive PI Controller (FSA-PIC) For Wind Turbine System Based On Doubly-Fed Induction Generator (DFIG) <i>Amira, Aggoune*; Berrezek, Farid; Khelil, Khaled</i>	ICNEP'2023 ID_86
16h00- 16h15	The Fabrication of Floating Titania Co-Doped Fe/Diatomite Granule Catalyst with Enhanced Photocatalytic Efficiency Under Visible Light Irradiation <i>REZIG, Walid*</i>	ICNEP'2023 ID_33
16h15- 16h30	The Carbon Nanotubes and Graphene Nanoparticles their Oxygen Modified Forms and Composites <i>Shi, Yuli; Hrebena, Yuliia; Demianenko, Eugeniy; Makhno, Stanislav; Ivanenko, Kateryna; Hamamda, Smail; Terets, Mariya; Kartel, Mykola; Sementsov, Yuri*</i>	ICNEP'2023 ID_12

Coffee Break: 16h30 - 16h45

Monday 09th, October 2023

Space 1

Session 03: POSTER SESSION

Chairs: Pr. Smail Hamamda and Pr. Ahcene Kara Ali

16h45- 18h00	Synthesis and characterization of CaTiO₃ powder prepared by Sol-Gel <i>Besma, MIHOUBI*, Ahcene Kara Ali</i>	ICNEP'2023 ID_01
16h45- 18h00	Synthesis and characterization of amorphous nanocrystalline Fe₇₃Si₁₅Ti₅B powders by mechanical alloying <i>Abdelhak, Chebli*</i>	ICNEP'2023 ID_06
16h45- 18h00	Synthesis and Characterization of ZnO(1-x) Ni(x=0.01-0.03) Nanofilms under Specific Conditions: Enhancement of Red Emission, and Photodegradation Retarding Behavior <i>ouhaibi, abdelhalim*; Bachir eddine, MESSAID; serhane, rafik; Zoukel, Abdelhalim; ZELLAGUI, Abderzak</i>	ICNEP'2023 ID_16
16h45- 18h00	X ray diffraction study of structural properties of Fe₈₆Cr₁₄ mechanical alloys, Effect of process control agent <i>Ayad, Mohammed Elamine*</i>	ICNEP'2023 ID_44
16h45- 18h00	Synthesis and Carcterisation of Magnesium Oxide Thin Film Nano-Material by Sol-Gel Method <i>AOUATI, Redha*</i>	ICNEP'2023 ID-45
16h45- 18h00	Synthesis, Crystal Structures, Luminescence and Magnetic Properties of Isostructural Fe (II) and Co (II) Complexes Based on a Tetradentate Ligand <i>Saadallah, Yaakoub*; setifi, zouaoui; Addala, Abderezak; setifi, fatima</i>	ICNEP'2023 ID-46
16h45- 18h00	Synthesis, crystal structure and Hirshfeld surface analysis of a new coordination complex with 4-nitroaniline <i>rouag, raounek*</i>	ICNEP'2023 CSE-54



16h45- 18h00	Nonlinear optical response in aluminum nitride nanocages <i>zaidi, meriem*; hannachi, douniazed; chermette, henry</i>	ICNEP'2023 ID-55
16h45- 18h00	Synthesis of copper with sodium ascorbate and its application in malachite green degradation <i>Meriem , Hamidani*</i>	ICNEP'2023 ID-72
16h45- 18h00	Synthesis, characterization and chemical-sensor applications of zinc oxide-graphene nanocomposite <i>Boutamine, Meriem*</i>	ICNEP'2023 ID-77
16h45- 18h00	Synthesis and Characterization of Fe₃O₄ Nanoparticles using Solvothermal Method <i>Esmâ Aliouat</i>	ICNEP'2023 ID-99
16h45- 18h00	Synthesis and characterization of pure BaTiO₃ Na-noparticles and doped with La³⁺ and Mn²⁺ prepared by Sol-Gel method <i>Bazine Abdelmajide</i>	ICNEP'2023 ID-102
16h45- 18h00	Synthesis and characterization of pure CaTiO₃ powders and doped by Mg²⁺ and Mn²⁺ prepared by Sol-Gel route <i>Nada Belmokhi</i>	ICNEP'2023 ID-103

Monday 09th, October 2023

Space 2

Session S3: POSTER SESSION

Chairs: Pr. Smail Hamamda and Pr. Ahcene Kara Ali

16h45 - 18h00	Structural, electronic, optical and thermodynamic properties of SrxCa1-xO, BaxSr1-xO and BaxCa1-xO alloys <i>Amine, ghebouli Mohamed*</i>	ICNEP'2023 ID_04
16h45 - 18h00	Ab initio calculations of electronic properties of non-stoichiometric CdmTen clusters <i>Deva, Liliya; Semkiv, Ihor; Kashuba, Andrii*</i>	ICNEP'2023 ID_27
16h45 - 18h00	Stability Analysis of Gradient Zone of a Solar Pond <i>Ouzani, Riadh*</i>	ICNEP'2023 ID_35
16h45 - 18h00	Ab-initio calculations of the structural and electronic properties for t-Se and t-Se containing a defect <i>MEKAHLIA, Mahira L*</i>	ICNEP'2023 ID-51
16h45 - 18h00	Ab-initio calculations of the structural and electronic properties of the t-Se1-xTex system for low concentration (x = 0.03, 0.04 and 0.08) <i>MEKAHLIA, Mahira L*</i>	ICNEP'2023 ID-52
16h45 - 18h00	Preparation and characterization of Novel Hybrid Semiconducting nanocomposite <i>AIT RADi, Massillia*</i>	ICNEP'2023 ID_63
16h45 - 18h00	Fe₂HfZ (Z=Si, Ge, Sn), promising new candidates materials for electronic and thermoelectric applications <i>DJENNANE, KHAOUALA*; Dehimi, Nour El Houda; MELIANI, KAWTHER; Dehbaoui, Mourad</i>	ICNEP'2023 ID_65



16h45 - 18h00	Physical properties of TiO₂ Nanotubes grow in different electrolytes by varying anodizing parameters <i>FRAOUCENE, Henia*</i>	ICNEP'2023 ID_70
16h45 - 18h00	Optical and structural properties of self- organized TiO₂ nanotubes <i>FRAOUCENE, Henia*</i>	ICNEP'2023 ID_74
16h45 - 18h00	First-principles calculations of structural, elastic and electronic properties of cubic CsBeI₃ compound <i>Meziani, Amel*</i>	ICNEP'2023 ID_90
16h45 - 18h00	Electronic Properties and Magnetic Stability in Binary Iron Pnictide <i>Nabila, BENMEDDAH*</i>	ICNEP'2023 ID_91
16h45 - 18h00	Improvement of the optical and photocatalytic properties of ZnAl₂O₄: 1% La³⁺, x% Pb²⁺nanoparticles synthesized by citrate sol-gel route <i>Hichem Filali</i>	ICNEP'2023 ID_100
16h45 - 18h00	Correlation between structural and Optical properties of CuO nanoparticule prepared by Sol-Gel method: Degradation of Mythylene blue <i>Fouzia Abbas</i>	ICNEP'2023 ID_116

Monday 15th, October 2022

Space 3

Session 03: POSTER SESSION

Chairs: Pr. Smail Hamamda and Pr. Ahcene Kara Ali

16h45 - 18h00	Optimizing Maximum Power Point Tracking of Partially Shaded Photovoltaic Module using hybrid P&O-FPA MPPT <i>bettahar, fares*</i>	ICNEP'2023 ID_02
16h45 - 18h00	formulation and optimization of sustained release microparticles of ketoprofen <i>BADAoui, FATIMA ZOHRa*</i>	ICNEP'2023 ID_13
16h45 - 18h00	Modeling of the elements of the photovoltaic pumping system <i>karima, chebli ch*</i>	ICNEP'2023 ID_14
16h45 - 18h00	High photovoltaic performance of InGa_N solar cells <i>ANNAB, Nassima M*</i>	ICNEP'2023 ID_20
16h45 - 18h00	Thermographic method of modeling the features of airflow in NPP air filters <i>Azarenkov, Mykola; Kolenov, Ivan*; Chupikov, Anatoly; Lytvynenko, Volodymyr V; Sokolenko, Volodymyr; Roskoshna, Olena; Shatov, Valeriy; Galuza, Alexey</i>	ICNEP'2023 ID_61
16h45 - 18h00	Design of a new photo-diode based on (α-PbO)/(α-SnO) lateral heterostructure <i>Bakhtatou, Ali*</i>	ICNEP'2023 ID_83



16h45 - 18h00	Heat Transfer by Natural Convection Under Constant Heat Flux Wall in a Semi-Annular Shaped Enclosure Filled with a Hybrid Nanofluid Allouche, Bilel*	ICNEP'2023 ID_88
16h45 - 18h00	A Comprehensive Analysis of MWCNT-Al Nanocomposites: Structural Properties soror, Saadallah sousou*; Smail, Hamamda; Kelthoum, Saadallah; Mohamed Cherif, Bouleklab	ICNEP'2023 ID_89
16h45 - 18h00	Structural and morphology characterization of an EVA/ZnO polymer in thin film form for solar applications Lyes, Maifi*; AYADI, AICHA; Ouided, Hioual; Zaina, MAZINE; kamel, agroui M; abdelhamid, Chari	ICNEP'2023 ID_96
16h45 - 18h00	Hybrid magnetic nanoparticles for antitumor drug delivery Kheira ZANOUNE	ICNEP'2023 ID_105
16h45 - 18h00	Multiwalled Carbon Nanotubes Concentration Influence on Aluminum Thermodynamics Properties Yassin Naoui	ICNEP'2023 ID_108
16h45 - 18h00	Environmental Protection by the Adsorptive Elimination of basic violet 3 dye from Water: equilibrium and kinetic study Kelthoum Saadallah	ICNEP'2023 ID_111
16h45 - 18h00	Hybrid systems in the various renewable energy sources Souad Belhour	ICNEP'2023 ID_113
16h45 - 18h00	Integration of photovoltaic panels and Biodigesters Souad Belhour	ICNEP'2023 ID_114
16h45 - 18h00	Analysis of Thermophysical and Structural Characteristics of Organosilica Nanocomposites Roman, Dinzhos*; Fialko, Nataliia; Lazarenko, Maxim; Parkhomenko, Olexander; Darmosiuk, Valentyna; Nedbaievska, Liudmyla; Mankus, Irina; Makhrovskiy, Volodymyr; Vasil'eva, Larisa	ICNEP'2023 ID_18
16h45 - 18h00	Non Isothermal Crystallization of Polymer Nanocomposites Based on Polycarbonate Filled with Carbon Nanotubes Roman, Dinzhos*; Fialko, Nataliia; Lazarenko, Maxim; Parkhomenko, Olexander; Darmosiuk, Valentyna; Nedbaievska, Liudmyla; Mankus, Irina; Makhrovskiy, Volodymyr; Vasil'eva, Larisa	ICNEP'2023 ID_19

Tuesday 10th, October 2022

Conference Room – 500 Places

Plenary Session 03

Chairs: Pr. Nadir Bellel and Dr. Tahar Dorbani

09h00 - 09h45	Estimation of The Percolation Threshold and its Influence on the Properties of Epoxy Resin-Based Polymer Composite Materials Filled Carbon Fibers and Carbon Nanotubes Prof. K. O. IVANENKO	ICNEP'2023 SP3
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Plenary Session 04

Chairs: Pr. Nadir Bellel and Dr. Tahar Dorbani

09h45 - 10h30	Experimental Investigation of Conductive Heat Transfer and Fire Protection in a Polymer-Based Plate Heat Exchanger Dr. Abdelhakim SETTAR	ICNEP'2023 SP4
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Coffee Break : 10h30 - 10h55

Tuesday 10th, October 2023

Space 1

Session 04: POSTER SESSION

Chairs: Pr. Nadir Bellel and Dr. Tahar Dorbani

10h55 - 12h00	Effect of calcination temperature on structural, morphological and optical properties of compound powder ZnO-Al₂O₃ <small>AYADI, AICHA*; Lyes, Maifi; ZAIBET, Esma; CHARI, ABDALHAMID</small>	ICNEP'2023 ID_17
10h55 - 12h00	Effect of fiber surface treatment on the mechanical properties of palm petiole fiber/LLDPE composites <small>Debabeche, Nadja*</small>	ICNEP'2023 ID_23
10h55 - 12h00	Effects of the Solvent and Calcination Temperature on LaFeO₃ Catalysts for Methanol Oxidation <small>Mahmoud, Lebid*</small>	ICNEP'2023 ID_24
10h55 - 12h00	Experimental Study on the Effect of Drying on the Kinetics of Cubic Beetroot Slices Using an Industrial Electric Food Dehydrator <small>boultif, soufounizia*; Belghar, Noureddine; Chabane, Foued</small>	ICNEP'2023 ID_39
10h55 - 12h00	Effect of silver doping on structural properties of (La, Sr) MnO₃ cathode material <small>boufenchouche, Ranya*; BOUDJADIA, Yazid; AMIRA, Abderrezak; VARILCI, Ahmet; POLAT-ALTINTAS, Sevgi</small>	ICNEP'2023 ID_40
10h55 - 12h00	Structure, Microstructure and Mossbauer studies of (Ni₆₀Co₄₀)_{100-x} Fex system Synthesized by Hydrothermal Method: Effect Fe content <small>BELKOFI, Reguia*</small>	ICNEP'2023 ID_41
10h55 - 12h00	Structural and hydrophobic properties of Cobalt doped ZnO thin films prepared by electrodeposition method <small>BELAMRI, Zehira*</small>	ICNEP'2023 ID_79
10h55 - 12h00	The effect of the marine environment on the durability of the precast concretes of the Taksebt dam <small>BEN AMMAR, Ben Khadda *</small>	ICNEP'2023 ID_97



10h55 - 12h00	Experimental investigation of conductive heat transfer and fire protection in a polymer-based plate heat exchanger <i>Bouchra Elarfaoui</i>	ICNEP'2023 ID_107
10h55 - 12h00	Optical and structural properties of Co doped ZnO thin films grown by spray pyrolysis method <i>Halima Djaaboube</i>	ICNEP'2023 ID_112
10h55 - 12h00	Effect of Ni -doping on ZnO nanostructures properties <i>Sonia Attaf</i>	ICNEP'2023 ID_115
10h55 - 12h00	The effect of precursor concentration on the morphological, phases and crystalline structures proprieties of iron oxides nanoparticles prepared via eco-friendly method <i>Leila Boumaza</i>	ICNEP'2023 ID_117

Tuesday 10th, October 2023

Space 2

Session 04: POSTER SESSION

Chairs: Pr. Nadir Bellel and Dr. Tahar Dorbani

10h55 - 12h00	Bifurcation in a Porous Cavity <i>Dalila, Menacer*</i>	ICNEP'2023 ID_03
10h55 - 12h00	Evaluation of the catalytic activity of two catalysts supported on crude and ground diatomite <i>Massinissa, ADJISSA*</i>	ICNEP'2023 ID_05
10h55 - 12h00	Preparation, structure and luminescence properties of "microcrystalline cellulose - K3Tb(PO4)2" composites <i>Chornii, Vitalii P*; Nedilko, Serhii G.; Terebilenko, Kateryna; Zozulia, Valeriia; Boyko, Volodymyr; Zhydachevskyy, Yaroslav; Suchocki, Andrzej</i>	ICNEP'2023 ID_21
10h55 - 12h00	Enhancing Photoluminescence and Crystallinity through Aluminum Doping in Sol-Gel Zinc Oxide Thin Films <i>Ibrahim Yaacoub, bouderbala*; Bouras, Imed Eddine</i>	ICNEP'2023 ID_37
10h55 - 12h00	Structural Characterization of Chlorine Doped Cuprous Oxide Thin Films by X-ray Diffraction and X-ray Fluorescence <i>Bouras, Imed Eddine*; Ibrahim Yaacoub, bouderbala</i>	ICNEP'2023 ID_38
10h55 - 12h00	Laser-assisted electrodeposition of composite carbon-containing nickel coatings <i>Tytarenko, Valentina*</i>	ICNEP'2023 ID_49
10h55 - 12h00	Advances of Mayer's cluster approach in quantitative theoretical description of phase transitions for various lattice models of matter <i>Ushcats, Michael V*; Ushcats, Svitlana; Kondratieva, Anna</i>	ICNEP'2023 ID_50
10h55 - 12h00	Comprehensive Investigation of ZnS: Structural Properties, Elastic Constants, and Their Crucial Role in Environmental Protection and Clean Energy Production <i>Benlakhdar, Faiza*</i>	ICNEP'2023 ID_53

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email : ICNEP2023@gmail.com



10h55 - 12h00	Electrochemical Measurements of Maghemite Nanostructured fibers for Energy Storage Applications <i>mounia, boufas*; Ouanassa, GUELLATI; Mohammed, guerioune; aicha, harat</i>	ICNEP'2023 ID _67
10h55 - 12h00	Elaboration and Characterization of Thermoelectric Materials <i>benidir, meriem*; Makhloufi, Sofiane; Omari, Mahmoud</i>	ICNEP'2023 ID _75
10h55 - 12h00	Elaboration and Thermoelectric Properties of NdCoO₃ Oxides <i>Bouaziz, Souhir*</i>	ICNEP'2023 ID _76
10h55 - 12h00	Gel polymer electrolyte materials based on polyethylene glycol, LiBF₄ and gelatin for renewable electrochemical devices <i>Lysenkov, Eduard A.*</i>	ICNEP'2023 ID _92
10h55 - 12h00	The Mathematical Modeling for Firocoxib Coo(Oh)-Assisted Determination in Milk and Meat Products <i>Tkach, Volodymyr V*; Kushnir, Marta; Ferrão da Paiva Martins, José Inácio; Garcia, Jarem Raul; Melnyk, Oleksii; Melnyk, Maria; KARAKOYUN, Necdet ; Melnyk, Oleg; Monteiro, Maria João; Ivanushko, Yana; Yagodynets, Petro</i>	ICNEP'2023 ID _28
10h55 - 12h00	The Theoretical Evaluation for Bromfenac Determination in Tears and Eye Drops over Copper Sulfide Nanoparticles <i>Tkach, Volodymyr V*; Kushnir, Marta; Ferrão da Paiva Martins, José Inácio ; Garcia, Jarem Raul; KARAKOYUN, Necdet ; Monteiro, Maria João; Ivanushko, Yana; Yagodynets, Petro; Melnyk, Oleg; Melnyk, Maria; Melnyk, Oleksii; Morozova, Tetiana</i>	ICNEP'2023 ID _29
10h55 - 12h00	The Theoretical Description of Letrozol Potentiometric Determination, Assisted by a Rhenium-Polymer Composite <i>Tkach, Volodymyr V*; Palytsia, Yulia; Ferrão da Paiva Martins, José Inácio; Garcia, Jarem Raul; Kushnir, Marta; de Oliveira, Silvio; LUGANSKA, OLGA; Kopiika, Vira; Yagodynets, Petro; Morozova, Tetiana</i>	ICNEP'2023 ID _30
10h55 - 12h00	The Mathematical Modeling for Sucralose (E955) Sweetener Potentiodynamic Cathodic Removal <i>Tkach, Volodymyr V*; Lavryk, Ruslan; Storoshchuk, Nataliia; Ferrão da Paiva Martins, José Inácio; Garcia, Jarem Raul; KARAKOYUN, Necdet ; Morozova, Tetiana; Ivanushko, Yana; Yagodynets, Petro</i>	ICNEP'2023 ID _31

Tuesday 10th, October 2023

Space 3

Session 04: POSTER SESSION

Chairs: Pr. Nadir Bellel and Dr. Tahar Dorbani

10h55 - 12h00	Hydrothermal synthesis and characterization of nanostructured CdSe: Effect of annealing treatment <i>BOUCHAREB, Hasna*</i>	ICNEP'2023 ID _09
10h55 - 12h00	The Efficiency of the Thermal Activation of a Biomaterial for the Elimination of Pollutants <i>CHERGUI, yamina*</i>	ICNEP'2023 ID _10
10h55 - 12h00	Numerical investigation of free convection inside a hexagonal enclosure filled with nanofluid (water-cu) under effect of the position of the inner obstacle	ICNEP'2023 ID _11

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	<i>benhanifia, kada*</i>	
10h55 - 12h00	Electronic properties of MAX phase materials Ti₂AlC and Ti₂AlB <i>Blilita, Sofiane*</i>	ICNEP'2023 ID _15
10h55 - 12h00	Preparation and investigation of structural properties of lanthanum cuprate doped with bismuth as cathode material for SOFCs <i>Mekimah, Meriem*</i>	ICNEP'2023 ID _56
10h55 - 12h00	Preparation and structural properties of lanthanum cuprate doped with bismuth as cathode material for SOFCs <i>Mekimah, Meriem*</i>	ICNEP'2023 ID _57
10h55 - 12h00	Morphology and superconductivity studies of BSCCO Sn doped <i>MENASSEL, SIHEM*</i>	ICNEP'2023 ID _80
10h55 - 12h00	Fabrication and characterizations of pure and doped Zinc Oxide thin films <i>Zaabat, Amina*; Boudine, Boubekur; Sebais, Miloud; Halimi, Ouahiba</i>	ICNEP'2023 ID _87
10h55 - 12h00	Natural Convection of a Nanofluid in a Sinusoidally Heated Square Cavity with an Opening <i>Allouche, Selmane*</i>	ICNEP'2023 ID _94
10h55 - 12h00	Structural and Quantum Study of the Geometry and Infrared Spectroscopy in Aniline-Substituted Chemicals <i>Ouarda, Brihi*</i>	ICNEP'2023 ID _95
10h55 - 12h00	Degradation of Hexamethylene Crystal Violet by Synthesized ZnAl₂O₄ Nanoparticles <i>Hichem filali</i>	ICNEP'2023 ID _101
10h55 - 12h00	Hirshfeld surface analysis, molecular conformation and in vitro study of anti-Fusarium oxysporum activity f. sp. lycopersici of methyl 2-(1,3-dithietan -2- ylidene)-3-oxobutanoate (MDYO) <i>Sabah. Kellou*, Hibet Errahmane Meroua. Akkache, Noujoud. Hamdouni, Ouarda. Brihi, Ali. Boudjada, AbdelAli. Fiala</i>	ICNEP'2023 ID _104
10h55 - 12h00	Hydrogels based on chitosan and glutaraldéhyde / Potential support for curcumin immobilization <i>Mohammed DELLALI</i>	ICNEP'2023 ID _106
10h55 - 12h00	Beta-phase formation in thin P(VDF-TrFE) films obtained by spincoating <i>Ivanchuk, Sofiia*; Makarenko, Oleksii V; Yampolskyi, Andrii L</i>	ICNEP'2023 ID _58
10h55 - 12h00	The Theoretical Description for the Indirect Synthesis of a New Mushroom-Based Material for Heavy Metal Removal <i>Tkach, Gennadii; Melnyk, Oleg; Melnyk, Maria; Melnyk, Oleksii; Tkach, Volodymyr V*; Kushnir, Marta; Ferrão da Paiva Martins, José Inácio; Garcia, Jarem Raul; KARAKOYUN, Necdet ; Monteiro, Maria João; Ivanushko, Yana; Yagodynets, Petro</i>	ICNEP'2023 ID _59
10h55 - 12h00	Economical and Green Acetaldehyde to Glyoxal Electroorganic Conversion in Potentiodynamic Constant Voltage Mode: a Theoretical Study <i>Morozova, Tetiana; Tkach, Gennadii; Melnyk, Oleg ; Melnyk, Maria; Melnyk, Oleksii; Tkach, Volodymyr V*; Kushnir, Marta; Ferrão da Paiva Martins, José Inácio; Garcia, Jarem Raul; KARAKOYUN, Necdet ; Ivanushko, Yana; Pochenchuk, Galyna; Yagodynets, Petro</i>	ICNEP'2023 ID _60



10h55 - 12h00	Synthesis of porous silicon matrices for studying the properties of substances in pores <i>Shevchenko, Viktoriia B.*; Polishchuk, Elysaveta; Teselko, Petro; Lazarenko, Maksym</i>	ICNEP'2023 ID _64
10h55 - 12h00	Interatomic mechanisms of interaction between cellulose molecules and carbon nanostructures <i>Hizhnyi, Yuriy*; Borysyuk, Viktor; Isokov, Tymur; Nedilko, Serhii G.; Zhydachevskyy, Yaroslav; Suchocki, Andrzej</i>	ICNEP'2023 ID _68
10h55 - 12h00	Electronic structure and optical properties of glass-ceramic system "potassium-bismuth molybdate crystal – phosphate-molybdate glass" <i>Hizhnyi, Yuriy*; Chornii, Vitalii P; Nedilko, Serhii G.; Zhydachevskyy, Yaroslav; Suchocki, Andrzej</i>	ICNEP'2023 ID _69
10h55 - 12h00	Effect of carbon nanotubes on optical and electrical properties of nanocellulose composites <i>Gomenyuk, Olga*; Nedilko, Serhii G.; Zhydachevskyy, Yaroslav; Schifano, Ramon</i>	ICNEP'2023 ID _71
10h55 - 12h00	Synergistic Enhancement of Electrical and Structural Properties in PEDOT: PSS Polymer Matrices via Carbon Nanotube Reinforcement <i>Zhydenko, Illia; Klym, Halyna*; Chalyy, Dmytro; Karbovnyk, Ivan</i>	ICNEP'2023 ID _73
10h55 - 12h00	Alcohol-salt solutions droplet evaporation kinetic and shell formation <i>Brytan, Andrii V.*; Verbinska, Galyna; Vasylyuk, Svetlana Viktorivna</i>	ICNEP'2023 ID _81
10h55 - 12h00	Influence of the structure of amylose and amylopectin on their dielectric properties <i>Sosnovska, Mariia*; Lazarenko, Maksym; Alekseev, Sergei; Alekseev, Oleksandr; Klepko, Valeriy; Nessin, Stanislav; Mosia, Oleksandr; Yablochkova, Kateryna; Lazarenko, Mykhailo; Gregirchak, Nataliia; Varukha, Antonina; Andrusenko, Dmytro</i>	ICNEP'2023 ID _82
10h55 - 12h00	Wind Turbine Energy Production Based on Event-Triggered Speed Control <i>Abdelmalek Zahaf and Abdelhamid Bounemour</i>	ICNEP'2023 ID_119
10h55 - 12h00	Solid Oxide Fuel Cell Performance for Power Generation: Adaptive Fuzzy Fault-Tolerant Control <i>Abdelhamid Bounemour and Abdelmalek Zahaf</i>	ICNEP'2023 ID_120

CLOSING and LUNCH - 12h00

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The 2nd

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ABSTRACTS

Evaluation of the catalytic activity of two supported catalystson Crude ground diatomite.

ADJISSA, Massinissa¹ ; BOUZIDI, Nedjima, ¹ ; IKKOUR, Kahina² ; OUHNIA, Salim² ;
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Abstract. The objective of this work is to study the influence of the granulometry and the amorphous phase of the Algerian diatomite supports from the Sig region (Mascara) on the reactivity of the catalysts and their stabilities during the dry reforming reaction of methane (DRM) by CO₂. The raw product of diatomite, was prepared mechanically until obtaining the supports with heterogeneous grain sizes (of the micrometric and nanometric sizes) then subjected to several investigation techniques (granulometric analysis, XRF, XRD, SEM). The supports obtained were taken to prepare the Ni impregnation test and its application in the catalysis process. The nickel-Ni catalysts supported on the diatomite supports by the impregnation method were applied to the dry reforming reaction of methane with CO₂ to obtain the synthesis gas (CO/H₂). Investigative methods such as (XRF, XRD, SEM) were used to study the qualities of the prepared catalysts. The results of the dry methane reforming reaction with CO₂ proved the stability of all the catalysts during the MDR reaction and the rate of conversion to synthesis gas is dependent on the particle size and morphology of the impregnated supports. The 15Ni/D7-700 catalyst supported on a crushed support for 3h showed the highest conversions with a 30% rate for CH₄ and CO₂ and stability for 6h of reaction.

Keywords: particles size, structure, supports, catalysts, impregnation, syngas.

Correlation between structural and Optical properties of CuO nanoparticle prepared by Sol-Gel method : Degradation of Methylene blue

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Abstract. Highly feature Copper Oxide CuO nanoparticles were prepared by sol–gel method at different temperature (400°C, 500°C). The Copper chloride dihydrate, ethanol and citric acid were used as precursor, solvent and stabilizer, respectively. The influence of annealing temperature on the structural and optical properties of CuO nanoparticle was also investigated. In order to determine the information on our samples several characterizations were carried out: Structural characterization: X-ray diffraction (XRD); Optical properties: optical absorption and photodegradation of blue methylene of nanopowder. X-ray diffraction shows monoclinic structure with high crystallinity of all powder with preferential orientation and crystallite size is 22 nm. The intensity of peaks greatly increased with increasing of annealing temperature. An extreme absorption onset has been observed for all powder in the region between 380 and 650 nm. This attributed to the absorption of light by copper oxide (CuO) nanoparticle. The band gap was determined to be 1.47-1.39 eV (decreased with annealing temperature) that is significantly smaller than the band gap of bulk copper. These CuO nanoparticle show an excellent

degradation of MB reach to 95 % by advanced oxidation using H_2O_2 which enhanced the photocatalysis applications.

Keywords: CuO, Nanoparticles, Structural properties, Photocatalysis.

Finite-control-set model predictive control (FCS-MPC) and fuzzy self-adaptive PI controller (FSA-PIC) for wind turbine system based on doubly-fed induction generator (DFIG)

Aggoune Amira, Berrezek Farid and Khelil Khaled

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Abstract. This paper aims at conducting a comparative analysis between two control strategies, namely the finite-control-set model predictive control (FCS-MPC) and the fuzzy self-adaptive proportional-integral controller (FSA-PIC), for regulating the rotor side converter (RSC) in a wind turbine system (WTS) based on a doubly-fed induction generator (DFIG). This study seeks to assess the performance of these strategies with regard to precision and stability when faced with random variations in wind speed and changes in system parameters. To achieve this objective, numerous numerical tests have been carried out within the MATLAB/Simulink environment, employing a 1.5 MW WTS model. The results obtained from these tests consistently demonstrate that the FCS-MPC outperforms the FSA-PIC in terms of accuracy, robustness, and the minimization of power fluctuations across all operational scenarios.

Keywords: wind turbine system, doubly-fed induction generator, fuzzy self-adaptive PI controller, finite-control-set model predictive control

Enhanced Photocatalytic Degradation of an organic Dye Using Novel Heterojunction p-n: Experimental and Theoretical Investigations

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Abstract. Photocatalysis is a process that utilizes light energy to drive chemical reactions. It involves the use of a photocatalyst, typically a semiconductor material, which absorbs light and generates highly reactive species. These species can then initiate various chemical transformations, such as pollutant degradation or hydrogen production. Photocatalysis holds promise for sustainable applications and has gained significant attention for its potential in addressing environmental and energy-related challenges.

This study introduces the use of sol-gel auto-combustion method for the synthesis of a spinel $ZnMn_2O_4$. The as-prepared material is characterized by physicochemical and electrochemical techniques. The prepared nanoparticles exhibit remarkably low charge transfer resistance, leading to enhanced charge transfer and superior separation of charge carriers. The

heterojunction p-n ($\text{ZnMn}_2\text{O}_4\text{-TiO}_2$) exhibited a high photocatalytic activity under solar light irradiation. The theoretical investigation focused on exploring the molecule's geometry, predicting sites susceptible to electrophilic, nucleophilic, and radical attacks, and assessing overall reactivity using Density Functional Theory (DFT) calculations. Furthermore, molecular dynamics (MD) simulations investigated the dynamic behavior of the organic pollutant during adsorption on the p and n surface materials in an aqueous medium. Significantly, a strong correlation was observed between the experimental and theoretical results.

Keywords: Pollution, Water treatment, Photocatalysis, DFT, MD.

Preparation and characterization of Novel Hybrid Semiconducting nanocomposite

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Abstract. The present research describes the preparation and characterization of novel semi-conductive nanocomposite based on poly(cinnamaldehyde-co-thiophene) and copper nanoparticles. The copolymer was obtained via the polycondensation of cinnamaldehyde with thiophene catalyzed by sulfuric acid at room temperature for 24h using chloroform as solvent. The nanocomposites were prepared by a solution mixture of the copolymer synthesized with a well-defined amount of copper nanoparticles for 24h. FTIR, UV-Vis and XRD were used to characterize the nanocomposite prepared and the electrical conductivity was determined using the four-point probe method.

Keywords: cinnamaldehyde, thiophene, semiconducting nanocomposite, solution mixture

Effect of dip-coating Seed Layer on the Morphological and Optical Properties of ZnO Nanorods Growth by Hydrothermal Method

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Laboratoire Microsystèmes et Instrumentation (LMI), Université Frères Mentouri Constantine 1, Faculté des Sciences de La Technologie, Route de Ain El Bey, Constantine, 25017, Algeria

Abstract. This paper presents the fabrication and characteristic analysis of ZnO nanorods grown on glass substrates using a two-step approach involving dip-coating for the seed layer and hydrothermal growth for ZnO nanorods. The study systematically investigates the effects of different dip-coating cycles on the morphology, crystal structure, and optoelectrical of the nanorods utilizing advanced characterization techniques, including field-emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD) analysis, and UV-VIS double beam spectrometer. The ZnO nanorods exhibit a hexagonal morphology, with average diameters

ranging from 60 nm to 450 nm through control of the dip-coating cycles. X-ray diffraction analysis reveals improved crystallinity with increasing dip-coating cycles. The UV transmittance spectra show characteristic absorption peaks in the UV range (360-380 nm) for all samples, with a decreasing band gap observed as the number of dip-coating cycles increases. These findings provide valuable insights into tailored ZnO nanorod synthesis and their potential applications in areas such as photocatalysis and optoelectronics. The study contributes to the fundamental understanding of nanomaterial properties, offering pathways for optimizing ZnO nanorod-based devices and technologies.

Keywords: dip-coating, hydrothermal, zno, nanorods

Synthesis and Characterization of Fe₃O₄ Nanoparticles using Solvothermal Method

E. Aliouat¹, N. Belmokhi¹, B. Mihoubi¹, H. Filali¹, R. Bouhroum² and N. Boukheit¹

¹ Laboratory of Thermodynamic and surface Treatment of Materials surface, Department of Physics, Faculty of Exact Sciences, Mentouri Brothers University, Constantine, Algeria.

² Laboratory of Innovative Techniques and Environmental Preservation, Mentouri Brothers University, Constantine, Algeria.

Abstract. Over the past 20 years, research on nanomaterials has made remarkable progress not only in the controlled synthesis and the study of novel properties, but also in the multiple applications of matter at the nanoscale. Currently, Fe₃O₄ magnetite nanoparticles continue to pose an enigma, as the understanding of certain fundamental properties remains unclear despite vigorous efforts and substantial progress in research. In fact, these materials have attracted considerable attention in the fields of new technology with different but complementary motivations using various types of experimental techniques and theoretical approaches. In this work, we present the results obtained from a thorough analysis of Fe₃O₄ nanoparticles with various Nickel concentrations synthesized through a simple solvothermal method. Characterization methods are mainly structural (XRD, SEM) and physical (UV-Vis, FTIR, ...). The SEM images show that the prepared NPs exhibit spherical shape with nanometric size confirmed by X-ray diffraction. Furthermore, the Nickel substitution of iron cations into the crystalline structure had an impact on the average crystallite size. Raman spectra of Fe₃O₄ magnetite nanoparticles are very consistent with the literature.

Keywords: Magnetite, Magnetic Properties, Nanoparticles.

Heat Transfer by Natural Convection Under Constant Heat Flux Wall in a Semi-Annular Shaped Enclosure Filled with a Hybrid Nanofluid

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¹Department of Physics, Faculty of Exact Sciences, Energy Physics Laboratory, Frères Mentouri Constantine1 University, Constantine, Algeria

² Department of Mechanical Engineering, Faculty of Sciences and Technology, Energy Physics Laboratory, Mohamed El Bachir El Ibrahimi University, Bordj Bou Arreridj, Algeria

Abstract. The study presented in this article focuses on the natural convection of Ag-MgO/water hybrid nanofluids in an eccentric semi-annular enclosure. The flow dynamics are simulated using

dimensionless parameters. The outer wall is maintained at a constant temperature T_c , while the inner circular wall undergoes a constant heat flux (q), and the other two walls are thermally insulated. The governing equations of the system are solved using the finite volume method with a Gauss-Seidel method using an under-relaxation process. The fixed parameters include the annulus radius ratio and the eccentricity. The study presents the results in the form of isotherms, streamlines, and average Nusselt number. The results show that the average Nusselt number increases with an increase in the Rayleigh number. The addition of hybrid nanoparticles to the base fluid enhances the heat transfer rate in the semi-annular enclosure.

Keywords: Natural convection, Hybrid nanofluid, Eccentric semi-annular enclosure

Natural Convection of a Nanofluid in a Sinusoidally Heated Square Cavity with an Opening

S. Allouche, M. Djezzar, B. Allouche, T. Tayebi

Abstract. The phenomenon of natural convection was investigated numerically in a square cavity containing an opening located in the middle of the right vertical wall and saturated with a nanofluid Cu-water. The left vertical wall undergoes non-uniform heating and the rest of the enclosure is kept at a cold temperature. The mathematical model that governs the two-dimensional stationary thermal natural convection of a laminar flow is formulated in cartesian coordinates using the stream-function/vorticity formulation. The partial differential equations obtained are solved with their boundary conditions by an iterative method using a FORTRAN code based on the finite volume method. As per the results, it appears that the heat transfer rate improves with increasing nanoparticle volume fraction and opening size.

Keywords: natural convection; nanofluid; open cavity; finite volume method

Synthesis and Characterisation of Magnesium Oxide Thin Film Nano-Material by Sol-Gel Method

Redha Aouati, Halima Djaaboube, Abderrahmane Bouabellou

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Abstract. thin film of Magnesium oxide (MgO) was prepared on glass substrate by dip-coating method. We have investigated the morphological, structural and optical properties of the film. The obtained thin layer of MgO was characterized by X-ray diffraction, the XRD spectra exhibit that the film was a cubic structure along (200) and (220) directions. The sample of MgO film has good transmittance with value between 70 –95% in visible region. The value of the optical gap was 3.90 eV. The morphology of the sample was similar to islands in shapes with homogeneous distribution. EDX analysis confirmed the presence of Magnesium and Oxygen elements, the film has good stoichiometric.

Keywords: Thin film, Magnesium, sol-gel, morphology, optical band gap.

High photovoltaic performance of InGaN solar cells

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Abstract. The ternary alloy **In_xGa_{1-x}N** is a promising candidate for modern electronics. Due to its modulation of energy band gap from UV to visible spectrum band gap (0.7 eV - 3.4 eV) and its interesting absorption coefficient, it can be considered as a potential candidate for high efficiency solar cells. In this work we have successfully developed a solar cell structure based on (In_xGa_{1-x}N) using SCAPS-1D software. The structure of the simulated cell is therefore: In_xGa_{1-x}N (p)/In_xGa_{1-x}N (i)/ZnO (n); x the composition of indium.

We optimized various photovoltaic parameters under some structural and optoelectronic effects and we obtained an interesting photovoltaic efficiency. This study investigates the great potential of InGaN solar cells and can be used for the design and manufacture of high efficiency III nitride solar cells.

Keywords—: In_xGa_{1-x}N; Photovoltaic efficiency; Solar cell; Band gap.

X ray diffraction study of structural properties of Fe₈₆Cr₁₄ mechanical alloys, Effect of process control agent

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Abstract. Fe-14%Cr nanoparticles with different PCA content (Acetone, Methanol and Ethanol) were elaborated by mechanical ball milling process during 72 h at room temperature. The PCA has been included in the Fe-14%Cr matrix with 5 wt.% of the total mass of each sample. From x-ray diffraction analysis indicated the formation of bcc and Trigonal phases, the lattice parameter remained constant while the grain size D changed with changing on the different of PCA.

Keywords: Mechanically alloying materials, ball milling process, process control agent, X ray diffraction, structural properties.

Effect of calcination temperature on structural, morphological and optical properties of compound powder ZnO-Al₂O₃

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Abstract. Zinc oxide nanoparticules is generally studied for numerous applications such as a photocatalyst, a working electrode for dye-sensitized solar cells and for thermoelectric devices. In this work studies the effect of calcination temperature on structural, morphological and optical properties of the compound powder ZnO-30% Al_2O_3 . Pure ZnO nanopowders and the compound ZnO-30% Al_2O_3 were synthesized by sol-gel route. Then they were annealed for 2 hours at 450°C, 700°C and 900°C temperatures. These powders were analyzed by X-ray diffraction (XRD), scanning electron microscopy technique, and photoluminescence. The results show that the pure ZnO powder has a hexagonal structure (Wurtzite) and a spinel phase with a cubic structure was revealed in the ZnO-30% Al_2O_3 nano-composites. This phase causes a reduction in the crystallite sizes. Analysis by scanning electron microscopy confirms that when the calcination temperature increases the size of the grains increase as expected from the results (XRD) and the incorporation of aluminium does modify the morphology, the shape spherical of particles become nanotubes on surface. Photoluminescence shows that the optical quality degrades progressively in the presence of Al content and the annealing effect improves the optical properties.

Keywords: ZnO, Sol-Gel, nanopowders, spinel phase

Effect of Ni -doping on ZnO nanostructures properties

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Abstract. In this work we have prepared and characterized nanoparticles of zinc oxides (ZnO) pure and doped with Nickel by the Sol Gel method. This non-costly, easy method makes it possible to have more homogeneous powders with a finer particle size. XRD analysis confirmed hexagonal wurtzite-like structure of ZnO nanoparticles. Sizes of these nanoparticles are in an order of magnitude of a few tens of nanometers. The doping of ZnO nano-powders with 5% Ni improved the crystalline quality; this is revealed by the increase in the intensity of the peaks. The infrared absorption spectroscopy (FTIR) made it possible to identify the nature of the bonds present in the nano-powders of ZnO. FT-IR spectra confirmed two characteristic bands attributed to Zn-O stretching bands. The degradation rate of methylene blue (D) of pure ZnO reaches 99.6% after 90 min. Nickel doping greatly reduced the degradation (D) from 99.6% to 21%.

Keywords: ZnO, doping, Sol Gel, nanoparticles, photocatalytic activity

Thermographic Method of Modeling the Features of Airflow in NPP Air Filters

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Abstract. The work is devoted to the tasks of safe operation of nuclear power plants, namely the prevention of inert radioactive gases, iodine, and its compounds from entering the air. The latter is particularly dangerous because it is radioactive and its compounds, in particular, methyl

iodide, are toxic. One of the methods of air purification is the use of air filters filled with activated carbon granules that have undergone preliminary treatment of thermal expansion and impregnation. At the same time, there is a problem with evaluating the change in local aerodynamic resistance as a result of the shape change of granules and their compaction when activated carbon is filled into the filter. For this purpose, the model that calculates the spatial field of movement of ventilation gases through a chamber that simulates an adsorber of the AU-1500 type filled with carbon granules was created. To verify the model, it was necessary to develop approaches to the assessment of the topology of the intergranular space and to draw up ideas about the possible inhomogeneities of such topology due to inhomogeneities in the compaction of granules during backfilling and vibration effects during operation. Therefore, an experimental model based on the assumption that air passage channels are spatially contiguous with electric current passage channels if a potential difference is applied to the "input-output" sections was proposed. Clusters of areas with heterogeneous packing by measuring the temperature distribution, which is released in the form of Joule heat were identified. Correlations between the characteristics of the spread of temperature fields and modes of current transmission have been established. It is shown that the obtained experimental data correlate with theoretical calculations of the flow of ventilation gases. The created set of methods allows optimization of the aerodynamic characteristics of the filter to improve their functional properties.

Keywords: thermography, air filters, active carbon, air flow

Formulation and Optimization of sustained release Microparticles of ketoprofen

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Abstract. Microparticles are one of the drug delivery systems used to sustain the release. The objective of our work was to produce sustained-release microparticles of ketoprofen (KTP). The microparticles were prepared by the method of emulsion-diffusion of the solvent using the design of experiments, the MINITAB 16 was used to analyze the results. EC:KTP mass ratio (%), PVA concentration (m/v %) and stirring speed (rpm) were selected as factors. Encapsulation efficiency rate (EE%) and *in vitro* release after 6h (REL6%) were selected as responses. For the optimization of our results we chose the central composite design. The latter show that the optimal formulation has an EE= 78, 89%, REL6 %= 39,98% for a EC: KTP mass ratio: EC = 80,59%, PVA concentration= 0,52% and stirring speed= 477,11 rpm. It was possible to observe the morphology of the microparticles which is characterized by a spherical shape using an optical microscope. The *in vitro* dissolution at 35°C in a medium with pH=7.4 gives a sustained release in which 36.98% of ketoprofen was released after 6 hours. According to the results obtained, the microparticles of ketoprofen can be used for the ocular sustained release.

Keywords: Ketoprofen, sustained release, Design of experiment, Korsmeyer-Peppas

Design of a new photo-diode based on (α -PbO)/(α -SnO) lateral heterostructure

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Abstract. α -PbO and α -SnO monolayers are stable nanostructures that are separately synthesized by epitaxial growth on the same oxidized silicon substrate (SiO₂/Si) with superior functionalities, making them industrially important material for many applications. We theoretically designed new lateral heterostructures (α -PbO)_m/(α -SnO)_m formed by periodically repeating narrow PbO and SnO strips joined along their adjacent one dimensional interface and investigated the structural, mechanical and electronic properties by using the first-principles calculations. We demonstrate that creating these lateral heterostructure by α -PbO and by α -SnO monolayer materials will allows for adjusting various physical and chemical parameters such as tunable band gap, which are required to fit wide spectral range in optoelectronics applications. We obtained that the (α -PbO)₇/(α -SnO)₇ heterostructure shows an Anderson type-II band alignment where CBM and VBM are located separately at α -PbO and α -SnO stripes respectively. Consequently, the photon-generated electron-hole pairs spatially separated, resulting in much longer exciton lifetime than that in the two monolayers separately which needs to be confirmed by further experimental measurements. This new structure could function as a forward p-n diode and can offer optoelectronic properties and quantum structures leading to device applications with interesting functionalities as a photo-diode.

Keywords: Two-dimensional materials, α -PbO monolayer, α -SnO monolayer, Lateral heterostructures, Band alignment.

Production and application of nanocellulose from non-wood plant raw materials in the production of cardboard and paper products

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Abstract. Environmentally friendly pulp production process from various representatives of non-woody plant materials (NWRM) is described. The method of acid hydrolysis of organosolv cellulose with low consumption of sulfuric acid produced nanocellulose (NC), which was used as a strengthening additive in the production of cardboard and paper products. SEM data confirmed the destruction and decrease in the size of fibers of the studied plants during their thermochemical treatments. FTIR and XRD data showed that the influence of chemicals and temperature leads to a decrease in the content of residual lignin, the lateral order index, the apparent size of crystallites and an increase in the crystallinity index in cellulosic materials in the following order: NWRM - pulp after alkaline extraction - organosolv cellulose - NC. It was established that the NC from NWRM had a density in the range of 1.2 - 1.5 g/cm³, tensile strength from 43 MPa to 67 MPa, crystalline index from 75% to 87%. DLS, AFM, and TEM data confirmed that NC particles had a transverse size in the range of 5-65 nm and a length of up to several micrometers.

The effect of the consumption of NC in the fibrous mass and on the surface of cardboard and paper products on their physical and mechanical parameters of paper for packaging food products and cardboard for flat layers of corrugated cardboard was studied. It has been established that the addition of NC improves the quality indicators of paper and cardboard. It is

recommended to add 2% NC to the mass or 3g/m² to the surface of food packaging paper to meet the requirements of the standards. SEM data confirmed that the addition of NC to the surface of paper leads to the closing of voids between cellulose fibers and irregularities in the structure of the paper surface, which increases its grease resistance. It has been proven that hemp NC allows to reduce the consumption of phenoprint synthesized from oil by 50% and to obtain paper for packaging food products with less impact on the environment. The positive effect of the use of corn NC on the improvement of cardboard indicators and the reduction of the consumption of harmful chemical auxiliary substances is shown. It was established that the use of NC with a consumption of 5 kg/t leads to the receipt of cardboard with quality indicators that meet the requirements of the standard.

Synthesis and characterization of pure BaTiO₃ Nanoparticles and doped with La³⁺ and Mn²⁺ prepared by Sol-Gel method

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Abstract. In this study, BaTiO₃ Nanoparticles doped by La³⁺ (10 mol %) and different ratios of Mn²⁺ (0; 1; 4; 7 and 10 mol %) were prepared by the Sol-Gel method. To better understand the effects of dopant concentration on the structural, optical, and thermal properties of undoped and doped BaTiO₃ perovskite nanostructures, different characterization methods were used, such as powder X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, and differential scanning calorimetry (DSC). The experimental results show that all diffraction peaks can be assigned to the tetragonal structure of BaTiO₃, without any impurity phases. These results were confirmed using FTIR and Raman spectroscopy. The crystallite size calculated from the intense X-ray diffraction peak using the Scherrer equation is of the order of the nanoscale. Moreover, the high photocatalytic activity of the nano powders in the degradation of methylene blue and rhodamine B, shows that these materials could be used as photocatalysts and good adsorbents.

Keywords: BaTiO₃, Sol-Gel, Nanoparticle, Adsorption, Photocatalysis.

Structural and hydrophobic properties of Cobalt doped ZnO thin films prepared by electrodeposition method

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Abstract. In this work, thin films of undoped and cobalt-doped ZnO were prepared by thermal oxidation method of electrodeposited zinc on aluminum substrates for fabrication of hydrophobic coatings. XRD analysis shows the diffraction peaks of ZnO Wurtzite hexagonal structure without secondary phase for the cobalt-doped sample; this is confirmed by Raman spectroscopy. FE-SEM images reveal that the grains shape is spherical for cobalt-doped ZnO thin film, however the undoped sample exhibit a compact grains with nanostructured pyramidal shape. Incorporation of cobalt into zinc ions sites leads to the decrease of crystallites size from 39 to 31 nm and enhanced the hydrophobic property of studied ZnO thin film.

Keywords: Co-doped ZnO; nanostructure; thermal oxidation; hydrophobic; pyramidal shape

Hybrid systems in the various renewable energy sources

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Abstract. The integration and blending of various renewable energy sources serves as the foundation for hybrid renewable energy systems in this study. They are a fantastic option for installing autonomous energy systems and have the benefits of using less storage space and being more environmentally friendly. For the design and operation of hybrid energy systems, the problem is, given an estimate of the (RE) resources. This work aims to the optimization and determine the best combination of resources of renewable system to meet energy demand for a specific region. The problem can be formulated as a problem of optimal allocation with limited resources to meet a specific demand. The linear programming method was adopted to solve this problem. Typical examples are discussed by applying this technique to optimize the allocation of various given regions.

Keywords: Hybrid Energy, Renewable energy, Optimal Allocation of Resources, Linear programming.

Integration of photovoltaic panels and Biodigesters

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Abstract. Systems that integrate two or more renewable energy (RE) sources are known as hybrid systems. When combined, they can get around the drawbacks of using only one energy source. In order to maximize the exploitation of these readily available resources while satisfying specific energy demands, this study deals with an evaluation of the energetic potential of renewable energy resources that can be harvested from a given location. It then offers the determination of their repartition to optimize the exploitation of these available resources while meeting specific energy demands. The general problem can be formulated as the optimal allocation of limited resources constrained to meet specific demands. We specifically consider situations where the installed energetic capacity of each resource is continuous. The Simplex linear programming method is adopted to solve this problem. We consider the combination of two renewable energy resources, namely photovoltaic panels and biomass, with limited capacities to meet an energetic demand at a specific site at the lowest cost.

Keywords: Hybrid Systems, Renewable energy, Photovoltaic panels, Biomass.

Structure, Microstructure and Mossbauer studies of (Ni₆₀Co₄₀)_{100-x} Fe_x system Synthesized by Hydrothermal Method: Effect Fe content

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Abstract. In this work, we synthesized ternary metal compounds of iron-cobalt-nickel nanoparticles via the hydrothermal method, investigating the impact of iron content on the structural, microstructural and magnetic properties of the $(\text{Ni}_{60}\text{Co}_{40})_{100-x}\text{Fe}_x$ system ($x=0, 3, 5, 7, 10, 13.5$ and 15%). The results of X-ray diffraction (XRD) analysis indicate that all samples exhibit a face-centered cubic (Fcc) crystallographic structure. While, a cobalt-rich hexagonal (Hcp) structure that appears at low iron content. The Mossbauer Spectroscopy analysis indicates the presence of two distinct iron atomic surroundings

Keywords: Nanostructured NiCoFe, hydrothermal method, Mossbauer Spectroscopy, Hyperfine Interactions.

Synthesis and Characterization of doped and c-doped ZnAl_2O_4 Nanoparticles using Sol-Gel Method

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Abstract. Samples of pure zinc aluminate (ZnAl_2O_4) and co-doped ZnAl_2O_4 with Chromium (Cr^{3+}) at different ratios (2, 4, 6, 8, 10 mol%) and a constant amount of Cobalt (Co^{2+} : 10 mol%), were synthesized by the citrate sol-gel technique, and then annealed at 900°C for 3h. To investigate the structural, and thermal properties, different characterization methods were used such as powder X-ray diffraction (XRD), differential scanning calorimetry (DSC), the Fourier transform infrared spectroscopy (FTIR) and the Raman spectroscopy. Analysis by X-ray diffraction revealed the presence, in all samples, of the cubic, single-phase ZnAl_2O_4 without any impurity phases, with a nanometric crystallite size. These results were confirmed using the Fourier transform infrared and the Raman spectroscopy. Furthermore, the photocatalytic study for different samples of ZnAl_2O_4 revealed their potential as proficient photocatalysts and adept adsorbents for the degradation of hexamethyl crystallized violet dye in aqueous solutions.

Topics: Zinc Aluminate, Nanoparticles, Sol-Gel, Photocatalysis, Adsorption.

Keywords: Zinc Aluminate, Nanoparticles, Sol-Gel, Photocatalysis.

Synthesis and Characterization of doped and c-doped ZnAl_2O_4 Nanoparticles using Sol-Gel Method

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Abstract. Samples of pure zinc aluminate (ZnAl_2O_4) and co-doped ZnAl_2O_4 with Chromium (Cr^{3+}) at different ratios (2, 4, 6, 8, 10 mol%) and a constant amount of Cobalt (Co^{2+} : 10 mol%), were synthesized by the citrate sol-gel technique, and then annealed at 900°C for 3h. To investigate the structural, and thermal properties, different characterization methods were used such as powder X-ray diffraction (XRD), differential scanning calorimetry (DSC), the Fourier transform infrared spectroscopy (FTIR) and the Raman spectroscopy. Analysis by X-ray diffraction revealed the presence, in all samples, of the cubic, single-phase ZnAl_2O_4 without any impurity phases, with a nanometric crystallite size. These results were confirmed using the Fourier transform infrared and the Raman spectroscopy. Furthermore, the photocatalytic study for different samples of ZnAl_2O_4 revealed their potential as proficient photocatalysts and adept adsorbents for the degradation of hexamethyl crystallized violet dye in aqueous solutions.

Keywords: Zinc Aluminate, Nanoparticles, Sol-Gel, Photocatalysis.

The effect of the marine environment on the durability of the precast concretes of the Taksebt dam

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Abstract. The study presented deals with the mechanical consequences and the degradations caused by the external attack of sulphates from the marine environment on the prefabricated concretes of the spillway and the dyke of the Taksebt dam in Tizi-ouzo (Algeria), concrete produced by solar curing and renewable energy all year round. Three different external sulphate attack protocols were applied for three types of concrete based on crushed aggregates (dry concrete at 45°C , ordinary concrete (28 days), water-hardened concrete at 28 days, the samples are immersed in a 5% H_2SO_4 solution.

The results show that the impact of the age of the material on its degradation in contact with the sulfuric acid solution was highlighted, visual observations then a rapid and brutal degradation on the surface then in depth towards the core then a loss of mass and cracking and finally the ruin of the material.

Keywords: Taksebt dam, precast concrete, external sulphate attack, degradation.

Numerical investigation of free convection inside a hexagonal enclosure filled with nanofluid (water-cu) under effect of the position of the inner obstacle

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Abstract. The present paper aims to investigate the natural convection of nanofluid (water-cu) inside a hexagonal enclosure shape embedded with a square obstacle with the presence of hot and cold side walls, The governing equations were solved in a non-uniform unstructured grid by

employing the Galerkin finite element method using software COMSOL Multiphysics. The objective of this study is to analyze the influence of Rayleigh number ($103 < Ra < 105$), the position of the obstacle which is located in three different positions (center, bottom, and top side), and the effect of Nanoparticles volume concentration ($0 < \phi < 0.2$) on the thermal behavior inside the enclosure. The results are reported as contours of isotherms, streamlines, and average Nusselt numbers. The obtained results illustrate that the increase in the Rayleigh number (Ra) and the Nanoparticles concentration (ϕ) leads to an increase in the Nusselt number (Nu average) that signifies the rate of heat transfer in the studied enclosure, in addition to the best performance observed with the position of obstacle that is located at the middle of the enclosure, where has a high effect in improving the heat transfer along the enclosure comparatively with the rest different positions.

Keywords: Natural Convection, Nanofluid (Water-Cu), Hexagonal enclosure, Nusselt numbers, Rayleigh Number.

Elaboration and Characterization of Thermoelectric Materials

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Abstract. The thermoelectric (TE) materials are one of the promising candidates for environmental friendly technologies. Thermoelectric materials can directly convert waste heat into electric energy. New mixed oxides of $Na_{0.74-x}Nd_xCoO_2$ ($x = 0, 0.1$) materials were successfully synthesized using a sol-gel method and characterized by several techniques such as: X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and various thermoelectrical properties (Resistivity, Seebeck coefficient and Power factor). The results showed that the undoped $Na_{0.74}CoO_2$ pellet sintered at 1123K for 12H crystallized with hexagonal symmetry, while the doped samples show the formation a second phase ($NdCoO_3$). SEM analysis showed that the porosity of the samples decreases with increasing Neodymium (Nd) content. The resistivity of the undoped sample and doped sample with $x=0.1$ increases with increasing temperature range while the resistivity of the sample with $x=0.1$ increases in the temperature range $307K \leq T \leq 419.5K$ and then decreases with rest of temperature range. The Seebeck values of the samples are between 61.6-137.5 $\mu V/K$ and positive at all temperature range. The highest power factor value of 0.4425 mW/mK^2 at 1070.5K is obtained for $x=0.1$ sample.

Keywords: sol-gel; thermoelectric materials; X-ray diffraction; oxides mixes; Scanning Electron Microscopy.

Electronic Properties and Magnetic Stability in Binary Iron Pnictide

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Abstract. In this work, we presented a first-principle study of the structural, electronic and magnetic properties of iron selenide in its pure state. The calculations were performed by the Pseudo-Potential method which is based on the density functional formalism (DFT), using the

local spin density approximation (LSDA). The lattice parameters and total energy of FeSe were calculated for three different cases of magnetism in order to examine magnetic stability and electronic properties. We discussed the most stable state as well as the one closest to the creation of the phenomenon of superconductivity in this binary iron pnictide.

Keywords: Magnetism, Superconductivity, DFT study, Fe-pnictides, Band structures, Fermi surfaces.

Optimizing Maximum Power Point Tracking of Partially Shaded Photovoltaic Module using hybrid P&O-FPA MPPT

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Abstract. Efficient power generation from photovoltaic (PV) modules is crucial for sustainable energy systems. Environmental factors like temperature, irradiance, and shading cause power output fluctuations, necessitating robust Maximum Power Point Tracking (MPPT) methods. The hybrid Perturb and Observe and Flower Pollination Algorithm (P&O-FPA) shows promise in optimizing PV array performance. However, its applicability in tracking the maximum power point of partially shaded PV modules remains uncertain. This research delves into the application of the hybrid P&O-FPA for MPPT in shaded conditions. Through extensive Matlab /Simulink simulations, we systematically compare the hybrid P&O-FPA with the Flower Pollination Algorithm (FPA), and conventional Perturb and Observe (P&O). Results reveal that the P&O-FPA algorithm outperforms both FPA and P&O in accurately tracking the global maximum power point of shaded PV modules. These results underscore the significant potential of the P&O-FPA algorithm to enhance photovoltaic performance, particularly in situations where partial shading is a concern. Moreover, this research contributes to the advancement of efficient PV systems.

Keywords: PV system, P&O-FPA, DC-DC Boost converter and partial shading condition (PSC).

Effect of Fe₂O₄ nanoparticle on electronic cooling: Numerical investigation of nanofluid flow through a heat sink

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Abstract. Nanotechnology has become necessary in electronics to keep up with recent rapid developments in this field, where precision and high performance are required. To learn about how adding nanoparticles affects heat transfer, the flow of water and nanofluid inside a heat sink filled with copper foam was compared numerically in this paper. Fe₂O₄-H₂O nanofluid was selected as a coolant with constant concentration and diameter of nanoparticles. Eulerian two-phase modeling is used to predict the behavior of nanofluid. Results clearly confirmed that nanofluid improved heat transfer by 41-50% and surface temperature by up to 14°C compared with water.

Keywords: Electronic cooling, heat sink, nanoparticles, nanofluid.

Elaboration and Thermoelectric Properties of NdCoO₃ Oxides

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Abstract. The present work demonstrates the effect of replacing some Co with Ni on the structural, morphology and thermoelectric properties. NdCo_{1-x}Ni_xO₃ pellets sintering at 1200°C for 12h was synthesized using sol-gel method and comprehensively characterized using X-ray diffraction), scanning electron microscopy and various thermoelectric measurements (resistivity, Seebeck coefficient and power factor). The results showed that the NdCo_{1-x}Ni_xO₃ samples had a pure orthorhombic crystal structure throughout the entire substitution range. The electrical resistivity changes upon doping. Overall, The Power factor of best performing is 0,204 μ W/m.K² was achieved for NdCo_{0.9}Ni_{0.1}O₃ sample at 417K .

Keywords: Perovskite, Seebeck coefficient, Resistivity, Power factor.

Hydrothermal synthesis and characterization of nanostructured CdSe: Effect of annealing treatment

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Abstract. Semiconductor nanoparticles also known as quantum dots, have diameters ranging from several nanometers and consist of only hundreds to a few thousand atoms. The CdSe nanoparticles have interesting physical and chemical properties and potential importance as nonlinear optical materials. They are semiconductors with quantum size effect and can be used for electroluminescent devices and sputtering target to produce photoconductive films and infrared filters. The CdSe, because of its high photosensitive nature, is widely preferred in the fabrication of different optoelectronic devices, photoconductors, thin film transistors, gamma ray detectors, etc. In this study, we have successfully synthesized ZnSe nanoparticles using a facile solvothermal method in mixed solvent of ethylenediamine and hydrazine hydrate, followed by thermal treatment. The powder X-ray Diffraction (PXRD) analysis revealed that the diffractogram of the powder, did not exhibit the desired CdSe phase, necessitating a thermal treatment. Consequently, the resulting powder was annealed for 4 hours at a temperature of 200°C, leading to the formation of a dark brown precipitate suitable for characterization.

The X-ray diffraction pattern displayed the growth of wurtzite CdSe phase with a hexagonal crystal structure. Further characterization using Environmental Scanning Electron Microscopy (ESEM) confirmed the presence of nano-sized crystallites, which exhibited a granular morphology with some stick-like particles forming a cotton-like shape. Additionally, Energy Dispersive X-Ray (EDX) spectroscopy of the CdSe powder confirmed the presence of only two chemical elements, Cd and Se, representing the crystallized CdSe phase. The measured concentration of Cd and Se were found to be in good agreement with the nominal concentrations. Validating the results

obtained through PXRD and ESEM analyses.

Keywords: Annealed, CdSe Nanoparticles, Hydrothermal synthesis, Semiconductor

Enhancing Photoluminescence and Crystallinity through Aluminum Doping in Sol-Gel Zinc Oxide Thin Films

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Abstract. This study investigates to see how aluminum (Al) doping affects the optical and photoluminescent properties of sol-gel zinc oxide (ZnO) thin films. The sol-gel method was used to produce Al-doped ZnO films, which were further investigated using X-ray diffraction, UV-VIS spectrophotometry, and photoluminescence studies. According to the findings, increased Al doping concentrations resulted in reduced crystallinity and a blue shift in the UV emission peak, which was ascribed to the Moss-Burstein effect. Al doping prohibited the visible emission band, but higher annealing temperatures enhanced film quality and the UV-to-visible emission ratio. This research looks at the link between Al doping, crystallinity, and photoluminescence in Al-doped ZnO thin films.

Keywords: Aluminum Doping, Zinc Oxide Thin Films, Photoluminescence.

Effect of silver doping on structural properties of (La, Sr)MnO₃ cathode material

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Abstract. In this study, we elaborated by sol-gel method a cathode material of perovskite structure $\text{La}_{1-y}\text{Sr}_y\text{Mn}_{1-x}\text{Ag}_x\text{O}_3$ for fuel cell doped with ($x = 0, 0.1, 0.2$ and 0.3). The aim of this work is to study the effect of doping by Ag^+ on the formation phase as well as its structural properties. The samples sintering at temperature of 1200°C were characterized by the X-ray diffraction and infrared spectroscopy (FTIR). The X-ray diagrams are attested to a formation of the main phase with the presence of secondary phases. Reitveld refinement has shown that all the samples were indexed in the rhombohedral structure with the space group ($R\bar{3}C$), and the crystalline size was around of (20-33 nm.) The cell parameters a , b and V are decreased with doping which can be attributed to the change in MnO distance due to change in charge carriers in the crystalline system with the doping by a monovalent element (Ag^+) on the site of a divalent element (Mn^{3+}) and an increased in the parameter c which can be explained by the substitution of Ag^+ with ionic radius of 1.15 \AA at Mn^{2+} site of 0.58 \AA . The FTIR analysis allowed us to identify the bands of Mn-O, Mn-O-Mn which confirm the formation of $\text{La}_{1-y}\text{Sr}_y\text{Mn}_{1-x}\text{Ag}_x\text{O}_3$.

Keywords: SOFC, Cathode, Sol-gel method, LSM, Agdoping

Electrochemical Measurements of Maghemite Nanostructured fibers for Energy Storage Applications

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Abstract. In this investigation, we report a one-pot facile, impurity-free hydrothermal method to synthesize nanostructure iron oxide type (γ -Fe₂O₃). Extensive materials characterization, using X-ray diffraction, scanning/transmission electron microscopy and Raman spectroscopy measurements, revealed very interesting Maghemite formation possessing nanofibers morphology with mean diameter around 32 nm. The capacitive property of these products obtained at optimized conditions was investigated by cyclic voltammetry (CV), galvanostatic charge-discharge and electrochemical impedance spectroscopy (EIS) tests in KOH electrolyte. The best prepared electrodes showed γ -Fe₂O₃ and γ -Fe₂O₃/AC, with an excellent specific capacitance (or capacity) values of $\sim 1200 \text{ F.g}^{-1}$ (166 mAh.g^{-1}) and 1400 F.g^{-1} (199 mAh.g^{-1}), at 5 mV.s^{-1} (1 A.g^{-1}). Furthermore, these electroactive iron oxide based nanofibers exhibit excellent cycling stability with good capacity retention of 73 % and 99.8% after 2000 cycles at 30 A.g^{-1} , respectively.

Keywords: Hydrothermal synthesis; Iron oxide; Nanofibers; Activated carbon; Energy storage, Supercapacitors.

Degradation of Hexamethylene Crystal Violet by Synthesized ZnAl₂O₄ Nanoparticles

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Abstract. This paper is investigated samples of pure zinc aluminate (ZnAl₂O₄), in addition of the doped ZnAl₂O₄ with Erbium (Er²⁺; 1%) and Lanthanum (La³⁺; 1%). The amount of Lanthanum is constant (La³⁺: 1% mol) and different ratios of Erbium (1.5 and 2 % mol). All samples are synthesized by the citrate sol-gel technique, followed by thermal treatment at 900 °C for 2h. Meanwhile, structural and thermal properties of particles are investigated by X-ray diffraction (XRD), thermo- gravimetric analysis (TG) and differential scanning calorimetry (DSC). Additionally, the photocatalytic and catalytic activities are evaluated in the degradation of organic pollutant in aqueous solution under ultra-violet light. The results of different samples of ZnAl₂O₄ showed that they could be used as adsorbents and photocatalysts for the degradation of a Hexamethyl Crystallized Violet (HCV) dye in an aqueous solution.

Keywords: nanoparticles, Sol-gel, photocatalysis, Adsorption.

Thermodynamic study of thermoplasticPE containing different quantities of carbon nanotubes

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Abstract. The addition of fillers and in particular carbon nanotubes into polymers with aim to enhance their specific properties and functionality is a current and utterly important subject. Thus, the obtained nanocomposites are light, resistant to corrosion, their elasticity and ease work and shaping promote them to be competitive in various fields of technology. Polyethylene is a widely used thermoplastic material, with immediate availability, low cost and good processability, polyethylene is also a promising material as a matrix for composites. The major focus on these materials regarded toward carbon nanotubes which possess an excellent mechanical property, good electrical and thermal conductivity. The spectrum of potential applications for polymer/CNT nanocomposites is very wide, from energy storage, environmental protection to medicine. This summary aim at the thermodynamic study of polyethylene with the introduction of multiwalled carbon nanotubes (0.01, 0.04, 0.07 and 0.09%MWCNTs). The coefficient of thermal expansion (CTE) was measured following both radial (R) and axial (Z) directions. The CTE $\alpha(T)$ in the axial direction (Z) reveals similar shapes with identical behavior, while in the radial direction (R) is very different from that of the (Z) direction. The anomalies are absent and only one curve has a very intense peak. Along the radial direction, the relative dimensional variations overlap over a wide temperature range. Those in the axial direction are practically identical. On the other hand, whatever the concentration and/or direction, all the curves each contain a peak whose intensity depends on the concentration. The DSC signal of the samples have the same tendency with the presence of common anomaly. Thermogravimetry shows three stages with a relatively similar weight loss. The first level shows a fast weight drop, while the second change contained a common anomaly between all the samples. At the end the signal flattened which implies a sample stabilization. The results within this study shows the importance and the positive role of CNTs, aimed to replace heavy and expensive materials as fillers in nanocomposites base polyethylene.

Keywords: PE, Carbon nanotubes, Thermal Expansion, Calorimetry, Thermogravimetry.

The Influence of Milling Time & Multiwalled Carbon Nanotubes Concentrations on the Thermal-Structural Behavior of Iron–Copper Nanocomposites

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Abstract. In this work we aim to study the effect of incorporating different concentrations of multiwalled carbon nanotubes into Iron–Copper — Fe–Cu with a ratio of 4:1; MWCNTs of 0.5, 1 and 2% in volume— nanocomposites —prepared via high-energy ball milling of different grinding times of 1 and 2 hours, respectively— on the thermal and structural properties. The characterization conducted was heat flow, weight change, relative linear expansion ($\Delta L/L_0$) and coefficient of thermal expansion (CTE) for the thermal behavior, as for the structural changes and assessments, x-ray diffraction, and Raman spectroscopy were applied. Several temperature ranges were distinguished for the Fe–Cu–MWCNTs nanocomposite by the $\Delta L/L_0$ (T) and CTE temperature dependences. Effect of CNTs on the $\Delta L/L_0$ and CTE temperature dependences are different for different temperature ranges, and the magnitude of the effect depends on the CNTs content. The heat flow and thermogravimetry show thermal stability and higher calorific capacity for the samples with longer milling time and containing a higher concentration of CNTs. As for the coefficient of thermal expansion, an improvement in CTE of the Fe–Cu-1% MWCNTs milled for 2 h time. The provided x-ray diffraction patterns show a grain refinement for the 2 h milling time, also a homogenous distribution of CNTs (the absence of CNTs clusters appearing as carbon graphite)

Raman spectroscopy reveals a higher defect density with a longer milling time, except for the 1 h samples, showing a lower defect density which indicates the healing and the recovery of CNTs.

Keywords: Carbon nanotube, Fe–Cu nanocomposite, Thermal expansion, Mechanical milling, Heat flow.

Experimental Study on the Effect of Drying on the Kinetics of Cubic Beetroot Slices Using an Industrial Electric Food Dehydrator.

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Abstract. Due to their high moisture content, fresh beetroots must be preserved, or they will rot and need to be thrown away. One of the most effective methods of preservation is drying. This experiment aims to investigate the impact of an industrial electric food dehydrator on a cubic beetroot slice of 4*3 with 3mm, 4mm, and 5mm thickness. Their respective beginning weights were 30 g, 32 g, and 45 g when they were subjected to a 50 °C air flow for 225 minutes. The final results revealed that the beetroot weight drastically fell to 05 g, 02 g, and 06 g, respectively, and was shaped like chips, while the color remained the same. This shows that this electric food dehydrator is very efficient on these three levels.

Keywords : Drying, Electric Food Dehydrator, Beetroot, kinetics, Chips, Efficient.

The effect of precursor concentration on the morphological, phases and crystalline structures proprieties of iron oxides nanoparticles prepared via eco-friendly method

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Abstract. Iron oxide nanoparticles (IO-Nps) were synthesized successfully via a green synthesis method using Geranium Rosat (GR) “Pelargonium graveolens” plant extract and ferric chloride hexahydrate ($\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$) as a reducing and stabilizing solvent and as a precursor respectively. In this work, we investigated the effect of precursor concentration on the morphological properties and crystalline structure of the as synthesized samples. It appears that, by simple changing of the precursor concentration, two different phases of iron oxides nanoparticles can be synthesized using the same procedures. X-Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), An Energy Dispersive X-Ray (EDX) analyses and Raman Spectroscopy are used to characterize IO-Nps. The XRD data revealed a rhombohedral structure of the hematite $\alpha\text{-Fe}_2\text{O}_3$ phase for low precursor concentration (0.025M) and the orthorhombic structure of the goethite $\alpha\text{-FeO(OH)}$ phase for high precursor concentrations (0.2M). As well as the transformation of goethite to hematite was observed for the heat-treated samples. FE-SEM images shows a nanorice morphology for hematite and needle like for goethite of dried product. Raman spectroscopy was used to determine the phonon modes of the hematite and goethite phases as well as to demonstrate that we had successfully synthesized these pure phases.

Keywords: nanoparticles, Iron oxide, hematite, goethite, geranium rosat (GR), leaves extract, nanorice, needle like.

Structural Characterization of Chlorine Doped Cuprous Oxide Thin Films by X-ray Diffraction and X-ray Fluorescence

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Abstract. This study investigates the structural changes in Cl-doped Cu_2O thin films through X-ray diffraction (XRD). The incorporation of Cl^- ions into the Cu_2O lattice is analyzed at varying concentrations. XRD patterns reveal shifts in the (111) peak due to Cl^- ion interaction, indicative of interstitial and substitutional incorporation. The lattice parameter and interatomic distance are compared between theoretical and experimental values, reflecting volume changes caused by Cl^- ion presence. At lower concentrations, interstitial incorporation contracts the lattice, while higher concentrations lead to lattice expansion through substitutional incorporation. These findings provide insights into the structural modifications induced by Cl^- doping, crucial for understanding the conductive properties of the thin films.

Keywords: Cu₂O Thin Films, Cl-doping, Structural Modification.

Synthesis, characterization and chemical-sensor applications of zinc oxide-graphene nanocomposite

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Abstract. The proposed study focuses on the development of a gas sensor utilizing a quartz crystal microbalance (QCM) as the sensing platform. The sensor incorporates a nanocomposite of Zinc Oxide (ZnO) and Graphene as the sensitive layer. The synthesis of this nanocomposite involves a chemical method for thin film deposition on QCM using spray pyrolysis technique. To evaluate the sensor's sensitivity, the frequency shift (Δf) of the coated QCM electrode is monitored when exposed to different gas concentrations such as ethanol, propane, and humidity. The frequency shift serves as an indicator of the gas concentration being detected. The isotherm response characteristics demonstrate good reproducibility and reversibility, suggesting the reliability of the sensor. Several techniques are employed to analyze various aspects of the coated QCM electrodes. Contact angle measurements (CA) are utilized to assess the surface wettability, providing information on how the nanocomposites interact with the surrounding environment. Chemical compositions of the coated electrodes have been investigated by employing attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy. Scanning electron microscopy (SEM) is utilized to study the surface morphology of the coated QCM electrodes, providing detailed information on the structure and topography of the sensor's sensitive layer.

Keywords: Spray pyrolysis deposition, Zinc oxide, Graphene, Gas sensor, quartz crystal micro-balance (QCM), Nanocomposites.

Structural and Quantum Study of the Geometry and Infrared Spectroscopy in Aniline-Substituted Chemicals.

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Abstract. In the context of this study, we present the results of calculations for determining the molecular conformation of substituted aminobenzenes obtained through theoretical calculations based on Density Functional Theory (DFT). This calculation result, which determines the molecular conformation of the isolated molecule at 0K for benzene-derived products, is achieved

using the GAUSSIAN03 program suite, employing exchange-correlation functionals such as B3LYP and MPW1PW91, along with sufficiently extensive basis sets tailored for organic products to perform highly precise geometry optimizations. The molecular internal modes are calculated using the MPW1PW91 and B3LYP functionals, along with the 6-311G and LanL2DZ basis sets, as employed in the geometry optimization. We conclude this study by comparing the calculation results of the molecular conformation obtained from these two functionals with the experimental crystal structures from X-ray diffraction.

Keywords: benzene-derived products, DFT, Conformation, spectroscopy.

Alcohol-salt solutions droplet evaporation kinetic and shell formation

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Abstract. In the report it was represented the experimental data of the alcohol (butanol, pentanol, hexanol) solutions of metal salt (LiCl, CaCl₂) droplets evaporation kinetics. The experiments were conducted for 1 mol/1 kg (1 M) initial solution concentration and gas medium different pressure values (740, 400 and 200 mm Hg) and the medium temperature value of 20 C. The experimental and the theoretically calculated time dependences of the droplet surface area were compared. It was shown that the modified Maxwell model can be used for modelling the salt solution droplets evaporation kinetic. It was observed, that during the evaporation of butanol, pentanol and hexanol CaCl₂ solution and in hexanol LiCl the forming of a shell around the droplet is possible when the solution inside droplets becomes oversaturated, and it leads to an almost complete cessation of the evaporation.

Keywords: nanomaterials, salt solution, evaporation, droplets

Synthesis and characterization of amorphous-nanocrystalline

Fe₇₃Si₁₅Ti₅B powders by mechanical alloying

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Abstract. Fe₇₃Si₁₅Ti₅B₇ (wt. %) alloy powders were synthesized from pure elemental powders by a mechanical alloying (MA) method under argon atmosphere. The evolution in particles morphology, chemical composition, crystalline structure, magnetic and hyperfine

properties of the mixture elements during MA(0-80 h) were investigated by scanning electron microscopy (SEM) attached with energy dispersive spectroscopy (EDS), X-ray diffraction (XRD), vibrating sample magnetometer magnetization measurements (VSM) and Mössbauer spectroscopy (MS). The Rietveld refinement of the XRD pattern of the sample milled 5 h shows the formation of several structures; Fe₃Si, α -Fe nanostructured, Fe₂Ti and Fe₂B, in addition, that the structure became much more amorphous together with increasing milling time at 80 h. The thermal stability of powder milled was characterized by differential scanning calorimetry (DSC). The annealing of sample milled 80 h shows that the crystallization of the amorphous phases and the activation energy determined by using Kissinger's equation was 462.23 ± 16.11 kJ mol⁻¹. Moreover, the results from XRD and DSC for 80 h of milling were approved by the Mössbauer spectroscopy, and the spectra revealed that the sample Fe₇₃Si₁₅Ti₅B₇ is fully amorphous. The saturation magnetization (M_s) and coercivity (H_c) values were of about 151 emu/g, 38.5 G after 80 h of milling.

Keywords: Mechanical alloying; thermal analysis; Mössbauer spectroscopy; Fe-based metallic glass.

Modeling of the elements of the photovoltaic pumping system

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Abstract. At the present time, the demand for water has become very important, especially in isolated and rural areas where traditional energy is difficult to access, most of these areas are very sunny and water is available in groundwater, which is the same case with us, where pumping water using solar photovoltaic energy represents the ideal applicable solution. And economical for the problem of water shortage, sizing is a necessary step in improving renewable energy systems, and in this work we present a study a technical study has been prepared for each element of the solar pumping system according to choosing the appropriate sizing and simulating the solar system on MATLAB.

Keywords: photoelectric pumping system, solar PV, charge regulator MPPT.

Elaboration of a reduced graphene oxide–chitosan biocomposite

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Abstract. In this work, to develop a graphene-chitosan (Gr-Cs) biocomposite by solution intercalation and cyclic voltammetry, we used reduced graphene oxide (rGO) and chitosan. We have synthesized reduced graphene oxide (rGO), from recycled, processed and activated graphite

extracted from batteries or carbon from electric motors, by electrochemical process using KOH as electrolyte and by chemical oxidation according to the two-step method HUMMERS modified. In the first stage, we obtain by chemical exfoliation with KMnO_4 as an oxidizing agent in an acid medium H_2SO_4 ; graphene oxide which is reduced to rGO with hydrazine; We have extracted Chitosan from shrimp shells chemically in two steps:

- * Extraction of chitin by demineralization, deproteinization and discoloration of shrimp shells

- * Then by deacetylation we obtain chitosan of off-white color, soluble in acetic acid and non-conductive and with a viscosity of 3.267 Pas with a good yield and a DDA of 72%, which indicates the good quality of the chitosan produced;

- * Using elaborated chitosan and commercial chitosan, graphene-chitosan (Gr-Cs) composites were synthesized;

- * The produced samples are characterized by FTIR and UV-Vis spectroscopy, by cyclic voltammetry and by rheology in addition to conductivity and solubility tests.

Key words: biocomposite, reduced graphene oxide, chitosane, exfoliation

Development of tubular membranes from local terracotta clays – Guelma

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Abstract. Clays represent an interesting alternative for water treatment, especially in underdeveloped countries. This is due to their abundance, low cost and their properties (chemical, mechanical, thermal and ease of implementation) suitable for use as membrane supports. Our work aims to use local materials based on local clays (from the Bendjerrah - Guelma region) to prepare tubular membrane supports, after heat treatment at different temperatures, and ultimately used for the filtration of wastewater and see the characteristics of the water before and after filtration (appearance, pH, salinity, conductivity, etc.). The different physical parameters such as: apparent density, total porosity, shrinkage, humidity level, grain fineness, were determined for the different stages of membrane manufacturing. The visual appearance of filtered water is very clear compared to used wastewater; it is quite close to the appearance of tap water. The filtered waters have conductivity, salinity and TDS values lower than the values of the starting solutions, which indicates to us that the membranes used have a capacity to retain the salts found in the starting solution.

Key words: Membranes, Local clay, Terracotta.and filtration.

The efficiency of the thermal activation of a biomaterial for the elimination of pollutants

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Abstract. This study consists in evaluating activated carbon for the discoloration of water contaminated by Malachite Green and Brillant Green used in its natural state and without activation by studying its adsorption capacity of these dyes. After determining the effect of various factors affecting adsorption, such as pH, initial concentration and amount of activated carbon, a study of isotherms and adsorption kinetics was made. At the end of this study, it was established that the experimental results of dye adsorption on activated carbon are well represented by Langmuir, Freundlich model and pseudo-second order model.

Keywords: Malachite Green, activated carbon, adsorption, adsorption isotherms, adsorption kinetics

Preparation, structure and luminescence properties of “microcrystalline cellulose -K₃Tb(PO₄)₂” composites

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Abstract. The continuous development of technologies has some negative effects, in particular, as impact of large amount of environmentally harmful wastes. Therefore, eco-friendly and easy recyclable materials are of great interest for elaboration of modern electronic devices. Cellulose and its derivatives are actively studied as such kind of materials. It is known, that dielectric, mechanical, and optical properties of the cellulose materials can be improved by adding of some fillers, particularly in the form of micro/nanosized particles. The interaction between the cellulosic matrix and fillers can lead to the emergence of new physical properties of such composite materials.

This work is devoted to study of structure and optical properties of composites consisting of microcrystalline cellulose (MCC) filled with polycrystalline luminescent oxide K₃Tb(PO₄)₂. The samples were prepared in the form of disk-shaped tablets by pressing a mixture of MCC and oxide powder. The mixture was prepared by simultaneous long-term low-energy grinding in a ball mill.

It was found that oxide particles are redistributed over all the sample's volume quite evenly. The oxide modifies the diffuse reflectance spectra of MCC in ultraviolet and violet spectral regions. The photoluminescence (PL) spectra of composites are highly dependent on excitation wavelength: 1) the direct PL excitation of Tb³⁺ ions at the region of their *f-f* electronic transitions results in strong linear spectra of these rare-earth ions emission in the green and red spectral regions; 2) the PL excitation at the region of cellulose-related light absorption is resulted in simultaneous PL of the cellulose and Tb³⁺ ions.

It was concluded that the studied materials can be considered as eco-friendly luminescent converters for light emitting diodes and solar cells.

Effect of fiber treatment on the mechanical properties of palm petiole fiber reinforced LLDPE composites

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Abstract. The present study examines the influence of successive treatments on the fiber surface (NaOH, hydrogen peroxide). The palm petiole fibers were incorporated as reinforcement in linear low-density polyethylene (LLDPE) composites loading 15 wt% and evaluated for mechanical, morphological properties.

The effect of treatments on fiber surfaces has been confirmed using FTIR. The scanning electron microscopy (SEM) results showed that the enhanced interfacial adhesion between the fibers and the matrix makes treated composites more rigid and homogeneous, which means that the fibers are distributed uniformly. The tensile modulus and flexural strength were enhanced by adding 15% of untreated palm petiole fibers, recorded at 598 MPa and 15.56 MPa, respectively, while the tensile strength decreased. We concluded that successive treatments improve the performance of the palm petiole fiber residue and have the potential to create a new type of sustainable and eco-friendly material for various applications.

Keywords: Palm petiole fibers · Linear low-density polyethylene · Chemical treatment · Morphological · Dynamic mechanical

Hydrogels based on chitosan and *glutaraldéhyde*/Potential support for curcumin immobilization

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Abstract. In this work, we have been interested in the synthesis of new hydrogels in the form of films intended for use in the biomedical field. These films are obtained from a chitosan polysaccharide (CS) (biocompatible and biodegradable) in the presence of the crosslinking agent *glutaraldéhyde* (GA). The reaction between the amino groups of chitosan ($-NH_2$) and the aldehyde groups ($-CH=O$) of *glutaraldéhyde* takes place by the formation of imine groups by forming covalent bridges of the Schiff base type ($-C=N$) between the chains of these two compounds. Hydrogel films were prepared based on CS and GA by crosslinking using different volume ratios between the aldehyde groups of GA and the amino groups of CS. Several influencing factors such as the volume ratio, the cross-linking temperature, and time were studied. The selected films were characterized by the analyzes of FTIR, SEM, TGA, mechanical resistance. Curcumin was immobilized in the films obtained based on CS/GA. The release kinetics of curcumin from the films obtained and the permeability of the skin membrane were evaluated in vitro in two different pH solutions (pH=5.5 and pH=7.4) using a diffusion cell Franz. Hydrogel films can be optimized to obtain delivery systems with dermatological applications.

Keywords: Skin cancer; Hydrogel film; polysaccharide; Curcumin; Immobilization, release system.

Ab initio calculations of electronic properties of non-stoichiometric Cd_mTe_n clusters

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Abstract. Non-stoichiometric Cd_mTe_n ($m \neq n$: $\text{Cd}_{13}\text{Te}_4$, $\text{Cd}_4\text{Te}_{13}$, $\text{Cd}_{19}\text{Te}_{16}$, $\text{Cd}_{16}\text{Te}_{19}$, $\text{Cd}_{38}\text{Te}_{28}$ and $\text{Cd}_{28}\text{Te}_{38}$) clusters with spherical form and diameter (D) 1, 1.4 and 1.6 nm are studied. These Cd_mTe_n clusters have T_d of point group symmetry. All calculations including geometry optimization and energy spectra of the Cd_mTe_n clusters were made using density functional theory (DFT). Density functional GGA+PBE was used to describe the exchange–correlation energy of the electronic subsystem with Hubbard corrections (GGA+ U). Structural properties, bond length, symmetry and electronic properties like the HOMO-LUMO gap, binding energy, and electronegativity have been analysed.

Keywords: non-stoichiometric CdTe clusters; HOMO-LUMO gap; binding energy; electronegativity

Ab initio calculations of electronic properties of non-stoichiometric Cd_mTe_n clusters

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Abstract. Non-stoichiometric Cd_mTe_n ($m \neq n$: $\text{Cd}_{13}\text{Te}_4$, $\text{Cd}_4\text{Te}_{13}$, $\text{Cd}_{19}\text{Te}_{16}$, $\text{Cd}_{16}\text{Te}_{19}$, $\text{Cd}_{38}\text{Te}_{28}$ and $\text{Cd}_{28}\text{Te}_{38}$) clusters with spherical form and diameter (D) 1, 1.4 and 1.6 nm are studied. These Cd_mTe_n clusters have T_d of point group symmetry. All calculations including geometry optimization and energy spectra of the Cd_mTe_n clusters were made using density functional theory (DFT). Density functional GGA+PBE was used to describe the exchange–correlation energy of the electronic subsystem with Hubbard corrections (GGA+ U). Structural properties, bond length, symmetry and electronic properties like the HOMO-LUMO gap, binding energy, and electronegativity have been analyses.

Keywords: non-stoichiometric CdTe clusters; HOMO-LUMO gap; binding energy; electronegativity.

Heat Transfer Enhancement in a Parabolic Trough Solar Collector Using Inner wall Fins and Nanofluids

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Abstract. In this study, two different absorber tube geometries (smooth absorber tube, absorber tube with inner wall fins at the bottom) are modeled and investigated using engineering equation solver. Primarily we investigate the effects of nanoparticle additions (Al_2O_3 and SiO_2) to the base fluid, Syltherm 800. The nanoparticles are introduced at concentrations of 1%, 2%, 3%, and 4% within a smooth tube. Additionally, the study explores their impact when introduced in a tube with inner wall fins at the bottom. The investigation focuses on two-dimensional heat transfers under turbulent flow conditions (Reynolds numbers ranging from 60000 to 150000) during forced convection. The thermophysical properties of the working fluids are integrated using User-Defined Functions (UDFs). The research reveals noteworthy observations. The incorporation of nanofluids results in a 4.90% increase in the Nusselt number for the smooth tube configuration. Furthermore, the friction factor sees a 2.64% increase, and the PEC (Performance Evaluation Criterion) improves by 1.04. Interestingly, a combination of SiO_2 with Syltherm 800 and the addition of fins exhibit even better performance, showcasing an 88.76% enhancement compared to individual nanofluids. This configuration leads to a Nusselt number and PEC increase of 1.80, while the friction factor initially decreases by 9.10% at Reynolds numbers below 100000, and subsequently increases by 16.73%.

Keywords: Parabolic trough collector, nanofluid, receiver Tube, forced convection, Nusselt number.

Analysis of thermophysical and structural characteristics of organosilica nanocomposites

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Abstract. The work is devoted to theoretical and experimental studies of the dependence of the heat of crystallization of polymer nanocomposites on such factors as the mass fraction of the filler and the cooling rate of composites from the melt. The kinetics of non-isothermal crystallization of isotactic polypropylene (PP) and nanocomposites containing from 0.4 to 5.0 vol. % of air force. An analysis of crystal formation parameters was performed depending on the percentage of aerosol. A systematic increase in the crystallization barrier of lamellar crystallization of polypropylene in polymer nanocomposites is shown, which corresponds to a strong limitation of the transport of PP segments across the melt/lamella interface. The peculiarities of the influence of the structure of polymer nanocomposites on their thermophysical properties have been studied. It was established that the morphology of the PP lamellae remains unchanged depending on the cooling rate from the melt or the content of aerosols.

Keywords: polymer nanocomposite, crystallization parameters, crystallization mechanism.

Optical and structural properties of Co doped ZnO thin films grown by spray pyrolysis method

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Abstract. Optical and structural properties of Co doped ZnO thin films grown by spray pyrolysis method. High quality of pure and cobalt doped ZnO thin films with different concentrations ($\text{Co}_x\text{Zn}_{1-x}\text{O}$ ($x=0.00, 0.02$ and 0.06)) have been successfully prepared using spray pyrolysis method. The microstructure and optical properties of the obtained thin films were investigated using X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), and UV-vis spectroscopy. Wurtzite phase of undoped as well as doped ZnO thin films was confirmed through XRD patterns. The lattice parameters a , c and the volume of unit cell increase with Co content indicating that the Zn^{2+} ions were substituted by the Co^{2+} ions. The UV-Vis investigation displayed high transmittance in the visible region with an increase in the absorption bands. The optical gap energy decreased from 3.19 eV to 2.78 eV. The micro-Raman spectra of pure and Co doped ZnO thin films exhibited Raman-active peaks attributed to the optical phonons of wurtzite ZnO, crystal imperfection and defects.

Keywords: Thin films, ZnO, Co doped, Optical structure, Spectroscopy.

Fe_2HfZ ($Z=\text{Si, Ge, Sn}$), promising new candidate materials for electronic and thermoelectric applications

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Abstract. Full-Heusler materials have attracted intensive attention of scientific research in recent years due to their physical properties, the materials are considered potential candidates for high performance thermoelectric applications. Structural, elastic, and electronic properties of Full-Heusler Fe_2HfZ ($Z=\text{Si, Ge, Sn}$) compounds have been studied using a pseudopotential plane-wave method within the framework of density functional theory, the exchange correlation effects have been treated using the generalized gradient approximation GGA-PBEsol as implemented in the CASTEP code. The calculated results for lattice constant, bulk modulus (B) and its pressure derivative B_0'

are in good agreement with the theoretical data. We have calculated the elastic constants and checked the mechanical stability of the Fe_2HfZ ($Z=\text{Si, Ge, Sn}$) materials. Fe_2HfZ ($Z=\text{Si, Ge, Sn}$) are found to be mechanically stable. Independent single-crystal elastic properties like bulk modulus, shear modulus, Young's modulus and universal index for the corresponding polycrystalline phase indicate that $\text{Fe}_2\text{HfZ}(\text{Si, Ge})$ are brittle and Fe_2HfSn is ductile. The values of Young's modulus demonstrate that, among the investigated materials, Fe_2HfSi is the stiffer one. The anisotropy factor differs significantly from zero, indicating that our materials are elastically anisotropic. We also calculated electronic band structures, total and partial electronic density of states. According to our calculations, $\text{Fe}_2\text{HfZ}(Z=\text{Si, Ge, Sn})$ compounds are not spin polarized. While Fe_2HfSn have a metallic behavior, Fe_2HfSi and Fe_2HfGe exhibit a semiconductor behavior with indirect band gaps of 0.325 eV, 0.113 eV respectively. The partial densities of states show that the valence bands due to Fe-d orbitals and the conduction band due to Fe-d and Hf-d orbitals.

Keywords: Full Heusler compounds; Density Functional Theory; GGA-PBEsol; Structural properties; Elastic Properties; Electronic Properties.

Experimental investigation of conductive heat transfer and fire protection in a polymer-based plate heat exchanger

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Abstract. Polymer-based heat exchangers offer several attractive features for thermal management applications such as low-cost, lightweight, antifouling, and anti-corrosion characteristics. However, their thermal performance is compromised primarily by the low thermal conductivity and high-flammability. This work consists of developing new Polymer-based Plate Heat Exchangers (PPHE), which are made from epoxy resin reinforced by banana fibres and manufactured using the Vacuum Bag Resin Transfer Moulding (VBRTM) technique. The aim of this research is to improve both the heat transfer efficiency and thermal protection of PPHEs. The proposed approach involves incorporating 8 wt.% Silicon Carbide (SiC) into the samples to increase their thermal conductivity, and applying an Intumescent Fire Retardant (IFR) coating to improve their capacity to withstand heat and flames. To determine the efficacy of this approach, a cone calorimetry test was performed to examine the thermal distribution within the PPHE samples and to assess fire reaction parameters during a fire scenario. The results of the test revealed a notable increase in thermal conductivity of approximately 36 %, due to the addition of SiC powder. Furthermore, the IFR coating substantially improved the samples' thermal resistance. This result has been verified by thermogravimetric analysis (TGA) conducted during this study. These findings suggest that using banana fibres-reinforced epoxy resin, combined with SiC powder and IFR coating, has the potential to enhance the overall thermal performances of PPHEs, demonstrating the feasibility of utilizing sustainable and biodegradable materials to create heat exchangers that are more efficient and eco-friendlier.

Keywords: Biocomposite; Heat transfer; Polymer heat exchanger; Cone calorimetry; Thermal conductivity, Process safety.

Improvement of the Optical and Photocatalytic Properties of ZnAl_2O_4 : 1% La^{3+} , x% Pb^{2+} Nanoparticles Synthesized by Citrate Sol-Gel Route.

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Abstract. Samples of pure zinc aluminate (ZnAl_2O_4) and doped ZnAl_2O_4 with both lead (Pb^{2+}) at different ratios (0, 0.5, 1, 1.5, 2, 2.5 mol %) and a constant amount of lanthanum (La^{3+} : 1 mol %), were prepared by the citrate sol–gel technique, and then annealed at 900°C for 2 h. To study the structural, optical, and thermal properties, different characterization methods were used such as powder X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, the Fourier transform infrared spectroscopy and the Raman spectroscopy. Analysis by X-ray diffraction revealed the presence, in all samples, of the cubic, single-phase ZnAl_2O_4 without any impurity phases, with a crystallite size between 19 and 25 nm. These results were confirmed using the Fourier transform infrared and the Raman spectroscopy. Also ultraviolet spectra indicated that the bandgap of the doped samples decreases and exhibits a redshift with increasing concentration of Pb^{2+} ion. In addition, the photocatalytic study for different samples of ZnAl_2O_4 showed that they could be used as photocatalysts and good adsorbents for the degradation of a hexamethyl crystallized violet dye in an aqueous solution.

Keywords: nanoparticles, sol–gel, photocatalysis, adsorption.

Physical properties of TiO_2 Nanotubes grow in different electrolytes by varying anodizing parameters

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Abstract. Highly ordered TiO_2 nanotubes (TiO_2 NTs) were successfully prepared by electrochemical anodization process. Titanium (Ti) foil was anodized at 20V in three different electrolyte; one organic consist on glycerol containing NH_4F and water, and two aqueous solution [$(\text{NH}_4)_2\text{SO}_4$ and Na_2SO_4] containing different amount of NH_4F at varying anodization time. The TiO_2 NTs were characterized using Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD) and UV-Visible spectrophotometer. SEM images shows homogeneous, regular and aligned TiO_2 NTs morphology obtained using organic solution, whereas not well nanotubular structure with lower ordering degree was produced in aqueous solution due to the high chemical dissolution rate of titanium dioxide (TiO_2) ensured by the high fluoride ions concentration; and by the extended anodization time. From the XRD analysis, the annealed samples at 450°C for 3h indicate apparition of a single anatase phase that exhibits a high optical absorption band edge for the TiO_2 NTs developed in glycerol electrolyte where the morphological parameters are well improved.

Keywords: anodization process, electrolyte, nanomaterials, properties, TiO₂ nanotubes.

HMDSO/ZnO-graphene heterostructure coated quartz crystal microbalance transducer for VOCs Sensing

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Abstract. Accurate, reliable and fast, detection of different harmful volatile organic compounds (VOCs) is crucial criterion for medical, industrial, agricultural and environmental applications. To address the issue, in this study, porous HMDSO/ZnO-graphene heterostructure has been used as a sensitive layer. The thin HMDSO and ZnO-graphene nanocomposite layers have been deposited on quartz crystal microbalance (QCM) transducer by plasma enhanced chemical vapor deposition (PECVD) and spray pyrolysis technique, respectively. The synthesized heterostructure was characterized by Fourier transform infrared spectroscopy (FTIR) and atomic force microscopy (AFM). The sensing performance of the coated QCM-based sensor was evaluated by exposing it to various concentrations of organic molecules. The coated QCM sensor demonstrated high sensitivity values of 1.26, 1.05, 1.58 and 0.90 Hz/ppm and low detection limit of 2.38, 2.58, 1.90 and 3.33 for toluene, ethanol, benzene and methanol, respectively. The sensing performance of the elaborated sensor correlates well its chemical and morphological properties. The observed results demonstrate the successful strategy of retaining the excellent property of graphene (high specific surface area) with plasma surface activation to provide more active sites for gas absorption.

Keywords: QCM, VOCs sensor, heterostructure, ZnO-graphene, HMDSO.

Effect of carbon nanotubes on optical and electrical properties of nanocellulose composites

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Abstract. Some advantages of cellulose based materials, e.g. the simple easy ways of their production, high mechanical characteristics and chemical hardness allow to use them in various applications. The combination in one solid body of the characteristics of the fiber structure, several crystalline and at least one amorphous phases makes cellulose a very complex and at the same time very interesting object of scientific and technological research. Cellulose is dielectric material, but it can be observed as wide gap semiconductor (measured forbidden band E_g is in the range 3.5 – 4.0 eV). If a non-conductive dielectric cellulose material is combined with a conductive agent, it can be obtained a composite material which under certain conditions can exhibit the optical and electrical properties of a dielectric or a conductor/semiconductor. In this work, an influence of multilayer carbon nanotubes (MWCNT) on the optical properties and electrical conductivity of a composite material created on the basis of a nanocellulose matrix

filled with a complex luminescent dielectric oxide powder has been studied. The water suspensions of MWCNTs and nanocellulose obtained from wheat straw pulp were used to produce a series of samples with varying MWCNT content. Aqueous mixtures of the above mentioned components were dried in the glass vessels at temperature of 60 °C with the formation of films up to 1 mm of the thickness and up to 15 mm in diameter. The analysis of the obtained data on diffuse light reflection, photoluminescence, and electrical conductivity of the studied samples was performed taking into account changes in the structure and phase composition of the studied materials.

Acknowledgements. The research was financed by National Research Foundation of Ukraine (project № 2022.01/0168) and supported by Institute of Physics of Polish Academy of Sciences.

Structural, electronic, optical and thermodynamic properties of $\text{Sr}_x\text{Ca}_{1-x}\text{O}$, $\text{Ba}_x\text{Sr}_{1-x}\text{O}$ and $\text{Ba}_x\text{Ca}_{1-x}\text{O}$ alloys

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Abstract. The structural, electronic, optical and thermodynamic properties of $\text{Sr}_x\text{Ca}_{1-x}\text{O}$, $\text{Ba}_x\text{Sr}_{1-x}\text{O}$ and $\text{Ba}_x\text{Ca}_{1-x}\text{O}$ ternary alloys in NaCl phase were studied using pseudo-potential plane-wave method within the density functional theory. We modeled the alloys at some selected compositions with ordered structures described in terms of periodically repeated supercells. The dependence of the lattice parameters, band gaps, dielectric constants, refractive indices, Debye temperatures, mixing entropies and heat capacities on the composition x were analyzed for $x = 0, 0.25, 0.50, 0.75$ and 1 . The lattice constant for $\text{Sr}_x\text{Ca}_{1-x}\text{O}$ and $\text{Ba}_x\text{Sr}_{1-x}\text{O}$ exhibits a marginal deviation from the Vegard's law, while the $\text{Ba}_x\text{Ca}_{1-x}\text{O}$ lattice constant exhibits an appreciable upward bowing. A strong deviation of the bulk modulus from linear concentration dependence was observed for the three alloys. The microscopic origins of the gap bowing were detailed and explained. The composition dependence of the dielectric constant and refractive index was studied using different models. The thermodynamic stability of these alloys was investigated by calculating the phase diagram. The thermal effect on some macroscopic properties was investigated using the quasi-harmonic Debye model. There is a good agreement between our results and the available experimental data for the binary compounds which may be a support for the results of the ternary alloys reported here for the first time.

Keywords: Ternary alloys; Ab initio calculations; Structural properties; Band structures; Optical constants; Thermodynamic properties.

Interatomic mechanisms of interaction between cellulose molecules and carbon nanostructures

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Abstract. Nanocomposites based on cellulose and carbon nanostructures (CNS) are studied as perspective multifunctional materials. Despite intensive studies, some open questions regarding the peculiarities of the interaction of the components of nanocomposites "cellulose-CNS" still exist. In particular, the questions regarding the types of bonds formed in the material between components, the mutual influence of the components on their physical properties, the role of individual components in formation of the materials properties remain unclear. The aim of this work is to find some answers to these questions using theoretical research and comparison of their results with experimental data. Theoretical studies are carried out in the form of calculations of the electronic structure performed by the quantum chemical method in the DFT approximation. The calculations revealed the mechanisms of adsorption of molecular cellulose on the surface of carbon nanotubes CNT(5,5) and single-layered graphene sheets, both bare and doped with boron or nitrogen. Binding energies and inter-nuclear distances between adsorption components are calculated and analyzed. The types of interatomic bonds between adsorbed cellulose molecules and carbon surfaces are elucidated. It was found that adsorption of cellulose molecules on the surface of undoped CNTs should generally be considered unlikely, as calculations show the absence of covalent interatomic bonds. In general, interaction of cellulose components with the surfaces of carbon components of composite materials should be considered as relatively weak. However, this interaction is enhanced by additional doping of carbon surfaces or their functionalization by oxygen-containing surface groups. Results of calculations are discussed in comparison with experimental data obtained from optical diffuse reflection, Raman scattering, FTIR absorption, and photoluminescence measurements performed for "nanocellulose"-graphene" nanocomposites.

Hirshfeld surface analysis, molecular conformation and in vitro study of anti-Fusariumoxysporum activity f. sp. lycopersicofmethyl 2-(1,3-dithietan -2-ylidene)-3-oxobutanoate (MDYO).

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Abstract. The aim of our study is to understand the behavior of CH₃ groups in organic products with biological interest. One of studied products by our group is the methyl 2-(1,3-dithietan -2-ylidene)-3-oxobutanoate, which has been synthesized, and characterized by single crystal x-ray diffraction XRD. This compound is one of the derivatives of ketene dithioacetal which have a high capacity to inhibit copper corrosion in nitric acid solutions. A Hirshfeld surface calculation on the asymmetric unit of the C₇H₈O₃S₂ was carried out using Crystal Explorer 3.1 to get a better understanding of the intermolecular interactions and their roles in the crystal cohesion and stabilization. The theoretical calculation of MDYO on molecular conformations based on density functional theory (DFT) are undertaken using the Gaussian 03 program package in gas phase, which has guided to optimization results close to the experience. We are also studying in this work the antifungal power of MDYO. In order to seek other alternatives for the control of the fungus *Fusariumoxysporum* f. sp. *radicis-lycopersici* (F.O.L), this ability was researched in vitro, on a PDA medium (Potato, Dextrose, Agar).

Keyword: DFT, Ketene Dithioacetal Derivatives, DRX, Hirshfeld Surface, Antifungal activity.

Deposition of copper oxide thin films by spray pyrolysis technique and by copper chloride solution for different spray number

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Abstract. In this study, nanostructured cupric oxide (CuO) thin films were deposited using simple spray pyrolysis technique on glass substrates with a fixed temperature at 350 °C. The films were deposited at 0.1 M using ($\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$) as precursor and a spray number that varies between 25 and 150 spray with a step of 25 spray to see the effect of this parameter on the structural properties of our material. The characterizations used such as X-ray diffraction (XRD) shows the formation of pure polycrystalline CuO with tenorite phase which belongs to a monoclinic structure with a preferential direction according to the plane (002). The parameter of the monoclinic cell a varies according to the spray number between 4.78 Å, 4.67 Å. also c varies according to the spray number between 5.12 Å, 5.3 Å. the variation in parameters was due to stresses. and the optical characterization was done by Raman spectroscopy. Raman spectroscopy confirms what we obtained in XRD.

Keywords: CuO, XRD, spray pyrolysis, spectroscopy Raman, spray number.

Impact of High temperature and Germanium rate on the electrical performance of the SiGe Heterojunction Bi-polar Transistor with DPSA-SEG architecture

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Abstract. The aim of this work is to model and analyze the electrical characteristics of a SiGe Heterojunction Bipolar Transistor HBT integrated in BiC-MOS055 technology with DPSA-SEG (Double Poly silicon, Self-Aligned, Selective Epitaxial Growth) architecture, using COMSOL Multiphysics software. The goal is to analyze the impact of high temperatures on component characteristics in the range from 300K to 450K. At high temperatures, electrical performances decrease considerably, the maximum oscillation frequency/transition frequency drops from 397/334GHz to 343/268GHz when the temperature ranges from 300K to 450K. Secondly, we optimized the impact of the Germanium fraction rate introduced into the SiGe base of the HBT on electrical properties. For Germanium concentration less than 20%, static and dynamic performances improved but these performances decreased when germanium concentration is over 20%.

Keywords: SiGe, HBT, BiCMOS55nm, DPSA-SEG, COMSOL, High temperature, germanium fraction rate.

Numerical investigation of laminar forced convection heat transfer nanofluids flow using different base fluids

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Abstract. In this paper, Numerical investigation of laminar forced convection heat transfer nanofluids flow through a horizontal circular pipe under a constant heat flux using different base fluids. In the first part, it has been studied the effect of using several base fluids such as water, engine oil and mercury at different temperature ranging from 280 K to 320 K and at different Reynolds number values ranging from 100 to 2100 on average Nusselt number and pressure drop. In the second part, it has been studied the effect of suspended of Al₂O₃ at 3% volume fraction, 295 K and Reynolds number equal 1460 on heat transfer coefficient and local Nusselt number. The governing equations have been modeled using finite volume method approach with SIMPLE algorithm helping with ANSYS FLUENT software. The results indicate that the average Nusselt number and pressure drop for all base fluids increase as Reynolds number increase and decrease as temperature decrease. Engine oil has a higher average Nusselt number and pressure drop while mercury has a small average Nusselt number and pressure drop. Also, mercury has a small change with temperature. Moreover, average Nusselt number is only function of Prandtl and Reynolds number but pressure drop varies with Reynolds number. Add of Al₂O₃ nanoparticle to the base fluids enhanced the heat transfer coefficient and local Nusselt number for all nanofluids. It has been found that mercury has a higher heat transfer coefficient and small Nusselt number due to higher thermal conductivity and small thermal boundary layer thickness.

Keywords: heat transfer; fluid flow; nanofluids; transport phenomenon

The mathematical modeling for sucralose (e955) sweetener potentiodynamic cathodic removal

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Sucralose (Fig. 1) is an extremely stable artificial sweetener up to 1000 times as sweet as common sugar. Its effects on human and animal organisms hasn't been completely studied yet. Moreover, being hardly metabolized, it is accumulated in the environment. Also, the organisms capable to metabolize it transform the sucralose transform it into toxic chloroorganic derivatives like dioxines and tetrachlorodibenzofurans, reason why the sucralose removal from the environment is also actual.

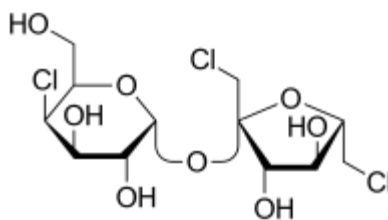


Fig. 1. Sucralose.

Taking into account the presence of organic chlorine in sucralose, the AOP may not be compatible for its removal, due to the formation of toxic chlorine oxides. Cathodic dehalogenation is to be used instead. It leads to the chlorine substitution by hydrogen, leading to the chloride-ion formation. Also, in order to impede the chloride ion passage towards the anodic electrolyte, a membrane, impeding its permeability, is posed to divide the cell into cathodic and anodic electrolyte. Vanadium (III) oxyhydroxide, acting as a strong reductant in neutral, basic and mildly acidic media may be potentially an interesting candidate for cathode modification for sucralose removal.

In this work, the theoretical description for sucralose and chloropicrin cathodic removal is given. In potentiodynamic mode, the behavior of this system will be described by a trivariate equation-set (1):

$$\begin{cases} \frac{ds}{dt} = \frac{2}{\delta} \left(\frac{D}{\delta} (s_0 - s) - r_1 \right) \\ \frac{dv}{dt} = \frac{1}{V} (r_1 - r_3) \\ \frac{dq}{dt} = -\frac{U}{AR} - i_F \end{cases} \quad (1)$$

Its analysis confirms that the behavior of the system in potentiodynamic mode becomes more unstable than for potentiostatic and galvanostatic mode. Despite of general efficiency of VO(OH) as cathode modifier for sucralose removal, the potentiostatic mode is the most effective for sucralose cathodic elimination.

Effects of the Solvent and Calcination Temperature on LaFeO₃ Catalysts for Methanol Oxidation

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Abstract. In this work, two types of solvents ethanol or water were used in preparation of the LaFeO₃ catalysts by citrate sol gel method. The obtained samples were subjected to various calcination temperatures in order to study the catalytic activity and stability for methanol electro-oxidation by XRD, cyclic voltammetry and chronoamperometry. The crystallinity of the LaFeO₃ phase in both cases is improved with increasing calcination temperature. The samples prepared using ethanol exhibit higher catalytic properties than those prepared in water for different calcination temperatures. Moreover, the catalyst prepared in ethanol and calcined at 1050 °C, exhibits a high catalytic activity in methanol electro-oxidation and is ~ two times greater than that obtained at 750 °C.

Keywords: LaFeO₃; Solvent effect; Calcination temperature; Methanol oxidation.

Gel polymer electrolyte materials based on polyethylene glycol, LiBF₄ and gelatin for renewable electrochemical devices

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Abstract. Gel polymer electrolytes are promising materials for the manufacture of modern renewable electrochemical devices. The development and improvement of the properties of such materials is an urgent task today. Using the methods of differential scanning calorimetry, impedance spectroscopy, the thermophysical and electrical properties of the developed polymer electrolytes based on polyethylene glycol (PEG), gelatin and lithium tetrafluoroborate were investigated. The analysis of thermophysical data showed that the melting point and crystallinity of the studied polymer electrolytes decrease with increasing salt content. The addition of gelatin to the composition of the system further reduces the melting point and crystallinity due to the formation of a gel network. At 20% salt content, polyelectrolyte systems are completely amorphized, which is explained by the formation of electrostatic complexes between cations and ether oxygens of the polymer macromolecules. Analysis within the framework of the classical theory of polymer solutions showed that PEG has a better dissolving capacity than the PEG-gelatin system, due to its lower molecular weight and the absence of a gel network. Values for entropy, enthalpy and Gibbs energy of solvation were obtained. The analysis of these parameters showed that dissolution occurs spontaneously in the polyether-salt system. The higher Gibbs energy values for the PEG-gelatin-salt system indicate that the gel network of gelatin hinders the processes of salt dissolution, therefore, it is likely to reduce the mobility of charges inside the polymer matrix.

Keywords: gel polymer electrolytes, electrical conductivity, melting point, crystallinity, gelatin

Structural and morphology characterization of an EVA/ZnO polymer in thin film form for solar applications

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Abstract. "The objective of this work is to develop and study the structural properties, as well as the morphology of thin films of ZnO nano powders prepared by the sol-gel method, based on the fact that reducing grain size to the nanoscale introduces new physical characteristics and opens promising prospects for solar applications. The first part is an experimental study on the fabrication of ZnO. The second part is an experimental study on the organic polymer EVA. We used THF-soluble EVA and doped it with In₂O₃. Experimental analysis using XRD and SEM techniques is conducted to examine the doping rate, efficiency, and performance of the materials."

Keywords: MCP, EVA, ZnO, Photovoltaic, Panels.

Estimation of the percolation threshold and its influence on the properties of epoxy resin-based polymer composite materials filled carbon fibers and carbon nanotubes

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Abstract. Carbon fillers are widely used in the polymer composite materials to control electrophysical properties, which makes them promising for shielding/absorbing electromagnetic radiation in various bands, protection against radio interference and antistatic coatings, etc. However, the low ability of polymers to dissipate heat limits their use in thermal management, so it is important that the electro-thermally conductive filler forms a continuous network. The study of percolation transitions in such materials is a priority for such tasks. In order to create polymer coatings with specified electrophysical and mechanical characteristics, epoxy resin-carbon fiber (ER-CF) and epoxy resin-carbon fiber-carbon nanotubes (ER-CF-CNT) systems with different filler contents were investigated. Electrophysical studies were carried out in the frequency range of 8–12 GHz by the non-contact method, and electrical conductivity at low frequencies of 0.1, 1 and 10 kHz was measured by the two-contact method. The bending strength was tested on a 2167 P-50 tensile tester. It was found that: the electrical conductivity at low frequencies and the complex permittivity at 9 GHz of the composites change significantly in the range of 0.001–0.005 volume fraction of the combined filler, i.e., a percolation transition is observed; in this region, the values of the real and imaginary components of the complex dielectric constant of the composites are ~ 50 , which indicates a significant level of interaction between the components of the system and a uniform distribution of the conductive component in the composite; the maximum values of the relative flexural strength are observed at the content of CF-CNT proportional to the percolation threshold in the systems. The composites have a high level of strength at a low content of fillers, which, taking into account their electrophysical properties, makes them attractive for use as protective coatings for absorbing or shielding from microwave EMFs.

Keywords: epoxy resin, carbon fibres, carbon nanotubes, electrical conductivity, dielectric constant

ab-initio calculations of the structural and electronic properties for t-Se and t-Se containing a defect

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Abstract. In this research, we explore the effect of the helical chain constants of trigonal Selenium (*t*-Se) on the optical gap value utilizing WIEN2k code. Based on structural properties and highlighting the helical chain constants of *t*-Se, it turns out that the distances of the two nearest neighbors (d_1) and of the third neighbors (d_3), the valency angle (Θ) and the dihedral angle (ϕ) are very identical to the experimental results. On the other hand, our defect did not affect d_1 , whereas, d_3 and Θ decrease, ϕ increases. The electronic properties show the semiconductor nature of the both *t*-Se and *t*-Se(D), it also turns out that the gap decreases when we introduce the defect in *t*-Se, this is mostly due to the change in the p-orbital. Hence, intra-

if the horse, from which they are prepared, has taken firocoxib and the problem of its determination in the mentioned products becomes really actual, and the electrochemical methods may provide it a good service.

Considering the structure of the drug, the cathodic determination becomes more viable, due to the presence of highly accepting groups, although the anodic route is also possible. In this case, cobalt (III) oxyhydroxide may be used as an anode modifier, in pair with *in situ* formed cobalt dioxide. The tetravalent cobalt particle provides an efficient firocoxibelectrooxidation by either cyclopropanic or aromatic ring.

In this case, for amperometric mode, the behavior of this system will be described by a bivariate equation-set (1):

$$\begin{cases} \frac{df}{dt} = \frac{2}{\delta} \left(\frac{\Phi}{\delta} (f_0 - f) - r_1 - r_2 \right) \\ \frac{dc}{dt} = \frac{1}{c} (r_3 - r_1 - r_2) \end{cases} \quad (2)$$

Its analysis confirms the efficiency of CoO(OH) as an anode modifier for firocoxib electrochemical determination in animal biological liquids and in animal products like milk and meat.

The theoretical evaluation for bromfenac determination in tears and eye drops over copper sulfide nanoparticles.

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Bromfenac (Fig. 1) is a NSAID, analogous top diclophenac, but with more specific use. It is used to treat eye inflammation and pain in post-operative states. It is used as an ophthalmic solution for eye drops. It has shown to reduce macular edema and retinal thickness, augmenting the visual acuity.

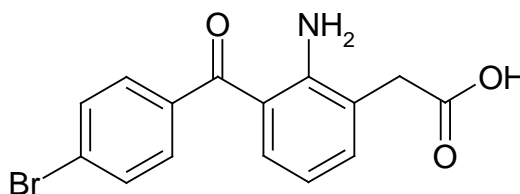


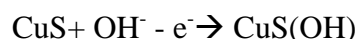
Fig. 1. Bromfenac

Its mechanism of action is somehow analogous to that of diclophenac and aceclophenac, but in basic eye solution the phenolization with following quinone-hydroquinone oxidation becomes more expressed.

Bromfenac is contraindicated to people, which do not tolerate NSAIDS. Its side effects include eye irritations and mild erosion of cornea. Moreover, the use of bromfenac in exceeded doses or in other inflammatory processes except of ocular may provoke hepatic disorders. For this and other reasons, the determination of bromfenac is actual in order to control the adequate medical care for the post-surgery ophthalmologic patients.

Being similar in either chemical structure or biological action to diclophenac, bromfenac is electroactive. Therefore, its electrochemical behavior will become similar and, considering that diclophenac is very popular analyte for electroanalytical processes, the same methods will be acceptable for bromfenac. Taking this into account, we may conclude that copper (II) sulfide nanoparticles, yet used for similar compounds, may also be applied as electrode modifier for bromfenac determination in tears.

Therefore, in this work we describe theoretically the electrochemical determination of bromfenac on anode, modified by CuS. In alkaline medium, correspondent to the tears and some of pharmaceutical formulations, copper sulfide is oxidized, yielding *in situ* trivalent copper derivative:



Which thereby oxidizes bromfenac, mimicking partially its metabolic path in ocular tissue.

The correspondent mathematical model confirms that, despite of high double electric layer impact of each of the stages, including the analyte hydrolysis, copper sulfide may be suitable for the bromfenac electrochemical determination in tears and eye drops.

First-principles calculations of structural, elastic and electronic properties of cubic CsBeI3 compound

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Abstract: Structural, elastic and electronic properties of the cubic CsBeI3 compound are calculated using the full potential linearized augmented plane wave (FP-LAPW) based on the density functional theory (DFT). The exchange-correlation potential is evaluated using the generalized gradient approximation (GGA-PBE). The modified Becke–Johnson potential (mBJ-GGA) potential is employed in the calculation of band structure. We have calculated structural properties (the equilibrium lattice constant, the bulk modulus and its pressure derivative) and they are in good agreement with the available data. The elastic properties such as elastic constants, Zener anisotropy factor, shear modulus, Young's modulus, Poisson's ratio and Debye temperature are obtained for the first time. We have obtained the electronic band structure and the density of states, and CsBeI3 is an indirect band gap material. The estimated band gap value is 0.4628 eV.

Keywords: DFT, FP-LAPW, electronic properties, elastic properties, CsBeI3

Synthesis and characterization of pure CaTiO₃ powders and doped by Mg²⁺ and Mn²⁺ prepared by Sol-Gel route

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Abstract. In this work, CaTiO₃ powders doped with Mg²⁺ (10 mol %) and different ratios of Mn²⁺ (0; 2; 4; 6; 8 and 10 mol %) were prepared by the Sol-Gel citrate route. The as synthesized nanopowders obtained from this method were calcined at 900°C for 3 hours. To better understand the effects of dopant concentration on the structural, optical, and thermal properties of undoped and doped CaTiO₃ perovskite nanostructures, different characterization methods were used, such as powder X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), differential scanning calorimetry (DSC-TG), Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy. The experimental results show that all diffraction peaks can be assigned to the orthorhombic phase of CaTiO₃, without any impurity phases. These results were confirmed using FTIR and Raman spectroscopy. The crystallite size calculated from the intense X-ray diffraction peak using the Scherrer equation is of the order of the nanoscale. Moreover, the high photocatalytic activity of the nanopowders in the degradation of methylene blue and Hexamethyle crystal violet, indicates that these nanostructures could be used as photocatalysts and good adsorbents.

Keywords: CaTiO₃, Sol-Gel, Photocatalysis, Adsorption

Economical and Green Acetaldehyde to Glyoxal Electroorganic Conversion in Potentiodynamic Constant Voltage Mode: a Theoretical Study

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Glyoxal [1-4] is the simplest dialdehyde, frequently used by pharmaceutical and cosmetical industry for the production of drugs, food additives, lipsticks, chewing gums. Its formula is represented on Fig. 1:

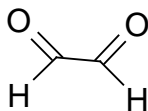
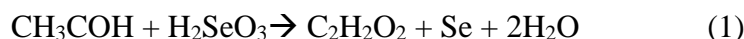
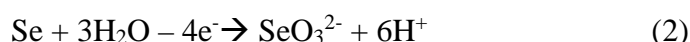


Figure 1. Glyoxal.

Glyoxal may be obtained in the industrial scale by different manners, including the electrooxidation of ethylene glycol [5], acetylene [6], and acetaldehyde, using highly specific oxidant – selenite-ion, according to the equation:



All of these processes involve poisonous, expensive, and ecologically dangerous substances. The last process is used for glyoxal synthesis in the laboratory and in a low industrial scale. Its high-industrial use is impeded by both toxicity and expense of tetravalent selenium derivatives. This problem may be resolved by the development of the electrochemical analogs of the process, described by the reaction (1). In this process, the selenite-ion is hosted in carbon or conducting polymer matrix, as in [8–16], oxidizing acetaldehyde into glyoxal. Furtherly, it will be regenerated by the electrochemical reaction (2):



In our previous works we analyzed the behavior of this process in potentiostatic and galvanostatic modes. Nevertheless, the frequent use of potentiodynamic modes requires the analysis of the potentiodynamic behavior of this system.

Setting the cell voltage as constant, we describe the behavior of this system by a trivariant equation-set (3):

$$\begin{cases} \frac{da}{dt} = \frac{2}{\delta} \left(\frac{A}{\delta} (a_0 - a) - r_1 \right) \\ \frac{ds}{dt} = \frac{1}{s} (r_1 - r_2) \\ \frac{dq}{dt} = -\frac{U}{AR} - i_F \end{cases} \quad (3)$$

Its analysis confirms that, despite of more dynamic behavior and more probable realization of electrochemical oscillations, the potentiodynamic mode may be efficiently used for ethanal electrochemical conversion to glyoxal.

First *a priori* theoretical evaluation of the electroanalytical anodic determination of antibiotic flavocillin in milk on cobalt (III) oxyhydroxide

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Abstract. The discovery of penicillin by Alexander Flemming in 1929 has changed the history of medicine forever. The cure for many dangerous diseases became more efficient and safe, as it didn't need any dangerous compounds like corrosive sublimate or salvarsan anymore. Penicillins were nearly the first antibiotics successfully applied to the vast variety of infections caused by staphylococci and streptococci. They are still widely used worldwide. Nevertheless, many types of bacteria have developed resistance, due to β -lactamase enzyme action. In this aspect, penicillin antibiotic structure undergoes modification, in order to provide β -lactamase inhibition.

Flavocillin (Fig. 1) is an antibiotic, newly reported by Mustafa Pehlivan and his group. Containing both flavone and penicillin derivatives, it is claimed to either increase the susceptibility of various bacteria to β -lactam group, or relieve the oxidative stress, due to the flavonoid group antioxidant properties. Nevertheless, the independent investigation of flavocillin properties are still in course. Moreover, the investigation of side and adverse effect is still pending. Also, the possibility of its veterinary use, by which it will be detected in animal products (milk and meat) is also viable.

Either way, the development of an efficient quantification methodology for flavocillin is really actual, and the electrochemical methods, yet applied to both flavonoids and penicillin may be easily applied to it.

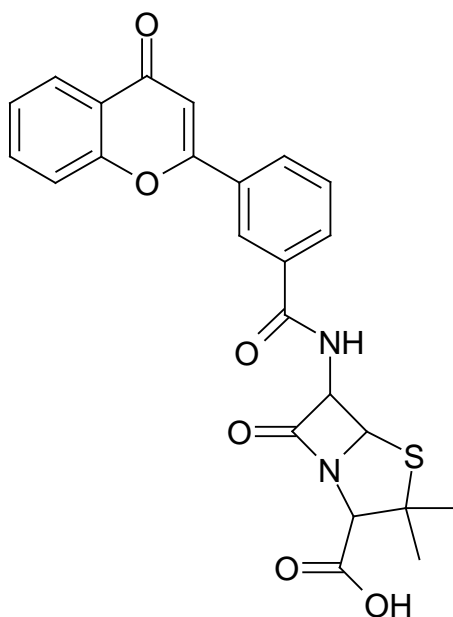


Fig. 1. Flavocillin

Considering the flavocillin structure, we may conclude that both anodic and cathodic determination may be viable for this molecule, being the cathodic route the most preferable, due to the presence of strong acceptors. Nevertheless, the anodic process may also be carried out on strong oxidants, like cobalt (III) oxyhydroxide in pair with cobalt dioxide. For this reason, the aim of this work is to investigate *a priori* the possibility for flavocillin electrochemical determination on cobalt (III) oxyhydroxide-modified electrode, which includes the mechanism suggestion and the correspondent mathematical model investigation with the comparison of the behavior of this system with that of the similar ones.

Multiwalled Carbon Nanotubes Concentration Influence on Aluminum Thermodynamics Properties

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Abstract. The objective of this note is the calorimetric and dilatometric study of the Al+X%MWCNTs nanocomposite with different concentrations of multiwall carbon nanotubes (X= 0.1, 0.25, 1.0 and 1.5% MWCNTs). The behavior of the heat capacity is strongly dependent on the quantities of carbon nanotubes added to the aluminum matrix. Which they are responsible for significant changes in the intensities and temperature shifts of precipitation sequences. Each nanomaterials displays a different calorimetry from the others, confirming the significant role of the CNTs quantity. The DSC signal of Aluminum without CNTs and Al+1%MWCNTs are similar over the temperature range. As for Al+0.1%MWCNTs and Al+0.25%MWCNTs, they show an intense calorific signal intensity indicating that the sample has a higher calorific value four folds compared to the samples with higher CNTs concentrations. This shows that the highest concentration has great absorption capability. Overall, the appearances of the four DSC curves have practically the same shapes. The coefficient of thermal expansion α_T and the relative dimensional variations $\Delta L/L_0$ of the four samples reveal different behaviors dependent on the concentration to another. This situation does not differ from that of the heat capacity. An interesting result observed is the drastic reduction in the expansion coefficient of all studied samples regardless of the concentration. The obtained CTE is of the same order of magnitude of the nanotubes themselves. This shows the essential role of the nanotubes which suggests to govern the expansion. The results obtained in this work are of great interest and a definite contribution to the field of nanotechnology. They highlight the important role of multi-walled carbon nanotubes in aluminum.

Keywords: Aluminum, Carbon nanotube, Expansion, Calorimetry, Thermogravimetry.

Study of interphases in dielectric nanocomposites: Luminescent aspect.

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Abstract. It is known that by changing the phase composition of materials it is possible to control and manage their properties. In reality, certain intermediate regions (interphase layers) are formed in the composite between the “pure” original components. Thus, the composition and structure of these layers do not correspond to the composition and structure of the initial phases. The contribution of the interphase to the material properties and the interaction between the components of the composite can be clarified by the difference in the characteristics of the separated starting components and the composite materials. The role of interphases in

determining the macrocharacteristics of various nanocomposite materials is discussed in the contribution. Suitable literature data and the results of our own experimental and computer simulation studies were used. The main direction of interphase behaviour in composite material study is a determination of the relationships between the properties of the material, on the one hand, and the atomic and energy structure, composition of the object, the size of its components, - on the other hand. Although the mechanisms of interaction between any possible components of the composite, in principle, are predictable, nevertheless, their role and contribution in the case of a particular type, especially – nanoscale composite material (nanocomposite) containing oxides fillers needs to be clarified. These issues are discussed here on the base of results obtained for nanocomposites where nanocrystalline luminescent oxides fillers were embedded into: 1) some glass oxide dielectric matrices; 2) polymer microcrystalline and nanocellulose 49ykhailo. Optical, electron and atomic force scanning microscopy methods as well as XRD, diffuse optical reflectance and photoluminescence methods were used to study mechanisms of phase interactions and their impact on optical and luminescent macro-characteristics of the noted nanocomposite materials.

Stability Analysis of Gradient Zone of a Solar Pond

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Abstract. Linear stability theory is applied to study the effect of feedback control on the onset of double diffusion convection in the non-convective layer of a solar pond. The system is stabilized using sensors and actuators that modify the intensity of the heat flow. The sensors are positioned at a given height of the layer. The influence of the application of active control on the appearance of convection in the case of an infinite layer is analyzed. The results show that the position optimal vertical position of the collectors is located in the center of the nonconvective layer.

Keywords: active control; solar pond; double diffusion; linear stability

Synthesis and Characterization of ZnO(1-x)Ni(x=0.01-0.03) Nanofilms Under Specific Conditions: Enhancement of Red Emission, and Photodegradation Retarding Behavior

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Abstract. In this work, undoped and Nickel (1%, 2%, and 3%) doped ZnO nanofilms were synthesized on glass substrates by ultrasonic spray pyrolysis method. Optical properties of samples were analyzed by photoluminescence (PL) spectroscopies. The structure was studied by X-ray diffraction (XRD). Subsequently, sprayed nanofilms were used as catalysts in an experiment for the degradation of methylene blue (MB) under UV irradiation. XRD spectra confirm the hexagonal 'wurtzite' structure with polycrystalline nature of undoped and Ni doped nanofilms, and revealed that no compound containing Nickel appeared confirming the good quality of the structures. Photoluminescence spectra showed that all samples exhibited strong UV emission with blue emission. The absence of green emission (mainly due according to the literature to the lack of oxygen) in all the spectra is obvious and unexpected. A regular red emission (very rare in the literature) is strangely observed in the spectra of doped nanofilms only which can be exploited by the development of photo or electroluminescent devices based on ZnO_Ni. Photodegradation of undoped ZnO exhibited high degradation rate activity by 87.1% compared to 61.4%, 49.7%, 72.7% of ZnO: Ni (1%, 2%, and 3%) respectively. Therefore, Ni doping lowered the photocatalytic efficiency. Hence, a thorough and in-depth study of this phenomenon is favorable to find a field of application of the reverse effect of the degradation by the ZnO doped Ni photocatalyst.

The theoretical description of letrozol potentiometric determination, assisted by a rhenium-polymer composite

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Letrozole (Fig. 1) is an aromatase inhibitor, used in the treatment of different types of breast cancer. From the chemical point of view, it is a triazolic derivative, containing two cyanic moieties

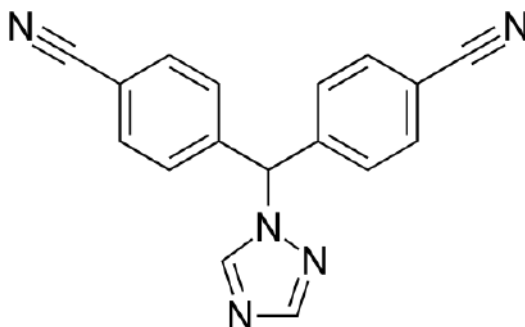
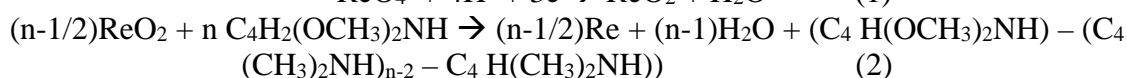


Fig. 1. Letrozole

Besides of its use as an anti-cancer drug, it is used also in the treatment of the infertility, as an ovarian stimulation. It has less side effects than clomiphene and gives less chances of multiple gestation. Nevertheless, besides of its direct action as anti-cancer and reproductive drug, it possesses different dose-related adverse effects, like arthralgia, fatigue. Its excessive use in females may provoke the ovarian hyperstimulation syndrome. Its lasting use may provoke osteoporosis. Thus, the development of the methods for its determination is really actual.

Recently, some methods for Letrozole electrochemical determination have been developed. The electroanalytical process has been realized via a cathodic reaction, including the reduction of the lateral cyanic groups. Thus, for an efficient electrochemical determination of letrozole, it is possible to develop a stable, reproducible and long-life catalyzer, like a composite, obtained by the reaction sequence:



Two models have been developed for galvanostatic composite synthesis and the electroanalytical processes. Despite of a more dynamic behavior than for the potentiostatic mode, both of the processes are efficient, and the steady-state is easily stabilized. The oscillatory and monotonic instabilities, for their turn, are also possible, due to the double electric layer capacitance changes during the both processes.

The fabrication of floating titania co-doped Fe/diatomite granule catalyst with enhanced photocatalytic efficiency under visible light irradiation

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Abstract. Iron (III) nitrate nanohydrate $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and titanium dioxide TiO_2 degussa P25 surface modification treatments were performed on ferric raw diatomite to create the titanium-modified “TDF” material. Surface silica from diatomite and TiO_2 degussa P25 were partially dissolved in the iron (III) nitrate nanohydrate during the $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ treatment by means of x-ray fluorescence (XRF), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and UV-visible diffuse reflectance spectroscopy (DRS). The titanium prepared ferric diatomite modified “ TDF ” with gap band was $E_g = 1.1 \text{ eV}$ by UV-visible DRS technique. The colour removal of vat green 03 indanthren in different pH's using the diatomite modified TDF. It was observed that the vat green 03 indanthren textile dye degradation has pH dependency, the better result is at $\text{pH} = 10$.

Keywords: Iron, titanium, diatomite, gap band, dye, degradation.

Synthesis, crystal structure and Hirshfeld surface analysis of a new coordination complex with 4-nitroaniline

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Abstract. Aromatic amines play a crucial role in both biology and the chemical industry. Specifically, aniline and its derivatives find application in the synthesis of dyes, insecticides, and antioxidants. Certain para-substituted versions of aniline function as local anesthetics, and these compounds fall within this classification [1-3]. Within the scope of these aniline derivatives, 4-nitroaniline, also recognized as 1-amino-4-nitrobenzene, stands out as an organic compound denoted by the chemical formula $C_6H_6N_2O_2$. Exhibiting a yellow solid state, it represents one of the three isomeric forms of nitroaniline [4].

Moreover, 4-nitroaniline serves as a ligand or co-ligand in coordination chemistry alongside various metals such as Cu, Co, Ru, Pt, Pd, Ni, and Zn. The sole feasible coordination mode for the latter involves a monodentate configuration, utilizing the nitrogen atom from the aniline group [5-8]. During our investigation we synthesized a new coordination complex with (4-nitroaniline) and Cadmium nitrate. The coordination complex has been characterized by single crystal X-Ray diffraction. The structural study showed that the complex crystallises the monoclinic system in the $P2_1/c$ space group. To get a better insight into the molecular interaction we conducted the Hirshfeld surface analysis.

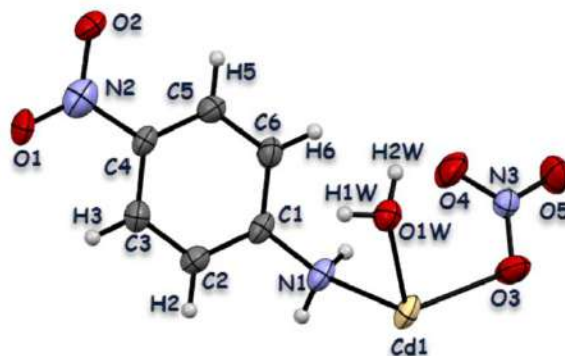


Fig.1 Asymmetric Unit of $[Cd^{II}(p-NA)_2(NO_3)_2(H_2O)]$

Environmental Protection by the Adsorptive Elimination of basic violet 3 dye from Water: equilibrium and kinetic study

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Abstract. The industrial sector is a significant source of persistent pollutants in water resources, and dyes are among the most harmful. These pollutants can have long-lasting effects on the environment and human health, underscoring the need for eco-friendly materials to treat dye-containing wastewater and prevent any adverse effects on water resources. This study focuses on the potential of using raw pine tree bark (RPTB) as an adsorbent to remove hazardous basic violet 3 dye (BV3) from aqueous solution. The study examines various physicochemical parameters, including contact time, concentration, adsorbent dosage, pH, and temperature, to understand their impact on batch-mode adsorption. The efficiency of RPTB for BV3 dye removal is evaluated through a wide range of basic violet 3 dye concentrations (15-150 mg/L), pH values (2-10), and temperatures (25-45°C), with the kinetics and adsorption isotherms of dyes studied systematically. The results indicate that the pseudo-second-order provides the most accurate fit to the data, and the Freundlich isotherm model accurately describes the experimental data. Based on these findings, it can be concluded that raw pine tree bark (RPTB) is a cost-effective, eco-friendly, and promising material for removing dye molecules from aqueous solutions. This material can effectively mitigate the adverse effects of dye-containing wastewater on the environment and water resources.

Keywords: adsorption, pine tree bark, basic violet 3, equilibrium, kinetics.

A Comprehensive Analysis of MWCNT-Al Nanocomposites: Structural Properties

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Abstract. This study aims to investigate the structural properties of multi-walled carbon nanotubes (MWCNT) that have been added to aluminium alloys, which are advanced composite materials that combine lightweight, strong aluminium with the unique properties of carbon nanotubes. Various techniques were used to characterize the materials, including X-ray diffraction analysis, which showed the presence of only the α -aluminium matrix, and ribbons that revealed the presence of alumina and aluminium carbide. Raman spectroscopy detected two bands, with the d band indicating disorder and the g band representing the vibration of the sp^2 sites, indicating an increase in defects. Infrared spectroscopy detected multiple functional groups, showing six pics: the hydroxyl group OH, hydrogen bonding due to oxygen-containing groups (CH...O) linked to carbon dioxide, the carboxyl functions, the CO₂ bond, and the aluminium oxide (Al₂O₃). The results obtained in this study are consistent with previous research.

Keywords: Nano-structures, Metal-matrix composites (MMCs), Structural Properties

Synthesis, Crystal Structures, Luminescence and Magnetic Properties of Isostructural Fe (II) and Co (II) Complexes Based on a Tetradentate Ligand

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Abstract. Mixed-metal compounds with bridging ligands have been of interest for quite some time [1–3], both because of their magnetic exchange interactions and because similar units occur in nature in a variety of proteins and enzymes. Among these compounds iron(II) and cobalt (II) coordination compounds are prominent in having an oxide bridge, that may be either linear or bent. The interest in such iron(II) and cobalt (II) compounds largely stems from magnetic exchange interactions between the metal ions and many species having the Fe(II)-O-Fe(II) bridge structure are found in the Cambridge Crystallographic Database. In the last few decades interest has also arisen in homo- and hetero nuclear species bridged by a cyanide ligand. The versatility of cyanide ligands as bridges is based on their ability to often act as a rigid end-on ligand bridge and, due to the linear and rigid geometry of the CN groups, often rather co-linear M-CN-M species are found, although slight bending at the CN-M angle may occur. In order to explore the combination of oxido and cyanido bridging, we have used a mixture of Fe(II) and Co(II) in combination with the common tripodal tetradentate ligand tris(2-pyridyl-methyl)amine, abbreviated as tpa. Herein we report on the synthesis of a unique mixed-metal compound based on Co(II) and Fe(II). The characterization and structure determination of the compound has been performed by infrared spectroscopy, elemental analysis, thermogravimetric and differential scanning calorimetry, and single crystal X-ray crystallography. The magnetic properties were studied in detail upon cooling from 300 to 2 K in order to explore the dinuclear Fe(II) exchange interactions.

Keywords: bridging ligands; magnetic exchange; spin crossover; coordination chemistry; X-ray; single crystal.

The carbon nanotubes, graphene nanoparticles their oxygen modified forms and composites

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Abstract. Multilayered graphene nanoparticles (GNPs), with the number of up to dozens of layers, with its unique properties, have great potential for application in many fields. GNPs are more stable compared to single-layer graphene and are suitable for mass production by splitting various precursors with a graphite-like structure. The problem is not in the production of GNPs, but in the control of its characteristics. On the other hand, the practical application of GNPs is significantly hindered by their agglomeration due to van der Waals interactions. In order to avoid it, you need to create a certain gap between the GNPs. Carbon nanotubes (CNTs) are an ideal candidate for this. By connecting the GNPs, CNTs can significantly reduce the internal electrical resistance and improve the overall electrical conductivity. Therefore, the production of GNPs@CNTs hybrids has attracted great interest. In this work, we show a simple and cheap method for the synthesis of GNPs by anodic exfoliation of expanded graphite (EG) foil in a weak alkaline electrolyte. A two-level method of controlling the structure of GNPs by adjusting the nanoscale cluster structure of EG by changing the parameters of its production process and modes of "secondary intercalation", i.e., anodic oxidation of EG foil in an alkaline medium, is disclosed. The method of synthesis of composite dispersions of GNPs@CNTs in alkaline electrolyte and film materials from them is described. Some structural characteristics of GNPs, CNTs, and their composites determined by the methods of X-ray diffraction, LCS, Raman

spectroscopy, XPS, DTA, and TG are given. The energy effects of the interaction of partially oxidized graphene-like planes with each other have been clarified by quantum chemistry methods. It was established that thermodynamically, the reaction between the hydroxyl and aldehyde groups of two interacting graphene-like planes is the most probable.

Keywords: expanded graphite, carbon nanotubes, graphene nanoparticles, nanocomposite material, anodic and chemical oxidation

The theoretical description for the indirect synthesis of a new mushroom-based material for heavy metal removal

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Abstract. The term “heavy metals” has been 55ykhailo55d by german chemist Leopold Gmelin in 1817. This term became so popular that has given its name to the musical style, known as “heavy metal rock”. As for now, morethen forty definitions for the term “heavy metals” are commonly accepted, but generally all the metals beginning with vanadium are considered as “heavy”. Most of them are transition metals, capable to form stable complex compounds. The heavy metal cations are among of the most aggressive pollutants in the environment. They may occur even in food and drinks (including those of traditional recipes). These cations are highly toxic, provoking different intoxication symptoms. For this and other reasons, the heavy metals concentration determination and removal is really actual, and the electrochemical methods may be a good solution for this problem. Besides of the cathodic deposition, yet used in different systems of the wastewater treatment, anodic extraction may also be used. Generally, it is based on electrooxidation of a metallic cation or of a surface material in the presence of this cation, yielding thereby a more oxidized form and(or) a stable complex. In order to implement this function, the anode will be modified by a conjugated dye, its polymer or another conducting polymer, possessing complex-forming functional groups. Those monomers and polymers are generally synthetic, but they may be substituted by natural analogous compounds.

The Effect of Increasing the Thickness of an Annular Space Subjected to a Heat Flow Emitted by a Solar Panel on the Dynamic and Thermal Fields

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Abstract. The present work is a 3D numerical simulation, in an annular space between two horizontal concentric cylinders in which an incompressible fluid circulates. The wall of the inner cylinder is adiabatic while the wall of the outer cylinder is subjected to a constant thermal heat flux emitted by a solar panel. The model equations of continuity, momenta and energy are numerically solved by the finite volume method with a second order spatiotemporal discretization. The used mesh is $26 \times 44 \times 162$ nodes along the radial, angular and axial directions. The studied hydraulic diameters are: $D_h = 0.75, 1.0, \text{ and } 1.25 \text{ cm}$. The purpose of this work is to improve the heat transfer by increasing the thickness of the annular space, this allowed us to study the dynamic and thermal fields of the heat transfer fluid and make a comparison of average temperatures and Nusselt numbers for three different cases.

The results obtained show that despite the qualitative similarity of thermal and dynamic fields for the three studied cases, the heat transfer increases when the thickness of the annular space is increased, this is justified by the increase in the Nusselt number.

Keywords: Annular space, Mixed convection, 3D Numerical simulation.

Fluid Flow and Heat Transfer in Absorber Tube Subject to a Non-Uniform Heat Flow

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Abstract. The present work is a numerical simulation which concerns the effect of the incident angle solar radiation on the heat transferred to fluid in a solar collector. The working fluid is considered Newtonian and incompressible with thermo-dependent physical properties. The latter circulates in a horizontal absorber tube subjected to a non-uniform wall heat flow. The studied inclination angles are: $\alpha = 0^\circ, 30^\circ, 45^\circ \text{ and } 60^\circ$. The model equations of continuity, momenta and energy are numerically solved by the finite volume method with a second order spatiotemporal discretization. The Prandtl, the Reynolds and the Grashof numbers are fixed at 8.0, 500 and 10^5 respectively. The obtained results show that the dynamic and thermal fields for perpendicular solar radiation ($\theta=0$) are qualitatively and quantitatively different from those of inclined solar radiation. The heat transfer is quantified by the local and average Nusselt numbers. The obtained results also shows that the average Nusselt number at the tube interface increases with the decrease of incident radiation angle. We have tried modelling the average Nusselt number as a function of incident radiation angle. With the parameters used, the heat transfer is quantified by the correlation of the average Nusselt number: $Nu_A = 6.188 - [0.467 \, tg(\alpha) - 0.089]^2$.

Keywords: Cylindrical absorber, Non-uniform heat flow, Finite volume method.

Laser-assisted electrodeposition of composite carbon-containing nickel coatings

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Abstract. The paper presents the study of the structure, protective and mechanical properties of nickel composite coatings modified with ultradispersed diamonds, electrodeposited under conditions of external stimulation by laser radiation. An analysis of the cathodic polarization curves showed that the presence of dispersed particles with a concentration of 2–15 g/l in the aqueous electrolyte solution leads to a shift in the cathodic potential to the electronegative region by 108–340 mV, respectively, which indicates an increase in charge transfer resistance. Composite nickel coatings obtained by laser-assisted electrodeposition are characterized by a higher content of ultradispersed diamond particles in the coating (4,35÷5,10 wt.%) as compared to the mode of deposition without laser irradiation (2,24÷3,15 wt.%). In this case, the proportion of particles of smaller size $\sim 0,25 \div 1 \mu\text{m}$ increases in the coatings. The more intense penetration of dispersed phase particles into the forming coating during the laser stimulation of the electrodeposition process is due to the presence of a temperature gradient, which provides an additional supply of metal ions in the irradiation region. Increased concentration of the dispersed phase in composite nickel coatings promotes formation of a finer crystalline coating structure, enhanced hardness, corrosion resistance and wear resistance of the coatings.

Keywords: ultradispersed diamond particles, composite nickel coatings, laser-assisted electrodeposition, structure, mechanical and protective properties.

Advances of Mayer's cluster approach in quantitative theoretical description of phase transitions for various lattice models of matter

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Abstract. Modern achievements in the statistical theory of condensation based on Mayer's cluster expansion of the partition function are applied to discrete (lattice) models of matter. In particular, the presented approach allows evaluating the phase transition parameters for the condensation process in lattice gases, spontaneous magnetization in ferromagnets, and spinodal decomposition phenomenon in binary mixtures with high accuracy on the basis of the information about several irreducible cluster integrals (virial coefficients) of low orders. The results of calculations indicate qualitative and even quantitative universality in the behavior of the mentioned lattice systems with various geometry and dimensionality at the same values of a certain reduced temperature when that behavior is expressed in terms of some dimensionless parameters. An additional possibility to describe the order-disorder phase transitions in some other lattice systems (e.g., antiferromagnets and mixtures/alloys with a certain interaction potential) is also discussed in the paper.

Keywords: lattice model, Mayer's expansion, cluster integral, phase transition, condensation, magnetization, spinodal decomposition

Fabrication and characterizations of pure and doped Zinc Oxide thin films

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Abstract. Semiconductor thin-film oxides are increasingly invading the world due to the extraordinary contribution they make and the possibility of using materials in nanometric dimensions. The major advantage of their use lies in the modification of their original properties by quantum confinement effects. In this context, extensive research has been developed for the use of nanoscale semiconductors. In the form of thin layers, the latter allowed the integration of thousands of components, leading to the miniaturization of devices used in technological applications, such as light emitting diodes, laser devices and photovoltaic cells.

The present work consists of the development and characterization of pure and doped ZnO thin films. These films were fabricated using the sol gel method and deposited on glass matrix by the Dip-Coating technique. The drying temperature was set at 350 ° C and then we proceeded to determine where the optimal annealing temperatures reside using the stress calculation. The latter are all compressive with the exception of the 1% doped film and annealed at 400 ° C where they are extensive. Minimum values for annealing temperatures of 500 ° C and 550 ° C were found.

The structural characterization of the ZnO thin films by X-ray diffraction has confirmed the formation of ZnO crystallites of nanometric size and hexagonal structure (wurtzite). The XRD has shown that the crystallites of ZnO have adopted a preferential orientation in the [002] direction. The AFM images have shown that the layers are of nanometric size. Raman spectroscopy has then confirmed the formation of ZnO of hexagonal structure (wurtzite).

Visible UV spectroscopy has shown a shift of the absorption edge towards large energies.

Key words: thin-films, ZnO, nanometric, Sol-Gel, X-ray, optical absorption.

Nonlinear optical response in aluminum nitride nanocages

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Abstract. Aluminum nitride AlN based nanosystems is a favourable material for use in nanodevices, high-performance NLO materials and optoelectronics, accordingly doping Al₁₂N₁₂ nanocage by first row transition metals (TM) have unique electronic and nonlinear optical properties. These properties were explored using the most excellent computational method: density functional theory (DFT) calculations. These new inorganic compounds with high stability, TM@b64/b66Al₁₂N₁₂ (TM: Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu and Zn) were doped on the fullerene-like Al₁₂ N₁₂ nanocage, where transition metal is located over the Al –

N bond (b64 /b66 site). DFT/TD-DFT study with the B3LYP exchange – correlation functional reveals the electronic transition, charge transfer properties (charge, distance and dipole moment), hyper-Rayleigh scattering and depolarization ratios (static and dynamic) of these compounds.

Keywords: DFT, Nonlinear optical properties (NLO), nanocage, transition metal.

Hybrid magnetic nanoparticles for antitumor drug delivery

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Abstract. Cancer is one of the deadliest diseases in the world. Controlled drug delivery systems offers great opportunities for the development of new non-invasive strategies for the treatment of cancers and the main advantage of these systems is represented by their capacity to accumulate in tumors by enhanced permeability and retention effect. We focused our research on hybrid magnetic nanoparticles (nanospheres) based on chitosan obtained by double crosslinking in reverse emulsion. Hybrid nanoparticle consisting of a polymeric matrix in which is dispersed a magnetic nanoparticles material (magnetite (Fe₃O₄), maghemite (γ-Fe₂O₃), hematite (α-Fe₂O₃), etc.), are lately studied for use as target delivery systems of antitumor drugs. Selection of the matrix-forming polymer is based on the need for it to be biocompatible, biodegradable, mucoadhesive, possessing reactive functional groups in order to achieve the cross-linking process under mild reaction conditions. The hybrid nanoparticles nanospheres formed is characterized in order to determine their shape and size; these particles are from a few tens to a few hundred nanometers in diameter. SEM confirmed their nanometric size and their well-defined spherical shape. These nanospheres allowed the encapsulation of an increased amount of 5-Fluorouracil and presented a controlled drug release.

Keywords: Chitosan, nanospheres, Biomaterial, hybrid nanoparticles, magnetite, 5-Fluorouracil.

Wind Turbine Energy Production Based on Event-Triggered Speed Control

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Abstract. This improved strategy for efficient energy production is introduced based model predictive control with a precise control instance using event triggered mechanism. Aiming to optimize the wind turbine speed for energy production while accounting for uncertainties, disturbances, and sensor malfunctions. The proposed strategy leverages MPC, a powerful control technique known for its ability to optimize system performance by considering future predictions of power generation. In this context, MPC is utilized to formulate an optimal control sequence for wind turbine operation, accounting for various factors such as wind speed fluctuations, turbine dynamics, and power output constraints. Unlike traditional time-triggered control schemes, our approach employs event-triggered sampling, which means that control updates are triggered only when specific events or significant changes occur in the system, thereby reducing computational demands and improving efficiency.

Keywords: Wind Turbine, Speed Control, Sensor Fault.

Lebail and Rietveld Refinement of the XDR-Diffractogram and Crystallographic Related Parameters of a Lanthanum Based Double Layered Manganite Prepared at 1438K by Solid State Route

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Abstract: By means of a solid state reaction, lanthanum based double layered manganite material is prepared at 1438. The XRD diffractogram is refined by both Lebail and Rietveld refinement using Jana2006 and FullProf software. It is shown that the sample mostly crystallized in a tetragonal structure with an I4/mmm space group. As an impurity phase, it has been detected, in very small amount, a simple perovskite that crystallized in an orthorhombic structure with a Pbnm space group. The experimental local Jahn-Teller distortion, the cation mismatch, the Goldschmidt tolerance factor and the crystallite size have been determined and discussed. 3D crystallographic structure was established in different configurations.

Keywords: Layered manganites, solid state route, XRD, Rietveld and Lebail refinement, local Jahn-Teller distortion, the cation mismatch, the Goldschmidt tolerance factor

Solid Oxide Fuel Cell Performance for Power Generation: Adaptive Fuzzy Fault-Tolerant Control Strategy

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Abstract. In this paper, we introduce an efficient methodology for precise control of Solid Oxide Fuel Cell (SOFC) systems, aiming to optimize power generation while accounting for uncertainties, disturbances, sensor malfunctions, and nonlinear actuator issues. Our approach leverages Particle Swarm Optimization (PSO) to estimate adaptive parameters and initialize fuzzy values, resulting in a dependable controller capable of rapid adaptation to changing conditions. Fuzzy systems are employed for the estimation of unknown nonlinearities, nonaffine nonlinear actuator faults, and time-varying sensor errors. To mitigate approximation errors and handle external disturbances, we incorporate a robust control component. We address the issue of an algebraic loop through the utilization of a Butterworth low-pass filter. Furthermore, our robust scheme effectively manages external disturbances without relying on approximations, and the controller undergoes real-time updates through online reconfiguration. The stability of the overall closed-loop system is rigorously analyzed using Lyapunov theory. We provide simulation scenarios to illustrate the effectiveness and advantages of our proposed methodology.

Keywords: Solid Oxide Fuel Cell, Butterworth low-pass filter, Sensor Fault, Actuator Faults.

Exploring the Evolution of Ni/ZrO₂ Nanocomposites: A Comprehensive Study of Metal-Oxide Interaction and Catalytic Potential

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Abstract. The interface between metal and oxide materials has been a focal point of extensive experimental and theoretical investigations, given its pervasive significance across diverse technological domains, including microelectronics, laser optics, chemistry, high-pressure physics, and medicine.

This study undertakes a systematic exploration of the interplay between metal nanoparticles and oxide support. Utilizing the wet impregnation method, we synthesized M/Oxide (M=Ni, Oxide=ZrO₂) nanocomposites and subjected them to variable calcination temperatures. Comprehensive characterization encompassing Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), UV-visible spectroscopy, and Fourier-Transform Infrared Spectroscopy (FTIR) was employed. XRD analysis unveiled novel phases, including intermetallic ones, with NiZr₂ predominating, albeit diminishing at 750°C, succeeded by the emergence of Ni_{0.99}Zr_{0.01}. Furthermore, UV-Vis spectra documented an electronic transformation at 550°C of Ni⁺² ions to Ni⁺³ ions, reverting at 750°C with the resurgence of Ni⁺² ions. FTIR spectra probed the elemental bonding within the nanocomposite. In summation, this investigation provides a comprehensive insight into the synthesis and evolution of Ni/m-ZrO₂ nanocomposites, elucidating their potential as catalysts.

Keywords: Nanocomposite, Metal-Oxide Interaction, Nickel (Ni), Support Oxide, m-ZrO₂, Catalysis.

Study of the Mechanical, Physical and Chemical Properties of Aluminum-Based Alloys

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Abstract. Aluminum proves to be a good non-magnetic conductor of electricity, it naturally resists atmospheric corrosion because of the formation of a thin surface layer of Al₂O₃ alumina which protects it against the ravages of air, temperature, humidity and chemical attack. Pitting corrosion is a form of localized corrosion where cavities form on the surface of aluminum. It generally occurs in the presence of an electrolyte that contains dissolved salts, normally chlorides.

In this present work, some physical and mechanical properties as well as the corrosion resistance of the three aluminum alloys; undeformed, 10% deformed and 40% deformed were studied. The aggressive mediums chosen are; a solution of 0.05M H₂SO₄, seawater and rainwater.

The characterization techniques used are X-ray diffraction (XRD), differential scanning calorimetry (DSC), micro-hardness measurements, in addition to the chemical characterization of corrosion resistance.

The increase in hardness in aluminum-based alloys is related to the presence of the precipitated phase and to microstructural defects in the alloy studied. Very good corrosion resistance of aluminum in ambient environments; rainwater and seawater. Sulfuric acid strongly attacks aluminum, it is a poor cleaner for aluminum and its alloys.

Keywords: Aluminum alloys, Corrosion, DRX, DSC, Polarization technique

Estimation of interaction parameters in liquid-liquid ternary systems at different temperatures using the NRTL model

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Abstract. The estimation of interaction parameters is the key for the calculation of physicochemical properties and calculations related to ternary systems in liquid-liquid extraction. The equilibrium conditions between phases of chemical systems involved in liquid-liquid extraction can be considered among the most important applications in chemical process engineering, chemical engineering and industrial chemistry etc...

In this work, we will study liquid-liquid equilibria for some ternary systems at different temperatures. The equilibrium data of the following ternary systems: Trichloromethane-Acetic Acid-Water; Trichloromethane-Acetone-Water; Trichloromethane-Ethanol-Water

The validation of the experimental results allows to calculate the interaction parameters of these systems using the NRTL model. The calculations were performed using a computational code on MATLAB based on a hybrid algorithm (Nelder-Mead and the genetic algorithm).

It should be noted that the algorithms used in these calculations allow optimized interaction parameters.

Keywords: Liquid-liquid extraction, Genetic algorithm, interaction parameter, optimization

Synthesis and characterization of ZnO-based nanocomposites

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Abstract. The main objective of this work is to develop ZnO-based nanocomposites. A series of nanocomposites was prepared by hydrothermal method. The different obtained nanostructures were systematically characterized in terms of structure and morphology using X-ray diffraction (XRD), scanning electron microscopy (SEM) and Raman spectroscopy. The XRD diffractograms of all samples showed the crystallization of the hexagonal wurtzite structure of ZnO phase with nanoscale crystallites, and the clear appearance of the second phase Co₃O₄ when increasing the concentration of cobalt acetate, which was confirmed by SEM images. Energy-dispersive X-ray spectroscopy (EDS) spectra confirmed the formation of ZnO/Co₃O₄ nanocomposite without any impurities. The vibrational analysis by Raman spectroscopy confirmed the good crystallization of the wurtzite structure, as evidenced by the presence of the E₂ (low) mode observed at 99 cm⁻¹, and showed that the ZnO lattice was disrupted due to the increase in cobalt acetate concentration. The antibacterial test was conducted using the Kirby-Bauer agar diffusion method. The efficacy of these nanocomposites in the antibacterial test is negative when the concentration of cobalt acetate exceeds 30%.

Keywords: ZnO, ZnO/Co₃O₄ nanocomposite, antibacterial

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